



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2025 – 01:36 pm GMT

PDB ID : 9HDF / pdb\_00009hdf  
Title : Glucocorticoid Receptor Ligand Binding Domain in complex with dexamethasone  
Authors : Alegre-Marti, A.; Jimenez-Panizo, A.; Fuentes-Prior, P.; Estebanez-Perpina, E.  
Deposited on : 2024-11-12  
Resolution : 2.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

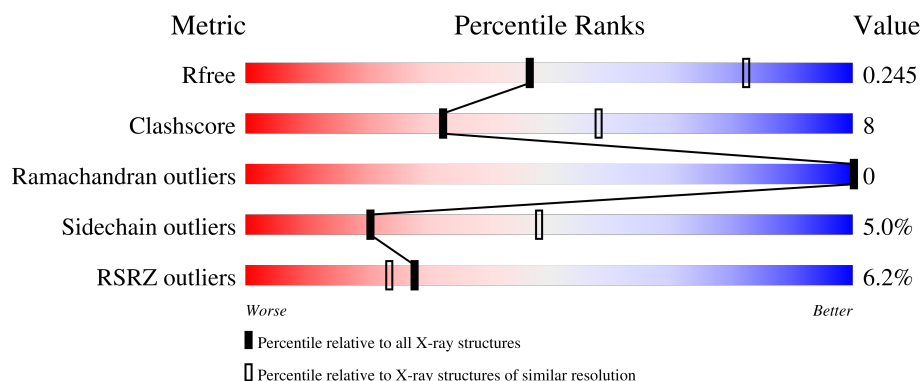
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	4924 (2.80-2.76)
Clashscore	180529	5458 (2.80-2.76)
Ramachandran outliers	177936	5386 (2.80-2.76)
Sidechain outliers	177891	5388 (2.80-2.76)
RSRZ outliers	164620	4926 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	248	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>..</div> </div> </div>
1	C	248	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>.</div> </div> </div>
1	D	248	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>
1	F	248	<div> <div>10%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	248	
1	H	248	
1	I	248	
1	L	248	
1	M	248	
1	P	248	
2	B	248	
2	E	248	
2	J	248	
2	K	248	
2	N	248	
2	O	248	
3	a	15	
3	b	15	
3	c	15	
3	d	15	
3	e	15	
3	f	15	
3	g	15	
3	h	15	
3	i	15	
3	j	15	
3	k	15	
3	l	15	
3	m	15	

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Mol	Chain	Length	Quality of chain
3	n	15	
3	o	15	
3	p	15	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	IMD	d	101	-	-	X	-
6	EPE	P	1002	-	-	X	-
7	GOL	C	1002	-	-	X	-
7	GOL	L	1004	-	-	X	-
7	GOL	P	1003	-	-	X	-
8	SO4	C	1006	-	-	X	-

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 34585 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ancestral Glucocorticoid Receptor2 ligand binding domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			2007	1297	328	365	17			
1	C	248	Total	C	N	O	S	0	0	0
			2007	1297	328	365	17			
1	D	248	Total	C	N	O	S	0	0	0
			2007	1297	328	365	17			
1	F	248	Total	C	N	O	S	0	1	0
			2008	1297	328	365	18			
1	G	248	Total	C	N	O	S	0	1	0
			2011	1299	329	366	17			
1	H	245	Total	C	N	O	S	0	0	0
			1986	1286	323	360	17			
1	I	248	Total	C	N	O	S	0	0	0
			2007	1297	328	365	17			
1	L	248	Total	C	N	O	S	0	0	0
			2007	1297	328	365	17			
1	M	248	Total	C	N	O	S	0	0	0
			2007	1297	328	365	17			
1	P	243	Total	C	N	O	S	0	0	0
			1974	1280	321	356	17			

- Molecule 2 is a protein called Ancestral Glucocorticoid Receptor2 ligand binding domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	1	0
			2010	1297	328	367	18			
2	E	244	Total	C	N	O	S	0	2	0
			1988	1287	323	360	18			
2	J	248	Total	C	N	O	S	0	1	0
			2014	1300	331	366	17			
2	K	245	Total	C	N	O	S	0	1	0
			1992	1288	324	362	18			

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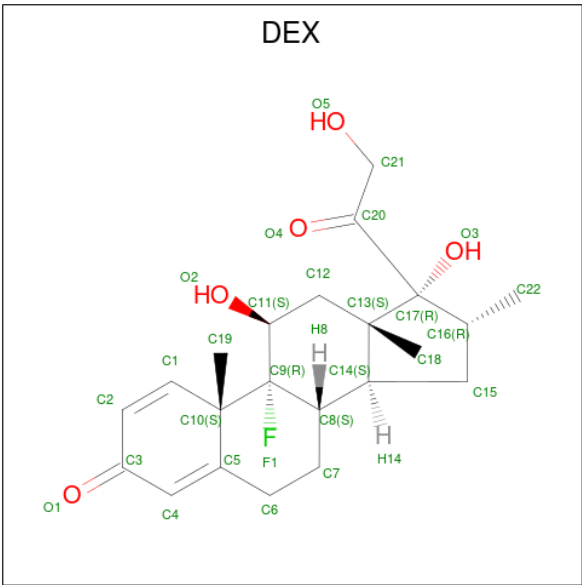
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	245	Total 1997	C 1290	N 327	O 362	S 18	0	2	0
2	O	244	Total 1986	C 1285	N 323	O 360	S 18	0	1	0

- Molecule 3 is a protein called Nuclear receptor subfamily 0 group B member 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	a	14	Total 104	C 68	N 17	O 19	0	0	0
3	b	14	Total 104	C 68	N 17	O 19	0	0	0
3	c	14	Total 104	C 68	N 17	O 19	0	0	0
3	d	14	Total 104	C 68	N 17	O 19	0	0	0
3	e	14	Total 104	C 68	N 17	O 19	0	0	0
3	f	13	Total 96	C 62	N 16	O 18	0	0	0
3	g	13	Total 96	C 62	N 16	O 18	0	0	0
3	h	13	Total 96	C 62	N 16	O 18	0	0	0
3	i	15	Total 109	C 71	N 18	O 20	0	0	0
3	j	14	Total 104	C 68	N 17	O 19	0	0	0
3	k	14	Total 104	C 68	N 17	O 19	0	0	0
3	l	14	Total 104	C 68	N 17	O 19	0	0	0
3	m	14	Total 104	C 68	N 17	O 19	0	0	0
3	n	15	Total 109	C 71	N 18	O 20	0	0	0
3	o	14	Total 104	C 68	N 17	O 19	0	0	0
3	p	14	Total 104	C 68	N 17	O 19	0	0	0

- Molecule 4 is DEXAMETHASONE (CCD ID: DEX) (formula: C<sub>22</sub>H<sub>29</sub>FO<sub>5</sub>).



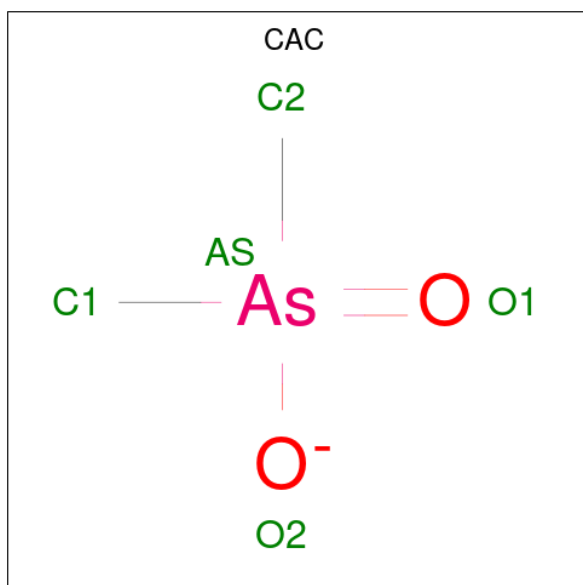
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	O	0	0
			28	22	1	5		
4	B	1	Total	C	F	O	0	0
			28	22	1	5		
4	C	1	Total	C	F	O	0	0
			28	22	1	5		
4	D	1	Total	C	F	O	0	0
			28	22	1	5		
4	E	1	Total	C	F	O	0	0
			28	22	1	5		
4	F	1	Total	C	F	O	0	0
			28	22	1	5		
4	G	1	Total	C	F	O	0	0
			28	22	1	5		
4	H	1	Total	C	F	O	0	0
			28	22	1	5		
4	I	1	Total	C	F	O	0	0
			28	22	1	5		
4	J	1	Total	C	F	O	0	0
			28	22	1	5		
4	K	1	Total	C	F	O	0	0
			28	22	1	5		
4	L	1	Total	C	F	O	0	0
			28	22	1	5		
4	M	1	Total	C	F	O	0	0
			28	22	1	5		
4	N	1	Total	C	F	O	0	0
			28	22	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	O	1	Total	C	F	O	0	0
			28	22	1	5		
4	P	1	Total	C	F	O	0	0
			28	22	1	5		

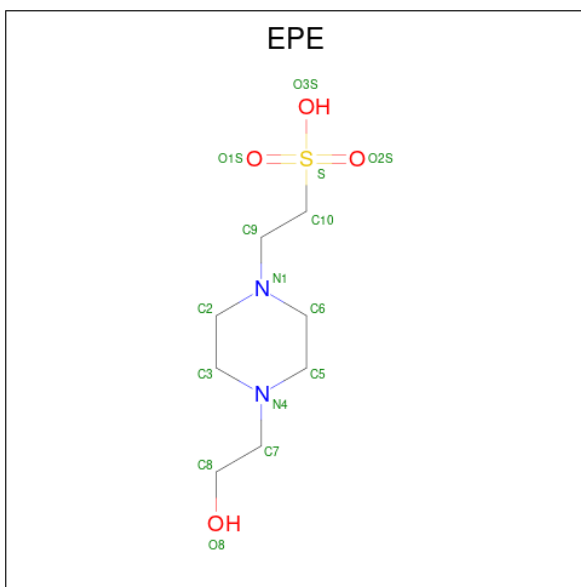
- Molecule 5 is CACODYLATE ION (CCD ID: CAC) (formula:  $C_2H_6AsO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	As	C	O	0	0
			5	1	2	2		
5	D	1	Total	As	C	O	0	0
			5	1	2	2		
5	E	1	Total	As	C	O	0	0
			5	1	2	2		
5	H	1	Total	As	C	O	0	0
			5	1	2	2		
5	I	1	Total	As	C	O	0	0
			5	1	2	2		
5	K	1	Total	As	C	O	0	0
			5	1	2	2		
5	M	1	Total	As	C	O	0	0
			5	1	2	2		
5	O	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	I	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	J	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	P	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



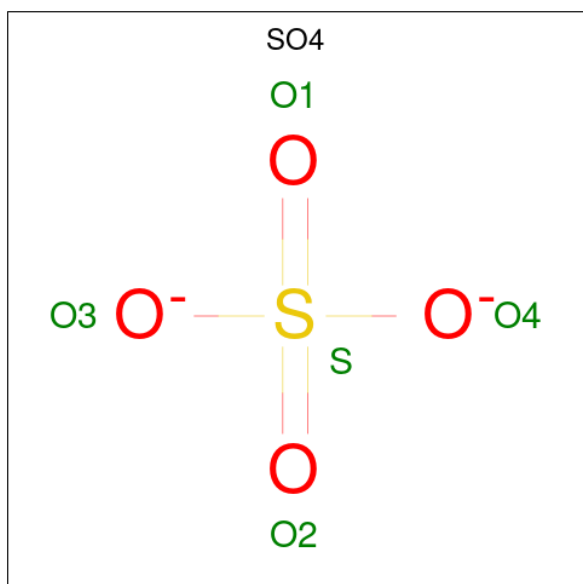
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	I	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		
7	K	1	Total	C	O	0	0
			6	3	3		
7	K	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			6	3	3		
7	L	1	Total	C	O	0	0
			6	3	3		
7	M	1	Total	C	O	0	0
			6	3	3		
7	N	1	Total	C	O	0	0
			6	3	3		
7	O	1	Total	C	O	0	0
			6	3	3		
7	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).

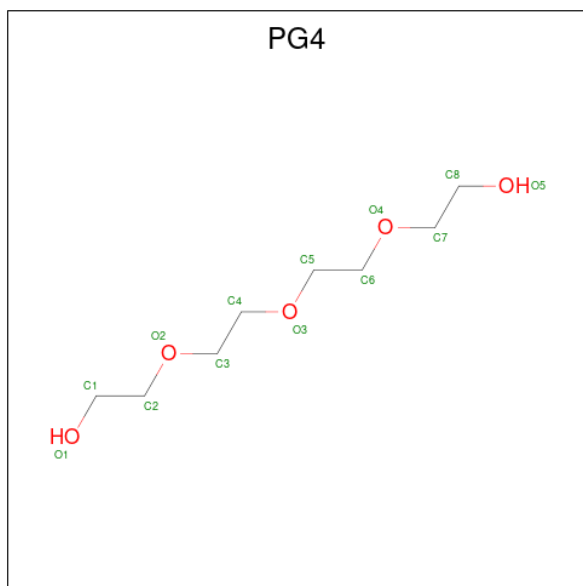


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	3	Total	Cl	0	0
			3	3		
9	C	1	Total	Cl	0	0
			1	1		
9	D	1	Total	Cl	0	0
			1	1		
9	E	1	Total	Cl	0	0
			1	1		
9	F	1	Total	Cl	0	0
			1	1		
9	J	1	Total	Cl	0	0
			1	1		
9	L	1	Total	Cl	0	0
			1	1		
9	M	1	Total	Cl	0	0
			1	1		
9	N	1	Total	Cl	0	0
			1	1		

- Molecule 10 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



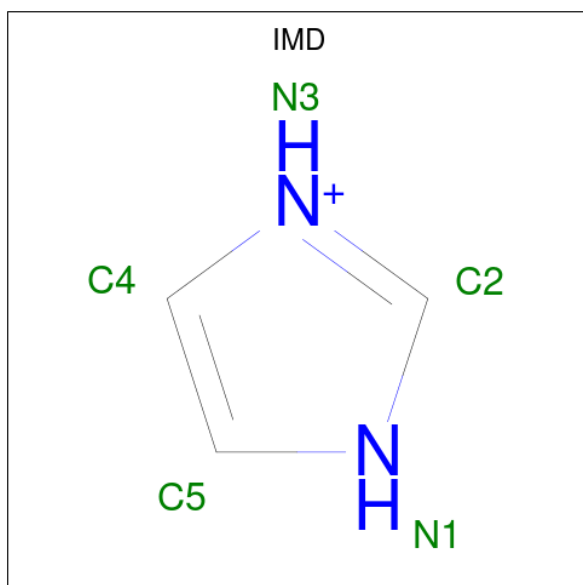
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			13	8	5		
10	D	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			13	8	5		
10	L	1	Total	C	O	0	0
			13	8	5		

- Molecule 11 is IMIDAZOLE (CCD ID: IMD) (formula:  $C_3H_5N_2$ ).



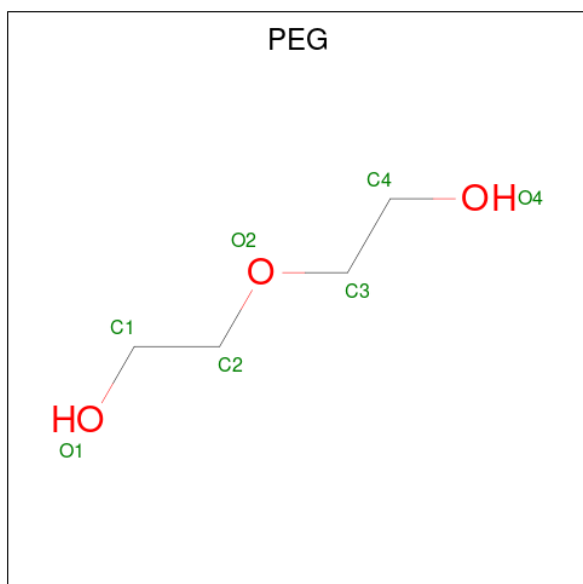
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	N	0	0
			5	3	2		
11	B	1	Total	C	N	0	0
			5	3	2		
11	C	1	Total	C	N	0	0
			5	3	2		
11	E	1	Total	C	N	0	0
			5	3	2		
11	F	1	Total	C	N	0	0
			5	3	2		
11	I	1	Total	C	N	0	0
			5	3	2		
11	J	1	Total	C	N	0	0
			5	3	2		
11	J	1	Total	C	N	0	0
			5	3	2		
11	L	1	Total	C	N	0	0
			5	3	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	N	0	0
			5	3	2		
11	M	1	Total	C	N	0	0
			5	3	2		
11	N	1	Total	C	N	0	0
			5	3	2		
11	O	1	Total	C	N	0	0
			5	3	2		
11	b	1	Total	C	N	0	0
			5	3	2		
11	d	1	Total	C	N	0	0
			5	3	2		

- Molecule 12 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	F	1	Total	C	O	0	0
			7	4	3		
12	I	1	Total	C	O	0	0
			7	4	3		
12	K	1	Total	C	O	0	0
			7	4	3		
12	M	1	Total	C	O	0	0
			7	4	3		

- Molecule 13 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total	C	O	0	0
			10	6	4		

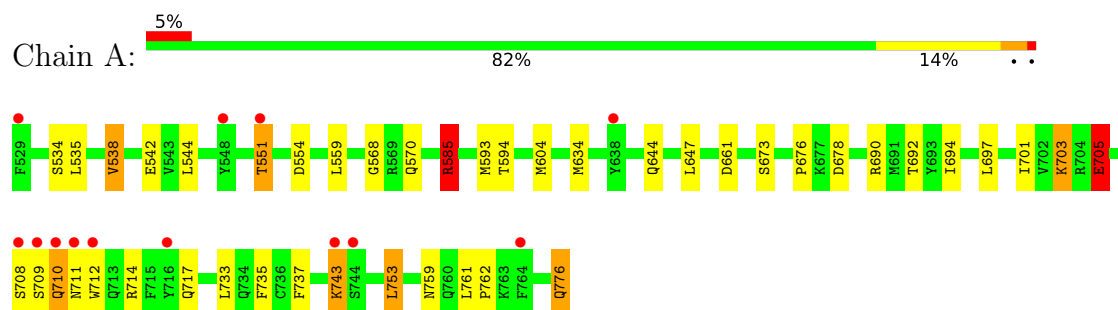
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	D	1	Total	O	0	0
			1	1		
14	I	3	Total	O	0	0
			3	3		
14	J	3	Total	O	0	0
			3	3		
14	K	1	Total	O	0	0
			1	1		
14	M	1	Total	O	0	0
			1	1		
14	O	2	Total	O	0	0
			2	2		
14	P	1	Total	O	0	0
			1	1		
14	i	1	Total	O	0	0
			1	1		

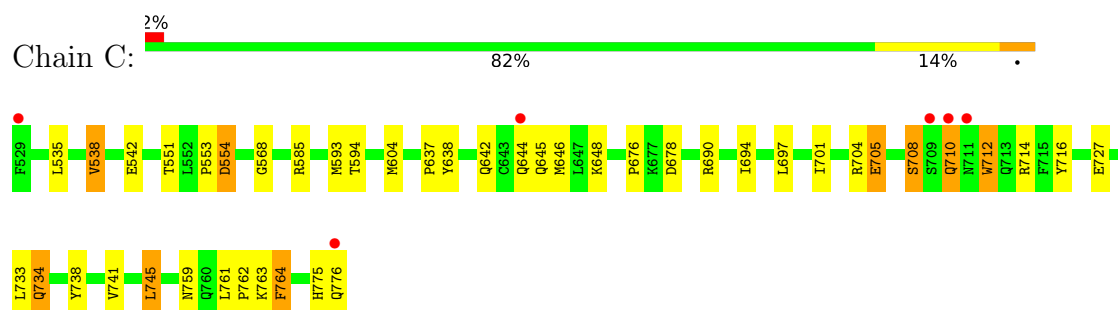
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

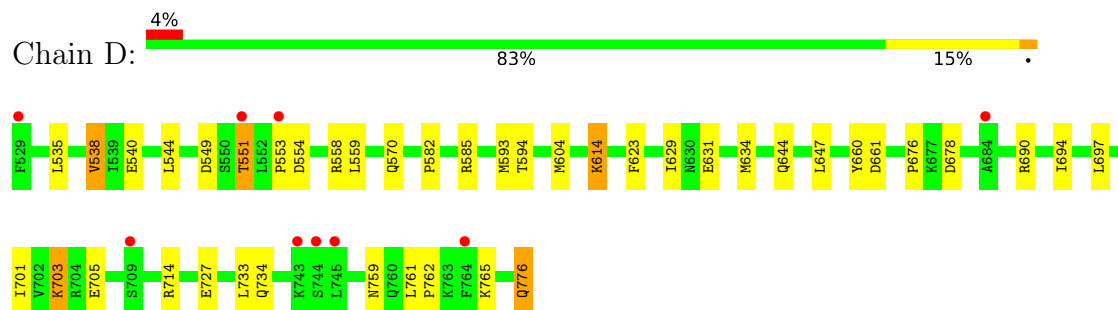
- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain



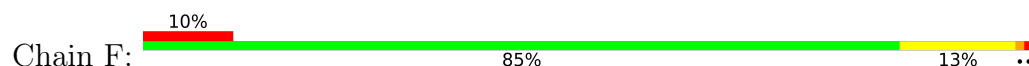
- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain



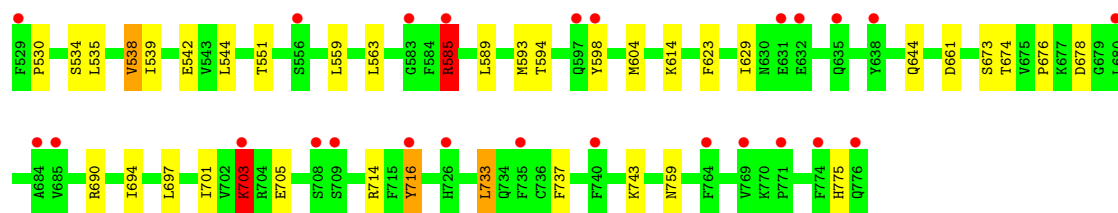
- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain



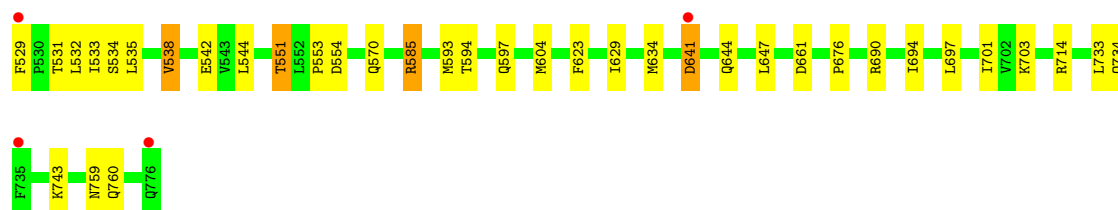
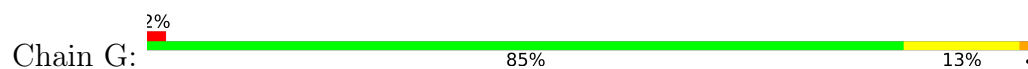
- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain



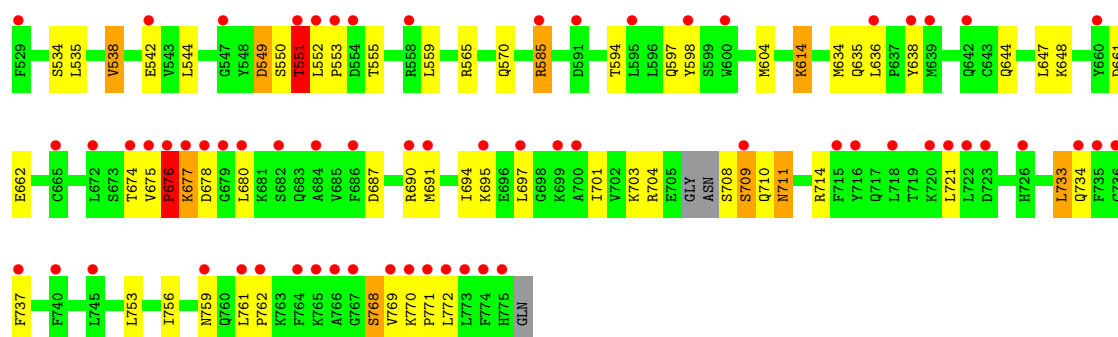
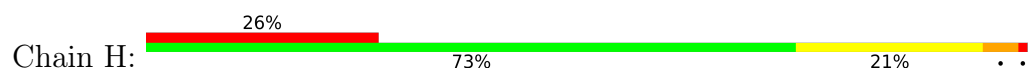




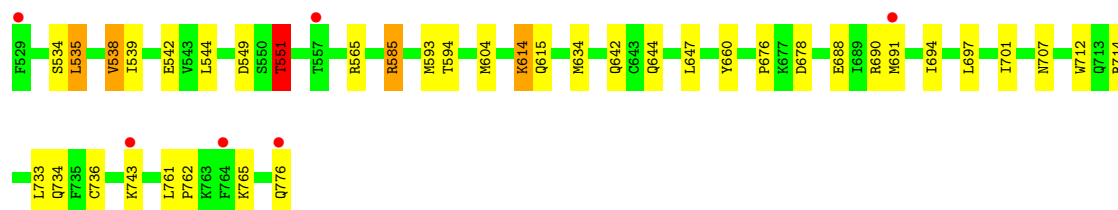
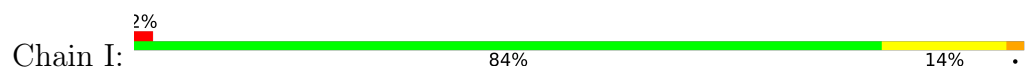
- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain



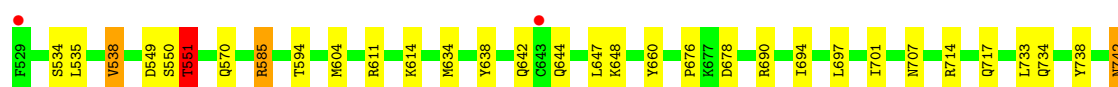
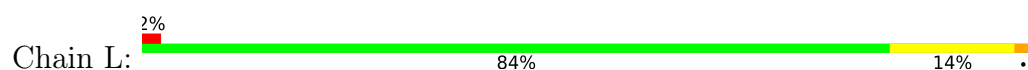
- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain



- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

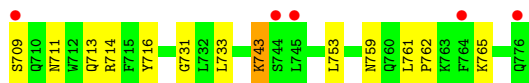
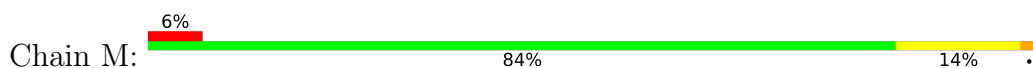


- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

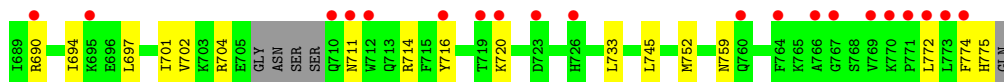
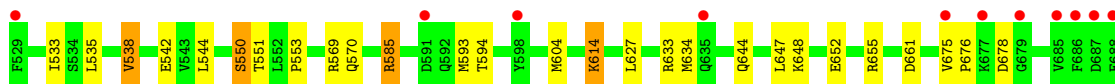
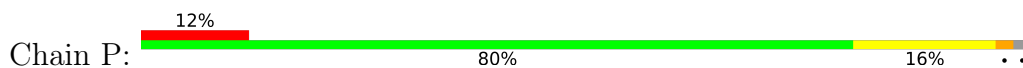




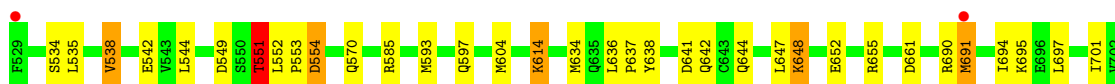
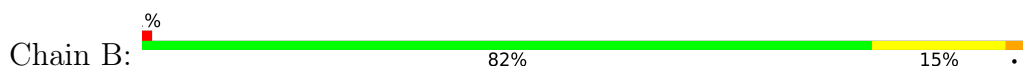
- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain



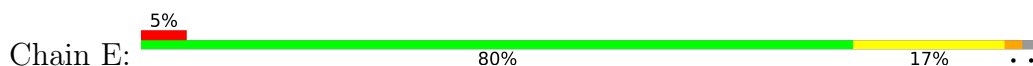
- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain



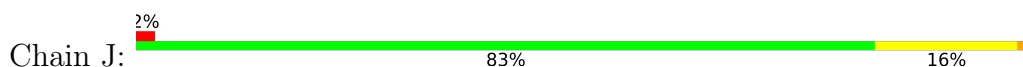
- Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain

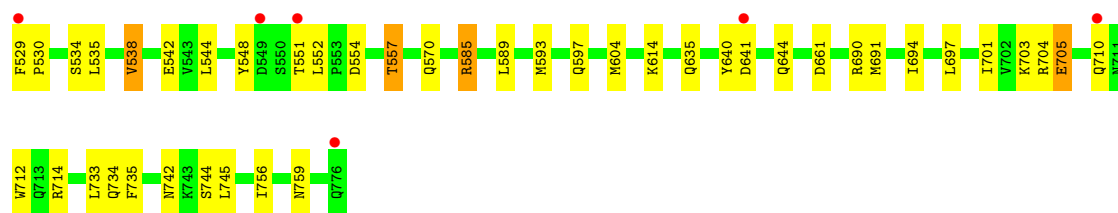


- Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain

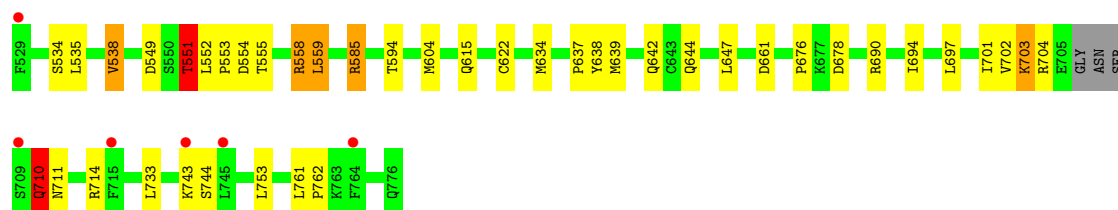
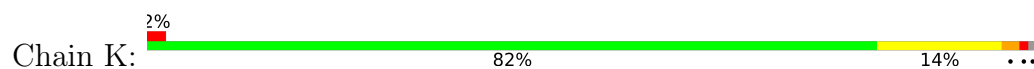


- Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain

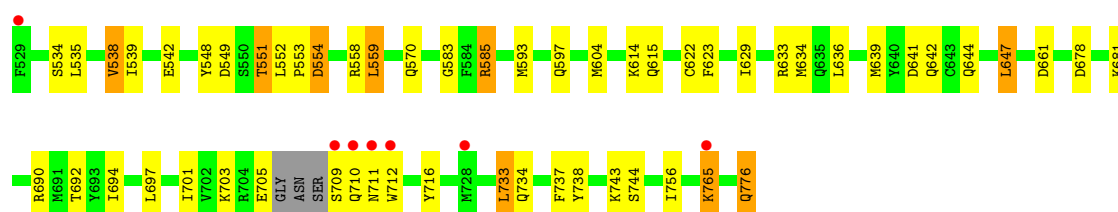
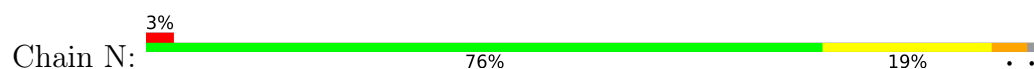




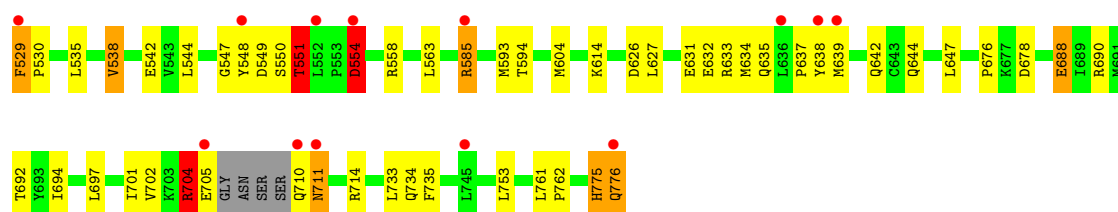
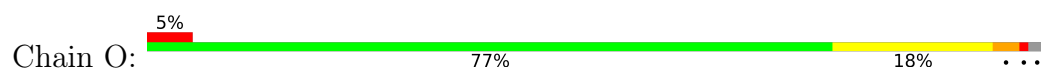
- Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain



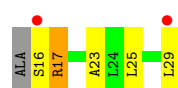
- Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain



- Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain

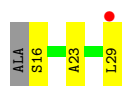


- Molecule 3: Nuclear receptor subfamily 0 group B member 2

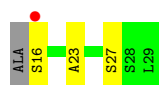
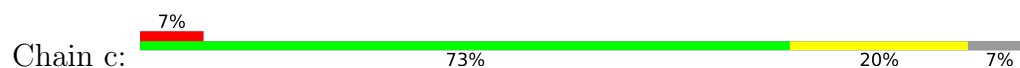


- Molecule 3: Nuclear receptor subfamily 0 group B member 2





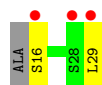
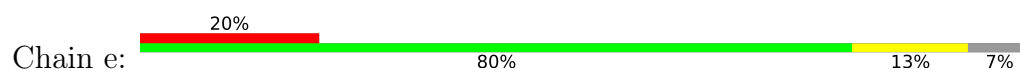
- Molecule 3: Nuclear receptor subfamily 0 group B member 2



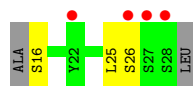
- Molecule 3: Nuclear receptor subfamily 0 group B member 2



- Molecule 3: Nuclear receptor subfamily 0 group B member 2



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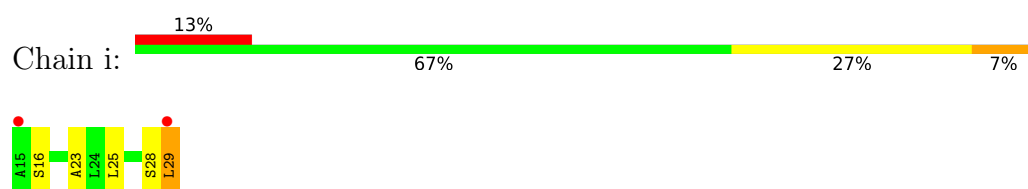
- Molecule 3: Nuclear receptor subfamily 0 group B member 2



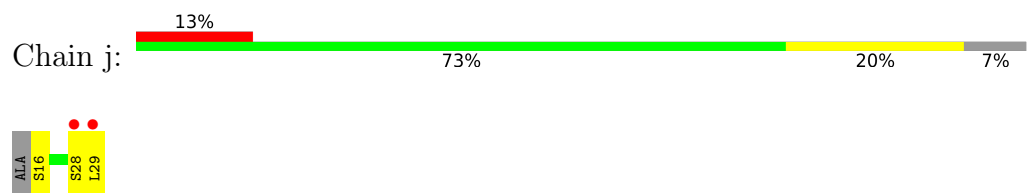
- Molecule 3: Nuclear receptor subfamily 0 group B member 2



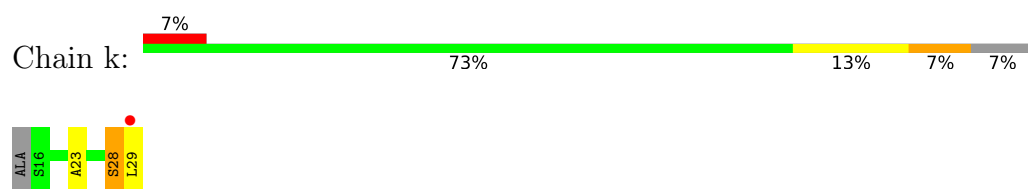
- Molecule 3: Nuclear receptor subfamily 0 group B member 2



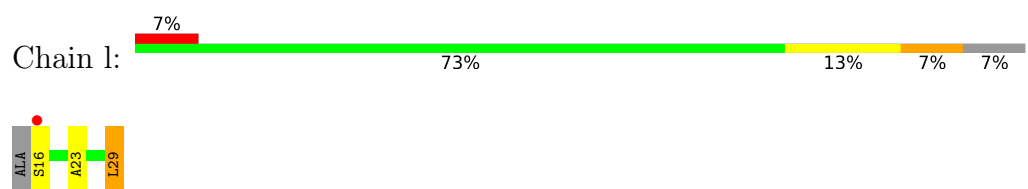
- Molecule 3: Nuclear receptor subfamily 0 group B member 2



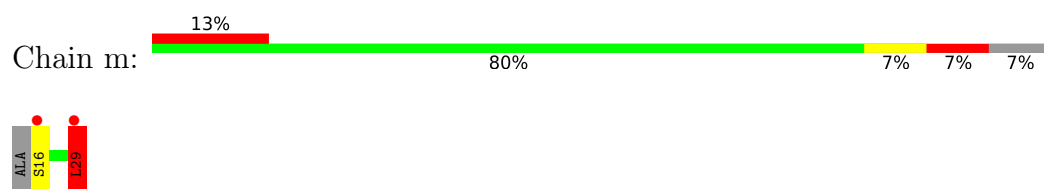
- Molecule 3: Nuclear receptor subfamily 0 group B member 2



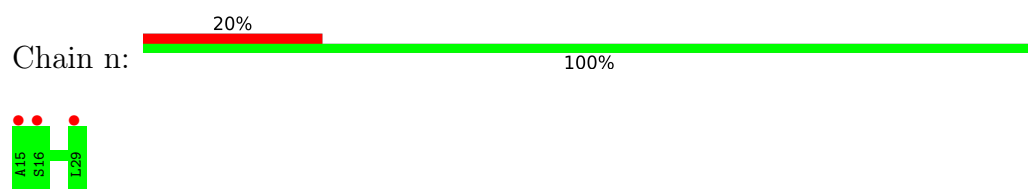
- Molecule 3: Nuclear receptor subfamily 0 group B member 2



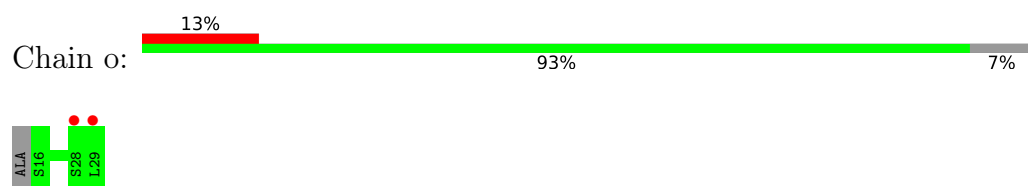
- Molecule 3: Nuclear receptor subfamily 0 group B member 2




- Molecule 3: Nuclear receptor subfamily 0 group B member 2



- Molecule 3: Nuclear receptor subfamily 0 group B member 2



- Molecule 3: Nuclear receptor subfamily 0 group B member 2

Chain p:  27% 80% 13% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	264.41Å 265.46Å 109.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.57 – 2.78 101.57 – 2.78	Depositor EDS
% Data completeness (in resolution range)	96.3 (101.57-2.78) 96.3 (101.57-2.78)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.211 , 0.244 0.211 , 0.245	Depositor DCC
$R_{free}$ test set	1946 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.6	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	34585	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, CSO, SO4, PGE, PEG, DEX, PG4, EPE, GOL, IMD, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.58	1/2051 (0.0%)	1.08	9/2769 (0.3%)
1	C	0.67	0/2051	1.14	5/2769 (0.2%)
1	D	0.57	0/2051	1.08	6/2769 (0.2%)
1	F	0.57	0/2057	1.12	4/2777 (0.1%)
1	G	0.53	0/2060	1.11	6/2781 (0.2%)
1	H	0.62	1/2029 (0.0%)	1.27	7/2738 (0.3%)
1	I	0.56	0/2051	1.08	4/2769 (0.1%)
1	L	0.58	0/2051	1.08	4/2769 (0.1%)
1	M	0.58	0/2051	1.16	10/2769 (0.4%)
1	P	0.58	0/2017	1.06	2/2722 (0.1%)
2	B	0.57	0/2044	1.06	3/2758 (0.1%)
2	E	0.61	0/2026	1.09	2/2733 (0.1%)
2	J	0.65	0/2055	1.09	6/2772 (0.2%)
2	K	0.61	0/2025	1.11	9/2731 (0.3%)
2	N	0.61	0/2036	1.12	6/2745 (0.2%)
2	O	0.62	0/2019	1.15	10/2723 (0.4%)
3	a	0.73	0/105	1.68	1/142 (0.7%)
3	b	0.58	0/105	0.98	0/142
3	c	0.68	0/105	0.99	0/142
3	d	0.67	0/105	1.03	0/142
3	e	0.58	0/105	0.99	0/142
3	f	0.64	0/97	0.94	0/131
3	g	0.73	0/97	1.06	0/131
3	h	0.63	0/97	1.79	1/131 (0.8%)
3	i	0.67	0/110	1.27	2/149 (1.3%)
3	j	0.75	0/105	0.99	0/142
3	k	0.73	0/105	1.07	1/142 (0.7%)
3	l	0.67	0/105	0.94	0/142
3	m	0.68	0/105	1.22	1/142 (0.7%)
3	n	0.67	0/110	0.96	0/149
3	o	0.57	0/105	0.96	0/142
3	p	0.56	0/105	0.95	0/142



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.60	2/34340 (0.0%)	1.12	99/46347 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3
1	F	0	1
1	H	0	2
1	M	0	1
2	J	0	1
2	O	0	3
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	709	SER	CA-CB	-5.48	1.45	1.52
1	A	709	SER	CA-CB	-5.33	1.45	1.53

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	676	PRO	CA-C-O	-23.80	88.75	122.31
1	H	676	PRO	CB-CA-C	20.69	142.46	111.22
3	a	17	ARG	CG-CD-NE	15.72	146.58	112.00
1	F	585	ARG	CG-CD-NE	15.50	146.10	112.00
1	M	552	LEU	N-CA-C	-15.28	88.40	108.11
3	h	17	ARG	CG-CD-NE	14.86	144.70	112.00
2	N	711	ASN	CB-CA-C	14.71	129.32	111.22
1	G	641	ASP	CA-CB-CG	14.46	127.06	112.60
1	I	585	ARG	CG-CD-NE	11.87	138.12	112.00
2	O	688	GLU	CB-CG-CD	10.60	130.63	112.60
1	D	727	GLU	CB-CG-CD	10.19	129.92	112.60
1	H	585	ARG	CG-CD-NE	9.56	133.03	112.00
2	O	554	ASP	CA-CB-CG	-9.01	103.59	112.60
1	H	676	PRO	N-CA-CB	-8.74	91.89	103.42
2	K	710	GLN	N-CA-C	8.38	123.09	109.76
2	K	637	PRO	N-CA-CB	8.33	112.23	103.15
1	M	633	ARG	CB-CG-CD	8.28	130.34	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	642	GLN	CB-CG-CD	8.22	126.57	112.60
1	M	548	TYR	CB-CA-C	8.18	123.30	109.72
1	H	768	SER	CA-C-O	8.15	129.61	119.59
1	M	585	ARG	CB-CG-CD	7.99	129.69	111.30
1	F	551	THR	CB-CA-C	7.85	125.06	110.70
2	E	711	ASN	CA-CB-CG	7.76	120.36	112.60
1	C	705	GLU	CB-CA-C	7.74	125.82	110.42
2	O	633	ARG	CG-CD-NE	-7.68	95.11	112.00
1	C	551	THR	CB-CA-C	7.63	124.67	110.70
1	P	551	THR	CB-CA-C	7.60	124.61	110.70
2	O	554	ASP	CB-CA-C	7.59	126.12	110.40
2	O	704	ARG	O-C-N	-7.55	111.22	122.39
1	M	551	THR	O-C-N	-7.45	113.14	122.82
2	B	551	THR	CA-CB-OG1	-7.28	98.68	109.60
2	N	551	THR	CA-CB-OG1	-7.28	98.68	109.60
2	J	705	GLU	CB-CA-C	7.23	124.80	110.42
2	O	711	ASN	CB-CA-C	7.17	123.54	111.22
3	i	28	SER	CA-C-N	7.13	134.54	121.70
3	i	28	SER	C-N-CA	7.13	134.54	121.70
2	J	557	THR	CA-CB-OG1	7.09	120.24	109.60
3	m	29	LEU	CB-CA-C	7.01	123.41	110.10
2	K	551	THR	CA-CB-OG1	-6.99	99.12	109.60
1	H	551	THR	CA-CB-OG1	-6.94	99.20	109.60
1	L	551	THR	CA-CB-OG1	-6.93	99.20	109.60
1	D	551	THR	CA-CB-OG1	-6.88	99.28	109.60
2	E	551	THR	CA-CB-OG1	-6.86	99.31	109.60
1	M	552	LEU	N-CA-CB	6.82	120.25	110.77
2	O	551	THR	CA-CB-OG1	-6.76	99.46	109.60
1	A	551	THR	CA-CB-OG1	-6.72	99.52	109.60
2	O	642	GLN	CB-CG-CD	6.69	123.98	112.60
1	G	734	GLN	CB-CA-C	6.67	121.45	110.90
1	G	551	THR	CA-CB-OG1	-6.67	99.59	109.60
2	K	637	PRO	CA-C-O	-6.59	109.64	120.05
1	I	551	THR	CA-CB-OG1	-6.59	99.72	109.60
1	H	676	PRO	N-CA-C	-6.52	102.09	111.22
1	C	554	ASP	CA-CB-CG	6.46	119.06	112.60
3	k	28	SER	N-CA-C	6.27	121.01	113.23
1	A	705	GLU	CB-CA-C	6.25	122.87	110.42
1	D	538	VAL	CA-CB-CG2	6.16	120.87	110.40
1	G	585	ARG	CB-CG-CD	-6.01	97.47	111.30
2	O	538	VAL	CA-CB-CG2	5.99	120.57	110.40
1	A	710	GLN	CA-C-N	5.91	128.47	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	710	GLN	C-N-CA	5.91	128.47	120.38
1	F	703	LYS	CG-CD-CE	5.91	124.88	111.30
2	B	554	ASP	CA-CB-CG	5.83	118.43	112.60
2	N	712	TRP	CB-CA-C	5.81	122.14	109.99
2	N	710	GLN	CB-CA-C	5.80	121.33	111.35
2	B	765	LYS	CB-CG-CD	5.79	124.62	111.30
1	L	734	GLN	CA-CB-CG	5.79	125.67	114.10
1	C	712	TRP	CB-CA-C	5.75	121.22	109.55
1	F	716	TYR	CA-CB-CG	5.64	124.06	113.90
1	C	538	VAL	CA-CB-CG2	5.63	119.97	110.40
1	M	765	LYS	CB-CG-CD	5.62	124.22	111.30
2	K	710	GLN	CB-CG-CD	5.58	122.09	112.60
1	M	551	THR	N-CA-C	-5.58	97.11	107.71
1	A	712	TRP	CB-CA-C	5.55	121.60	109.99
1	M	551	THR	CA-CB-OG1	-5.45	101.42	109.60
2	J	712	TRP	CB-CA-C	5.41	121.30	109.99
1	D	554	ASP	CA-CB-CG	5.36	117.96	112.60
1	D	554	ASP	CB-CA-C	-5.36	100.47	109.53
1	P	538	VAL	CA-CB-CG2	5.35	119.50	110.40
1	G	554	ASP	CA-CB-CG	5.35	117.95	112.60
1	D	765	LYS	CB-CG-CD	5.28	123.44	111.30
2	J	551	THR	CA-CB-OG1	5.25	117.48	109.60
1	M	716	TYR	CA-CB-CG	5.24	123.34	113.90
2	K	585	ARG	CG-CD-NE	5.22	123.48	112.00
2	K	711	ASN	CA-C-O	5.18	126.31	120.92
2	J	551	THR	CA-CB-CG2	5.17	119.29	110.50
1	A	585	ARG	CB-CG-CD	5.15	123.14	111.30
2	K	558	ARG	NE-CZ-NH1	-5.13	116.37	121.50
2	N	554	ASP	CB-CA-C	-5.11	100.91	109.65
1	A	717	GLN	CB-CG-CD	5.10	121.27	112.60
1	I	707	ASN	CA-C-N	5.10	127.36	120.38
1	I	707	ASN	C-N-CA	5.10	127.36	120.38
1	G	554	ASP	CB-CA-C	-5.09	100.92	109.53
2	K	554	ASP	CB-CA-C	-5.06	101.60	109.84
1	A	554	ASP	CB-CA-C	-5.04	101.01	109.53
2	J	548	TYR	CA-CB-CG	5.04	122.97	113.90
1	A	743	LYS	CB-CG-CD	5.03	122.87	111.30
1	L	707	ASN	CA-C-N	5.03	127.02	120.28
1	L	707	ASN	C-N-CA	5.03	127.02	120.28
2	O	639	MET	N-CA-CB	5.03	118.05	110.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	704	ARG	Peptide
1	C	708	SER	Peptide
1	C	738	TYR	Sidechain
1	F	775	HIS	Sidechain
1	H	549	ASP	Sidechain
1	H	676	PRO	Mainchain
2	J	704	ARG	Peptide
1	M	551	THR	Mainchain
2	O	554	ASP	Peptide
2	O	704	ARG	Peptide
2	O	775	HIS	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2007	0	2030	31	0
1	C	2007	0	2029	43	0
1	D	2007	0	2030	30	0
1	F	2008	0	2031	29	0
1	G	2011	0	2034	28	0
1	H	1986	0	2012	66	1
1	I	2007	0	2030	27	0
1	L	2007	0	2030	31	0
1	M	2007	0	2030	29	0
1	P	1974	0	2002	51	0
2	B	2010	0	2031	40	0
2	E	1988	0	2016	31	0
2	J	2014	0	2039	32	0
2	K	1992	0	2016	32	0
2	N	1997	0	2021	50	1
2	O	1986	0	2010	42	0
3	a	104	0	113	4	0
3	b	104	0	113	3	0
3	c	104	0	113	3	0
3	d	104	0	113	9	0
3	e	104	0	113	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	f	96	0	102	2	0
3	g	96	0	102	3	0
3	h	96	0	102	2	0
3	i	109	0	118	4	0
3	j	104	0	113	3	0
3	k	104	0	113	4	0
3	l	104	0	113	3	0
3	m	104	0	113	3	0
3	n	109	0	118	0	0
3	o	104	0	113	0	0
3	p	104	0	113	3	0
4	A	28	0	29	1	0
4	B	28	0	29	4	0
4	C	28	0	29	3	0
4	D	28	0	29	0	0
4	E	28	0	29	3	0
4	F	28	0	29	2	0
4	G	28	0	29	0	0
4	H	28	0	29	1	0
4	I	28	0	29	2	0
4	J	28	0	29	2	0
4	K	28	0	29	2	0
4	L	28	0	29	1	0
4	M	28	0	29	1	0
4	N	28	0	29	2	0
4	O	28	0	29	2	0
4	P	28	0	29	0	0
5	A	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	H	5	0	0	1	0
5	I	5	0	0	0	0
5	K	5	0	0	0	0
5	M	5	0	0	0	0
5	O	5	0	0	0	0
6	A	15	0	18	0	0
6	B	15	0	18	1	0
6	D	15	0	18	1	0
6	I	15	0	18	2	0
6	J	15	0	18	0	0
6	L	15	0	18	1	0
6	P	15	0	18	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	12	0	16	1	0
7	B	6	0	8	0	0
7	C	12	0	16	8	0
7	E	18	0	24	0	0
7	I	6	0	8	1	0
7	J	18	0	24	0	0
7	K	12	0	16	0	0
7	L	12	0	16	5	0
7	M	6	0	8	0	0
7	N	6	0	8	1	0
7	O	6	0	8	0	0
7	P	6	0	8	4	0
8	A	5	0	0	1	0
8	B	5	0	0	0	0
8	C	10	0	0	3	0
8	J	5	0	0	0	0
9	B	3	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	J	1	0	0	0	0
9	L	1	0	0	1	0
9	M	1	0	0	0	0
9	N	1	0	0	0	0
10	B	13	0	18	0	0
10	D	13	0	18	1	0
10	H	13	0	18	1	0
10	L	13	0	18	0	0
11	B	10	0	10	0	0
11	C	5	0	5	0	0
11	E	5	0	5	0	0
11	F	5	0	5	0	0
11	I	5	0	5	0	0
11	J	10	0	10	0	0
11	L	10	0	10	2	0
11	M	5	0	5	0	0
11	N	5	0	5	2	0
11	O	5	0	5	1	0
11	b	5	0	5	0	0
11	d	5	0	5	4	0
12	F	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	I	7	0	10	0	0
12	K	7	0	10	1	0
12	M	7	0	10	0	0
13	M	10	0	14	2	0
14	D	1	0	0	0	0
14	I	3	0	0	1	0
14	J	3	0	0	0	0
14	K	1	0	0	0	0
14	M	1	0	0	0	0
14	O	2	0	0	0	0
14	P	1	0	0	0	0
14	i	1	0	0	1	0
All	All	34585	0	35127	544	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (544) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:711:ASN:HB2	6:P:1002:EPE:C6	1.19	1.65
1:P:711:ASN:CB	6:P:1002:EPE:H62	1.30	1.56
1:P:711:ASN:CB	6:P:1002:EPE:C6	1.84	1.50
1:P:711:ASN:CG	6:P:1002:EPE:H62	1.40	1.44
1:C:763:LYS:NZ	8:C:1006:SO4:O4	1.59	1.32
1:I:551:THR:O	1:P:553:PRO:HB3	1.16	1.25
2:J:742:ASN:OD1	2:N:552:LEU:HD21	1.40	1.18
2:J:640:TYR:CE2	2:K:744:SER:HB2	1.82	1.14
1:I:585:ARG:NH2	3:i:25:LEU:O	1.83	1.12
2:J:640:TYR:HE2	2:K:744:SER:HB2	0.98	1.08
1:P:716:TYR:HE1	1:P:775:HIS:CD2	1.71	1.08
1:P:711:ASN:HB3	6:P:1002:EPE:H92	1.29	1.08
2:J:742:ASN:OD1	2:N:552:LEU:CD2	2.02	1.07
1:H:598:TYR:HE2	1:H:676:PRO:HB3	1.17	1.03
1:H:676:PRO:HD3	1:H:680:LEU:HD21	1.37	1.03
1:I:551:THR:O	1:P:553:PRO:CB	2.08	1.00
1:H:759:ASN:ND2	3:h:16:SER:O	1.96	0.99
1:H:598:TYR:CE2	1:H:676:PRO:HB3	1.96	0.99
1:M:711:ASN:HB3	13:M:804:PGE:H4	1.42	0.97
1:P:711:ASN:CB	6:P:1002:EPE:H61	1.68	0.97
1:P:759:ASN:ND2	3:p:16:SER:O	1.99	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:677:LYS:N	1:H:768:SER:O	2.01	0.93
1:G:585:ARG:NH2	3:g:25:LEU:O	2.01	0.92
1:L:660:TYR:HB2	6:L:1003:EPE:H101	1.52	0.90
1:D:593:MET:SD	3:d:21:LEU:HD13	2.12	0.90
2:E:759:ASN:ND2	3:e:16:SER:O	2.04	0.90
1:H:676:PRO:CD	1:H:680:LEU:CD2	2.51	0.89
1:P:716:TYR:CE1	1:P:775:HIS:CD2	2.61	0.88
2:O:548:TYR:CD2	2:O:627:LEU:HD13	2.09	0.87
1:H:676:PRO:CD	1:H:680:LEU:HD21	2.04	0.87
1:I:565:ARG:NH1	14:I:1101:HOH:O	2.04	0.87
1:P:711:ASN:HB2	6:P:1002:EPE:H61	0.87	0.86
1:P:711:ASN:HB3	6:P:1002:EPE:C6	2.06	0.86
2:J:640:TYR:HE2	2:K:744:SER:CB	1.86	0.86
2:B:553:PRO:HD2	1:C:638:TYR:OH	1.76	0.85
1:P:716:TYR:CE1	1:P:775:HIS:NE2	2.45	0.85
1:H:675:VAL:O	1:H:676:PRO:O	1.96	0.83
3:j:28:SER:O	3:j:29:LEU:HB2	1.79	0.82
1:L:759:ASN:ND2	3:l:16:SER:O	2.12	0.82
1:P:716:TYR:HE1	1:P:775:HIS:NE2	1.78	0.82
1:P:711:ASN:HB3	6:P:1002:EPE:C9	2.10	0.81
1:H:676:PRO:C	1:H:768:SER:O	2.24	0.80
1:D:759:ASN:ND2	3:d:16:SER:O	2.14	0.80
1:H:676:PRO:HA	1:H:768:SER:O	1.80	0.80
2:O:775:HIS:O	2:O:776:GLN:HG3	1.81	0.80
3:i:16:SER:HB2	14:i:101:HOH:O	1.82	0.79
2:K:559:LEU:CD2	2:K:639:MET:HE2	2.13	0.78
1:H:676:PRO:HD3	1:H:680:LEU:CD2	2.13	0.78
1:H:676:PRO:CG	1:H:680:LEU:HD23	2.14	0.77
2:N:641:ASP:HB3	2:O:637:PRO:CD	2.14	0.76
1:H:675:VAL:C	1:H:676:PRO:O	2.18	0.76
2:N:692:THR:HG21	3:m:29:LEU:HD12	1.67	0.76
2:B:637:PRO:HB3	1:H:553:PRO:HG3	1.66	0.76
1:C:763:LYS:NZ	8:C:1006:SO4:S	2.52	0.76
1:H:676:PRO:CD	1:H:680:LEU:HD23	2.16	0.76
3:k:28:SER:O	3:k:29:LEU:HB2	1.85	0.76
2:N:641:ASP:HB3	2:O:637:PRO:HD2	1.68	0.76
1:P:704:ARG:NH2	1:P:714:ARG:NH1	2.33	0.75
1:C:712:TRP:CE2	1:M:713:GLN:HG3	2.22	0.75
2:N:738:TYR:CD2	2:O:635:GLN:HG3	2.22	0.74
1:H:677:LYS:HB2	1:H:768:SER:HA	1.70	0.73
2:O:690:ARG:O	2:O:694:ILE:HG13	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:648:LYS:NZ	1:H:638:TYR:OH	2.20	0.73
1:L:690:ARG:O	1:L:694:ILE:HG13	1.89	0.73
2:E:690:ARG:O	2:E:694:ILE:HG13	1.88	0.73
2:N:690:ARG:O	2:N:694:ILE:HG13	1.89	0.72
1:A:690:ARG:O	1:A:694:ILE:HG13	1.89	0.72
2:B:690:ARG:O	2:B:694:ILE:HG13	1.89	0.72
1:F:690:ARG:O	1:F:694:ILE:HG13	1.88	0.72
1:G:690:ARG:O	1:G:694:ILE:HG13	1.89	0.72
1:I:690:ARG:O	1:I:694:ILE:HG13	1.89	0.72
1:P:690:ARG:O	1:P:694:ILE:HG13	1.89	0.72
2:K:690:ARG:O	2:K:694:ILE:HG13	1.89	0.72
2:J:690:ARG:O	2:J:694:ILE:HG13	1.90	0.71
1:M:690:ARG:O	1:M:694:ILE:HG13	1.89	0.71
1:D:690:ARG:O	1:D:694:ILE:HG13	1.89	0.71
2:N:623:PHE:CE2	2:N:629:ILE:HD12	2.25	0.71
1:C:690:ARG:O	1:C:694:ILE:HG13	1.90	0.71
1:H:690:ARG:O	1:H:694:ILE:HG13	1.89	0.70
1:P:711:ASN:CG	6:P:1002:EPE:C6	2.36	0.70
2:N:765:LYS:HE3	11:N:1003:IMD:HN3	1.55	0.70
1:C:727:GLU:OE2	2:E:738:TYR:OH	2.10	0.69
1:H:604:MET:HE2	1:H:604:MET:HA	1.74	0.69
1:A:759:ASN:ND2	3:a:16:SER:O	2.21	0.69
1:F:623:PHE:CE2	1:F:629:ILE:HD12	2.27	0.69
1:C:568:GLY:HA3	7:C:1002:GOL:C3	2.23	0.69
1:D:623:PHE:CE2	1:D:629:ILE:HD12	2.28	0.69
1:G:623:PHE:CE2	1:G:629:ILE:HD12	2.28	0.69
2:N:559:LEU:HD23	2:N:639:MET:HE2	1.76	0.68
1:P:604:MET:HE2	1:P:604:MET:HA	1.75	0.68
1:L:604:MET:HA	1:L:604:MET:HE2	1.76	0.68
1:F:604:MET:HE2	1:F:604:MET:HA	1.76	0.68
1:P:711:ASN:OD1	6:P:1002:EPE:H62	1.92	0.68
2:K:604:MET:HE2	2:K:604:MET:HA	1.74	0.68
1:H:598:TYR:HE2	1:H:676:PRO:CB	1.99	0.67
2:E:604:MET:HA	2:E:604:MET:HE2	1.76	0.67
2:B:604:MET:HE2	2:B:604:MET:HA	1.77	0.67
2:J:742:ASN:OD1	2:N:552:LEU:HD22	1.95	0.67
1:G:604:MET:HE2	1:G:604:MET:HA	1.76	0.67
2:J:604:MET:HA	2:J:604:MET:HE2	1.77	0.66
1:I:604:MET:HE2	1:I:604:MET:HA	1.77	0.66
1:M:604:MET:HE2	1:M:604:MET:HA	1.76	0.66
1:C:554:ASP:OD1	1:H:551:THR:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:589:LEU:HD23	2:J:589:LEU:O	1.95	0.66
2:N:738:TYR:CG	2:O:635:GLN:HG3	2.31	0.66
2:O:604:MET:HA	2:O:604:MET:HE2	1.78	0.66
2:N:641:ASP:HB3	2:O:637:PRO:HG2	1.79	0.65
2:O:585:ARG:NH1	1:P:585:ARG:HG3	2.10	0.65
2:J:589:LEU:HD23	2:J:589:LEU:C	2.22	0.65
2:N:604:MET:HE2	2:N:604:MET:HA	1.78	0.65
2:B:637:PRO:CB	1:H:553:PRO:HG3	2.27	0.65
2:K:559:LEU:HD23	2:K:639:MET:HE2	1.76	0.65
1:A:604:MET:HE2	1:A:604:MET:HA	1.77	0.65
1:C:568:GLY:C	7:C:1002:GOL:H31	2.21	0.65
1:C:604:MET:HA	1:C:604:MET:HE2	1.77	0.64
1:D:604:MET:HE2	1:D:604:MET:HA	1.79	0.64
2:O:638:TYR:HB3	2:O:735:PHE:HZ	1.62	0.64
1:D:553:PRO:HA	1:G:553:PRO:HB3	1.80	0.64
1:H:687:ASP:O	1:H:691:MET:HG2	1.97	0.64
1:H:674:THR:HG23	1:H:769:VAL:HG13	1.79	0.64
1:H:674:THR:CG2	1:H:769:VAL:HG13	2.28	0.63
1:M:759:ASN:ND2	3:m:16:SER:O	2.28	0.63
1:H:676:PRO:CG	1:H:680:LEU:CD2	2.77	0.63
2:N:776:GLN:OE1	2:N:776:GLN:HA	1.98	0.62
11:O:1004:IMD:HN1	1:P:569:ARG:HE	1.47	0.62
1:C:568:GLY:HA3	7:C:1002:GOL:H31	1.82	0.62
1:D:660:TYR:HB2	6:D:804:EPE:H101	1.81	0.62
1:F:589:LEU:HD23	1:F:589:LEU:O	2.00	0.61
1:L:776:GLN:HA	1:L:776:GLN:OE1	2.00	0.61
2:N:641:ASP:HB3	2:O:637:PRO:CG	2.30	0.61
2:N:623:PHE:HE2	2:N:629:ILE:HD12	1.63	0.61
1:D:553:PRO:HA	1:G:553:PRO:CB	2.30	0.61
1:L:638:TYR:HD1	7:L:1004:GOL:H2	1.66	0.61
1:G:531:THR:HG22	1:G:533:ILE:H	1.65	0.61
1:D:701:ILE:HG23	1:D:714:ARG:HG2	1.83	0.61
4:E:1001:DEX:O2	4:E:1001:DEX:H821	2.01	0.61
2:B:701:ILE:HG23	2:B:714:ARG:HG2	1.83	0.60
2:J:710:GLN:OE1	2:J:710:GLN:N	2.34	0.60
1:P:704:ARG:NH2	1:P:714:ARG:HH12	1.97	0.60
1:H:594:THR:HG21	1:H:676:PRO:HG3	1.84	0.60
1:F:589:LEU:HD23	1:F:589:LEU:C	2.26	0.60
1:D:623:PHE:HE2	1:D:629:ILE:HD12	1.67	0.60
1:M:701:ILE:HG23	1:M:714:ARG:HG2	1.84	0.60
1:F:701:ILE:HG23	1:F:714:ARG:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:585:ARG:HH11	1:L:585:ARG:HE	1.51	0.59
2:K:638:TYR:CD2	2:K:638:TYR:N	2.70	0.59
1:G:534:SER:O	1:G:538:VAL:HG13	2.02	0.59
1:M:534:SER:O	1:M:538:VAL:HG13	2.02	0.59
1:F:534:SER:O	1:F:538:VAL:HG13	2.02	0.59
1:H:534:SER:O	1:H:538:VAL:HG13	2.02	0.59
1:L:642:GLN:HB2	4:L:1001:DEX:C22	2.33	0.59
2:J:534:SER:O	2:J:538:VAL:HG13	2.03	0.59
2:K:534:SER:O	2:K:538:VAL:HG13	2.03	0.59
1:D:776:GLN:OE1	1:D:776:GLN:HA	2.01	0.59
1:C:775:HIS:O	1:C:776:GLN:C	2.46	0.59
2:E:534:SER:O	2:E:538:VAL:HG13	2.02	0.59
1:G:701:ILE:HG23	1:G:714:ARG:HG2	1.84	0.58
1:A:534:SER:O	1:A:538:VAL:HG13	2.02	0.58
2:B:549:ASP:OD1	2:B:551:THR:HB	2.04	0.58
2:N:554:ASP:HB3	2:N:636:LEU:HD11	1.85	0.58
1:L:638:TYR:CD1	7:L:1004:GOL:H2	2.38	0.58
1:I:534:SER:O	1:I:538:VAL:HG13	2.03	0.58
2:K:535:LEU:HD11	3:L:23:ALA:HB1	1.85	0.58
2:K:615:GLN:HB2	2:K:622[B]:CSO:OD	2.04	0.58
2:N:559:LEU:CD2	2:N:639:MET:HE2	2.34	0.58
1:L:534:SER:O	1:L:538:VAL:HG13	2.03	0.58
1:I:701:ILE:HG23	1:I:714:ARG:HG2	1.86	0.58
2:B:534:SER:O	2:B:538:VAL:HG13	2.03	0.57
2:B:642:GLN:OE1	4:B:802:DEX:O3	2.18	0.57
2:J:701:ILE:HG23	2:J:714:ARG:HG2	1.86	0.57
2:N:534:SER:O	2:N:538:VAL:HG13	2.03	0.57
1:L:701:ILE:HG23	1:L:714:ARG:HG2	1.85	0.57
2:O:632:GLU:OE1	2:O:632:GLU:N	2.38	0.57
3:j:28:SER:O	3:j:29:LEU:CB	2.50	0.57
1:A:776:GLN:OE1	1:A:776:GLN:HA	2.04	0.57
2:K:549:ASP:OD1	2:K:551:THR:HB	2.04	0.57
1:C:716:TYR:CE1	1:M:709:SER:HB3	2.40	0.56
1:C:701:ILE:HG23	1:C:714:ARG:HG2	1.87	0.56
1:D:593:MET:SD	3:d:21:LEU:CD1	2.91	0.56
2:E:642:GLN:OE1	4:E:1001:DEX:O3	2.12	0.56
1:G:585:ARG:HD2	1:H:585:ARG:NH1	2.20	0.56
1:L:745:LEU:HD21	7:L:1005:GOL:H12	1.87	0.56
1:C:764:PHE:HB2	7:C:1003:GOL:C3	2.35	0.56
1:P:711:ASN:HB2	6:P:1002:EPE:C5	2.22	0.56
2:B:553:PRO:HD2	1:C:638:TYR:CZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:GLY:CA	7:C:1002:GOL:H31	2.36	0.56
1:L:549:ASP:OD1	1:L:551:THR:HB	2.04	0.56
2:N:765:LYS:HE3	11:N:1003:IMD:N3	2.20	0.56
2:O:549:ASP:OD1	2:O:551:THR:HB	2.05	0.56
2:E:549:ASP:OD1	2:E:551:THR:HB	2.05	0.56
1:A:585:ARG:NH2	3:a:25:LEU:O	2.29	0.56
1:I:549:ASP:OD1	1:I:551:THR:HB	2.05	0.56
6:I:1004:EPE:O8	7:I:1005:GOL:H11	2.06	0.56
2:O:701:ILE:HG23	2:O:714:ARG:HG2	1.86	0.56
2:O:702:VAL:HG22	2:O:710:GLN:HA	1.87	0.55
1:P:652:GLU:OE2	1:P:655:ARG:NH1	2.39	0.55
2:E:691:MET:HG2	1:I:688:GLU:HB2	1.88	0.55
1:A:701:ILE:HG23	1:A:714:ARG:HG2	1.88	0.55
2:O:529:PHE:N	2:O:530:PRO:HD2	2.22	0.55
2:B:652:GLU:OE2	2:B:655:ARG:NH1	2.40	0.55
2:K:549:ASP:O	2:K:558:ARG:NH1	2.40	0.55
2:B:549:ASP:OD2	2:B:552:LEU:HD13	2.07	0.55
2:B:641:ASP:OD2	1:H:636:LEU:HD22	2.07	0.55
1:F:585:ARG:NH1	3:f:25:LEU:O	2.40	0.55
1:M:652:GLU:OE2	1:M:655:ARG:NH1	2.41	0.54
1:M:743:LYS:H	1:M:743:LYS:CD	2.20	0.54
1:L:742:ASN:HD22	1:L:742:ASN:C	2.14	0.54
2:O:710:GLN:HG3	2:O:711:ASN:N	2.22	0.54
1:H:676:PRO:CA	1:H:768:SER:O	2.54	0.54
1:H:708:SER:CB	1:H:710:GLN:HG3	2.38	0.54
1:H:662:GLU:CD	1:H:714:ARG:HH21	2.15	0.54
2:O:529:PHE:N	2:O:530:PRO:CD	2.71	0.54
1:C:710:GLN:N	1:C:710:GLN:OE1	2.41	0.53
2:B:691:MET:HE3	2:B:695:LYS:HE2	1.89	0.53
1:F:623:PHE:HE2	1:F:629:ILE:HD12	1.72	0.53
4:K:802:DEX:O2	4:K:802:DEX:H821	2.08	0.53
2:B:641:ASP:OD2	1:H:555:THR:HA	2.09	0.53
1:A:568:GLY:HA2	1:A:753:LEU:HD13	1.91	0.53
1:F:661:ASP:OD2	1:F:703:LYS:HE2	2.08	0.53
1:C:763:LYS:CE	8:C:1006:SO4:O4	2.53	0.53
1:D:540:GLU:OE2	10:D:803:PG4:H22	2.08	0.53
2:J:745:LEU:HD11	2:N:552:LEU:HB3	1.89	0.53
1:A:708:SER:CB	1:A:710:GLN:OE1	2.56	0.53
1:A:708:SER:OG	1:A:710:GLN:OE1	2.23	0.53
3:k:28:SER:O	3:k:29:LEU:CB	2.54	0.53
2:O:544:LEU:HD22	1:P:542:GLU:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:583:GLY:HA2	3:m:29:LEU:HD22	1.91	0.52
2:B:759:ASN:ND2	3:b:16:SER:O	2.30	0.52
2:J:529:PHE:N	2:J:530:PRO:CD	2.72	0.52
2:K:702:VAL:HG22	2:K:710:GLN:HB2	1.92	0.52
1:M:711:ASN:CB	13:M:804:PGE:H4	2.29	0.52
1:L:742:ASN:O	1:L:742:ASN:ND2	2.31	0.52
1:P:533:ILE:CG1	1:P:661:ASP:OD2	2.57	0.52
1:G:531:THR:HG21	1:G:533:ILE:HG22	1.91	0.52
2:K:559:LEU:HD22	2:K:639:MET:HE2	1.91	0.52
1:L:717:GLN:HG2	9:L:1008:CL:CL	2.46	0.52
2:O:548:TYR:CG	2:O:627:LEU:HD13	2.44	0.52
1:P:550:SER:OG	7:P:1003:GOL:O1	2.27	0.52
1:C:712:TRP:NE1	1:M:713:GLN:HG3	2.25	0.51
1:G:623:PHE:HE2	1:G:629:ILE:HD12	1.73	0.51
1:H:711:ASN:OD1	10:H:803:PG4:H52	2.10	0.51
1:P:633:ARG:NH1	7:P:1003:GOL:H12	2.25	0.51
1:G:544:LEU:HD22	1:H:542:GLU:HG3	1.92	0.51
2:B:641:ASP:OD2	1:H:636:LEU:CD2	2.58	0.51
1:G:531:THR:CG2	1:G:533:ILE:HG22	2.40	0.51
1:P:627:LEU:HA	7:P:1003:GOL:H11	1.93	0.51
4:F:1001:DEX:H821	4:F:1001:DEX:O2	2.11	0.51
1:M:544:LEU:CD2	2:N:542:GLU:HG3	2.40	0.51
1:G:542:GLU:HG3	1:H:544:LEU:CD2	2.41	0.51
1:M:544:LEU:HD22	2:N:542:GLU:HG3	1.93	0.51
2:E:542:GLU:HG3	1:F:544:LEU:HD22	1.93	0.50
2:J:597:GLN:HG2	2:J:756:ILE:HG23	1.93	0.50
1:C:775:HIS:HA	1:M:708:SER:OG	2.11	0.50
2:E:542:GLU:HG3	1:F:544:LEU:CD2	2.41	0.50
1:C:716:TYR:CD1	1:M:709:SER:CB	2.95	0.50
1:H:535:LEU:HD11	3:g:23:ALA:HB1	1.93	0.50
1:M:743:LYS:H	1:M:743:LYS:HD3	1.76	0.50
1:C:716:TYR:CE1	1:M:709:SER:CB	2.95	0.50
1:C:542:GLU:HG3	1:D:544:LEU:HD22	1.93	0.50
1:F:697:LEU:O	1:F:701:ILE:HG13	2.12	0.50
1:M:697:LEU:O	1:M:701:ILE:HG13	2.12	0.50
1:G:759:ASN:ND2	3:g:16:SER:O	2.34	0.49
2:J:744:SER:O	2:N:558:ARG:HD2	2.12	0.49
1:D:661:ASP:OD1	1:D:703:LYS:HE3	2.12	0.49
2:J:535:LEU:HD11	3:i:23:ALA:HB1	1.94	0.49
2:N:641:ASP:CB	2:O:637:PRO:HD2	2.41	0.49
2:E:576:LYS:NZ	1:F:539:ILE:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:633:ARG:HH12	7:P:1003:GOL:H12	1.77	0.49
2:B:638:TYR:OH	1:C:553:PRO:HG2	2.13	0.49
1:L:697:LEU:O	1:L:701:ILE:HG13	2.12	0.49
2:B:697:LEU:O	2:B:701:ILE:HG13	2.12	0.49
2:E:697:LEU:O	2:E:701:ILE:HG13	2.12	0.49
1:A:697:LEU:O	1:A:701:ILE:HG13	2.13	0.49
2:N:554:ASP:CB	2:N:636:LEU:HD11	2.42	0.49
2:O:542:GLU:HG3	1:P:544:LEU:CD2	2.43	0.49
1:P:697:LEU:O	1:P:701:ILE:HG13	2.13	0.49
1:A:542:GLU:HG3	2:B:544:LEU:CD2	2.42	0.49
4:B:802:DEX:H931	4:B:802:DEX:O2	2.12	0.49
2:O:547:GLY:N	2:O:626:ASP:OD2	2.42	0.49
3:d:21:LEU:HD22	3:d:21:LEU:O	2.13	0.49
1:A:585:ARG:NH1	8:A:1006:SO4:O1	2.46	0.49
1:C:759:ASN:ND2	3:c:16:SER:O	2.42	0.49
1:G:544:LEU:CD2	1:H:542:GLU:HG3	2.43	0.49
1:H:634:MET:HE1	1:H:647:LEU:HD11	1.95	0.49
2:O:544:LEU:CD2	1:P:542:GLU:HG3	2.42	0.49
2:B:634:MET:HE1	2:B:647:LEU:HD11	1.95	0.48
1:C:697:LEU:O	1:C:701:ILE:HG13	2.13	0.48
1:M:629:ILE:HG23	1:M:633:ARG:HB3	1.95	0.48
4:N:1001:DEX:O2	4:N:1001:DEX:H931	2.13	0.48
2:O:638:TYR:HB3	2:O:735:PHE:CZ	2.44	0.48
1:G:697:LEU:O	1:G:701:ILE:HG13	2.12	0.48
1:I:697:LEU:O	1:I:701:ILE:HG13	2.13	0.48
4:A:1001:DEX:H931	4:A:1001:DEX:O2	2.13	0.48
2:B:661:ASP:OD2	2:B:703:LYS:HE3	2.13	0.48
4:J:802:DEX:H821	4:J:802:DEX:O2	2.14	0.48
2:B:736:CYS:HA	4:B:802:DEX:O4	2.14	0.48
1:C:594:THR:HG21	1:C:676:PRO:HG3	1.94	0.48
1:D:697:LEU:O	1:D:701:ILE:HG13	2.13	0.48
2:O:697:LEU:O	2:O:701:ILE:HG13	2.12	0.48
1:H:721:LEU:C	1:H:721:LEU:HD23	2.38	0.48
2:K:701:ILE:HG23	2:K:714:ARG:HG2	1.94	0.48
1:M:661:ASP:OD2	1:M:703:LYS:HE2	2.14	0.48
1:A:542:GLU:HG3	2:B:544:LEU:HD22	1.96	0.48
2:J:697:LEU:O	2:J:701:ILE:HG13	2.13	0.48
1:C:716:TYR:CD1	1:M:709:SER:HB3	2.48	0.48
1:H:708:SER:HB3	1:H:710:GLN:HG3	1.95	0.48
2:N:661:ASP:OD1	2:N:703:LYS:HE3	2.14	0.48
2:J:759:ASN:ND2	3:j:16:SER:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:697:LEU:O	2:K:701:ILE:HG13	2.13	0.47
1:H:676:PRO:HG3	1:H:680:LEU:CD2	2.44	0.47
1:L:535:LEU:HD11	3:k:23:ALA:HB1	1.96	0.47
1:A:735:PHE:HE2	7:A:1005:GOL:H32	1.79	0.47
1:H:697:LEU:O	1:H:701:ILE:HG13	2.13	0.47
3:d:29:LEU:C	11:d:101:IMD:H2	2.39	0.47
1:C:568:GLY:HA3	7:C:1002:GOL:H32	1.96	0.47
2:B:551:THR:HG22	2:B:552:LEU:HD12	1.97	0.47
1:G:531:THR:HG22	1:G:532:LEU:N	2.29	0.47
2:K:661:ASP:OD2	2:K:703:LYS:HE3	2.15	0.47
2:N:697:LEU:O	2:N:701:ILE:HG13	2.14	0.47
2:B:637:PRO:CA	1:H:553:PRO:HG3	2.45	0.47
1:F:563:LEU:HB3	4:F:1001:DEX:H11	1.97	0.47
2:O:634:MET:HE1	2:O:647:LEU:HD11	1.96	0.47
2:E:675:VAL:HG21	2:E:772:LEU:HD21	1.97	0.47
1:A:733:LEU:HD22	1:A:737:PHE:CZ	2.50	0.47
1:D:594:THR:HG21	1:D:676:PRO:HG3	1.97	0.47
2:O:585:ARG:HH11	1:P:585:ARG:HG3	1.78	0.47
1:D:535:LEU:HD11	3:c:23:ALA:HB1	1.97	0.46
1:G:593:MET:HB3	1:G:593:MET:HE3	1.79	0.46
1:H:674:THR:HG23	1:H:769:VAL:CG1	2.42	0.46
3:d:28:SER:O	11:d:101:IMD:H2	2.15	0.46
1:L:742:ASN:C	1:L:742:ASN:ND2	2.73	0.46
3:h:17:ARG:NH2	3:h:22:TYR:CZ	2.83	0.46
1:A:661:ASP:OD2	1:A:703:LYS:HE3	2.15	0.46
2:E:713:GLN:HA	1:I:712:TRP:CH2	2.51	0.46
1:H:661:ASP:OD2	1:H:703:LYS:HE2	2.15	0.46
2:O:593:MET:HE3	2:O:593:MET:HB3	1.79	0.46
1:C:642:GLN:HB2	4:C:1001:DEX:C22	2.46	0.46
1:C:734:GLN:OE1	2:E:638:TYR:N	2.45	0.46
2:N:634:MET:HE1	2:N:647:LEU:HD21	1.97	0.46
2:E:593:MET:HE3	2:E:593:MET:HB3	1.81	0.46
1:G:661:ASP:OD2	1:G:703:LYS:HE2	2.15	0.46
2:K:704:ARG:CZ	2:K:714:ARG:NH2	2.79	0.46
1:P:593:MET:HE3	1:P:593:MET:HB3	1.80	0.46
2:O:563:LEU:HB3	4:O:1001:DEX:H11	1.98	0.46
1:A:604:MET:HE2	1:A:604:MET:CA	2.46	0.46
1:F:604:MET:HE2	1:F:604:MET:CA	2.46	0.46
2:J:554:ASP:OD2	2:O:551:THR:HG23	2.16	0.46
4:J:802:DEX:O2	4:J:802:DEX:H931	2.15	0.46
2:N:593:MET:HE3	2:N:593:MET:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:544:LEU:CD2	1:F:542:GLU:HG3	2.46	0.45
1:A:678:ASP:OD2	1:A:678:ASP:N	2.50	0.45
1:A:692:THR:HG21	3:b:29:LEU:HD22	1.98	0.45
2:B:637:PRO:HA	1:H:553:PRO:HG3	1.97	0.45
2:E:544:LEU:HD22	1:F:542:GLU:HG3	1.98	0.45
1:H:676:PRO:HD2	1:H:680:LEU:CD2	2.42	0.45
1:M:678:ASP:OD2	1:M:678:ASP:N	2.49	0.45
2:K:559:LEU:HD23	2:K:639:MET:CE	2.45	0.45
1:F:733:LEU:HD22	1:F:737:PHE:CZ	2.51	0.45
1:I:544:LEU:HD22	2:J:542:GLU:HG3	1.99	0.45
1:I:736:CYS:HA	4:I:1001:DEX:O4	2.16	0.45
2:K:552:LEU:CD2	2:N:633:ARG:HB2	2.45	0.45
2:N:549:ASP:H	7:N:1002:GOL:H12	1.81	0.45
1:P:716:TYR:CE1	1:P:775:HIS:CE1	3.04	0.45
1:D:678:ASP:OD2	1:D:678:ASP:N	2.49	0.45
2:K:555:THR:HG22	2:N:553:PRO:HB3	1.97	0.45
1:H:711:ASN:N	1:H:711:ASN:HD22	2.14	0.45
1:M:594:THR:HG21	1:M:676:PRO:HG3	1.98	0.45
2:N:634:MET:HE1	2:N:647:LEU:CD2	2.46	0.45
1:A:593:MET:HE3	1:A:593:MET:HB3	1.84	0.45
2:J:661:ASP:OD2	2:J:703:LYS:HE3	2.17	0.45
1:L:611:ARG:HD2	11:L:1007:IMD:N1	2.32	0.45
1:I:542:GLU:HG3	2:J:544:LEU:CD2	2.47	0.45
1:C:642:GLN:HB2	4:C:1001:DEX:H222	1.98	0.45
1:G:542:GLU:HG3	1:H:544:LEU:HD22	1.99	0.45
1:G:634:MET:HE1	1:G:647:LEU:HD11	1.98	0.45
1:H:678:ASP:OD2	1:H:678:ASP:N	2.50	0.45
2:N:548:TYR:CE2	2:N:633:ARG:NH1	2.85	0.45
2:O:585:ARG:NH1	1:P:585:ARG:HE	2.13	0.45
1:H:549:ASP:OD1	1:H:552:LEU:HG	2.16	0.45
1:L:604:MET:HE2	1:L:604:MET:CA	2.45	0.45
2:K:678:ASP:OD2	2:K:678:ASP:N	2.49	0.44
1:L:594:THR:HG21	1:L:676:PRO:HG3	1.98	0.44
1:P:678:ASP:OD2	1:P:678:ASP:N	2.50	0.44
1:A:535:LEU:HD11	3:b:23:ALA:HB1	1.99	0.44
1:C:542:GLU:HG3	1:D:544:LEU:CD2	2.46	0.44
2:E:678:ASP:OD2	2:E:678:ASP:N	2.50	0.44
1:G:594:THR:HG21	1:G:676:PRO:HG3	1.99	0.44
1:I:594:THR:HG21	1:I:676:PRO:HG3	1.99	0.44
1:H:733:LEU:HD22	1:H:737:PHE:CZ	2.52	0.44
2:N:597:GLN:HG2	2:N:756:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:594:THR:HG21	2:O:676:PRO:HG3	2.00	0.44
2:E:585:ARG:HH22	1:F:585:ARG:HG3	1.83	0.44
2:O:678:ASP:N	2:O:678:ASP:OD2	2.50	0.44
1:D:604:MET:HE2	1:D:604:MET:CA	2.47	0.44
2:K:553:PRO:HG3	2:N:554:ASP:CG	2.42	0.44
1:C:604:MET:HE2	1:C:604:MET:CA	2.46	0.44
1:F:678:ASP:OD2	1:F:678:ASP:N	2.50	0.44
2:B:554:ASP:CB	2:B:636:LEU:HD11	2.48	0.44
1:P:533:ILE:HG12	1:P:661:ASP:OD2	2.18	0.44
1:D:582:PRO:HA	3:c:27:SER:O	2.18	0.44
2:E:594:THR:HG21	2:E:676:PRO:HG3	2.00	0.44
1:F:585:ARG:HD2	1:F:585:ARG:HA	1.75	0.44
2:B:614:LYS:HE2	6:B:804:EPE:H22	2.00	0.43
2:J:552:LEU:HD21	2:N:744:SER:OG	2.18	0.43
1:C:637:PRO:O	1:C:638:TYR:HB2	2.18	0.43
2:N:733:LEU:HD22	2:N:737:PHE:CZ	2.53	0.43
1:A:594:THR:HG21	1:A:676:PRO:HG3	2.00	0.43
2:B:554:ASP:HB3	2:B:636:LEU:HD11	2.00	0.43
2:E:675:VAL:CG2	2:E:772:LEU:HD21	2.48	0.43
1:F:530:PRO:HG2	1:F:535:LEU:HD21	2.01	0.43
1:G:604:MET:HE2	1:G:604:MET:CA	2.46	0.43
4:N:1001:DEX:O2	4:N:1001:DEX:H821	2.18	0.43
1:I:660:TYR:HB2	6:I:1004:EPE:H92	1.99	0.43
1:F:598:TYR:HD2	1:F:674:THR:HG22	1.84	0.43
1:H:542:GLU:H	5:H:801:CAC:C2	2.31	0.43
1:I:604:MET:HE2	1:I:604:MET:CA	2.46	0.43
2:J:604:MET:HE2	2:J:604:MET:CA	2.46	0.43
1:C:535:LEU:HD11	3:d:23:ALA:HB1	2.00	0.43
1:I:642:GLN:HB2	4:I:1001:DEX:C22	2.47	0.43
1:P:594:THR:HG21	1:P:676:PRO:HG3	2.00	0.43
1:F:593:MET:HE3	1:F:593:MET:HB3	1.82	0.43
2:N:615:GLN:HB2	2:N:622[A]:CSO:OD	2.19	0.43
2:O:705:GLU:OE1	2:O:705:GLU:HA	2.18	0.43
2:B:597:GLN:HG2	2:B:756:ILE:HG23	2.00	0.43
2:E:559:LEU:HD12	2:E:559:LEU:HA	1.89	0.43
2:E:615:GLN:HB2	2:E:622[A]:CSO:OD	2.18	0.43
1:P:701:ILE:HG23	1:P:714:ARG:HG2	2.01	0.43
2:N:604:MET:HE2	2:N:604:MET:CA	2.46	0.43
1:P:634:MET:HE1	1:P:647:LEU:HD11	2.01	0.43
2:B:552:LEU:HD23	1:C:745:LEU:HD13	1.99	0.43
4:C:1001:DEX:O2	4:C:1001:DEX:H931	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:585:ARG:HH11	1:L:585:ARG:NE	2.14	0.43
2:N:559:LEU:HD23	2:N:639:MET:CE	2.46	0.43
2:O:548:TYR:CE2	2:O:627:LEU:HD13	2.52	0.43
2:B:535:LEU:HD11	3:a:23:ALA:HB1	2.01	0.42
2:J:735:PHE:CZ	12:K:801:PEG:H22	2.55	0.42
1:L:611:ARG:HD2	11:L:1007:IMD:HN1	1.83	0.42
2:O:542:GLU:HG3	1:P:544:LEU:HD22	2.00	0.42
1:D:553:PRO:CA	1:G:553:PRO:CB	2.97	0.42
2:J:635:GLN:OE1	2:J:635:GLN:HA	2.19	0.42
3:a:29:LEU:HD23	3:a:29:LEU:HA	1.90	0.42
3:i:29:LEU:HD13	3:i:29:LEU:HA	1.87	0.42
2:B:593:MET:HB3	2:B:593:MET:HE3	1.81	0.42
1:L:738:TYR:CD2	7:L:1004:GOL:H32	2.53	0.42
1:P:652:GLU:CD	1:P:655:ARG:HH12	2.28	0.42
1:P:675:VAL:HG21	1:P:772:LEU:HD21	2.01	0.42
3:d:29:LEU:HA	11:d:101:IMD:H2	2.01	0.42
1:A:559:LEU:HD12	1:A:559:LEU:HA	1.90	0.42
2:B:604:MET:HE2	2:B:604:MET:CA	2.46	0.42
3:k:29:LEU:HD23	3:k:29:LEU:HA	1.88	0.42
2:E:701:ILE:HG23	2:E:714:ARG:HG2	2.00	0.42
2:J:593:MET:HE3	2:J:593:MET:HB3	1.80	0.42
3:l:29:LEU:HD12	3:l:29:LEU:HA	1.85	0.42
1:C:764:PHE:HB2	7:C:1003:GOL:O3	2.19	0.42
2:E:612:SER:HA	2:E:622[A]:CSO:SG	2.60	0.42
1:F:594:THR:HG21	1:F:676:PRO:HG3	2.02	0.42
1:I:614:LYS:HA	1:I:614:LYS:HD2	1.86	0.42
1:C:764:PHE:HB2	7:C:1003:GOL:H31	2.01	0.42
1:D:559:LEU:HD12	1:D:559:LEU:HA	1.90	0.42
3:d:29:LEU:CA	11:d:101:IMD:H2	2.50	0.42
2:B:642:GLN:HB2	4:B:802:DEX:H222	2.01	0.42
2:K:604:MET:HE2	2:K:604:MET:CA	2.48	0.42
1:L:738:TYR:CE2	7:L:1004:GOL:H32	2.55	0.42
2:O:604:MET:HE2	2:O:604:MET:CA	2.46	0.42
1:P:774:PHE:C	1:P:775:HIS:CG	2.98	0.41
1:C:678:ASP:OD1	1:C:678:ASP:N	2.53	0.41
1:H:597:GLN:HG2	1:H:756:ILE:HG23	2.01	0.41
2:N:570:GLN:HB3	2:N:604:MET:SD	2.60	0.41
1:P:614:LYS:HD2	1:P:614:LYS:HA	1.86	0.41
2:B:570:GLN:HB3	2:B:604:MET:SD	2.60	0.41
2:E:597:GLN:HG2	2:E:756:ILE:HG23	2.01	0.41
1:L:678:ASP:OD1	1:L:678:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:692:THR:HG21	3:p:29:LEU:HD11	2.02	0.41
1:A:570:GLN:HB3	1:A:604:MET:SD	2.61	0.41
4:E:1001:DEX:O2	4:E:1001:DEX:C18	2.66	0.41
1:G:597:GLN:CD	1:G:760[B]:GLN:HE21	2.25	0.41
1:H:761:LEU:HB3	1:H:762:PRO:CD	2.51	0.41
4:O:1001:DEX:O2	4:O:1001:DEX:H931	2.21	0.41
1:P:702:VAL:HA	1:P:711:ASN:HD21	1.85	0.41
1:D:761:LEU:HB3	1:D:762:PRO:CD	2.51	0.41
2:K:634:MET:HE1	2:K:647:LEU:HD11	2.02	0.41
1:M:753:LEU:HD23	1:M:753:LEU:HA	1.94	0.41
1:D:634:MET:HE1	1:D:647:LEU:HD11	2.02	0.41
2:E:604:MET:HE2	2:E:604:MET:CA	2.47	0.41
1:F:759:ASN:ND2	3:f:16:SER:O	2.34	0.41
1:H:604:MET:HE2	1:H:604:MET:CA	2.45	0.41
1:A:634:MET:HE1	1:A:647:LEU:HD11	2.03	0.41
1:A:708:SER:O	1:A:711:ASN:HB2	2.20	0.41
2:E:552:LEU:HB2	2:E:558:ARG:NH2	2.35	0.41
1:F:559:LEU:HD12	1:F:559:LEU:HA	1.90	0.41
1:I:761:LEU:HB3	1:I:762:PRO:CD	2.51	0.41
1:I:765:LYS:HD2	1:I:765:LYS:HA	1.82	0.41
2:K:594:THR:HG21	2:K:676:PRO:HG3	2.02	0.41
2:N:678:ASP:OD1	2:N:678:ASP:N	2.54	0.41
1:D:549:ASP:O	1:D:558:ARG:NH1	2.52	0.41
1:I:542:GLU:HG3	2:J:544:LEU:HD22	2.01	0.41
2:K:552:LEU:HD23	2:N:633:ARG:HB2	2.01	0.41
1:C:761:LEU:HB3	1:C:762:PRO:CD	2.51	0.41
1:G:570:GLN:HB3	1:G:604:MET:SD	2.61	0.41
1:H:559:LEU:HD12	1:H:559:LEU:HA	1.90	0.41
1:H:614:LYS:HA	1:H:614:LYS:HD2	1.89	0.41
1:H:635:GLN:HA	1:H:635:GLN:OE1	2.20	0.41
1:H:770:LYS:HA	1:H:771:PRO:HD2	1.94	0.41
1:I:634:MET:HE1	1:I:647:LEU:HD11	2.03	0.41
2:J:570:GLN:HB3	2:J:604:MET:SD	2.61	0.41
1:L:634:MET:HE1	1:L:647:LEU:HD11	2.03	0.41
2:N:629:ILE:HG23	2:N:633:ARG:HB3	2.03	0.41
1:P:570:GLN:HB3	1:P:604:MET:SD	2.61	0.41
1:H:570:GLN:HB3	1:H:604:MET:SD	2.61	0.41
2:K:761:LEU:HB3	2:K:762:PRO:CD	2.51	0.41
1:L:585:ARG:HD2	1:L:585:ARG:HA	1.89	0.41
3:p:29:LEU:HD23	3:p:29:LEU:HA	1.90	0.41
1:A:544:LEU:CD2	2:B:542:GLU:HG3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:MET:HE3	1:C:593:MET:HB3	1.83	0.40
1:D:593:MET:HE3	1:D:593:MET:HB3	1.82	0.40
2:E:570:GLN:HB3	2:E:604:MET:SD	2.60	0.40
1:I:593:MET:HE3	1:I:593:MET:HB3	1.83	0.40
4:M:802:DEX:H931	4:M:802:DEX:O2	2.21	0.40
2:N:585:ARG:HD2	2:N:585:ARG:HA	1.88	0.40
1:A:761:LEU:HB3	1:A:762:PRO:CD	2.51	0.40
1:D:570:GLN:HB3	1:D:604:MET:SD	2.61	0.40
4:H:802:DEX:O2	4:H:802:DEX:H821	2.21	0.40
1:I:535:LEU:O	1:I:539:ILE:HG12	2.22	0.40
1:I:678:ASP:OD1	1:I:678:ASP:N	2.53	0.40
1:L:570:GLN:HB3	1:L:604:MET:SD	2.61	0.40
1:M:761:LEU:HB3	1:M:762:PRO:CD	2.51	0.40
2:N:535:LEU:O	2:N:539:ILE:HG12	2.21	0.40
3:e:29:LEU:HD23	3:e:29:LEU:HA	1.87	0.40
1:A:705:GLU:OE1	1:A:711:ASN:ND2	2.50	0.40
2:E:554:ASP:HB3	2:E:636:LEU:HD11	2.04	0.40
1:H:708:SER:HB2	1:H:710:GLN:HG3	2.03	0.40
1:L:761:LEU:HB3	1:L:762:PRO:CD	2.52	0.40
1:M:604:MET:HE2	1:M:604:MET:CA	2.46	0.40
1:M:645:GLN:NE2	1:M:731:GLY:HA3	2.37	0.40
2:O:761:LEU:HB3	2:O:762:PRO:CD	2.52	0.40
2:B:761:LEU:HB3	2:B:762:PRO:CD	2.52	0.40
1:F:589:LEU:C	1:F:589:LEU:CD2	2.95	0.40
2:K:642:GLN:HB2	4:K:802:DEX:H212	2.03	0.40
1:M:634:MET:HE1	1:M:647:LEU:HD11	2.03	0.40
1:A:705:GLU:HG2	1:A:711:ASN:HD21	1.85	0.40
1:D:614:LYS:HD2	1:D:614:LYS:HA	1.91	0.40
1:H:711:ASN:N	1:H:711:ASN:ND2	2.69	0.40
2:J:585:ARG:HA	2:J:585:ARG:HD2	1.88	0.40
2:O:530:PRO:HG2	2:O:535:LEU:HD21	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:709:SER:OG	2:N:716:TYR:CD1[3_545]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/248 (99%)	238 (97%)	8 (3%)	0	100	100
1	C	246/248 (99%)	237 (96%)	9 (4%)	0	100	100
1	D	246/248 (99%)	238 (97%)	8 (3%)	0	100	100
1	F	247/248 (100%)	240 (97%)	7 (3%)	0	100	100
1	G	247/248 (100%)	240 (97%)	7 (3%)	0	100	100
1	H	241/248 (97%)	234 (97%)	7 (3%)	0	100	100
1	I	246/248 (99%)	238 (97%)	8 (3%)	0	100	100
1	L	246/248 (99%)	239 (97%)	7 (3%)	0	100	100
1	M	246/248 (99%)	237 (96%)	9 (4%)	0	100	100
1	P	239/248 (96%)	233 (98%)	6 (2%)	0	100	100
2	B	245/248 (99%)	238 (97%)	7 (3%)	0	100	100
2	E	240/248 (97%)	233 (97%)	7 (3%)	0	100	100
2	J	246/248 (99%)	239 (97%)	7 (3%)	0	100	100
2	K	240/248 (97%)	235 (98%)	5 (2%)	0	100	100
2	N	241/248 (97%)	234 (97%)	7 (3%)	0	100	100
2	O	239/248 (96%)	232 (97%)	7 (3%)	0	100	100
3	a	12/15 (80%)	12 (100%)	0	0	100	100
3	b	12/15 (80%)	12 (100%)	0	0	100	100
3	c	12/15 (80%)	12 (100%)	0	0	100	100
3	d	12/15 (80%)	12 (100%)	0	0	100	100
3	e	12/15 (80%)	12 (100%)	0	0	100	100
3	f	11/15 (73%)	10 (91%)	1 (9%)	0	100	100
3	g	11/15 (73%)	11 (100%)	0	0	100	100
3	h	11/15 (73%)	10 (91%)	1 (9%)	0	100	100
3	i	13/15 (87%)	12 (92%)	1 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	j	12/15 (80%)	12 (100%)	0	0	100	100
3	k	12/15 (80%)	12 (100%)	0	0	100	100
3	l	12/15 (80%)	12 (100%)	0	0	100	100
3	m	12/15 (80%)	12 (100%)	0	0	100	100
3	n	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
3	o	12/15 (80%)	12 (100%)	0	0	100	100
3	p	12/15 (80%)	12 (100%)	0	0	100	100
All	All	4092/4208 (97%)	3972 (97%)	120 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/227 (100%)	217 (96%)	10 (4%)	24	53
1	C	227/227 (100%)	213 (94%)	14 (6%)	15	39
1	D	227/227 (100%)	216 (95%)	11 (5%)	21	50
1	F	228/227 (100%)	218 (96%)	10 (4%)	24	53
1	G	228/227 (100%)	220 (96%)	8 (4%)	31	62
1	H	225/227 (99%)	209 (93%)	16 (7%)	12	32
1	I	227/227 (100%)	216 (95%)	11 (5%)	21	50
1	L	227/227 (100%)	215 (95%)	12 (5%)	19	46
1	M	227/227 (100%)	220 (97%)	7 (3%)	35	66
1	P	223/227 (98%)	212 (95%)	11 (5%)	21	49
2	B	226/226 (100%)	215 (95%)	11 (5%)	21	49
2	E	224/226 (99%)	210 (94%)	14 (6%)	15	38
2	J	227/226 (100%)	217 (96%)	10 (4%)	24	53
2	K	224/226 (99%)	215 (96%)	9 (4%)	27	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	225/226 (100%)	210 (93%)	15 (7%)	13	35
2	O	223/226 (99%)	207 (93%)	16 (7%)	12	31
3	a	12/12 (100%)	11 (92%)	1 (8%)	9	26
3	b	12/12 (100%)	12 (100%)	0	100	100
3	c	12/12 (100%)	12 (100%)	0	100	100
3	d	12/12 (100%)	11 (92%)	1 (8%)	9	26
3	e	12/12 (100%)	12 (100%)	0	100	100
3	f	11/12 (92%)	10 (91%)	1 (9%)	7	22
3	g	11/12 (92%)	11 (100%)	0	100	100
3	h	11/12 (92%)	10 (91%)	1 (9%)	7	22
3	i	12/12 (100%)	11 (92%)	1 (8%)	9	26
3	j	12/12 (100%)	12 (100%)	0	100	100
3	k	12/12 (100%)	12 (100%)	0	100	100
3	l	12/12 (100%)	11 (92%)	1 (8%)	9	26
3	m	12/12 (100%)	11 (92%)	1 (8%)	9	26
3	n	12/12 (100%)	12 (100%)	0	100	100
3	o	12/12 (100%)	12 (100%)	0	100	100
3	p	12/12 (100%)	12 (100%)	0	100	100
All	All	3804/3818 (100%)	3612 (95%)	192 (5%)	20	48

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	538	VAL
1	A	551	THR
1	A	585	ARG
1	A	644	GLN
1	A	673	SER
1	A	703	LYS
1	A	705	GLU
1	A	743	LYS
1	A	753	LEU
1	A	776	GLN
2	B	538	VAL
2	B	551	THR
2	B	585	ARG

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Mol	Chain	Res	Type
2	B	614	LYS
2	B	644	GLN
2	B	648	LYS
2	B	691	MET
2	B	703	LYS
2	B	733	LEU
2	B	734	GLN
2	B	743	LYS
1	C	538	VAL
1	C	585	ARG
1	C	644	GLN
1	C	645	GLN
1	C	646	MET
1	C	648	LYS
1	C	705	GLU
1	C	708	SER
1	C	710	GLN
1	C	733	LEU
1	C	734	GLN
1	C	741	VAL
1	C	745	LEU
1	C	764	PHE
1	D	538	VAL
1	D	551	THR
1	D	585	ARG
1	D	614	LYS
1	D	631	GLU
1	D	644	GLN
1	D	703	LYS
1	D	705	GLU
1	D	733	LEU
1	D	734	GLN
1	D	776	GLN
2	E	538	VAL
2	E	543[A]	VAL
2	E	543[B]	VAL
2	E	551	THR
2	E	558	ARG
2	E	585	ARG
2	E	644	GLN
2	E	705	GLU
2	E	711	ASN

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Mol	Chain	Res	Type
2	E	733	LEU
2	E	734	GLN
2	E	743	LYS
2	E	745	LEU
2	E	753	LEU
1	F	538	VAL
1	F	585	ARG
1	F	614	LYS
1	F	644	GLN
1	F	673	SER
1	F	703	LYS
1	F	705	GLU
1	F	716	TYR
1	F	733	LEU
1	F	743	LYS
1	G	529	PHE
1	G	535	LEU
1	G	538	VAL
1	G	551	THR
1	G	641	ASP
1	G	644	GLN
1	G	733	LEU
1	G	743	LYS
1	H	538	VAL
1	H	550	SER
1	H	551	THR
1	H	565	ARG
1	H	614	LYS
1	H	644	GLN
1	H	648	LYS
1	H	676	PRO
1	H	677	LYS
1	H	695	LYS
1	H	704	ARG
1	H	711	ASN
1	H	733	LEU
1	H	734	GLN
1	H	753	LEU
1	H	772	LEU
1	I	535	LEU
1	I	538	VAL
1	I	551	THR

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Mol	Chain	Res	Type
1	I	614	LYS
1	I	615	GLN
1	I	644	GLN
1	I	691	MET
1	I	733	LEU
1	I	734	GLN
1	I	743	LYS
1	I	776	GLN
2	J	538	VAL
2	J	557	THR
2	J	585	ARG
2	J	614	LYS
2	J	641	ASP
2	J	644	GLN
2	J	691	MET
2	J	705	GLU
2	J	733	LEU
2	J	734	GLN
2	K	538	VAL
2	K	551	THR
2	K	559	LEU
2	K	644	GLN
2	K	703	LYS
2	K	710	GLN
2	K	733	LEU
2	K	743	LYS
2	K	753	LEU
1	L	538	VAL
1	L	550	SER
1	L	551	THR
1	L	585	ARG
1	L	614	LYS
1	L	644	GLN
1	L	648	LYS
1	L	733	LEU
1	L	742	ASN
1	L	743	LYS
1	L	765	LYS
1	L	776	GLN
1	M	538	VAL
1	M	542	GLU
1	M	548	TYR

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Mol	Chain	Res	Type
1	M	644	GLN
1	M	708	SER
1	M	733	LEU
1	M	743	LYS
2	N	538	VAL
2	N	551	THR
2	N	559	LEU
2	N	585	ARG
2	N	614	LYS
2	N	644	GLN
2	N	647	LEU
2	N	681	LYS
2	N	705	GLU
2	N	709	SER
2	N	733	LEU
2	N	734	GLN
2	N	743	LYS
2	N	765	LYS
2	N	776	GLN
2	O	529	PHE
2	O	538	VAL
2	O	550	SER
2	O	551	THR
2	O	554	ASP
2	O	558	ARG
2	O	585	ARG
2	O	614	LYS
2	O	631	GLU
2	O	644	GLN
2	O	688	GLU
2	O	704	ARG
2	O	733	LEU
2	O	734	GLN
2	O	753	LEU
2	O	776	GLN
1	P	535	LEU
1	P	538	VAL
1	P	550	SER
1	P	585	ARG
1	P	614	LYS
1	P	644	GLN
1	P	648	LYS

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Mol	Chain	Res	Type
1	P	720	LYS
1	P	733	LEU
1	P	745	LEU
1	P	752	MET
3	a	17	ARG
3	d	21	LEU
3	f	26	SER
3	h	17	ARG
3	i	29	LEU
3	l	29	LEU
3	m	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	597	GLN
1	A	615	GLN
1	A	619	ASN
1	A	711	ASN
2	B	615	GLN
2	B	726	HIS
1	C	615	GLN
1	C	644	GLN
1	C	711	ASN
1	C	726	HIS
1	D	615	GLN
1	D	645	GLN
1	D	742	ASN
2	E	615	GLN
2	E	635	GLN
2	E	726	HIS
1	F	597	GLN
1	F	615	GLN
1	F	644	GLN
1	F	775	HIS
1	G	615	GLN
1	G	619	ASN
1	H	615	GLN
1	I	597	GLN
1	I	619	ASN
1	I	645	GLN
2	J	597	GLN

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Mol	Chain	Res	Type
2	J	615	GLN
2	J	619	ASN
2	J	645	GLN
2	J	711	ASN
2	K	615	GLN
2	K	726	HIS
2	K	742	ASN
1	L	570	GLN
1	L	597	GLN
1	M	615	GLN
1	M	619	ASN
1	M	645	GLN
1	M	776	GLN
2	N	644	GLN
2	O	597	GLN
2	O	711	ASN
2	O	726	HIS
1	P	615	GLN
1	P	711	ASN
1	P	726	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CSO	O	622[A]	-	3,6,7	0.53	0	0,6,8	-	-
2	CSO	E	622[B]	-	3,6,7	0.46	0	0,6,8	-	-
2	CSO	N	622[A]	-	3,6,7	0.55	0	0,6,8	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CSO	K	622[A]	-	3,6,7	0.57	0	0,6,8	-	-
2	CSO	B	622[B]	-	3,6,7	0.68	0	0,6,8	-	-
2	CSO	E	622[A]	-	3,6,7	0.46	0	0,6,8	-	-
2	CSO	B	622[A]	-	3,6,7	0.68	0	0,6,8	-	-
2	CSO	O	622[B]	-	3,6,7	0.53	0	0,6,8	-	-
2	CSO	N	622[B]	-	3,6,7	0.55	0	0,6,8	-	-
2	CSO	K	622[B]	-	3,6,7	0.57	0	0,6,8	-	-
2	CSO	J	622	2	3,6,7	0.87	0	0,6,8	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSO	O	622[A]	-	-	0/1/5/7	-
2	CSO	E	622[B]	-	-	0/1/5/7	-
2	CSO	N	622[A]	-	-	1/1/5/7	-
2	CSO	K	622[A]	-	-	1/1/5/7	-
2	CSO	B	622[B]	-	-	1/1/5/7	-
2	CSO	E	622[A]	-	-	1/1/5/7	-
2	CSO	B	622[A]	-	-	1/1/5/7	-
2	CSO	O	622[B]	-	-	1/1/5/7	-
2	CSO	N	622[B]	-	-	0/1/5/7	-
2	CSO	K	622[B]	-	-	1/1/5/7	-
2	CSO	J	622	2	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	622[B]	CSO	N-CA-CB-SG
2	E	622[A]	CSO	N-CA-CB-SG
2	K	622[B]	CSO	N-CA-CB-SG
2	O	622[B]	CSO	N-CA-CB-SG
2	B	622[A]	CSO	N-CA-CB-SG
2	J	622	CSO	N-CA-CB-SG
2	K	622[A]	CSO	N-CA-CB-SG
2	N	622[A]	CSO	N-CA-CB-SG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	622[A]	CSO	1	0
2	E	622[A]	CSO	2	0
2	K	622[B]	CSO	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 91 ligands modelled in this entry, 11 are monoatomic - leaving 80 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	GOL	N	1002	-	5,5,5	0.12	0	5,5,5	0.30	0
4	DEX	N	1001	-	31,31,31	0.41	0	52,53,53	1.18	3 (5%)
8	SO4	C	1005	-	4,4,4	0.36	0	6,6,6	0.06	0
11	IMD	J	807	-	3,5,5	0.29	0	4,5,5	0.79	0
7	GOL	C	1003	-	5,5,5	0.23	0	5,5,5	0.73	0
7	GOL	J	804	-	5,5,5	0.20	0	5,5,5	0.54	0
11	IMD	I	1006	-	3,5,5	0.30	0	4,5,5	0.66	0
4	DEX	I	1001	-	31,31,31	0.45	0	52,53,53	1.34	7 (13%)
10	PG4	H	803	-	12,12,12	0.34	0	11,11,11	0.19	0
7	GOL	P	1003	-	5,5,5	0.10	0	5,5,5	0.37	0
6	EPE	A	1003	-	15,15,15	0.65	1 (6%)	18,20,20	0.86	1 (5%)
8	SO4	A	1006	-	4,4,4	0.36	0	6,6,6	0.06	0
5	CAC	D	801	-	0,4,4	-	-	0,6,6	-	-
12	PEG	F	1002	-	6,6,6	0.35	0	5,5,5	0.27	0
10	PG4	L	1002	-	12,12,12	0.29	0	11,11,11	0.23	0
4	DEX	F	1001	-	31,31,31	0.46	0	52,53,53	0.85	1 (1%)
4	DEX	K	802	-	31,31,31	0.45	0	52,53,53	1.40	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	J	805	-	5,5,5	0.15	0	5,5,5	0.36	0
7	GOL	K	805	-	5,5,5	0.10	0	5,5,5	0.35	0
8	SO4	C	1006	-	4,4,4	0.39	0	6,6,6	0.10	0
10	PG4	D	803	-	12,12,12	0.41	0	11,11,11	0.27	0
4	DEX	P	1001	-	31,31,31	0.55	0	52,53,53	1.16	6 (11%)
4	DEX	J	802	-	31,31,31	0.45	0	52,53,53	1.19	5 (9%)
11	IMD	F	1003	-	3,5,5	0.34	0	4,5,5	0.77	0
7	GOL	K	804	-	5,5,5	0.13	0	5,5,5	0.40	0
7	GOL	A	1004	-	5,5,5	0.11	0	5,5,5	0.43	0
11	IMD	b	101	-	3,5,5	0.28	0	4,5,5	0.69	0
5	CAC	O	1002	-	0,4,4	-	-	0,6,6	-	-
7	GOL	J	806	-	5,5,5	0.22	0	5,5,5	0.70	0
11	IMD	B	806	-	3,5,5	0.30	0	4,5,5	0.68	0
4	DEX	H	802	-	31,31,31	0.47	0	52,53,53	1.02	2 (3%)
11	IMD	d	101	-	3,5,5	0.28	0	4,5,5	0.64	0
5	CAC	H	801	-	0,4,4	-	-	0,6,6	-	-
6	EPE	P	1002	-	15,15,15	0.68	1 (6%)	18,20,20	0.60	0
12	PEG	M	805	-	6,6,6	0.28	0	5,5,5	0.24	0
12	PEG	I	1003	-	6,6,6	0.38	0	5,5,5	0.31	0
4	DEX	M	802	-	31,31,31	0.42	0	52,53,53	1.17	5 (9%)
8	SO4	J	801	-	4,4,4	0.36	0	6,6,6	0.09	0
7	GOL	E	1003	-	5,5,5	0.14	0	5,5,5	0.41	0
4	DEX	A	1001	-	31,31,31	0.47	0	52,53,53	1.03	2 (3%)
11	IMD	N	1003	-	3,5,5	0.30	0	4,5,5	0.70	0
7	GOL	E	1005	-	5,5,5	0.16	0	5,5,5	0.52	0
4	DEX	L	1001	-	31,31,31	0.49	0	52,53,53	1.11	5 (9%)
5	CAC	I	1002	-	0,4,4	-	-	0,6,6	-	-
6	EPE	I	1004	-	15,15,15	0.84	1 (6%)	18,20,20	0.92	1 (5%)
7	GOL	E	1004	-	5,5,5	0.21	0	5,5,5	0.59	0
11	IMD	C	1004	-	3,5,5	0.28	0	4,5,5	0.67	0
13	PGE	M	804	-	9,9,9	0.18	0	8,8,8	0.15	0
4	DEX	D	802	-	31,31,31	0.49	0	52,53,53	1.39	8 (15%)
5	CAC	E	1002	-	0,4,4	-	-	0,6,6	-	-
11	IMD	L	1006	-	3,5,5	0.27	0	4,5,5	0.70	0
5	CAC	K	803	-	0,4,4	-	-	0,6,6	-	-
4	DEX	G	1001	-	31,31,31	0.61	1 (3%)	52,53,53	1.06	3 (5%)
11	IMD	L	1007	-	3,5,5	0.31	0	4,5,5	0.73	0
6	EPE	L	1003	-	15,15,15	0.87	1 (6%)	18,20,20	0.78	0
7	GOL	M	801	-	5,5,5	0.09	0	5,5,5	0.45	0
11	IMD	O	1004	-	3,5,5	0.39	0	4,5,5	0.86	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DEX	B	802	-	31,31,31	0.60	0	52,53,53	1.37	4 (7%)
7	GOL	L	1005	-	5,5,5	0.11	0	5,5,5	0.37	0
12	PEG	K	801	-	6,6,6	0.57	0	5,5,5	0.61	0
6	EPE	J	803	-	15,15,15	0.63	1 (6%)	18,20,20	0.68	0
6	EPE	B	804	-	15,15,15	0.73	1 (6%)	18,20,20	0.73	0
7	GOL	C	1002	-	5,5,5	0.33	0	5,5,5	1.12	0
4	DEX	E	1001	-	31,31,31	0.66	1 (3%)	52,53,53	0.96	3 (5%)
6	EPE	D	804	-	15,15,15	0.65	1 (6%)	18,20,20	0.86	0
11	IMD	E	1006	-	3,5,5	0.29	0	4,5,5	0.72	0
7	GOL	B	805	-	5,5,5	0.19	0	5,5,5	0.53	0
7	GOL	I	1005	-	5,5,5	0.18	0	5,5,5	0.52	0
7	GOL	L	1004	-	5,5,5	0.18	0	5,5,5	0.65	0
7	GOL	O	1003	-	5,5,5	0.08	0	5,5,5	0.41	0
11	IMD	M	806	-	3,5,5	0.32	0	4,5,5	0.78	0
4	DEX	C	1001	-	31,31,31	0.67	0	52,53,53	1.13	5 (9%)
10	PG4	B	803	-	12,12,12	0.45	0	11,11,11	0.33	0
11	IMD	J	808	-	3,5,5	0.27	0	4,5,5	0.72	0
11	IMD	B	807	-	3,5,5	0.28	0	4,5,5	0.73	0
7	GOL	A	1005	-	5,5,5	0.20	0	5,5,5	0.55	0
4	DEX	O	1001	-	31,31,31	0.61	0	52,53,53	1.26	6 (11%)
5	CAC	A	1002	-	0,4,4	-	-	0,6,6	-	-
5	CAC	M	803	-	0,4,4	-	-	0,6,6	-	-
8	SO4	B	808	-	4,4,4	0.35	0	6,6,6	0.15	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	N	1002	-	-	1/4/4/4	-
4	DEX	N	1001	-	-	2/8/84/84	0/4/4/4
11	IMD	L	1006	-	-	-	0/1/1/1
6	EPE	A	1003	-	-	3/9/19/19	0/1/1/1
4	DEX	G	1001	-	-	1/8/84/84	0/4/4/4
6	EPE	P	1002	-	-	4/9/19/19	0/1/1/1
12	PEG	M	805	-	-	2/4/4/4	-
11	IMD	J	807	-	-	-	0/1/1/1
12	PEG	I	1003	-	-	2/4/4/4	-
4	DEX	M	802	-	-	2/8/84/84	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	IMD	L	1007	-	-	-	0/1/1/1
6	EPE	L	1003	-	-	8/9/19/19	0/1/1/1
7	GOL	C	1003	-	-	4/4/4/4	-
7	GOL	M	801	-	-	2/4/4/4	-
12	PEG	F	1002	-	-	1/4/4/4	-
10	PG4	L	1002	-	-	4/10/10/10	-
4	DEX	F	1001	-	-	0/8/84/84	0/4/4/4
11	IMD	N	1003	-	-	-	0/1/1/1
11	IMD	O	1004	-	-	-	0/1/1/1
4	DEX	K	802	-	-	2/8/84/84	0/4/4/4
7	GOL	J	805	-	-	2/4/4/4	-
7	GOL	J	804	-	-	4/4/4/4	-
4	DEX	B	802	-	-	1/8/84/84	0/4/4/4
7	GOL	L	1005	-	-	0/4/4/4	-
12	PEG	K	801	-	-	1/4/4/4	-
7	GOL	E	1003	-	-	2/4/4/4	-
6	EPE	J	803	-	-	2/9/19/19	0/1/1/1
6	EPE	B	804	-	-	5/9/19/19	0/1/1/1
4	DEX	A	1001	-	-	2/8/84/84	0/4/4/4
7	GOL	C	1002	-	-	2/4/4/4	-
4	DEX	E	1001	-	-	2/8/84/84	0/4/4/4
7	GOL	E	1005	-	-	2/4/4/4	-
6	EPE	D	804	-	-	2/9/19/19	0/1/1/1
7	GOL	K	805	-	-	2/4/4/4	-
10	PG4	D	803	-	-	7/10/10/10	-
4	DEX	P	1001	-	-	1/8/84/84	0/4/4/4
11	IMD	E	1006	-	-	-	0/1/1/1
4	DEX	J	802	-	-	0/8/84/84	0/4/4/4
4	DEX	L	1001	-	-	2/8/84/84	0/4/4/4
7	GOL	B	805	-	-	2/4/4/4	-
11	IMD	I	1006	-	-	-	0/1/1/1
4	DEX	I	1001	-	-	2/8/84/84	0/4/4/4
11	IMD	F	1003	-	-	-	0/1/1/1
7	GOL	I	1005	-	-	3/4/4/4	-
7	GOL	K	804	-	-	2/4/4/4	-
7	GOL	L	1004	-	-	3/4/4/4	-
7	GOL	O	1003	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DEX	C	1001	-	-	2/8/84/84	0/4/4/4
11	IMD	M	806	-	-	-	0/1/1/1
7	GOL	A	1004	-	-	4/4/4/4	-
6	EPE	I	1004	-	-	6/9/19/19	0/1/1/1
10	PG4	B	803	-	-	8/10/10/10	-
11	IMD	B	807	-	-	-	0/1/1/1
7	GOL	E	1004	-	-	0/4/4/4	-
11	IMD	J	808	-	-	-	0/1/1/1
7	GOL	A	1005	-	-	2/4/4/4	-
10	PG4	H	803	-	-	6/10/10/10	-
11	IMD	C	1004	-	-	-	0/1/1/1
11	IMD	b	101	-	-	-	0/1/1/1
7	GOL	J	806	-	-	0/4/4/4	-
4	DEX	O	1001	-	-	0/8/84/84	0/4/4/4
11	IMD	B	806	-	-	-	0/1/1/1
13	PGE	M	804	-	-	3/7/7/7	-
7	GOL	P	1003	-	-	2/4/4/4	-
4	DEX	H	802	-	-	2/8/84/84	0/4/4/4
11	IMD	d	101	-	-	-	0/1/1/1
4	DEX	D	802	-	-	2/8/84/84	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	1004	EPE	O3S-S	2.34	1.55	1.47
6	P	1002	EPE	O3S-S	2.30	1.55	1.47
6	L	1003	EPE	O3S-S	2.28	1.55	1.47
6	B	804	EPE	O3S-S	2.27	1.55	1.47
6	D	804	EPE	O3S-S	2.25	1.55	1.47
6	J	803	EPE	O3S-S	2.22	1.55	1.47
6	A	1003	EPE	O3S-S	2.16	1.55	1.47
4	G	1001	DEX	C10-C9	-2.03	1.55	1.57
4	E	1001	DEX	C10-C9	-2.00	1.55	1.57

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	802	DEX	C6-C5-C10	4.73	118.52	115.61
4	I	1001	DEX	C9-C8-C14	4.35	112.64	109.26
4	O	1001	DEX	C6-C5-C10	4.04	118.10	115.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	802	DEX	C13-C17-C20	-4.03	108.62	112.89
4	K	802	DEX	F1-C9-C11	-4.02	99.23	102.72
4	D	802	DEX	C6-C5-C10	3.91	118.02	115.61
4	D	802	DEX	C1-C10-C5	-3.66	110.42	112.36
4	N	1001	DEX	C7-C8-C9	-3.46	107.75	110.94
4	G	1001	DEX	C6-C5-C10	3.30	117.64	115.61
4	K	802	DEX	C13-C17-C16	3.25	105.93	102.86
4	O	1001	DEX	C15-C14-C8	-3.17	116.12	119.07
4	C	1001	DEX	C13-C14-C8	-3.10	111.29	113.73
4	I	1001	DEX	F1-C9-C10	-3.01	101.64	104.19
4	A	1001	DEX	C6-C5-C10	2.98	117.45	115.61
4	N	1001	DEX	C12-C13-C14	-2.93	105.44	108.03
4	P	1001	DEX	C13-C17-C16	2.90	105.61	102.86
4	O	1001	DEX	C13-C17-C20	-2.86	109.86	112.89
4	G	1001	DEX	F1-C9-C10	-2.84	101.78	104.19
4	J	802	DEX	C9-C8-C14	2.77	111.41	109.26
4	K	802	DEX	C13-C17-C20	-2.73	110.00	112.89
4	J	802	DEX	C6-C5-C10	2.70	117.28	115.61
4	C	1001	DEX	C13-C17-C20	-2.68	110.05	112.89
6	A	1003	EPE	O3S-S-C10	-2.68	101.43	105.77
4	M	802	DEX	C7-C8-C9	-2.64	108.50	110.94
4	D	802	DEX	C19-C10-C5	2.63	111.01	107.76
4	I	1001	DEX	C13-C17-C16	2.62	105.34	102.86
4	P	1001	DEX	C17-C13-C14	-2.60	96.92	99.36
4	L	1001	DEX	C6-C5-C10	2.60	117.21	115.61
4	A	1001	DEX	C13-C17-C20	-2.60	110.14	112.89
4	I	1001	DEX	C5-C4-C3	-2.53	120.50	122.72
4	H	802	DEX	C13-C17-C16	2.52	105.24	102.86
4	J	802	DEX	C13-C17-C16	2.49	105.22	102.86
4	K	802	DEX	C10-C9-C11	2.49	117.34	115.52
4	O	1001	DEX	C13-C17-C16	2.47	105.19	102.86
4	I	1001	DEX	C10-C9-C11	2.45	117.31	115.52
4	P	1001	DEX	C7-C8-C9	-2.45	108.68	110.94
4	D	802	DEX	C12-C13-C14	-2.45	105.87	108.03
4	P	1001	DEX	C6-C5-C10	2.44	117.12	115.61
4	M	802	DEX	C13-C17-C16	2.40	105.14	102.86
4	M	802	DEX	C6-C5-C10	2.37	117.07	115.61
4	P	1001	DEX	C15-C14-C8	-2.36	116.88	119.07
4	B	802	DEX	C1-C10-C5	-2.36	111.11	112.36
4	E	1001	DEX	O2-C11-C9	-2.36	105.59	109.08
4	L	1001	DEX	C13-C17-C16	2.36	105.09	102.86
4	K	802	DEX	C1-C10-C5	-2.35	111.12	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	802	DEX	C15-C14-C13	2.35	106.39	103.97
4	J	802	DEX	F1-C9-C11	2.33	104.75	102.72
4	D	802	DEX	C2-C3-C4	-2.30	114.78	117.13
4	O	1001	DEX	C8-C9-C11	2.29	117.15	114.55
4	D	802	DEX	C13-C17-C16	2.29	105.02	102.86
4	K	802	DEX	C8-C9-C11	2.28	117.14	114.55
4	K	802	DEX	C7-C8-C9	-2.25	108.86	110.94
4	F	1001	DEX	C9-C8-C14	2.23	110.99	109.26
4	E	1001	DEX	C15-C14-C8	-2.22	117.01	119.07
4	D	802	DEX	C15-C14-C13	2.21	106.24	103.97
4	M	802	DEX	C8-C9-C11	2.19	117.04	114.55
4	C	1001	DEX	C15-C16-C17	2.19	106.65	105.07
4	N	1001	DEX	C13-C17-C20	-2.17	110.59	112.89
4	M	802	DEX	C15-C14-C13	-2.16	101.74	103.97
4	C	1001	DEX	C12-C13-C17	-2.14	113.81	115.57
4	K	802	DEX	C6-C7-C8	2.14	115.98	111.74
4	O	1001	DEX	F1-C9-C11	-2.12	100.88	102.72
4	H	802	DEX	C13-C14-C8	2.11	115.40	113.73
4	D	802	DEX	C19-C10-C1	-2.10	104.44	106.63
6	I	1004	EPE	O2S-S-C10	2.09	109.43	106.92
4	P	1001	DEX	F1-C9-C8	-2.08	104.08	105.95
4	I	1001	DEX	C22-C16-C15	-2.08	110.18	113.53
4	E	1001	DEX	C13-C12-C11	-2.07	110.21	113.19
4	K	802	DEX	C6-C5-C10	2.07	116.89	115.61
4	L	1001	DEX	C9-C8-C14	2.06	110.85	109.26
4	L	1001	DEX	C19-C10-C5	2.05	110.29	107.76
4	K	802	DEX	C2-C3-C4	-2.04	115.05	117.13
4	L	1001	DEX	C12-C13-C14	-2.03	106.23	108.03
4	C	1001	DEX	O2-C11-C9	-2.03	106.08	109.08
4	G	1001	DEX	C8-C9-C11	2.03	116.86	114.55
4	J	802	DEX	O2-C11-C9	-2.02	106.09	109.08
4	I	1001	DEX	C13-C17-C20	-2.00	110.77	112.89

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	DEX	C17-C20-C21-O5
4	A	1001	DEX	O4-C20-C21-O5
4	D	802	DEX	C17-C20-C21-O5
4	D	802	DEX	O4-C20-C21-O5
4	H	802	DEX	C17-C20-C21-O5

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Mol	Chain	Res	Type	Atoms
4	I	1001	DEX	C17-C20-C21-O5
4	I	1001	DEX	O4-C20-C21-O5
4	K	802	DEX	C17-C20-C21-O5
4	K	802	DEX	O4-C20-C21-O5
4	L	1001	DEX	C17-C20-C21-O5
4	L	1001	DEX	O4-C20-C21-O5
4	M	802	DEX	C17-C20-C21-O5
4	M	802	DEX	O4-C20-C21-O5
6	A	1003	EPE	C8-C7-N4-C5
6	A	1003	EPE	S-C10-C9-N1
6	B	804	EPE	C10-C9-N1-C2
6	B	804	EPE	C10-C9-N1-C6
6	B	804	EPE	S-C10-C9-N1
6	I	1004	EPE	C9-C10-S-O1S
6	J	803	EPE	S-C10-C9-N1
6	L	1003	EPE	C10-C9-N1-C6
6	P	1002	EPE	C8-C7-N4-C5
7	A	1004	GOL	O1-C1-C2-C3
7	A	1005	GOL	C1-C2-C3-O3
7	B	805	GOL	C1-C2-C3-O3
7	C	1003	GOL	O1-C1-C2-C3
7	E	1003	GOL	O1-C1-C2-C3
7	E	1005	GOL	C1-C2-C3-O3
7	I	1005	GOL	C1-C2-C3-O3
7	J	804	GOL	O1-C1-C2-C3
7	J	804	GOL	C1-C2-C3-O3
7	J	805	GOL	O1-C1-C2-C3
7	K	804	GOL	C1-C2-C3-O3
7	K	805	GOL	C1-C2-C3-O3
7	P	1003	GOL	O1-C1-C2-C3
10	D	803	PG4	O2-C3-C4-O3
10	B	803	PG4	O2-C3-C4-O3
7	K	804	GOL	O2-C2-C3-O3
10	H	803	PG4	O1-C1-C2-O2
10	L	1002	PG4	O4-C7-C8-O5
12	F	1002	PEG	O1-C1-C2-O2
6	D	804	EPE	N4-C7-C8-O8
6	L	1003	EPE	C9-C10-S-O3S
10	B	803	PG4	O1-C1-C2-O2
10	B	803	PG4	O4-C7-C8-O5
10	D	803	PG4	O1-C1-C2-O2
7	A	1004	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	C	1002	GOL	O1-C1-C2-C3
7	C	1003	GOL	C1-C2-C3-O3
12	M	805	PEG	O1-C1-C2-O2
10	L	1002	PG4	O3-C5-C6-O4
7	A	1004	GOL	O2-C2-C3-O3
7	B	805	GOL	O2-C2-C3-O3
7	C	1002	GOL	O1-C1-C2-O2
7	E	1005	GOL	O2-C2-C3-O3
7	I	1005	GOL	O2-C2-C3-O3
7	J	804	GOL	O2-C2-C3-O3
7	K	805	GOL	O2-C2-C3-O3
7	P	1003	GOL	O1-C1-C2-O2
6	A	1003	EPE	N4-C7-C8-O8
4	H	802	DEX	O4-C20-C21-O5
6	I	1004	EPE	C9-C10-S-O3S
4	C	1001	DEX	C17-C20-C21-O5
7	A	1005	GOL	O2-C2-C3-O3
7	E	1003	GOL	O1-C1-C2-O2
7	J	805	GOL	O1-C1-C2-O2
7	L	1004	GOL	O2-C2-C3-O3
10	B	803	PG4	O3-C5-C6-O4
10	D	803	PG4	O4-C7-C8-O5
6	J	803	EPE	N4-C7-C8-O8
6	L	1003	EPE	C10-C9-N1-C2
6	P	1002	EPE	C10-C9-N1-C6
6	I	1004	EPE	N4-C7-C8-O8
7	C	1003	GOL	O1-C1-C2-O2
7	C	1003	GOL	O2-C2-C3-O3
7	J	804	GOL	O1-C1-C2-O2
7	L	1004	GOL	O1-C1-C2-O2
7	M	801	GOL	O2-C2-C3-O3
10	B	803	PG4	C6-C5-O3-C4
10	D	803	PG4	C4-C3-O2-C2
10	D	803	PG4	C8-C7-O4-C6
6	L	1003	EPE	C8-C7-N4-C3
10	H	803	PG4	C1-C2-O2-C3
10	B	803	PG4	C5-C6-O4-C7
10	D	803	PG4	C6-C5-O3-C4
10	L	1002	PG4	C3-C4-O3-C5
7	N	1002	GOL	O1-C1-C2-O2
12	I	1003	PEG	C4-C3-O2-C2
10	B	803	PG4	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
10	H	803	PG4	C8-C7-O4-C6
6	D	804	EPE	C9-C10-S-O2S
6	I	1004	EPE	C9-C10-S-O2S
6	L	1003	EPE	C9-C10-S-O1S
6	L	1003	EPE	C9-C10-S-O2S
4	N	1001	DEX	C17-C20-C21-O5
7	A	1004	GOL	O1-C1-C2-O2
12	K	801	PEG	O1-C1-C2-O2
13	M	804	PGE	C6-C5-O3-C4
6	I	1004	EPE	C8-C7-N4-C3
6	L	1003	EPE	C8-C7-N4-C5
6	L	1003	EPE	N4-C7-C8-O8
4	C	1001	DEX	O4-C20-C21-O5
4	E	1001	DEX	O4-C20-C21-O5
4	G	1001	DEX	O4-C20-C21-O5
4	N	1001	DEX	O4-C20-C21-O5
6	I	1004	EPE	C8-C7-N4-C5
6	P	1002	EPE	C10-C9-N1-C2
13	M	804	PGE	C3-C4-O3-C5
12	M	805	PEG	C4-C3-O2-C2
12	I	1003	PEG	C1-C2-O2-C3
4	E	1001	DEX	C17-C20-C21-O5
7	I	1005	GOL	O1-C1-C2-C3
10	B	803	PG4	C3-C4-O3-C5
10	L	1002	PG4	O2-C3-C4-O3
4	P	1001	DEX	O4-C20-C21-O5
10	H	803	PG4	O3-C5-C6-O4
10	D	803	PG4	O3-C5-C6-O4
10	H	803	PG4	O2-C3-C4-O3
7	L	1004	GOL	C1-C2-C3-O3
7	M	801	GOL	C1-C2-C3-O3
13	M	804	PGE	O3-C5-C6-O4
4	B	802	DEX	C17-C20-C21-O5
6	B	804	EPE	C8-C7-N4-C3
6	B	804	EPE	C8-C7-N4-C5
6	P	1002	EPE	C8-C7-N4-C3
10	H	803	PG4	C3-C4-O3-C5

There are no ring outliers.

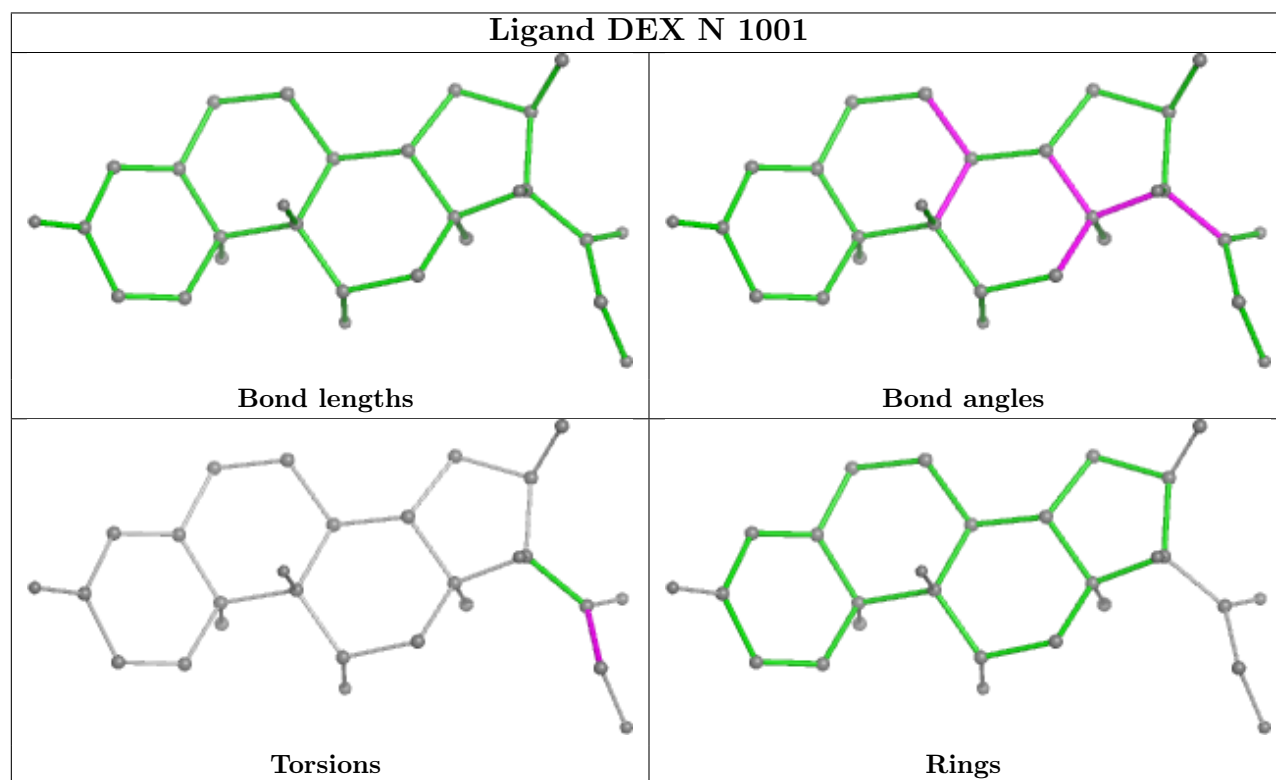
37 monomers are involved in 81 short contacts:

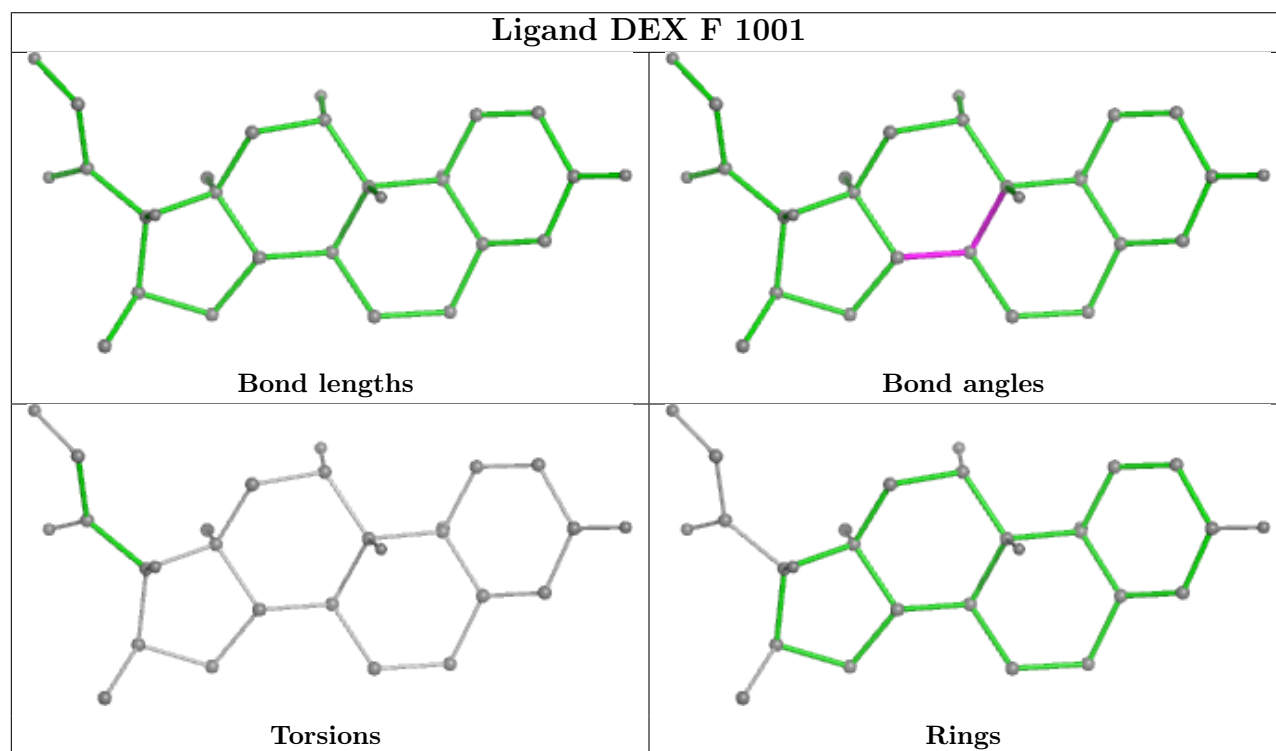
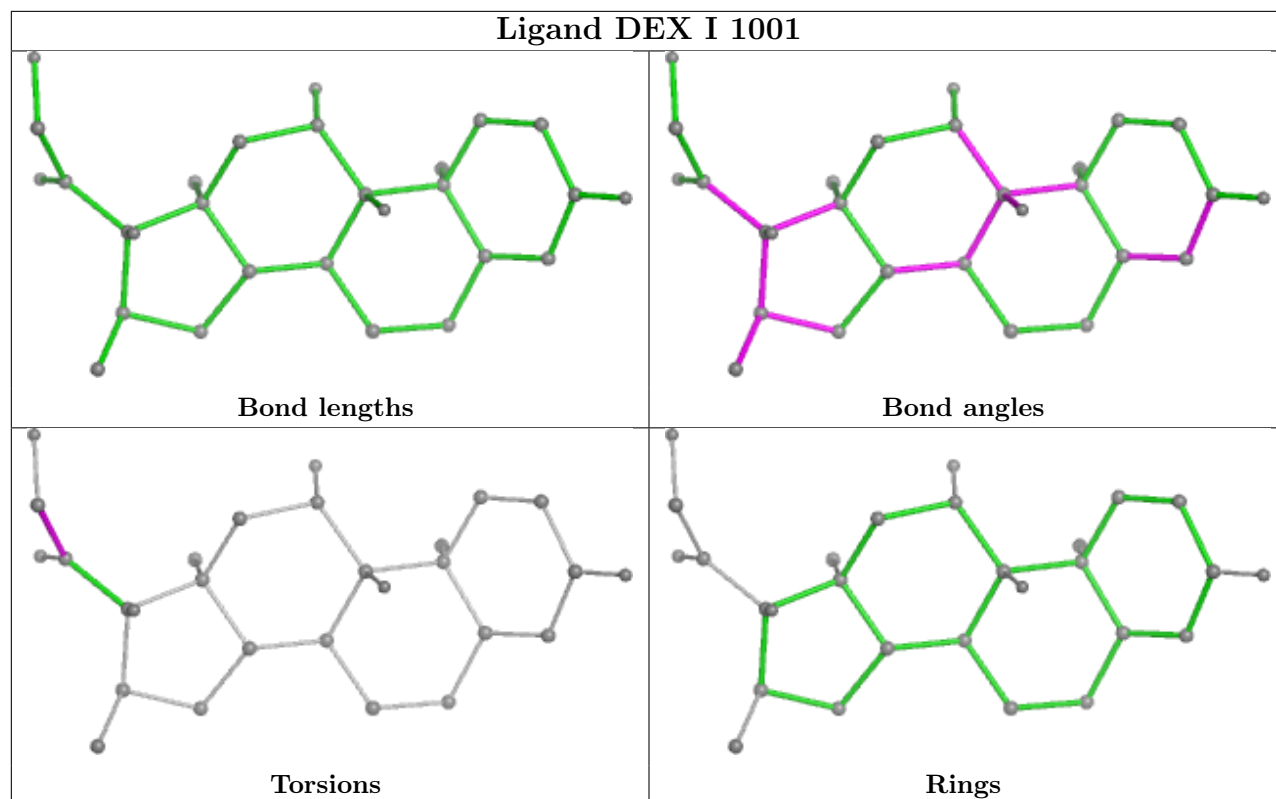


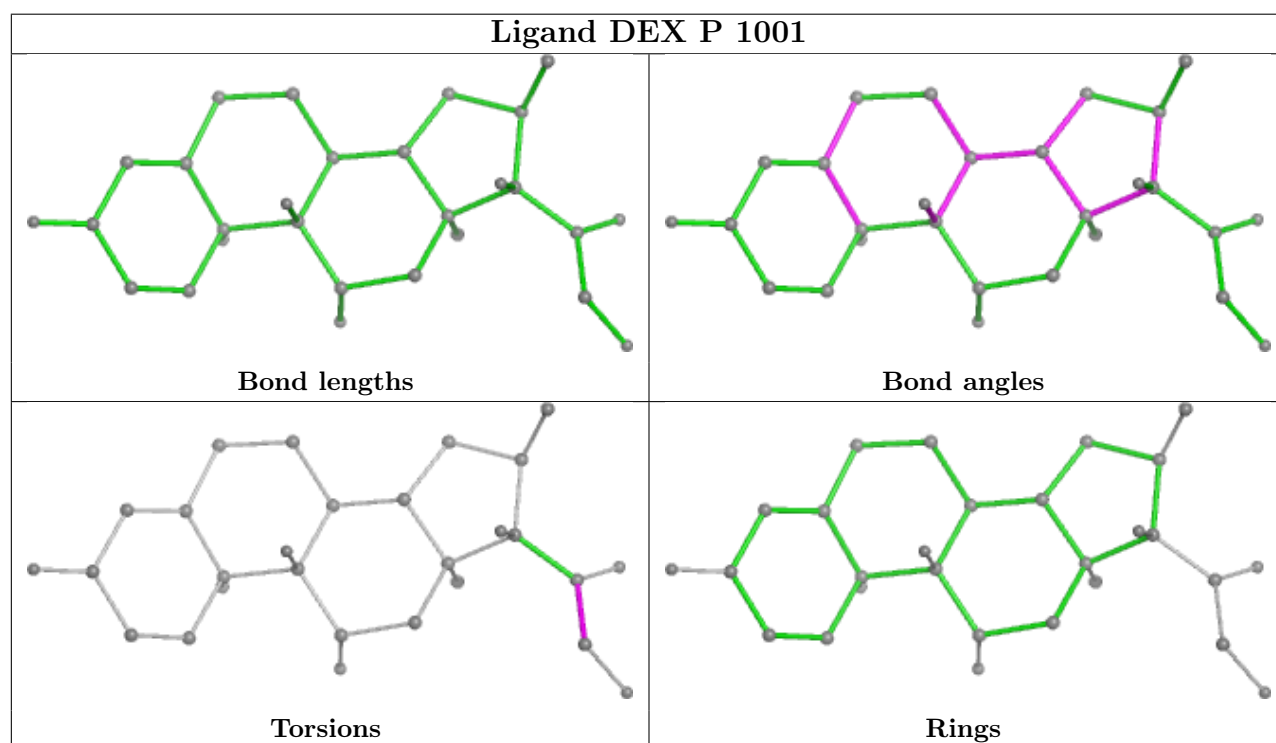
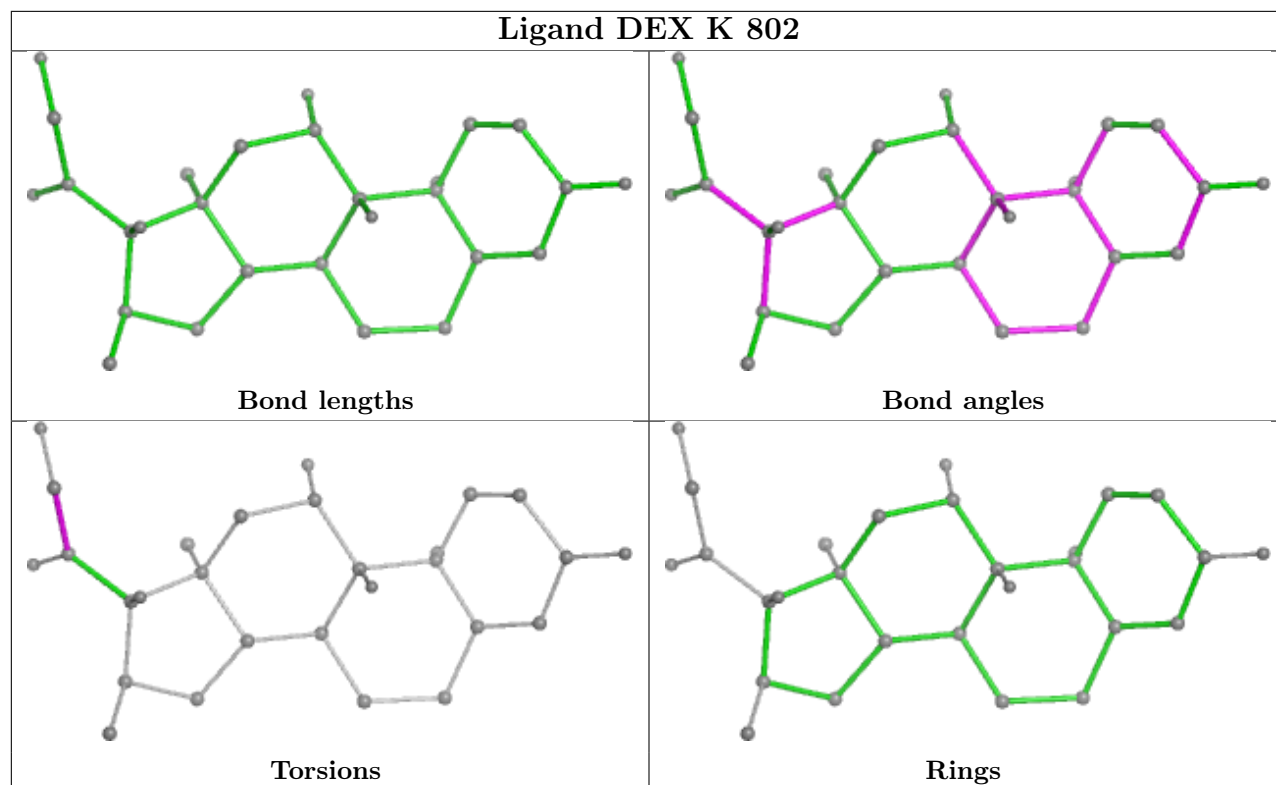
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	N	1002	GOL	1	0
4	N	1001	DEX	2	0
7	C	1003	GOL	3	0
4	I	1001	DEX	2	0
10	H	803	PG4	1	0
7	P	1003	GOL	4	0
8	A	1006	SO4	1	0
4	F	1001	DEX	2	0
4	K	802	DEX	2	0
8	C	1006	SO4	3	0
10	D	803	PG4	1	0
4	J	802	DEX	2	0
4	H	802	DEX	1	0
11	d	101	IMD	4	0
5	H	801	CAC	1	0
6	P	1002	EPE	12	0
4	M	802	DEX	1	0
4	A	1001	DEX	1	0
11	N	1003	IMD	2	0
4	L	1001	DEX	1	0
6	I	1004	EPE	2	0
13	M	804	PGE	2	0
11	L	1007	IMD	2	0
6	L	1003	EPE	1	0
11	O	1004	IMD	1	0
4	B	802	DEX	4	0
7	L	1005	GOL	1	0
12	K	801	PEG	1	0
6	B	804	EPE	1	0
7	C	1002	GOL	5	0
4	E	1001	DEX	3	0
6	D	804	EPE	1	0
7	I	1005	GOL	1	0
7	L	1004	GOL	4	0
4	C	1001	DEX	3	0
7	A	1005	GOL	1	0
4	O	1001	DEX	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

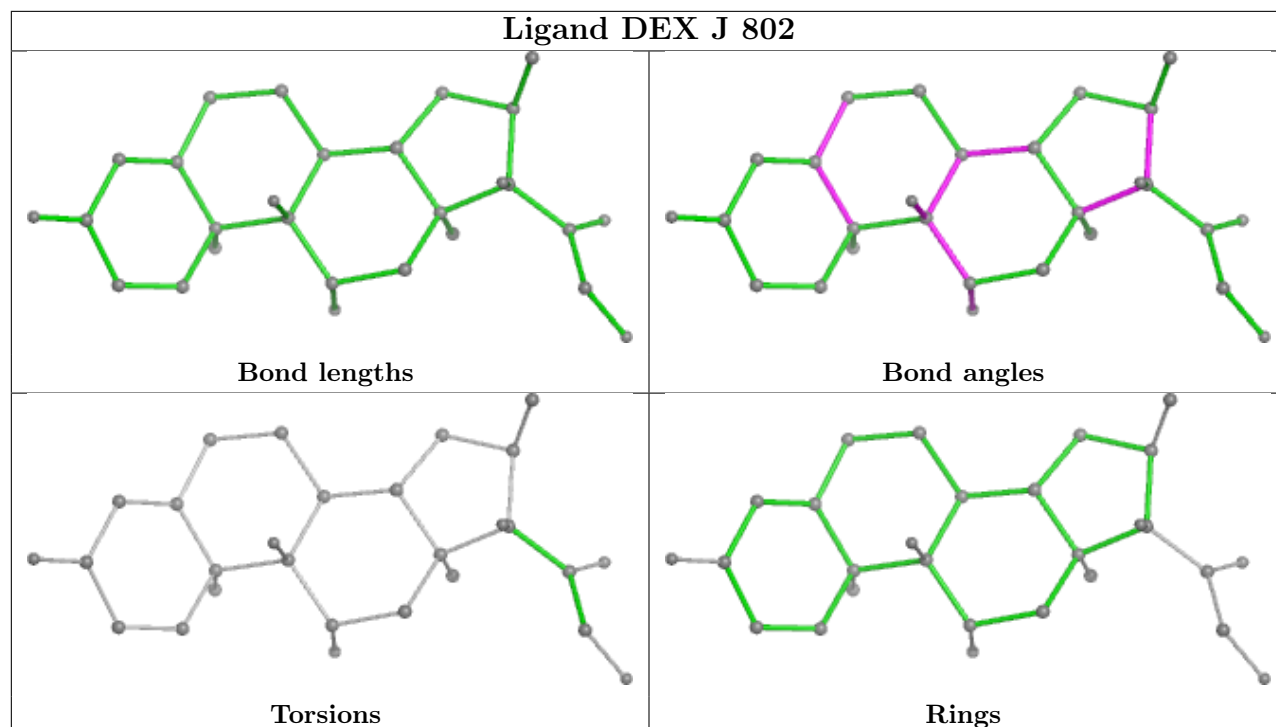
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



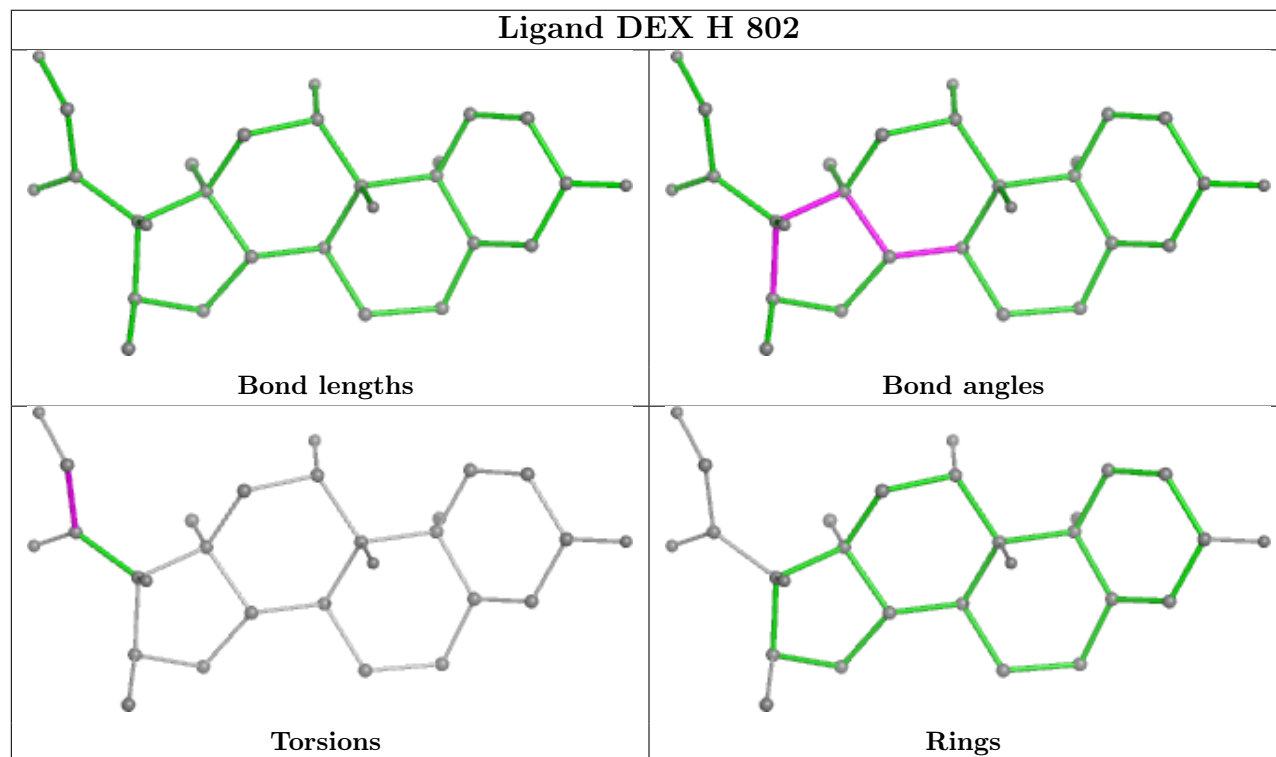


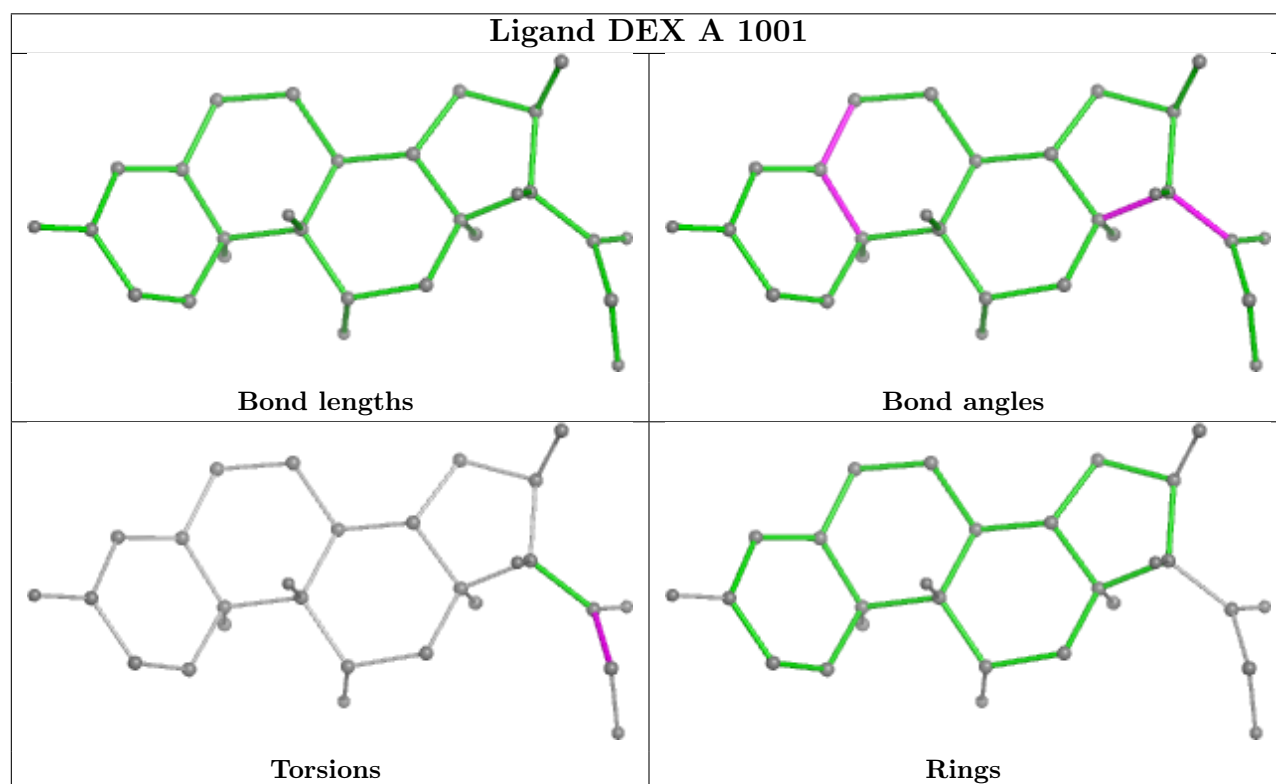
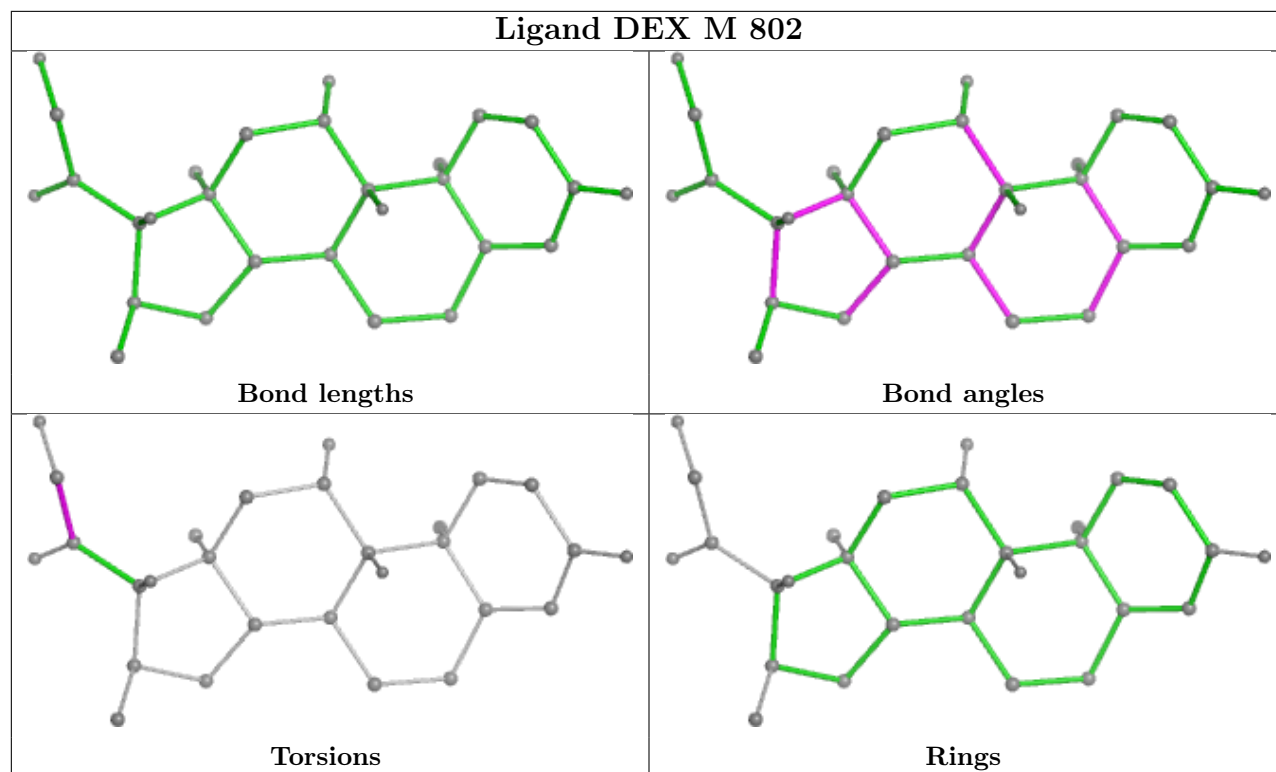


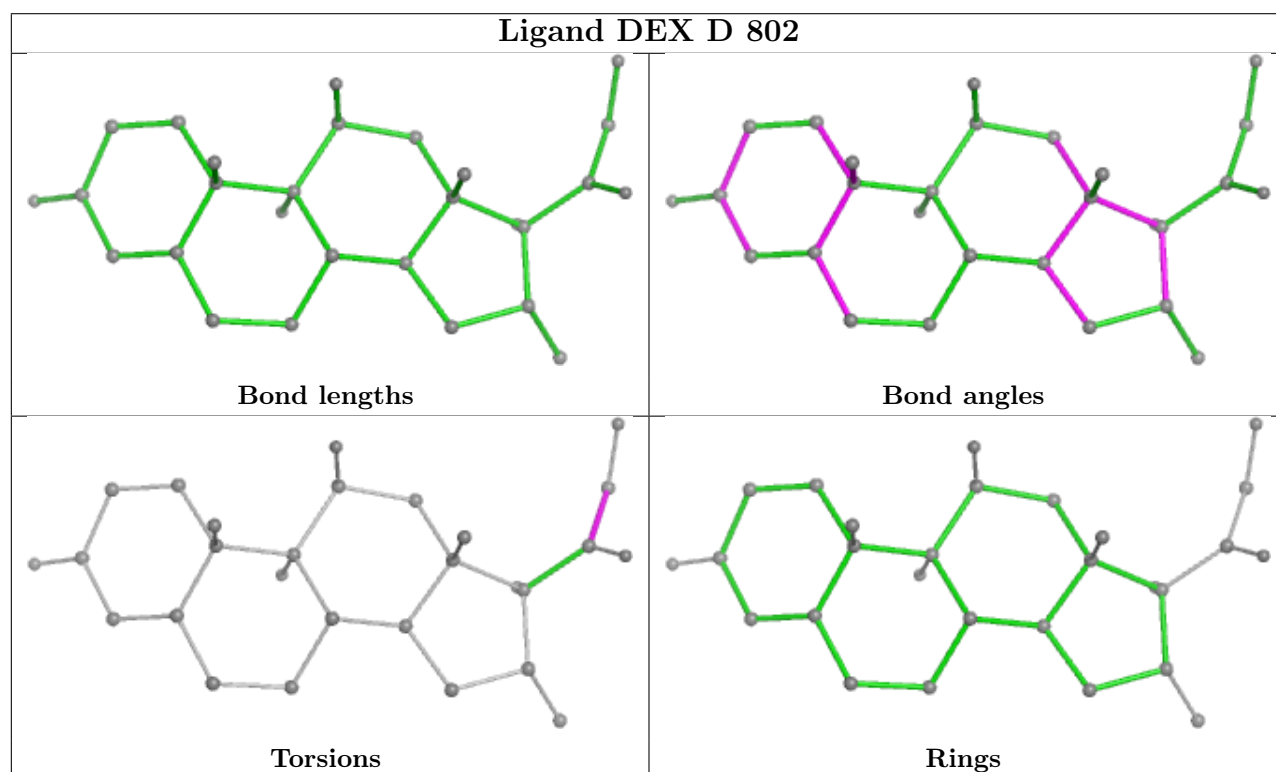
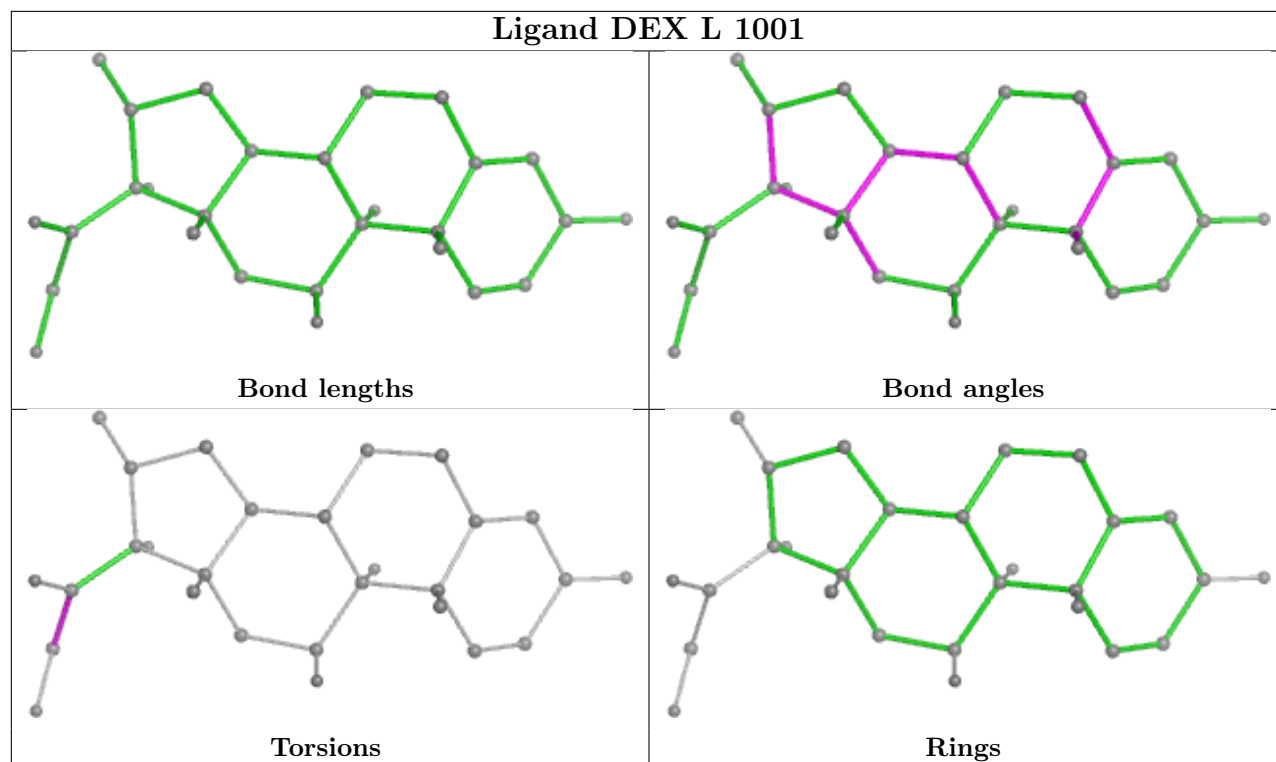
## Ligand DEX J 802



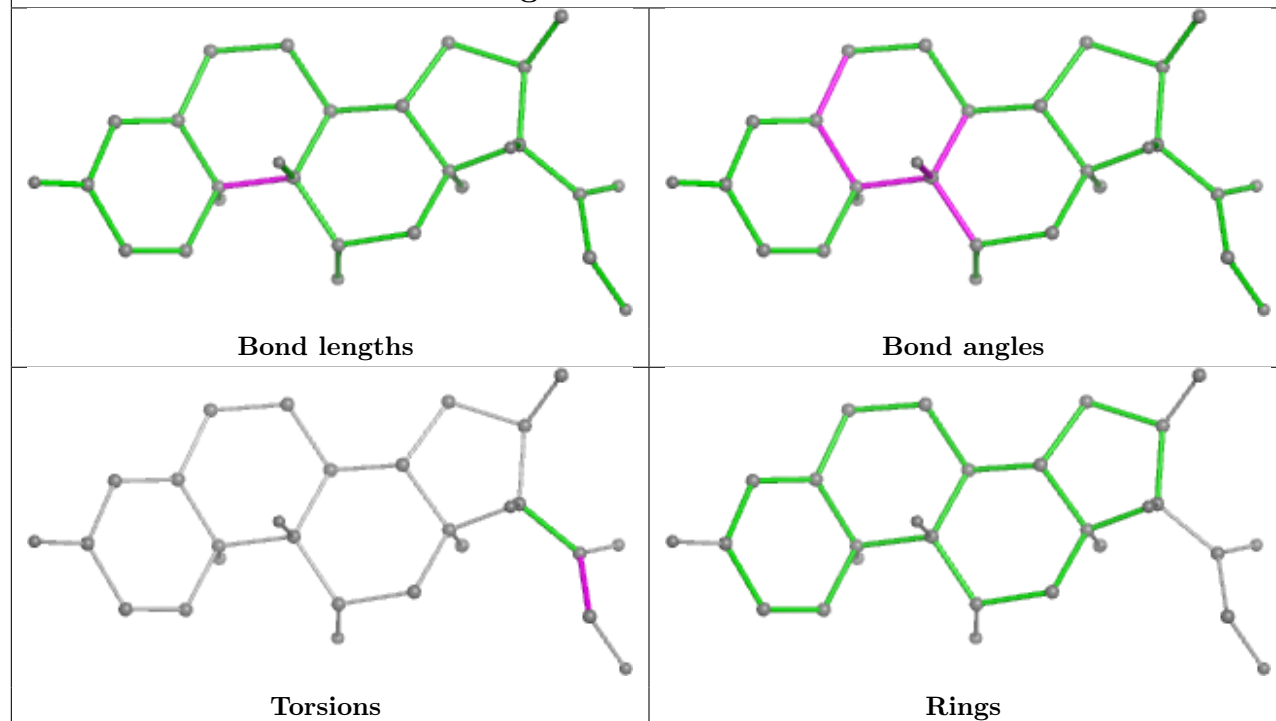
## Ligand DEX H 802



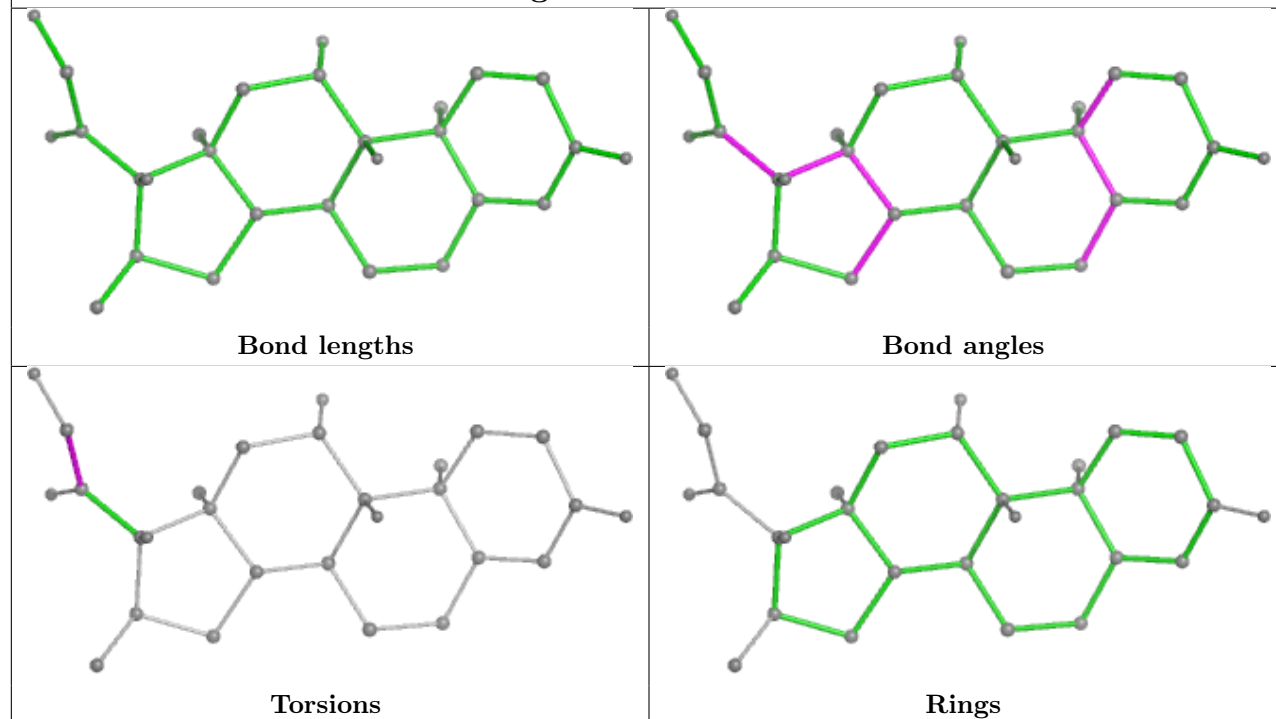




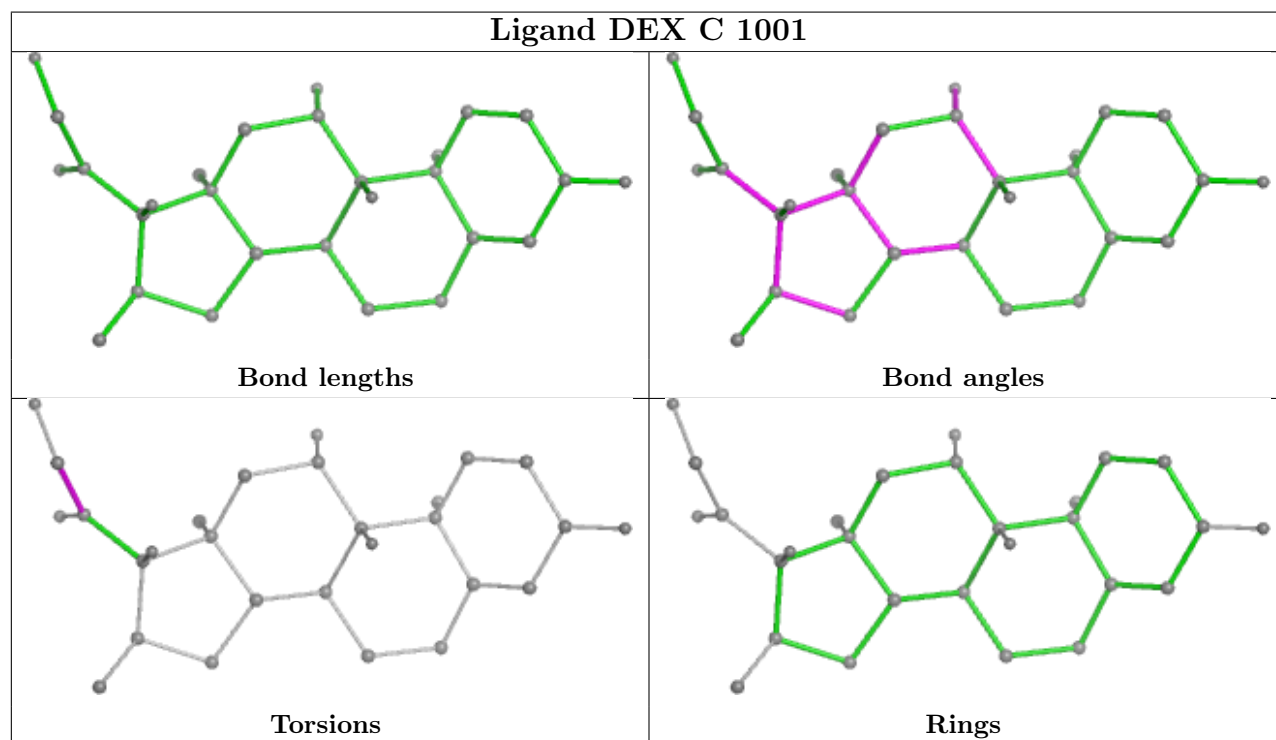
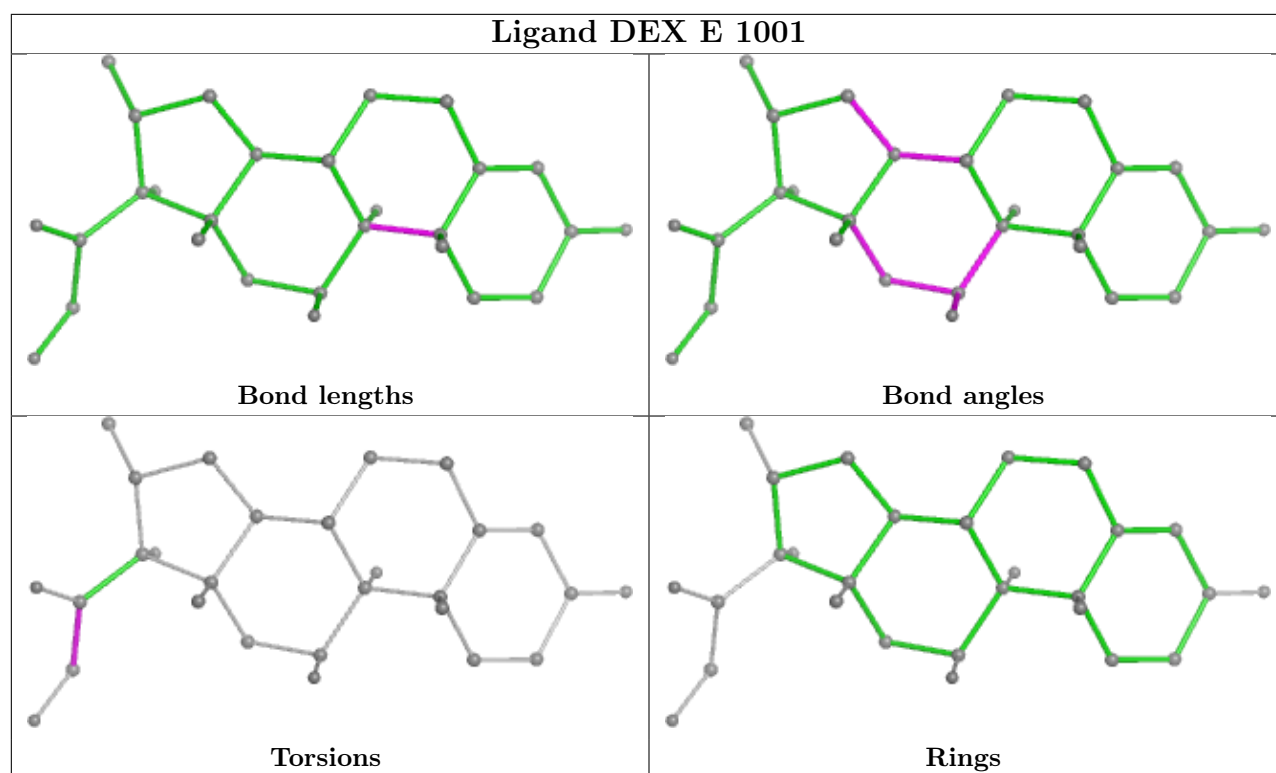
## Ligand DEX G 1001

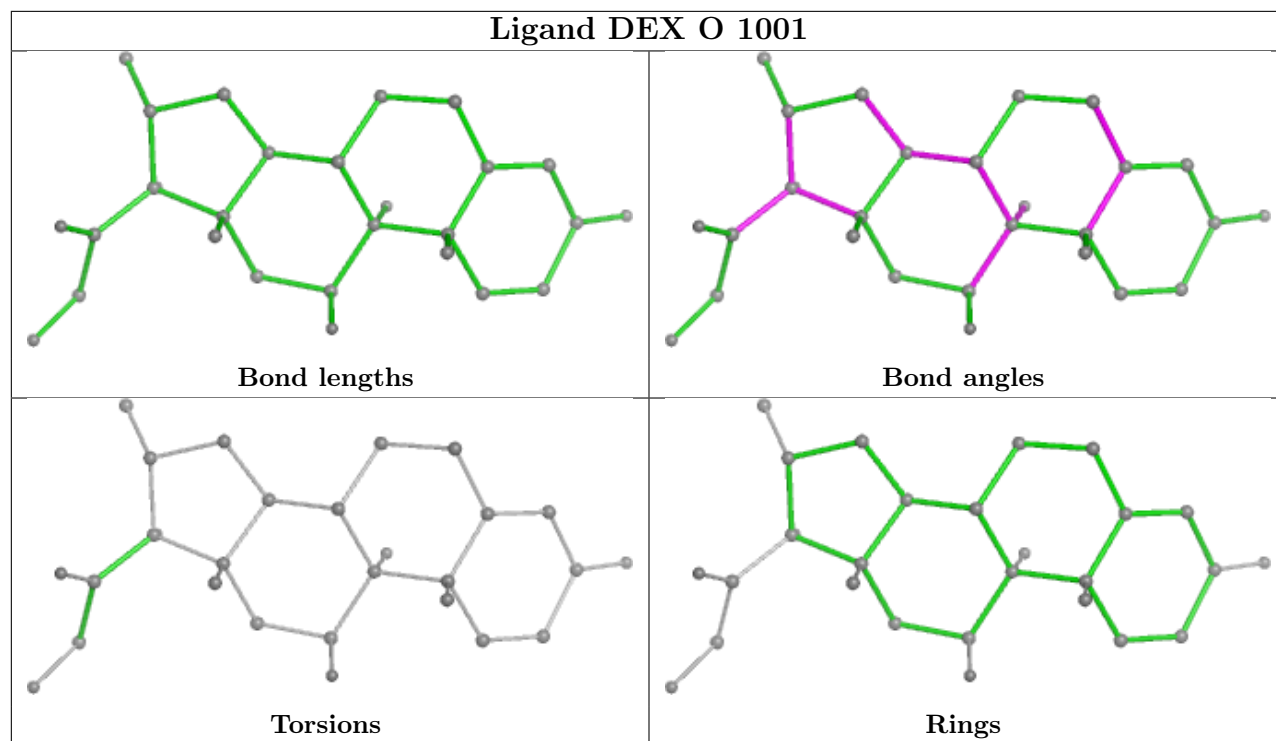


## Ligand DEX B 802









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	248/248 (100%)	0.07	13 (5%) 34 29	33, 63, 108, 155	0
1	C	248/248 (100%)	-0.24	6 (2%) 59 53	29, 51, 83, 126	0
1	D	248/248 (100%)	-0.09	9 (3%) 46 40	33, 57, 109, 141	0
1	F	248/248 (100%)	0.71	25 (10%) 14 12	44, 76, 122, 156	1 (0%)
1	G	248/248 (100%)	0.03	4 (1%) 70 65	37, 67, 111, 155	1 (0%)
1	H	245/248 (98%)	1.40	65 (26%) 2 2	44, 95, 146, 196	0
1	I	248/248 (100%)	-0.27	6 (2%) 59 53	33, 55, 95, 140	0
1	L	248/248 (100%)	-0.24	4 (1%) 70 65	34, 54, 89, 135	0
1	M	248/248 (100%)	0.28	16 (6%) 26 22	38, 67, 117, 166	0
1	P	243/248 (97%)	0.56	31 (12%) 9 9	37, 70, 115, 159	0
2	B	247/248 (99%)	-0.28	3 (1%) 76 72	30, 53, 96, 127	0
2	E	243/248 (97%)	0.33	12 (4%) 36 31	38, 63, 104, 140	1 (0%)
2	J	247/248 (99%)	-0.23	6 (2%) 59 53	29, 54, 94, 138	1 (0%)
2	K	244/248 (98%)	-0.07	6 (2%) 58 52	36, 63, 100, 150	0
2	N	244/248 (98%)	-0.15	7 (2%) 54 48	32, 60, 97, 134	1 (0%)
2	O	243/248 (97%)	0.19	13 (5%) 33 28	37, 65, 103, 129	0
3	a	14/15 (93%)	0.13	2 (14%) 7 7	41, 53, 115, 115	0
3	b	14/15 (93%)	0.05	1 (7%) 23 20	39, 55, 103, 117	0
3	c	14/15 (93%)	0.23	1 (7%) 23 20	43, 56, 114, 114	0
3	d	14/15 (93%)	0.33	1 (7%) 23 20	47, 63, 120, 126	0
3	e	14/15 (93%)	0.89	3 (21%) 3 3	53, 74, 130, 134	0
3	f	13/15 (86%)	1.42	4 (30%) 1 1	72, 96, 130, 135	0
3	g	13/15 (86%)	0.61	1 (7%) 21 18	50, 62, 120, 133	0
3	h	13/15 (86%)	1.17	1 (7%) 21 18	71, 94, 119, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	i	15/15 (100%)	0.45	2 (13%) 8 8	45, 61, 115, 125	0
3	j	14/15 (93%)	0.30	2 (14%) 7 7	40, 55, 106, 124	0
3	k	14/15 (93%)	0.26	1 (7%) 23 20	49, 60, 116, 129	0
3	l	14/15 (93%)	0.30	1 (7%) 23 20	48, 59, 109, 135	0
3	m	14/15 (93%)	0.43	2 (14%) 7 7	60, 72, 129, 137	0
3	n	15/15 (100%)	0.36	3 (20%) 3 3	47, 66, 120, 145	0
3	o	14/15 (93%)	0.97	2 (14%) 7 7	53, 78, 122, 140	0
3	p	14/15 (93%)	1.14	4 (28%) 1 2	59, 80, 123, 143	0
All	All	4163/4208 (98%)	0.15	257 (6%) 28 24	29, 63, 115, 196	5 (0%)

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	553	PRO	8.5
1	H	716	TYR	6.3
1	H	774	PHE	5.5
2	O	529	PHE	5.1
1	H	675	VAL	5.0
2	E	529	PHE	4.9
1	M	552	LEU	4.9
1	H	552	LEU	4.7
1	H	775	HIS	4.7
3	i	29	LEU	4.6
1	H	680	LEU	4.4
1	D	553	PRO	4.4
1	A	712	TRP	4.3
1	P	774	PHE	4.3
2	K	745	LEU	4.2
1	H	529	PHE	4.2
1	A	529	PHE	4.1
1	H	553	PRO	4.1
1	H	737	PHE	4.1
2	K	743	LYS	4.0
1	H	766	ALA	4.0
1	C	529	PHE	4.0
1	H	709	SER	4.0
1	P	529	PHE	4.0
2	K	709	SER	4.0
3	g	28	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	769	VAL	3.9
1	P	773	LEU	3.9
1	D	529	PHE	3.9
3	j	29	LEU	3.8
2	E	764	PHE	3.8
1	H	690	ARG	3.8
1	P	688	GLU	3.7
1	A	744	SER	3.7
1	H	686	PHE	3.7
1	G	529	PHE	3.7
1	H	722	LEU	3.6
1	H	726	HIS	3.6
1	I	743	LYS	3.6
1	F	684	ALA	3.6
1	H	676	PRO	3.6
1	A	711	ASN	3.5
1	H	764	PHE	3.5
1	P	771	PRO	3.5
1	H	679	GLY	3.5
2	N	728	MET	3.5
1	H	642	GLN	3.5
1	H	772	LEU	3.5
1	H	639	MET	3.5
1	M	529	PHE	3.4
1	F	709	SER	3.4
1	F	529	PHE	3.4
2	O	638	TYR	3.4
1	M	764	PHE	3.4
3	p	28	SER	3.4
1	H	761	LEU	3.3
3	h	22	TYR	3.3
2	K	529	PHE	3.3
1	P	679	GLY	3.2
3	f	26	SER	3.2
1	H	773	LEU	3.2
1	F	735	PHE	3.2
1	H	767	GLY	3.2
2	B	529	PHE	3.2
2	O	711	ASN	3.2
1	A	708	SER	3.2
1	F	680	LEU	3.2
2	E	585	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	591	ASP	3.2
1	M	745	LEU	3.1
1	H	674	THR	3.1
3	b	29	LEU	3.1
1	M	709	SER	3.1
2	E	679	GLY	3.1
1	H	723	ASP	3.1
1	P	675	VAL	3.1
1	M	551	THR	3.0
2	B	691	MET	3.0
1	F	703	LYS	3.0
1	H	551	THR	3.0
2	E	711	ASN	3.0
1	P	770	LYS	2.9
1	A	710	GLN	2.9
2	J	529	PHE	2.9
3	c	16	SER	2.9
1	F	585	ARG	2.9
2	N	712	TRP	2.9
1	H	695	LYS	2.9
1	A	638	TYR	2.9
1	M	684	ALA	2.9
2	N	711	ASN	2.9
1	P	716	TYR	2.9
1	M	549	ASP	2.9
3	p	29	LEU	2.9
1	A	743	LYS	2.8
3	o	28	SER	2.8
1	H	598	TYR	2.8
1	H	736	CYS	2.8
1	D	551	THR	2.8
1	M	638	TYR	2.8
1	H	745	LEU	2.8
2	E	691	MET	2.8
2	O	552	LEU	2.8
3	n	29	LEU	2.8
3	o	29	LEU	2.8
1	M	776	GLN	2.8
1	P	710	GLN	2.8
1	P	677	LYS	2.8
1	F	708	SER	2.8
3	f	28	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	691	MET	2.8
1	F	638	TYR	2.8
1	P	760	GLN	2.7
3	m	16	SER	2.7
1	P	764	PHE	2.7
2	O	705	GLU	2.7
1	H	771	PRO	2.7
1	D	745	LEU	2.7
1	P	767	GLY	2.7
1	C	644	GLN	2.7
3	p	22	TYR	2.7
1	P	687	ASP	2.7
1	G	735	PHE	2.7
1	H	595	LEU	2.7
1	I	529	PHE	2.7
1	M	744	SER	2.7
1	P	685	VAL	2.6
2	O	745	LEU	2.6
1	H	735	PHE	2.6
3	d	16	SER	2.6
2	O	548	TYR	2.6
1	C	711	ASN	2.6
1	H	672	LEU	2.6
1	H	600	TRP	2.6
3	f	27	SER	2.6
2	N	529	PHE	2.6
2	J	551	THR	2.6
3	l	16	SER	2.6
1	F	769	VAL	2.6
3	a	16	SER	2.5
1	F	597	GLN	2.5
1	H	554	ASP	2.5
2	J	549	ASP	2.5
3	n	15	ALA	2.5
1	F	740	PHE	2.5
1	H	715	PHE	2.5
1	H	720	LYS	2.5
1	A	551	THR	2.5
1	H	762	PRO	2.5
1	H	740	PHE	2.5
1	P	726	HIS	2.5
1	P	695	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	557	THR	2.5
1	P	772	LEU	2.4
1	H	585	ARG	2.4
1	A	716	TYR	2.4
1	F	598	TYR	2.4
1	M	558	ARG	2.4
1	C	709	SER	2.4
1	F	556	SER	2.4
2	O	639	MET	2.4
1	H	636	LEU	2.4
1	H	697	LEU	2.4
1	H	721	LEU	2.4
1	F	771	PRO	2.4
1	H	691	MET	2.4
1	F	774	PHE	2.4
1	I	764	PHE	2.4
1	P	635	GLN	2.4
2	J	641	ASP	2.4
3	e	29	LEU	2.4
1	L	743	LYS	2.4
1	P	769	VAL	2.4
1	D	709	SER	2.4
1	H	700	ALA	2.4
1	H	665	CYS	2.4
1	H	542	GLU	2.3
1	H	770	LYS	2.3
2	B	735	PHE	2.3
2	J	710	GLN	2.3
3	f	22	TYR	2.3
1	P	591	ASP	2.3
1	P	719	THR	2.3
1	F	632	GLU	2.3
1	L	529	PHE	2.3
1	D	744	SER	2.3
1	H	759	ASN	2.3
3	a	29	LEU	2.3
1	P	723	ASP	2.3
1	F	631	GLU	2.3
3	p	17	ARG	2.3
1	D	764	PHE	2.3
1	F	776	GLN	2.3
2	N	710	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	766	ALA	2.3
1	H	699	LYS	2.3
1	H	660	TYR	2.3
3	i	15	ALA	2.3
3	j	28	SER	2.3
3	n	16	SER	2.3
2	E	631	GLU	2.2
1	G	641	ASP	2.2
1	L	643	CYS	2.2
2	K	715	PHE	2.2
2	O	710	GLN	2.2
1	D	684	ALA	2.2
1	H	765	LYS	2.2
2	O	585	ARG	2.2
2	E	685	VAL	2.2
1	D	743	LYS	2.2
1	H	677	LYS	2.2
1	H	684	ALA	2.2
1	H	718	LEU	2.2
2	E	589	LEU	2.2
1	H	558	ARG	2.2
3	e	16	SER	2.2
3	e	28	SER	2.2
2	O	554	ASP	2.2
1	F	635	GLN	2.2
1	H	547	GLY	2.2
2	N	709	SER	2.2
1	P	686	PHE	2.2
1	P	711	ASN	2.1
1	L	765	LYS	2.1
1	F	726	HIS	2.1
1	A	709	SER	2.1
1	P	720	LYS	2.1
1	A	764	PHE	2.1
1	F	716	TYR	2.1
2	J	776	GLN	2.1
2	O	776	GLN	2.1
1	P	690	ARG	2.1
1	F	583	GLY	2.1
1	P	712	TRP	2.1
1	M	550	SER	2.1
2	N	765	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	710	GLN	2.1
1	C	776	GLN	2.1
1	H	734	GLN	2.1
1	I	776	GLN	2.1
2	E	678	ASP	2.1
3	k	29	LEU	2.1
1	M	703	LYS	2.1
1	F	685	VAL	2.1
1	F	764	PHE	2.1
2	O	636	LEU	2.1
3	m	29	LEU	2.1
1	M	708	SER	2.0
2	E	702	VAL	2.0
2	K	764	PHE	2.0
2	E	680	LEU	2.0
1	A	548	TYR	2.0
1	H	638	TYR	2.0
1	G	776	GLN	2.0
1	H	682	SER	2.0
1	H	678	ASP	2.0
1	P	598	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CSO	J	622	7/8	0.93	0.11	48,51,91,103	0
2	CSO	K	622[A]	7/8	0.93	0.11	43,48,57,63	2
2	CSO	K	622[B]	7/8	0.93	0.11	43,48,49,51	2
2	CSO	B	622[B]	7/8	0.94	0.10	40,44,64,67	2
2	CSO	B	622[A]	7/8	0.94	0.10	40,44,50,55	2
2	CSO	O	622[A]	7/8	0.94	0.11	39,44,48,59	2
2	CSO	O	622[B]	7/8	0.94	0.11	39,44,48,48	2
2	CSO	N	622[A]	7/8	0.95	0.10	43,44,50,51	2
2	CSO	N	622[B]	7/8	0.95	0.10	43,47,53,64	2
2	CSO	E	622[B]	7/8	0.96	0.08	39,42,50,58	2
2	CSO	E	622[A]	7/8	0.96	0.08	39,42,45,46	2

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	SO4	C	1006	5/5	0.68	0.17	143,144,166,175	0
8	SO4	C	1005	5/5	0.69	0.13	153,158,184,187	0
6	EPE	J	803	15/15	0.71	0.30	99,143,200,200	0
6	EPE	A	1003	15/15	0.72	0.22	112,127,165,176	0
6	EPE	P	1002	15/15	0.75	0.23	101,131,154,177	0
8	SO4	A	1006	5/5	0.77	0.11	163,165,175,185	0
11	IMD	J	807	5/5	0.77	0.25	103,104,108,117	0
6	EPE	B	804	15/15	0.78	0.22	74,113,165,185	0
6	EPE	L	1003	15/15	0.79	0.26	107,124,148,156	0
8	SO4	J	801	5/5	0.80	0.10	138,151,162,182	0
11	IMD	O	1004	5/5	0.81	0.28	77,92,101,103	0
7	GOL	J	806	6/6	0.83	0.18	74,85,96,97	0
11	IMD	B	807	5/5	0.83	0.26	92,99,101,108	0
11	IMD	F	1003	5/5	0.84	0.24	92,93,104,111	0
11	IMD	I	1006	5/5	0.84	0.23	116,117,126,126	0
7	GOL	O	1003	6/6	0.84	0.22	79,93,99,108	0
8	SO4	B	808	5/5	0.84	0.14	91,120,137,137	0
7	GOL	K	805	6/6	0.85	0.17	93,112,122,128	0
7	GOL	C	1002	6/6	0.85	0.21	63,85,91,99	0
11	IMD	J	808	5/5	0.85	0.26	101,102,112,113	0
11	IMD	L	1006	5/5	0.85	0.31	101,104,116,118	0
6	EPE	D	804	15/15	0.85	0.18	84,116,172,190	0
11	IMD	L	1007	5/5	0.86	0.29	106,112,115,117	0
7	GOL	N	1002	6/6	0.86	0.13	68,86,90,96	0
9	CL	F	1004	1/1	0.87	0.09	83,83,83,83	0
7	GOL	E	1003	6/6	0.87	0.18	98,106,119,123	0
6	EPE	I	1004	15/15	0.87	0.21	103,123,154,159	0
7	GOL	A	1005	6/6	0.88	0.16	59,79,82,86	0
7	GOL	E	1005	6/6	0.88	0.19	82,88,101,103	0
5	CAC	K	803	5/5	0.88	0.21	60,76,116,132	0
10	PG4	H	803	13/13	0.88	0.16	76,93,108,109	0
12	PEG	F	1002	7/7	0.88	0.17	64,82,92,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	A	1004	6/6	0.89	0.12	65,84,94,99	0
11	IMD	E	1006	5/5	0.89	0.28	106,106,112,113	0
7	GOL	K	804	6/6	0.89	0.12	87,92,97,98	0
10	PG4	D	803	13/13	0.89	0.18	70,83,95,103	0
11	IMD	b	101	5/5	0.89	0.21	87,93,95,95	0
7	GOL	C	1003	6/6	0.89	0.20	72,93,99,110	0
11	IMD	C	1004	5/5	0.90	0.31	106,116,125,128	0
12	PEG	K	801	7/7	0.90	0.14	47,58,63,65	0
7	GOL	B	805	6/6	0.91	0.12	67,78,89,92	0
11	IMD	M	806	5/5	0.91	0.18	95,97,106,113	0
12	PEG	I	1003	7/7	0.91	0.18	77,80,92,94	0
5	CAC	H	801	5/5	0.91	0.17	62,76,103,114	0
7	GOL	J	804	6/6	0.92	0.17	62,86,91,91	0
11	IMD	d	101	5/5	0.92	0.22	110,110,125,127	0
9	CL	J	809	1/1	0.92	0.17	81,81,81,81	0
10	PG4	B	803	13/13	0.92	0.19	77,89,98,101	0
7	GOL	J	805	6/6	0.92	0.12	54,76,82,83	0
9	CL	B	809	1/1	0.93	0.11	80,80,80,80	0
9	CL	E	1007	1/1	0.93	0.10	93,93,93,93	0
5	CAC	M	803	5/5	0.93	0.17	62,85,114,118	0
7	GOL	L	1004	6/6	0.93	0.11	51,51,54,57	0
9	CL	N	1004	1/1	0.93	0.14	87,87,87,87	0
7	GOL	M	801	6/6	0.93	0.12	65,65,68,69	0
7	GOL	I	1005	6/6	0.93	0.12	65,76,88,89	0
5	CAC	E	1002	5/5	0.93	0.15	58,63,92,99	0
12	PEG	M	805	7/7	0.93	0.15	66,70,82,88	0
7	GOL	L	1005	6/6	0.94	0.10	60,67,71,85	0
9	CL	B	810	1/1	0.94	0.12	94,94,94,94	0
5	CAC	A	1002	5/5	0.94	0.17	53,58,97,97	0
10	PG4	L	1002	13/13	0.94	0.16	63,75,93,102	0
5	CAC	I	1002	5/5	0.94	0.15	58,61,104,109	0
5	CAC	O	1002	5/5	0.94	0.17	68,93,105,112	0
7	GOL	P	1003	6/6	0.94	0.12	68,89,102,113	0
13	PGE	M	804	10/10	0.94	0.14	75,85,111,114	0
5	CAC	D	801	5/5	0.95	0.15	46,60,99,108	0
11	IMD	B	806	5/5	0.95	0.14	110,112,118,122	0
9	CL	M	807	1/1	0.95	0.09	85,85,85,85	0
11	IMD	N	1003	5/5	0.95	0.15	91,95,98,105	0
9	CL	D	805	1/1	0.96	0.18	82,82,82,82	0
9	CL	L	1008	1/1	0.96	0.08	84,84,84,84	0
4	DEX	H	802	28/28	0.96	0.09	57,68,78,83	0
9	CL	C	1007	1/1	0.96	0.08	75,75,75,75	0

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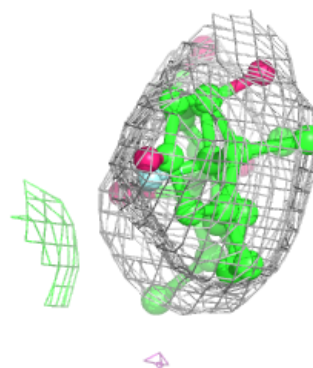
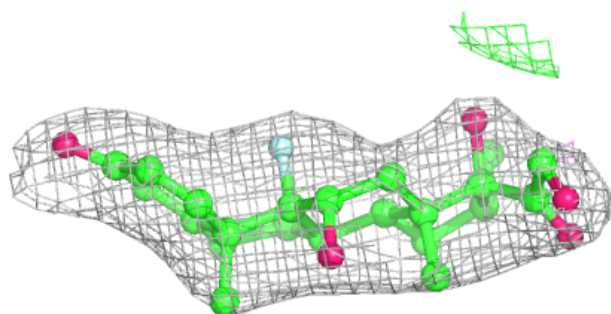
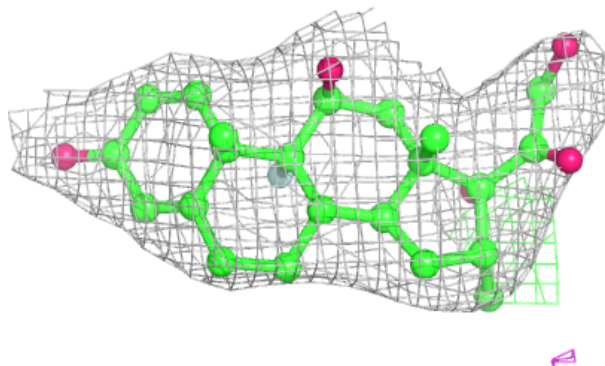
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DEX	F	1001	28/28	0.97	0.07	45,60,68,75	0
4	DEX	E	1001	28/28	0.97	0.07	36,40,47,57	0
4	DEX	K	802	28/28	0.97	0.07	32,44,57,65	0
7	GOL	E	1004	6/6	0.97	0.09	52,56,60,60	0
4	DEX	A	1001	28/28	0.98	0.06	35,43,60,65	0
4	DEX	B	802	28/28	0.98	0.07	32,41,49,52	0
4	DEX	G	1001	28/28	0.98	0.06	36,41,52,66	0
4	DEX	C	1001	28/28	0.98	0.06	32,39,46,58	0
9	CL	B	801	1/1	0.98	0.09	43,43,43,43	0
4	DEX	I	1001	28/28	0.98	0.06	33,38,50,65	0
4	DEX	J	802	28/28	0.98	0.05	26,34,47,61	0
4	DEX	D	802	28/28	0.98	0.06	36,41,52,63	0
4	DEX	L	1001	28/28	0.98	0.06	29,41,55,66	0
4	DEX	M	802	28/28	0.98	0.06	42,49,59,72	0
4	DEX	N	1001	28/28	0.98	0.06	33,43,51,53	0
4	DEX	O	1001	28/28	0.98	0.07	33,40,57,70	0
4	DEX	P	1001	28/28	0.98	0.07	38,45,56,60	0

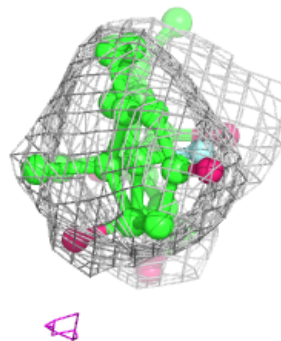
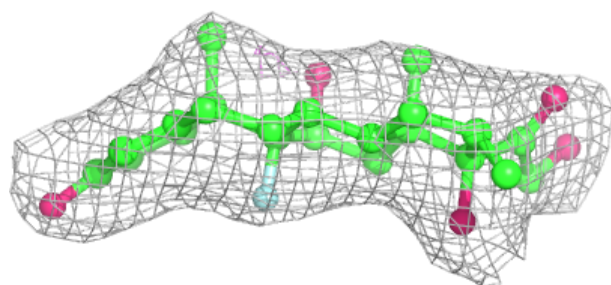
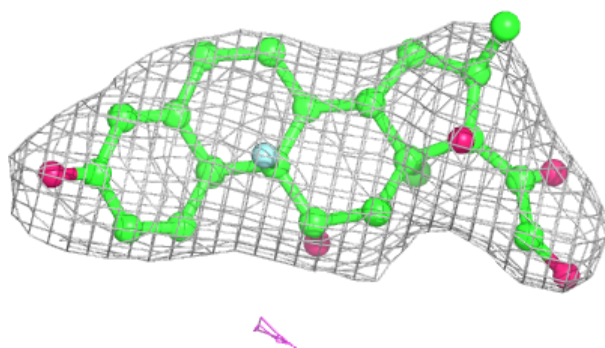
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around DEX H 802:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around DEX F 1001:**

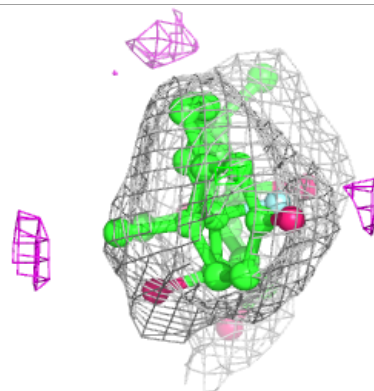
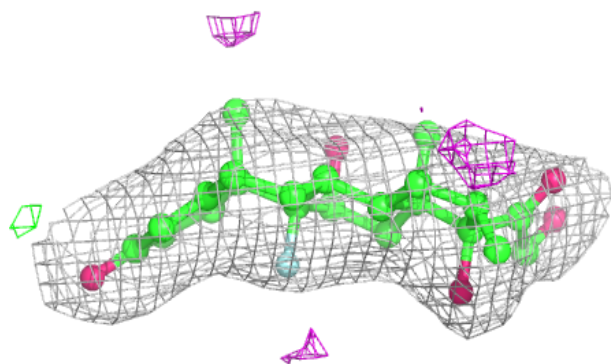
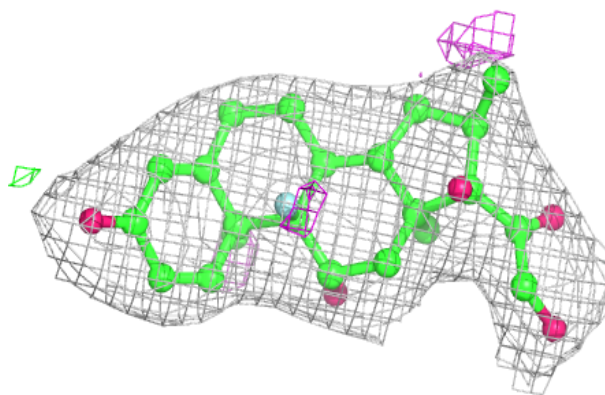
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



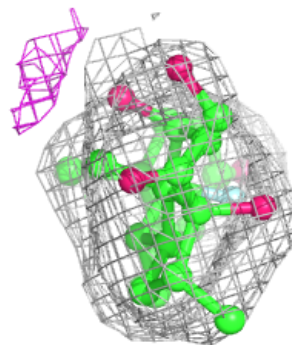
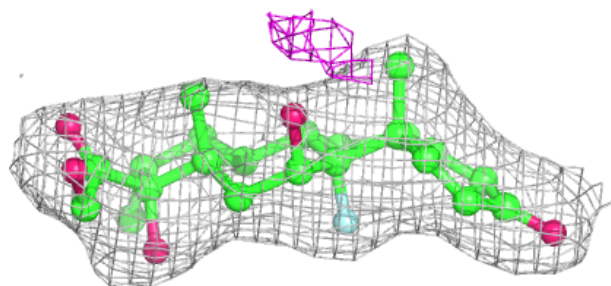
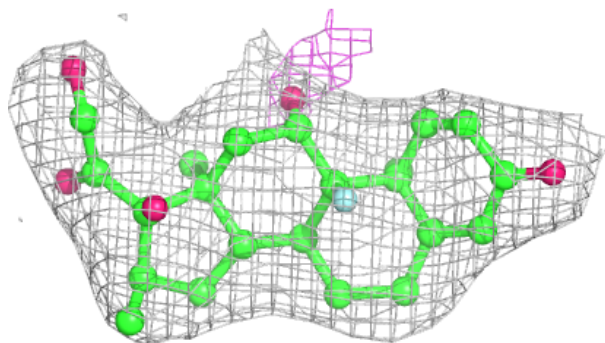


**Electron density around DEX E 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

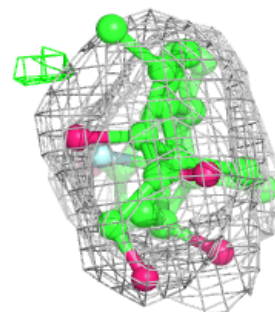
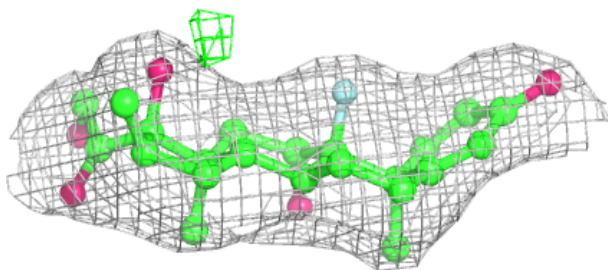
**Electron density around DEX K 802:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

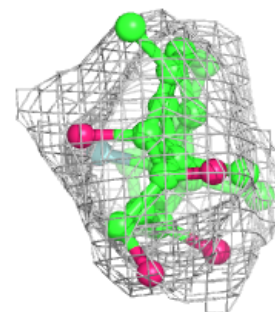
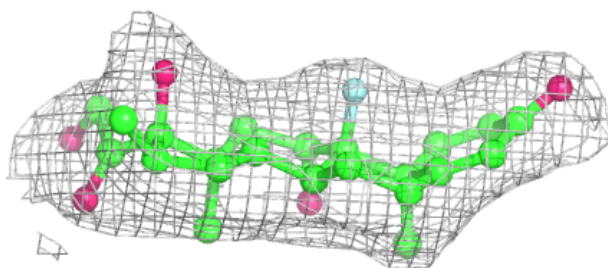
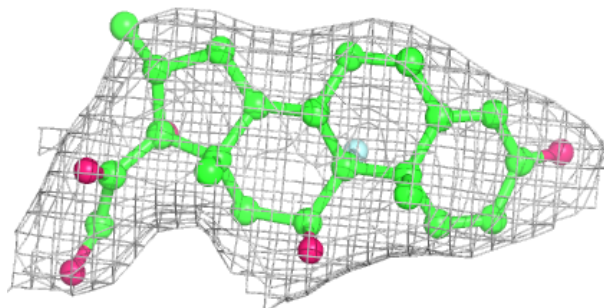


**Electron density around DEX A 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around DEX B 802:**

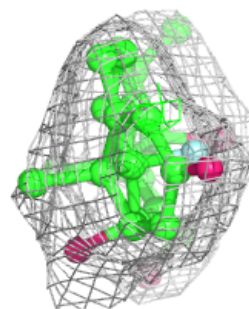
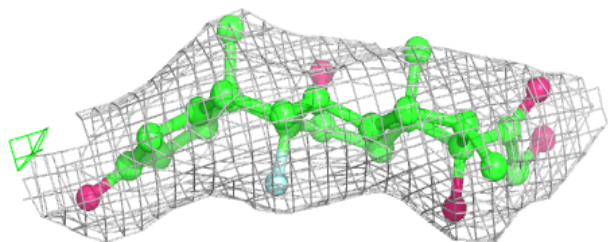
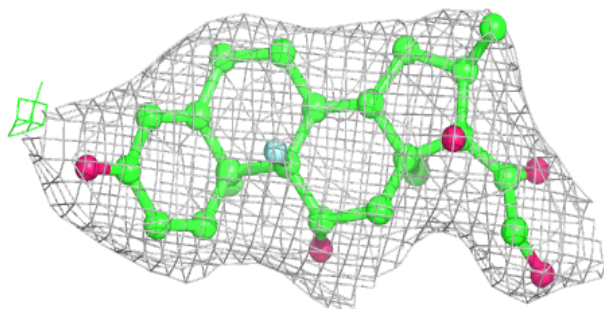
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



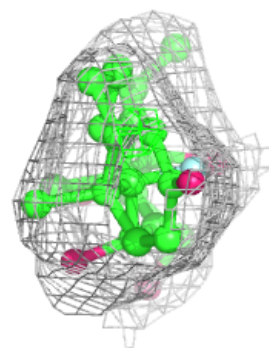
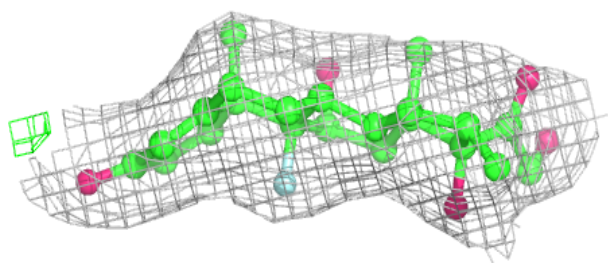
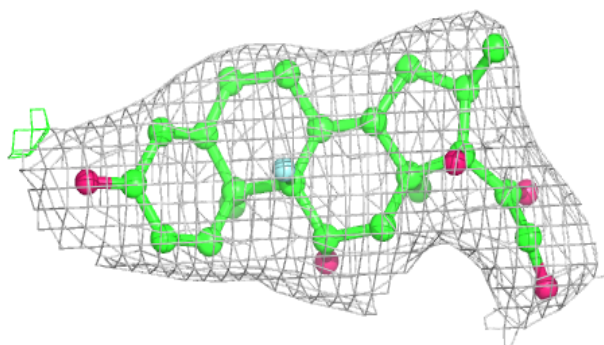


**Electron density around DEX G 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

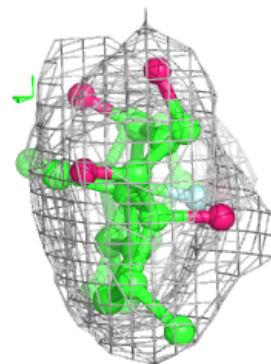
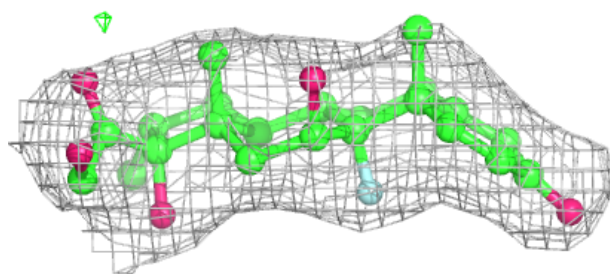
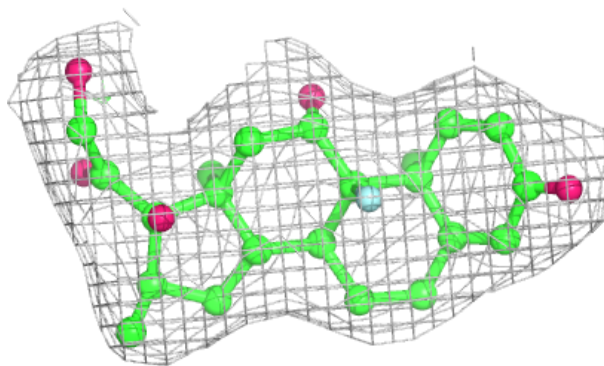
**Electron density around DEX C 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

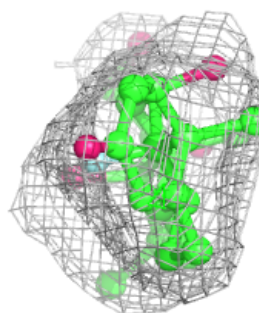
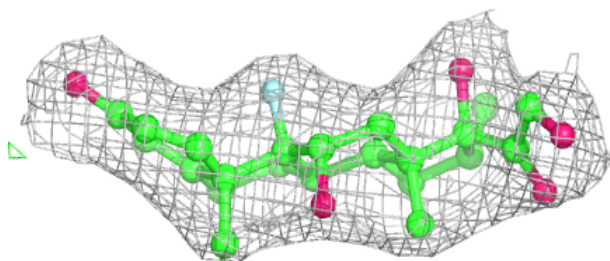
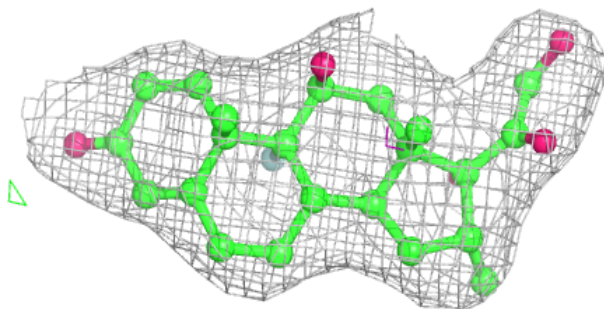


**Electron density around DEX I 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

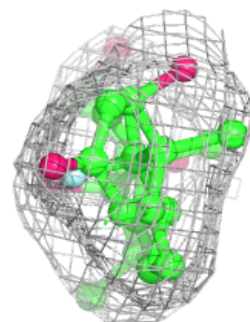
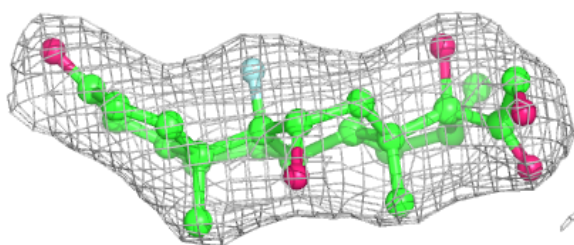
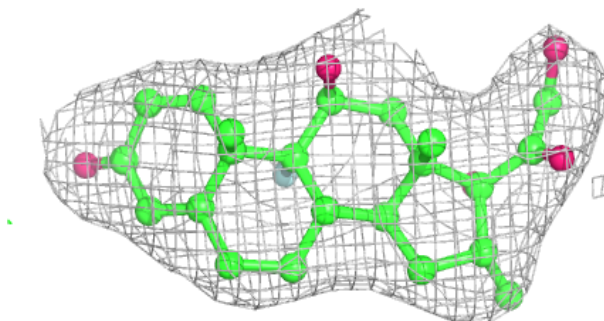
**Electron density around DEX J 802:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

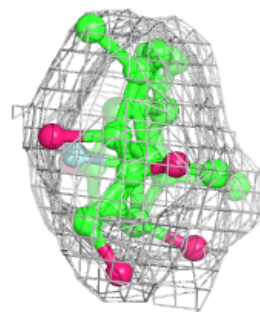
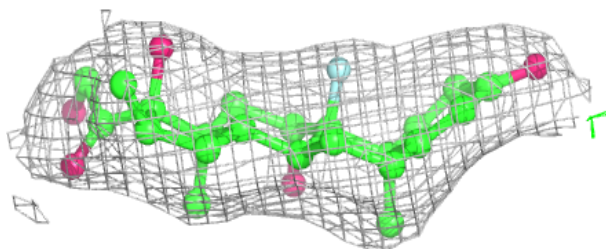
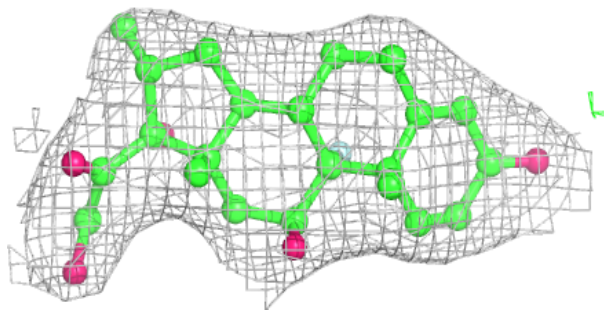


**Electron density around DEX D 802:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around DEX L 1001:**

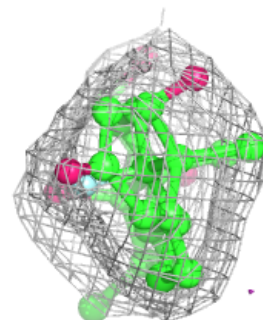
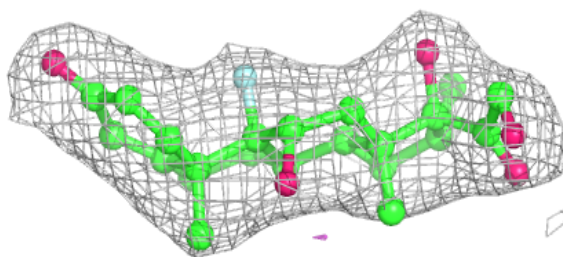
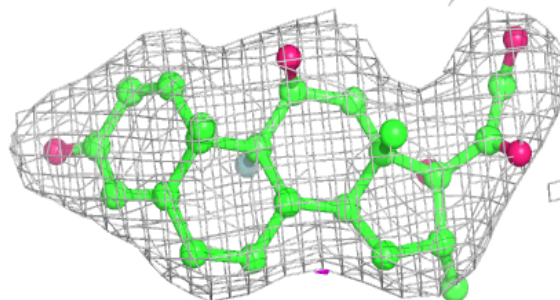
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



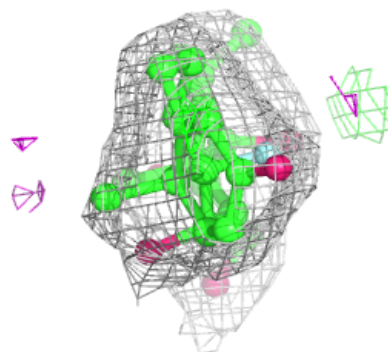
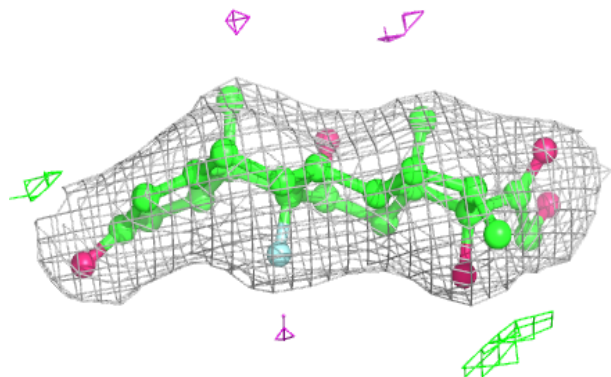
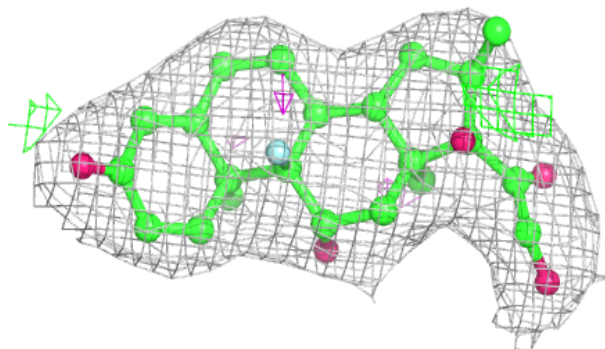


**Electron density around DEX M 802:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

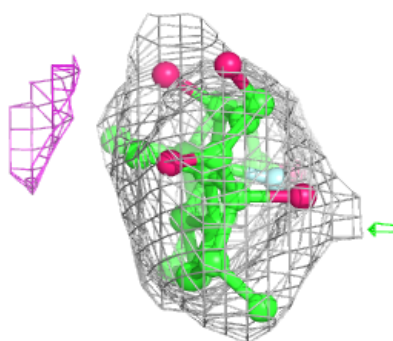
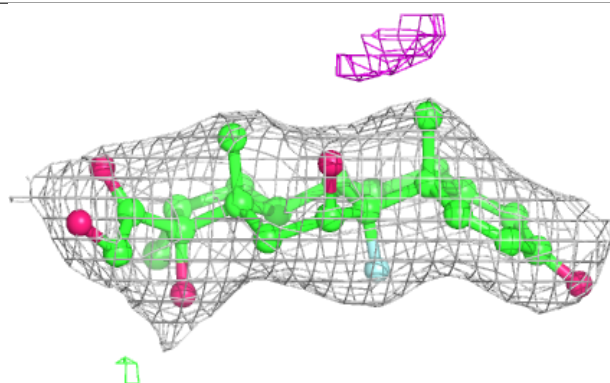
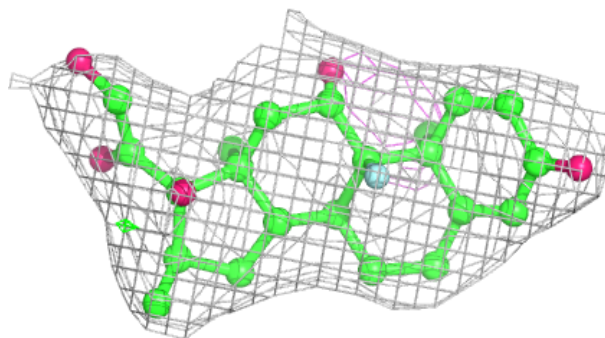
**Electron density around DEX N 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

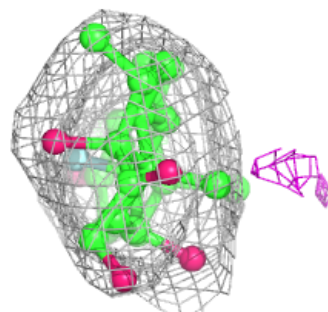
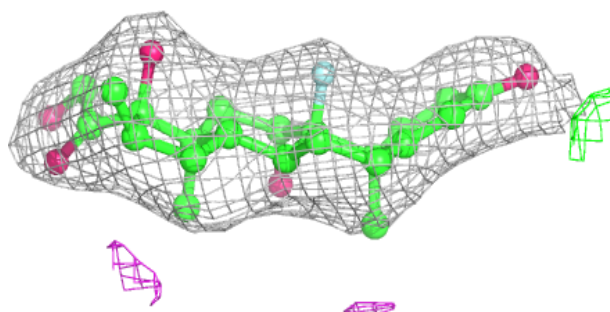


**Electron density around DEX O 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around DEX P 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.