



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2025 – 10:18 AM EDT

PDB ID : 9CBO / pdb\_00009cbo  
Title : Methionine synthase from *Thermus thermophilus* HB8, Folate and Cobalamin Domains, Pre-Catalytic Conformation (Pre-Fol-on)  
Authors : Yamada, K.; Mendoza, J.; Koutmos, M.  
Deposited on : 2024-06-19  
Resolution : 3.34 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 Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

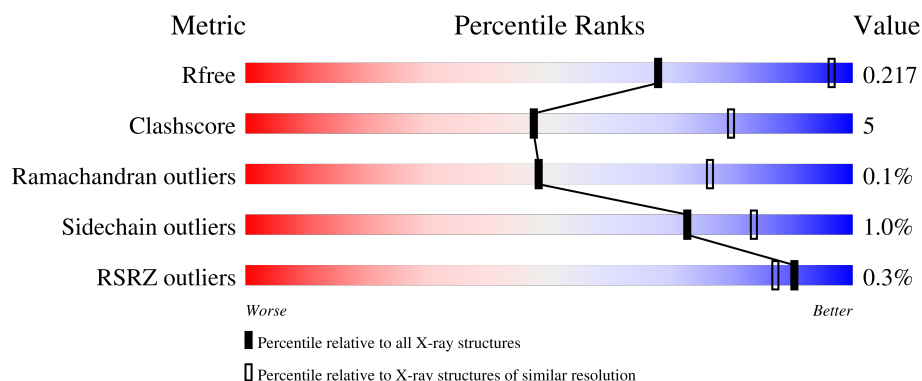
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.34 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	1325 (3.38-3.30)
Clashscore	180529	1376 (3.38-3.30)
Ramachandran outliers	177936	1376 (3.38-3.30)
Sidechain outliers	177891	1375 (3.38-3.30)
RSRZ outliers	164620	1325 (3.38-3.30)

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	511	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>.</div> </div> </div>
1	B	511	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div> </div>
1	C	511	<div> <div></div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>
1	D	511	<div> <div></div> <div> <div></div> <div>82%</div> <div>14%</div> <div>..</div> </div> </div>
1	E	511	<div> <div></div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	511	<div><div></div><div>84%</div><div>13%</div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24532 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.

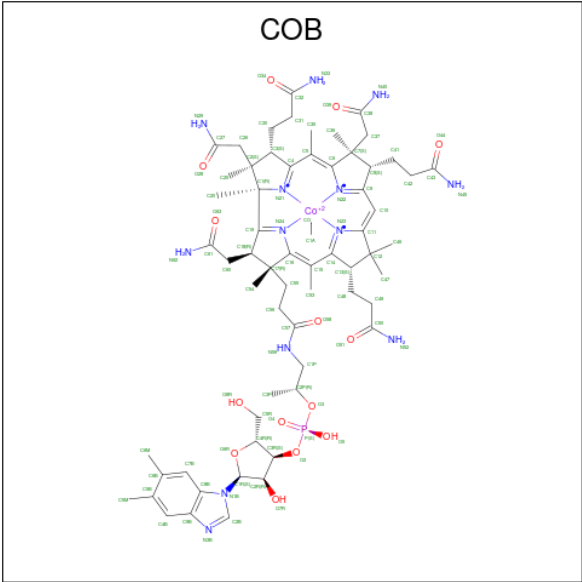
- Molecule 1 is a protein called Methionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			3978	2536	696	731	15			
1	B	510	Total	C	N	O	S	0	0	0
			3978	2536	696	731	15			
1	C	510	Total	C	N	O	S	0	0	0
			3978	2536	696	731	15			
1	D	507	Total	C	N	O	S	0	0	0
			3955	2523	692	725	15			
1	E	509	Total	C	N	O	S	0	0	0
			3969	2531	694	729	15			
1	F	510	Total	C	N	O	S	0	0	0
			3978	2536	696	731	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	759	ALA	ASP	engineered mutation	UNP Q5SKM5
B	759	ALA	ASP	engineered mutation	UNP Q5SKM5
C	759	ALA	ASP	engineered mutation	UNP Q5SKM5
D	759	ALA	ASP	engineered mutation	UNP Q5SKM5
E	759	ALA	ASP	engineered mutation	UNP Q5SKM5
F	759	ALA	ASP	engineered mutation	UNP Q5SKM5

- Molecule 2 is CO-METHYLCOBALAMIN (CCD ID: COB) (formula:  $C_{63}H_{91}CoN_{13}O_{14}P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Co	N	O	P	0	0
			92	63	1	13	14	1		
2	B	1	Total	C	Co	N	O	P	0	0
			92	63	1	13	14	1		
2	C	1	Total	C	Co	N	O	P	0	0
			92	63	1	13	14	1		
2	D	1	Total	C	Co	N	O	P	0	0
			92	63	1	13	14	1		
2	E	1	Total	C	Co	N	O	P	0	0
			92	63	1	13	14	1		
2	F	1	Total	C	Co	N	O	P	0	0
			92	63	1	13	14	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

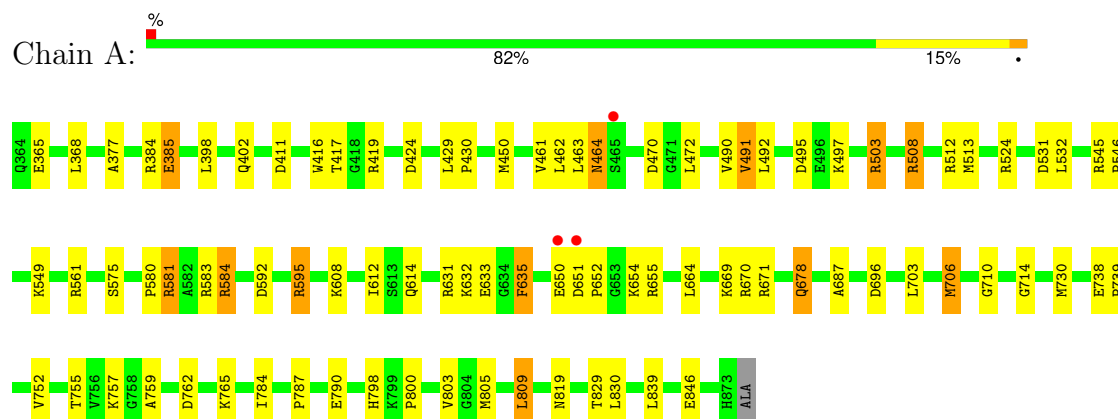
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	19	Total	O	0	0
			19	19		
4	C	26	Total	O	0	0
			26	26		
4	D	16	Total	O	0	0
			16	16		
4	E	6	Total	O	0	0
			6	6		
4	F	11	Total	O	0	0
			11	11		

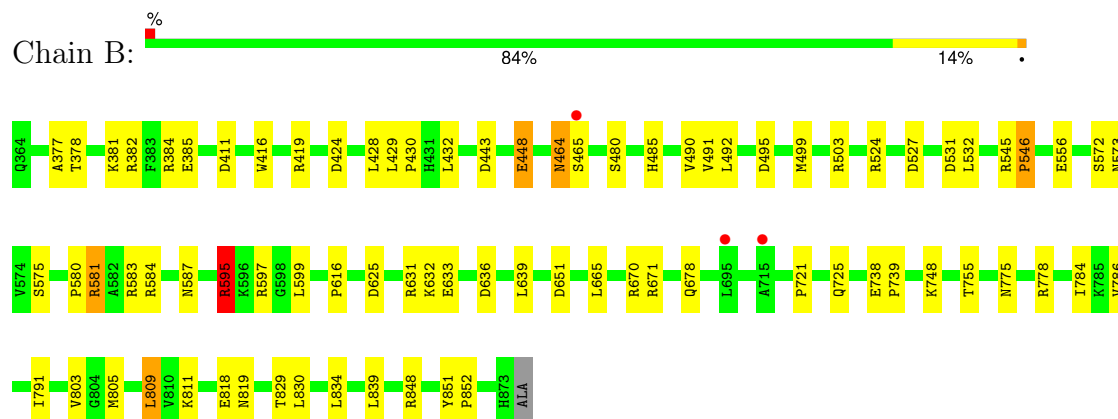
### 3 Residue-property plots [i](#)

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.

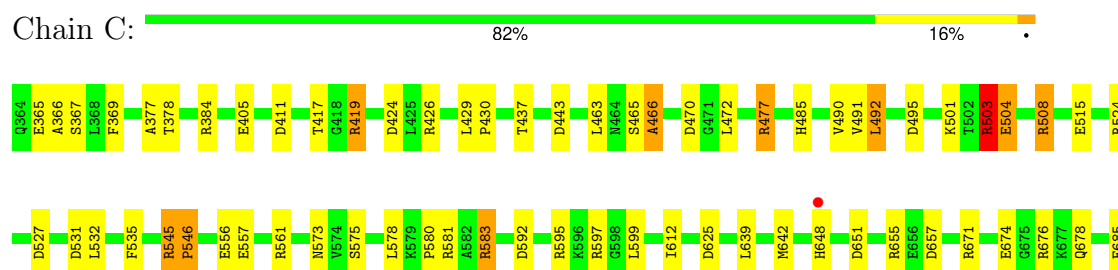
#### • Molecule 1: Methionine synthase

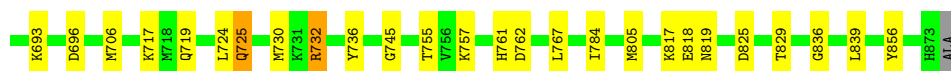


#### • Molecule 1: Methionine synthase



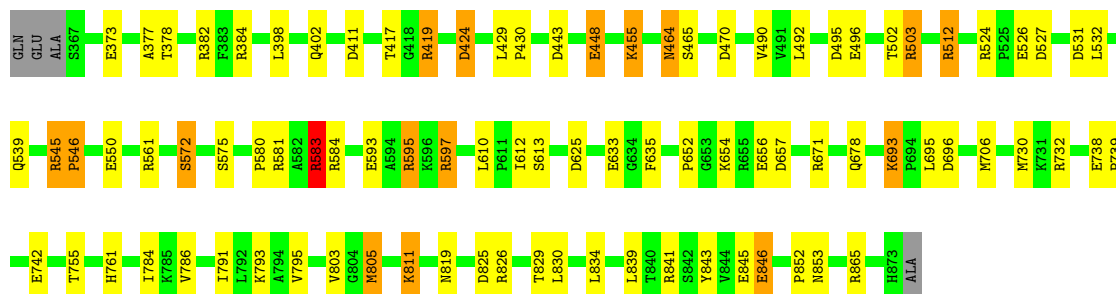
#### • Molecule 1: Methionine synthase





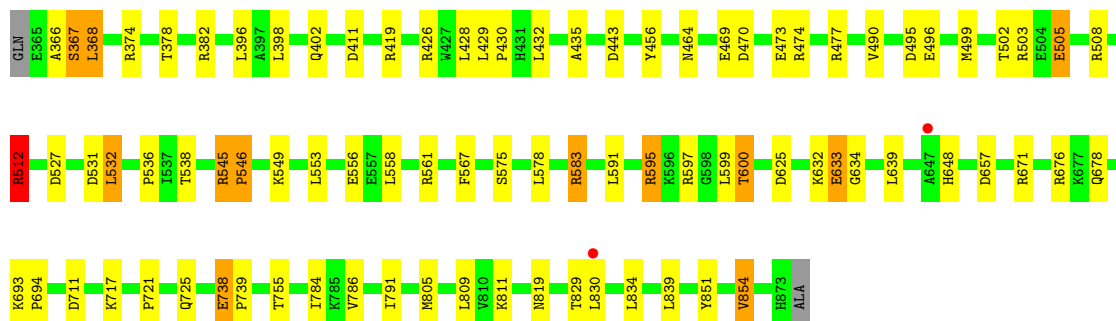
• Molecule 1: Methionine synthase

Chain D: 82% 14%



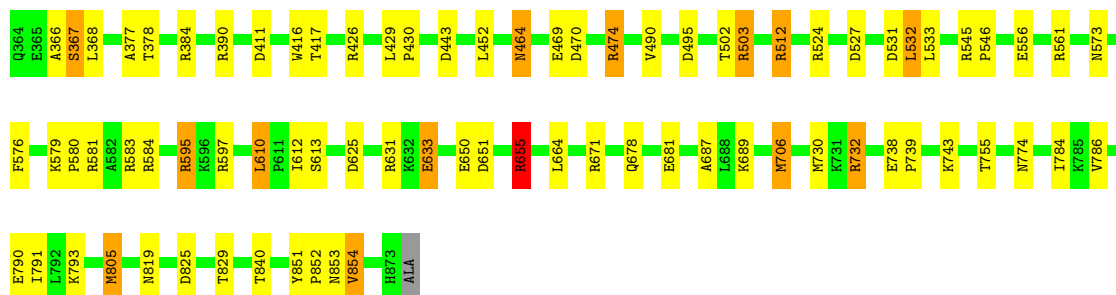
• Molecule 1: Methionine synthase

Chain E: 83% 14%



• Molecule 1: Methionine synthase

Chain F: 84% 13%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	187.77Å 187.77Å 325.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	163.18 – 3.34 162.65 – 3.34	Depositor EDS
% Data completeness (in resolution range)	99.9 (163.18-3.34) 99.9 (162.65-3.34)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.173 , 0.216 0.179 , 0.217	Depositor DCC
$R_{free}$ test set	4229 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	100.1	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 117.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	24532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: COB, GOL

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	0.93	3/4044 (0.1%)	1.50	35/5458 (0.6%)
1	B	0.88	2/4044 (0.0%)	1.41	25/5458 (0.5%)
1	C	0.89	1/4044 (0.0%)	1.46	39/5458 (0.7%)
1	D	0.87	3/4021 (0.1%)	1.47	50/5427 (0.9%)
1	E	0.79	0/4035	1.41	27/5446 (0.5%)
1	F	0.83	1/4044 (0.0%)	1.43	34/5458 (0.6%)
All	All	0.87	10/24232 (0.0%)	1.45	210/32705 (0.6%)

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	A	0	7
1	B	0	6
1	C	0	11
1	D	0	8
1	E	0	8
1	F	0	9
All	All	0	49

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	652	PRO	N-CD	8.31	1.59	1.47
1	D	496	GLU	CD-OE2	7.33	1.39	1.25
1	D	496	GLU	CD-OE1	6.66	1.38	1.25
1	B	485	HIS	CG-CD2	-6.65	1.28	1.35
1	B	503	ARG	NE-CZ	6.62	1.40	1.33
1	C	485	HIS	CG-CD2	-6.09	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	655	ARG	NE-CZ	5.89	1.39	1.33
1	D	545	ARG	C-O	-5.58	1.19	1.24
1	A	385	GLU	CD-OE1	5.48	1.35	1.25
1	A	512	ARG	CZ-NH2	-5.06	1.26	1.33

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	508	ARG	NE-CZ-NH1	-10.17	111.33	121.50
1	D	546	PRO	N-CA-C	10.07	126.90	114.92
1	D	841	ARG	NE-CZ-NH1	-9.39	112.11	121.50
1	D	546	PRO	N-CA-CB	-8.40	93.35	102.17
1	C	657	ASP	CA-CB-CG	8.34	120.94	112.60
1	A	495	ASP	CA-CB-CG	8.32	120.92	112.60
1	C	648	HIS	N-CA-C	8.30	120.62	110.91
1	D	502	THR	OG1-CB-CG2	-8.28	92.75	109.30
1	A	385	GLU	CG-CD-OE1	8.11	137.06	118.40
1	A	829	THR	CA-CB-OG1	-7.80	97.90	109.60
1	D	805	MET	CG-SD-CE	-7.79	83.77	100.90
1	C	508	ARG	NE-CZ-NH1	-7.74	113.76	121.50
1	A	417	THR	OG1-CB-CG2	-7.59	94.12	109.30
1	C	495	ASP	CA-CB-CG	7.59	120.19	112.60
1	E	368	LEU	N-CA-CB	-7.54	98.62	109.85
1	F	503	ARG	CG-CD-NE	7.42	128.33	112.00
1	B	495	ASP	CA-CB-CG	7.38	119.97	112.60
1	E	546	PRO	N-CA-CB	-7.22	94.59	102.17
1	D	532	LEU	N-CA-C	-7.20	100.35	110.50
1	C	378	THR	CA-CB-OG1	-7.15	98.87	109.60
1	C	532	LEU	N-CA-C	-7.14	100.43	110.50
1	D	654	LYS	CB-CG-CD	7.14	127.72	111.30
1	E	829	THR	CA-CB-OG1	-7.12	98.92	109.60
1	E	495	ASP	CA-CB-CG	7.08	119.69	112.60
1	A	503	ARG	NH1-CZ-NH2	-7.02	110.18	119.30
1	E	378	THR	CA-CB-OG1	-6.91	99.23	109.60
1	F	495	ASP	CA-CB-CG	6.91	119.50	112.60
1	F	378	THR	CA-CB-OG1	-6.89	99.26	109.60
1	A	411	ASP	CA-CB-CG	6.89	119.49	112.60
1	A	549	LYS	CG-CD-CE	-6.86	95.52	111.30
1	C	411	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	532	LEU	N-CA-C	-6.85	100.85	110.50
1	A	464	ASN	CA-C-N	-6.84	111.72	121.50
1	A	464	ASN	C-N-CA	-6.84	111.72	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	829	THR	CA-CB-OG1	-6.83	99.35	109.60
1	E	546	PRO	N-CA-C	6.75	122.96	114.92
1	D	841	ARG	NE-CZ-NH2	6.75	125.28	119.20
1	D	496	GLU	CG-CD-OE2	-6.73	102.92	118.40
1	C	503	ARG	CG-CD-NE	6.72	126.79	112.00
1	E	583	ARG	NE-CZ-NH2	6.62	125.16	119.20
1	B	411	ASP	CA-CB-CG	6.60	119.20	112.60
1	C	531	ASP	CA-CB-CG	6.59	119.19	112.60
1	F	829	THR	CA-CB-OG1	-6.56	99.76	109.60
1	D	845	GLU	CG-CD-OE1	6.54	133.44	118.40
1	A	635	PHE	N-CA-CB	-6.54	99.83	110.81
1	B	492	LEU	N-CA-CB	6.52	119.91	110.06
1	F	633	GLU	CB-CG-CD	6.51	123.66	112.60
1	B	595	ARG	NE-CZ-NH2	6.50	125.05	119.20
1	A	652	PRO	N-CA-CB	6.50	110.67	103.26
1	A	531	ASP	CA-CB-CG	6.49	119.09	112.60
1	D	825	ASP	CA-CB-CG	6.48	119.08	112.60
1	F	790	GLU	CG-CD-OE2	-6.45	103.57	118.40
1	E	531	ASP	CA-CB-CG	6.40	119.00	112.60
1	F	464	ASN	CA-C-N	-6.40	113.17	122.19
1	F	464	ASN	C-N-CA	-6.40	113.17	122.19
1	D	531	ASP	CA-CB-CG	6.37	118.97	112.60
1	D	496	GLU	OE1-CD-OE2	6.36	138.15	122.90
1	F	610	LEU	CD1-CG-CD2	-6.35	96.83	110.80
1	D	635	PHE	N-CA-CB	-6.33	100.20	110.71
1	C	829	THR	CA-CB-OG1	-6.33	100.10	109.60
1	D	805	MET	CB-CG-SD	6.33	131.69	112.70
1	B	378	THR	CA-CB-OG1	-6.30	100.15	109.60
1	E	600	THR	CA-CB-OG1	-6.29	100.17	109.60
1	D	512	ARG	NE-CZ-NH2	-6.26	113.56	119.20
1	A	696	ASP	CA-CB-CG	6.25	118.85	112.60
1	B	531	ASP	CA-CB-CG	6.25	118.85	112.60
1	A	464	ASN	N-CA-CB	6.23	118.94	110.10
1	E	499	MET	CG-SD-CE	6.22	114.58	100.90
1	F	443	ASP	CA-CB-CG	6.21	118.81	112.60
1	D	443	ASP	CA-CB-CG	6.20	118.80	112.60
1	F	853	ASN	OD1-CG-ND2	6.18	128.78	122.60
1	B	573	ASN	OD1-CG-ND2	6.16	128.76	122.60
1	F	411	ASP	CA-CB-CG	6.15	118.75	112.60
1	E	473	GLU	CB-CA-C	6.15	120.62	110.90
1	B	532	LEU	N-CA-C	-6.15	101.83	110.50
1	D	581	ARG	N-CA-CB	6.14	119.25	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	654	LYS	CD-CE-NZ	6.10	131.41	111.90
1	D	853	ASN	OD1-CG-ND2	6.10	128.70	122.60
1	E	411	ASP	CA-CB-CG	6.10	118.70	112.60
1	C	472	LEU	N-CA-CB	-6.08	100.94	110.30
1	F	651	ASP	CB-CA-C	6.08	118.80	109.50
1	A	491	VAL	N-CA-CB	-6.08	104.32	112.10
1	A	595	ARG	NE-CZ-NH2	6.07	124.67	119.20
1	D	625	ASP	CA-CB-CG	6.05	118.65	112.60
1	B	464	ASN	CA-C-N	-6.05	112.85	121.50
1	B	464	ASN	C-N-CA	-6.05	112.85	121.50
1	E	657	ASP	CA-CB-CG	6.05	118.65	112.60
1	A	492	LEU	N-CA-CB	6.04	119.19	110.06
1	C	503	ARG	NH1-CZ-NH2	-6.04	111.45	119.30
1	A	417	THR	CA-CB-CG2	6.03	120.74	110.50
1	B	448	GLU	N-CA-CB	6.01	118.96	110.12
1	D	829	THR	CA-CB-OG1	-6.01	100.58	109.60
1	B	818	GLU	CG-CD-OE1	-6.00	104.59	118.40
1	B	616	PRO	N-CA-CB	5.99	108.35	103.32
1	A	614	GLN	OE1-CD-NE2	5.98	128.58	122.60
1	F	512	ARG	NH1-CZ-NH2	5.94	127.02	119.30
1	D	378	THR	CA-CB-OG1	-5.94	100.70	109.60
1	C	503	ARG	NE-CZ-NH2	5.93	124.53	119.20
1	A	846	GLU	N-CA-CB	5.92	118.82	110.12
1	C	745	GLY	CA-C-O	-5.92	116.89	122.39
1	A	497	LYS	CA-CB-CG	5.90	125.91	114.10
1	A	470	ASP	CA-CB-CG	5.89	118.49	112.60
1	E	711	ASP	CA-CB-CG	5.89	118.49	112.60
1	F	527	ASP	CA-CB-CG	5.89	118.49	112.60
1	C	757	LYS	CG-CD-CE	5.86	124.78	111.30
1	D	852	PRO	N-CA-CB	-5.84	97.90	103.51
1	D	448	GLU	N-CA-CB	5.83	118.69	110.12
1	F	840	THR	OG1-CB-CG2	-5.81	97.69	109.30
1	C	732	ARG	CG-CD-NE	5.80	124.75	112.00
1	F	853	ASN	CB-CA-C	-5.79	103.93	111.40
1	F	689	LYS	CB-CG-CD	5.79	124.61	111.30
1	F	502	THR	OG1-CB-CG2	-5.78	97.74	109.30
1	B	581	ARG	CD-NE-CZ	5.78	132.49	124.40
1	C	470	ASP	CA-CB-CG	5.76	118.36	112.60
1	E	532	LEU	N-CA-C	-5.76	102.38	110.50
1	D	584	ARG	NH1-CZ-NH2	5.75	126.77	119.30
1	E	527	ASP	CA-CB-CG	5.74	118.34	112.60
1	C	527	ASP	CA-CB-CG	5.73	118.33	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	512	ARG	CG-CD-NE	5.72	124.59	112.00
1	C	717	LYS	CG-CD-CE	5.72	124.45	111.30
1	E	717	LYS	CG-CD-CE	5.70	124.40	111.30
1	B	491	VAL	N-CA-CB	-5.68	104.83	112.10
1	D	495	ASP	CA-CB-CG	5.68	118.28	112.60
1	C	466	ALA	N-CA-C	5.68	117.55	110.91
1	A	365	GLU	CB-CG-CD	5.67	122.24	112.60
1	A	472	LEU	N-CA-CB	-5.67	101.16	110.40
1	C	532	LEU	CA-C-O	-5.67	115.38	121.56
1	F	469	GLU	N-CA-CB	5.66	118.22	110.01
1	C	437	THR	OG1-CB-CG2	5.66	120.61	109.30
1	F	625	ASP	CA-CB-CG	5.66	118.26	112.60
1	C	463	LEU	CA-C-O	-5.64	114.28	120.43
1	E	382	ARG	CA-CB-CG	5.63	125.36	114.10
1	F	852	PRO	N-CA-CB	-5.61	98.12	103.51
1	D	742	GLU	CB-CG-CD	5.60	122.13	112.60
1	F	825	ASP	CA-CB-CG	5.59	118.19	112.60
1	C	546	PRO	N-CA-C	5.58	121.56	114.92
1	E	648	HIS	CB-CA-C	5.58	119.81	111.89
1	F	650	GLU	CG-CD-OE2	5.54	131.15	118.40
1	D	455	LYS	CB-CG-CD	5.54	124.04	111.30
1	A	584	ARG	NH1-CZ-NH2	5.54	126.50	119.30
1	D	657	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	612	ILE	O-C-N	5.53	127.45	121.87
1	B	465	SER	CB-CA-C	5.50	118.81	109.84
1	A	503	ARG	CG-CD-NE	5.50	124.10	112.00
1	C	503	ARG	N-CA-CB	5.49	118.02	110.07
1	C	825	ASP	CA-CB-CG	5.49	118.09	112.60
1	C	417	THR	CA-CB-OG1	-5.48	101.38	109.60
1	C	696	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	546	PRO	N-CA-C	5.47	121.68	114.68
1	C	818	GLU	CG-CD-OE1	-5.47	105.82	118.40
1	B	464	ASN	N-CA-CB	5.46	117.86	110.10
1	C	515	GLU	CG-CD-OE1	-5.46	105.84	118.40
1	D	464	ASN	CA-C-N	-5.46	113.69	121.50
1	D	464	ASN	C-N-CA	-5.46	113.69	121.50
1	F	595	ARG	CG-CD-NE	-5.45	100.01	112.00
1	C	693	LYS	CG-CD-CE	5.45	123.83	111.30
1	C	491	VAL	N-CA-CB	-5.43	105.15	112.10
1	C	725	GLN	CB-CG-CD	5.42	121.82	112.60
1	C	625	ASP	CA-CB-CG	5.40	118.00	112.60
1	C	492	LEU	N-CA-CB	5.39	118.20	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	853	ASN	CB-CA-C	-5.38	104.47	111.40
1	B	527	ASP	CA-CB-CG	5.37	117.97	112.60
1	E	625	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	368	LEU	N-CA-CB	-5.36	101.31	110.16
1	E	503	ARG	N-CA-CB	5.36	117.84	110.07
1	E	505	GLU	CB-CG-CD	5.36	121.71	112.60
1	D	419	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	F	584	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	D	411	ASP	CA-CB-CG	5.30	117.90	112.60
1	F	573	ASN	CA-CB-CG	-5.30	107.30	112.60
1	B	480	SER	CA-CB-OG	-5.30	100.51	111.10
1	D	696	ASP	CA-CB-CG	5.29	117.89	112.60
1	F	651	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	595	ARG	NH1-CZ-NH2	-5.27	112.45	119.30
1	A	829	THR	OG1-CB-CG2	5.27	119.83	109.30
1	C	573	ASN	OD1-CG-ND2	5.26	127.86	122.60
1	D	424	ASP	CA-CB-CG	5.26	117.86	112.60
1	D	492	LEU	N-CA-CB	5.26	118.00	110.06
1	D	826	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	E	633	GLU	CB-CG-CD	5.21	121.46	112.60
1	D	595	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	F	368	LEU	N-CA-CB	-5.21	101.41	109.48
1	C	504	GLU	CB-CG-CD	5.20	121.45	112.60
1	F	706	MET	CG-SD-CE	-5.20	89.45	100.90
1	D	465	SER	CB-CA-C	5.20	118.32	109.84
1	D	527	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	706	MET	CG-SD-CE	-5.18	89.50	100.90
1	D	846	GLU	N-CA-CB	5.16	117.71	110.12
1	F	532	LEU	CA-C-O	-5.16	113.13	120.51
1	D	811	LYS	CB-CA-C	5.15	119.29	110.74
1	D	503	ARG	N-CA-CB	5.14	117.77	110.16
1	A	503	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	B	378	THR	OG1-CB-CG2	5.11	119.52	109.30
1	C	443	ASP	CB-CA-C	5.11	120.01	111.22
1	B	625	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	592	ASP	CA-CB-CG	5.10	117.70	112.60
1	D	550	GLU	CB-CG-CD	5.09	121.25	112.60
1	C	817	LYS	CG-CD-CE	-5.08	99.61	111.30
1	E	583	ARG	NH1-CZ-NH2	-5.08	112.69	119.30
1	D	417	THR	CA-CB-OG1	-5.08	101.98	109.60
1	F	805	MET	CB-CG-SD	5.08	127.94	112.70
1	B	651	ASP	CA-CB-CG	5.05	117.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	532	LEU	N-CA-CB	5.05	119.03	110.49
1	D	841	ARG	CB-CG-CD	5.04	122.90	111.30
1	E	549	LYS	CD-CE-NZ	5.04	128.03	111.90
1	D	693	LYS	CB-CA-C	5.03	116.65	109.26
1	D	583	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	F	531	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	443	ASP	CA-CB-CG	5.01	117.61	112.60
1	E	443	ASP	CB-CA-C	5.00	119.83	111.22

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	503	ARG	Sidechain
1	A	508	ARG	Sidechain
1	A	524	ARG	Sidechain
1	A	561	ARG	Sidechain
1	A	581	ARG	Sidechain
1	A	595	ARG	Sidechain
1	A	631	ARG	Sidechain
1	B	524	ARG	Sidechain
1	B	584	ARG	Sidechain
1	B	595	ARG	Sidechain
1	B	631	ARG	Sidechain
1	B	670	ARG	Sidechain
1	B	778	ARG	Sidechain
1	C	419	ARG	Sidechain
1	C	426	ARG	Sidechain
1	C	477	ARG	Sidechain
1	C	503	ARG	Sidechain
1	C	508	ARG	Sidechain
1	C	524	ARG	Sidechain
1	C	545	ARG	Sidechain
1	C	561	ARG	Sidechain
1	C	581	ARG	Sidechain
1	C	583	ARG	Sidechain
1	C	732	ARG	Sidechain
1	D	382	ARG	Sidechain
1	D	503	ARG	Sidechain
1	D	512	ARG	Sidechain
1	D	561	ARG	Sidechain
1	D	583	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	595	ARG	Sidechain
1	D	597	ARG	Sidechain
1	D	732	ARG	Sidechain
1	E	374	ARG	Sidechain
1	E	419	ARG	Sidechain
1	E	508	ARG	Sidechain
1	E	512	ARG	Sidechain
1	E	545	ARG	Sidechain
1	E	561	ARG	Sidechain
1	E	595	ARG	Sidechain
1	E	676	ARG	Sidechain
1	F	390	ARG	Sidechain
1	F	474	ARG	Sidechain
1	F	503	ARG	Sidechain
1	F	512	ARG	Sidechain
1	F	524	ARG	Sidechain
1	F	561	ARG	Sidechain
1	F	581	ARG	Sidechain
1	F	595	ARG	Sidechain
1	F	655	ARG	Sidechain

## 5.2 Too-close contacts

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	3978	0	4096	45	0
1	B	3978	0	4096	34	0
1	C	3978	0	4096	42	0
1	D	3955	0	4077	34	0
1	E	3969	0	4088	41	0
1	F	3978	0	4096	33	0
2	A	92	0	87	13	0
2	B	92	0	87	8	0
2	C	92	0	85	11	0
2	D	92	0	87	8	0
2	E	92	0	86	5	0
2	F	92	0	86	9	0
3	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	1	0
3	C	12	0	16	1	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
4	A	30	0	0	6	0
4	B	19	0	0	3	0
4	C	26	0	0	2	0
4	D	16	0	0	1	0
4	E	6	0	0	1	0
4	F	11	0	0	1	0
All	All	24532	0	25115	270	0

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 5.

All (270) 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)
2:E:901:COB:H362	2:E:901:COB:H351	1.40	1.01
1:A:651:ASP:HB3	1:A:654:LYS:HB3	1.41	0.98
2:B:901:COB:H362	2:B:901:COB:H351	1.47	0.96
1:D:545:ARG:HB2	1:D:546:PRO:HD3	1.48	0.95
2:A:901:COB:H362	2:A:901:COB:H351	1.52	0.89
1:E:830:LEU:HB2	4:E:1006:HOH:O	1.73	0.89
2:F:901:COB:H362	2:F:901:COB:H351	1.55	0.89
2:D:901:COB:H362	2:D:901:COB:H351	1.57	0.85
2:F:901:COB:H252	2:F:901:COB:H601	1.60	0.81
1:A:669:LYS:HD3	4:A:1004:HOH:O	1.80	0.81
1:E:639:LEU:HD11	1:E:725:GLN:HG3	1.65	0.78
1:C:503:ARG:NH1	1:C:557:GLU:OE1	2.18	0.77
1:F:545:ARG:HG3	1:F:631:ARG:HH21	1.52	0.74
2:C:901:COB:H362	2:C:901:COB:H351	1.70	0.74
1:E:633:GLU:HG3	1:E:634:GLY:H	1.51	0.74
1:A:581:ARG:HD2	1:D:470:ASP:OD2	1.88	0.74
1:B:639:LEU:HD11	1:B:725:GLN:HG3	1.69	0.74
1:E:496:GLU:OE1	1:E:512:ARG:NH2	2.21	0.73
1:B:385:GLU:HB3	4:B:1002:HOH:O	1.88	0.73
2:C:901:COB:H252	2:C:901:COB:H601	1.70	0.72
2:E:901:COB:H601	2:E:901:COB:H252	1.72	0.71
1:B:545:ARG:HB2	1:B:546:PRO:HD3	1.73	0.71
1:E:538:THR:HB	1:E:578:LEU:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:901:COB:H351	2:E:901:COB:C36	2.14	0.68
2:D:901:COB:H252	2:D:901:COB:H601	1.76	0.67
2:C:901:COB:H552	2:C:901:COB:H531	1.76	0.67
1:F:545:ARG:HB2	1:F:546:PRO:HD3	1.76	0.67
2:B:901:COB:H351	2:B:901:COB:C36	2.22	0.67
1:A:632:LYS:HG2	1:A:633:GLU:H	1.61	0.66
1:F:681:GLU:OE2	1:F:732:ARG:HD3	1.98	0.65
1:F:579:LYS:HB2	4:F:1008:HOH:O	1.97	0.64
1:A:703:LEU:HA	1:A:730:MET:HE1	1.79	0.64
1:C:639:LEU:HD11	1:C:725:GLN:HG3	1.79	0.64
1:F:732:ARG:HH11	1:F:732:ARG:HB2	1.61	0.63
1:E:575:SER:OG	1:E:583:ARG:HD2	1.97	0.63
1:E:532:LEU:HD21	1:E:558:LEU:HD12	1.81	0.63
1:A:575:SER:OG	1:A:583:ARG:HD2	1.99	0.63
1:E:545:ARG:HB2	1:E:546:PRO:HD3	1.81	0.62
1:B:575:SER:OG	1:B:583:ARG:HD2	2.00	0.62
1:C:575:SER:OG	1:C:583:ARG:HD2	2.00	0.62
1:C:466:ALA:HB3	1:C:490:VAL:O	2.00	0.61
1:E:633:GLU:HG3	1:E:634:GLY:N	2.15	0.61
1:D:575:SER:OG	1:D:583:ARG:HD2	2.00	0.61
1:A:670:ARG:HD2	4:A:1004:HOH:O	1.99	0.61
1:E:428:LEU:HG	1:E:432:LEU:HD23	1.83	0.61
1:F:416:TRP:CG	1:F:417:THR:H	2.19	0.61
2:A:901:COB:H252	2:A:901:COB:H601	1.82	0.60
1:B:428:LEU:HG	1:B:432:LEU:HD23	1.82	0.60
1:C:365:GLU:HB2	1:C:369:PHE:CD1	2.37	0.59
1:E:469:GLU:HG3	1:E:470:ASP:OD1	2.03	0.59
2:D:901:COB:H552	2:D:901:COB:H531	1.83	0.58
2:A:901:COB:H561	2:A:901:COB:H531	1.84	0.58
1:C:365:GLU:HG2	1:C:366:ALA:H	1.67	0.58
1:A:632:LYS:HG2	1:A:633:GLU:N	2.19	0.57
2:A:901:COB:H351	2:A:901:COB:C36	2.27	0.57
1:D:865:ARG:HD3	4:D:1008:HOH:O	2.04	0.57
1:C:674:GLU:OE1	1:C:676:ARG:NH1	2.37	0.57
1:E:545:ARG:N	1:E:546:PRO:HD2	2.19	0.57
1:D:761:HIS:CE1	2:D:901:COB:N23	2.73	0.57
2:C:901:COB:H531	2:C:901:COB:C55	2.36	0.56
2:F:901:COB:H491	2:F:901:COB:H463	1.87	0.56
1:A:632:LYS:HB3	1:A:635:PHE:HB3	1.88	0.56
1:D:761:HIS:HE1	2:D:901:COB:N23	2.03	0.55
1:D:693:LYS:HE3	1:D:695:LEU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:901:COB:H252	2:B:901:COB:H601	1.88	0.55
2:E:901:COB:H531	2:E:901:COB:H552	1.89	0.55
2:F:901:COB:H552	2:F:901:COB:H531	1.88	0.55
1:C:366:ALA:HB1	4:C:1002:HOH:O	2.07	0.54
1:C:755:THR:HB	1:C:784:ILE:HA	1.90	0.54
1:E:538:THR:HB	1:E:578:LEU:CD1	2.37	0.54
1:E:693:LYS:HD2	1:E:694:PRO:HD2	1.89	0.54
1:A:803:VAL:HG23	1:A:830:LEU:HD11	1.89	0.54
1:D:545:ARG:HB2	1:D:546:PRO:CD	2.29	0.54
1:B:748:LYS:HE2	1:B:775:ASN:O	2.08	0.54
1:A:385:GLU:HB3	4:A:1008:HOH:O	2.08	0.54
1:D:803:VAL:HG23	1:D:830:LEU:HD11	1.91	0.53
1:A:461:VAL:HG12	1:A:463:LEU:HD12	1.91	0.53
1:B:636:ASP:OD2	1:B:639:LEU:HG	2.09	0.52
1:F:755:THR:HB	1:F:784:ILE:HA	1.91	0.52
1:A:416:TRP:HB3	1:A:419:ARG:HG3	1.91	0.52
1:F:612:ILE:HD12	1:F:613:SER:N	2.24	0.52
1:F:805:MET:HE1	1:F:819:ASN:HB2	1.91	0.52
1:F:545:ARG:N	1:F:546:PRO:CD	2.73	0.52
1:E:536:PRO:O	1:E:536:PRO:HG2	2.10	0.52
1:F:416:TRP:CG	1:F:417:THR:N	2.76	0.52
1:C:545:ARG:N	1:C:546:PRO:CD	2.73	0.52
1:B:419:ARG:NH2	1:B:424:ASP:OD1	2.43	0.52
1:B:852:PRO:HD2	4:B:1015:HOH:O	2.10	0.52
1:A:671:ARG:NH2	1:A:678:GLN:O	2.43	0.52
1:C:761:HIS:CE1	2:C:901:COB:H202	2.44	0.52
1:D:612:ILE:HD12	1:D:613:SER:N	2.24	0.51
1:A:714:GLY:CA	2:A:901:COB:H292	2.23	0.51
1:A:419:ARG:NH2	1:A:424:ASP:OD1	2.44	0.51
1:E:545:ARG:N	1:E:546:PRO:CD	2.73	0.51
2:C:901:COB:H301	2:C:901:COB:H203	1.93	0.51
1:A:450:MET:SD	1:A:463:LEU:HD23	2.51	0.51
1:C:545:ARG:N	1:C:546:PRO:HD2	2.26	0.50
1:B:545:ARG:N	1:B:546:PRO:HD2	2.26	0.50
1:D:755:THR:HB	1:D:784:ILE:HA	1.93	0.50
2:D:901:COB:H531	2:D:901:COB:C55	2.41	0.50
1:B:671:ARG:NH2	1:B:678:GLN:O	2.44	0.50
1:C:671:ARG:NH2	1:C:678:GLN:O	2.44	0.50
1:D:545:ARG:N	1:D:546:PRO:CD	2.75	0.50
1:A:651:ASP:HB3	1:A:654:LYS:CB	2.30	0.50
1:B:545:ARG:N	1:B:546:PRO:CD	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:632:LYS:O	1:E:633:GLU:HG2	2.12	0.50
1:D:545:ARG:N	1:D:546:PRO:HD2	2.27	0.50
1:D:671:ARG:NH2	1:D:678:GLN:O	2.44	0.50
2:A:901:COB:H561	2:A:901:COB:C53	2.41	0.49
1:C:419:ARG:NH2	1:C:424:ASP:OD1	2.46	0.49
1:C:612:ILE:N	1:C:612:ILE:HD12	2.27	0.49
1:D:593:GLU:O	1:D:597:ARG:HG2	2.12	0.49
2:A:901:COB:C53	2:A:901:COB:C56	2.89	0.49
1:C:465:SER:O	1:C:492:LEU:HD12	2.12	0.49
1:C:612:ILE:HD12	1:C:612:ILE:H	1.77	0.49
2:C:901:COB:H421	2:C:901:COB:H363	1.94	0.49
1:B:464:ASN:O	1:B:490:VAL:HB	2.13	0.49
1:A:710:GLY:HA3	2:A:901:COB:H602	1.95	0.49
2:B:901:COB:H531	2:B:901:COB:H552	1.94	0.49
1:E:809:LEU:HD12	1:E:811:LYS:HE2	1.94	0.49
1:E:755:THR:HB	1:E:784:ILE:HA	1.95	0.49
1:B:805:MET:HE1	1:B:819:ASN:HB2	1.94	0.48
1:E:671:ARG:NH2	1:E:678:GLN:O	2.45	0.48
1:D:524:ARG:HB3	1:D:526:GLU:HG2	1.96	0.48
1:A:710:GLY:HA2	2:A:901:COB:H542	1.96	0.48
1:F:655:ARG:HB2	1:F:655:ARG:NH1	2.29	0.48
1:B:755:THR:HB	1:B:784:ILE:HA	1.94	0.48
1:A:464:ASN:O	1:A:490:VAL:HB	2.14	0.48
1:C:836:GLY:O	4:C:1001:HOH:O	2.20	0.48
1:F:532:LEU:O	1:F:533:LEU:HG	2.14	0.48
1:F:671:ARG:NH2	1:F:678:GLN:O	2.47	0.48
1:A:429:LEU:N	1:A:430:PRO:CD	2.77	0.48
1:C:405:GLU:HG2	1:D:633:GLU:HG2	1.96	0.48
2:B:901:COB:H463	2:B:901:COB:H481	1.72	0.47
1:F:805:MET:HE1	1:F:819:ASN:CB	2.45	0.47
1:D:429:LEU:N	1:D:430:PRO:CD	2.77	0.47
2:F:901:COB:H533	2:F:901:COB:H481	1.94	0.47
1:E:426:ARG:NH1	1:E:456:TYR:OH	2.47	0.47
1:F:464:ASN:O	1:F:490:VAL:HB	2.14	0.47
1:A:706:MET:HE2	1:A:730:MET:HE2	1.96	0.47
1:F:366:ALA:O	1:F:367:SER:C	2.58	0.47
1:E:464:ASN:O	1:E:490:VAL:HB	2.15	0.47
1:A:759:ALA:HB1	4:A:1018:HOH:O	2.15	0.46
1:B:786:VAL:HG12	1:B:791:ILE:HG13	1.97	0.46
1:C:429:LEU:N	1:C:430:PRO:CD	2.78	0.46
1:E:429:LEU:N	1:E:430:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:706:MET:CE	1:D:730:MET:HB2	2.45	0.46
1:B:429:LEU:N	1:B:430:PRO:CD	2.78	0.46
1:F:426:ARG:HG3	1:F:452:LEU:HD21	1.97	0.46
1:D:419:ARG:NH2	1:D:424:ASP:OD1	2.49	0.46
1:D:464:ASN:O	1:D:490:VAL:HB	2.15	0.46
1:E:786:VAL:HG12	1:E:791:ILE:HG13	1.98	0.45
2:F:901:COB:H531	2:F:901:COB:C55	2.46	0.45
2:C:901:COB:C2B	2:C:901:COB:O7R	2.64	0.45
1:A:664:LEU:HD21	1:A:687:ALA:HB2	1.97	0.45
2:D:901:COB:H411	2:D:901:COB:H363	1.69	0.45
1:A:491:VAL:CG1	1:A:513:MET:SD	3.05	0.45
1:C:642:MET:HE2	1:C:719:GLN:NE2	2.31	0.45
1:F:416:TRP:HA	1:F:416:TRP:CE3	2.51	0.45
1:F:743:LYS:HE2	1:F:774:ASN:ND2	2.32	0.45
1:F:706:MET:CE	1:F:730:MET:HB2	2.45	0.45
1:A:706:MET:HB2	1:A:730:MET:HE2	1.98	0.45
1:C:592:ASP:OD1	1:C:595:ARG:NH1	2.43	0.45
1:C:762:ASP:H	2:C:901:COB:H522	1.64	0.45
1:C:805:MET:HE1	1:C:819:ASN:HB2	1.99	0.45
1:A:755:THR:HB	1:A:784:ILE:HA	1.98	0.45
1:B:499:MET:HE1	3:B:902:GOL:O2	2.17	0.45
1:D:652:PRO:O	1:D:656:GLU:HG2	2.17	0.45
1:E:396:LEU:CD1	1:E:435:ALA:HB1	2.47	0.45
2:A:901:COB:H531	2:A:901:COB:H543	1.98	0.44
1:F:786:VAL:HG12	1:F:791:ILE:HG13	1.98	0.44
1:D:373:GLU:OE1	1:D:572:SER:OG	2.35	0.44
1:E:502:THR:OG1	1:E:505:GLU:HG2	2.17	0.44
1:F:429:LEU:N	1:F:430:PRO:CD	2.80	0.44
1:A:545:ARG:N	1:A:546:PRO:CD	2.81	0.44
1:B:416:TRP:HB3	1:B:419:ARG:HG3	2.00	0.44
1:C:477:ARG:HD2	1:C:477:ARG:HA	1.71	0.44
1:C:651:ASP:O	1:C:655:ARG:HG2	2.17	0.44
1:E:834:LEU:HB3	1:E:839:LEU:HD11	1.99	0.44
1:E:474:ARG:O	1:E:477:ARG:HG2	2.17	0.44
1:F:556:GLU:OE1	1:F:597:ARG:NH1	2.51	0.44
1:B:381:LYS:HG2	1:B:384:ARG:NH2	2.33	0.44
1:D:398:LEU:O	1:D:402:GLN:HG3	2.18	0.44
1:D:834:LEU:HB3	1:D:839:LEU:HD11	2.00	0.44
1:A:787:PRO:HD2	1:A:790:GLU:CG	2.48	0.44
2:A:901:COB:H531	2:A:901:COB:C56	2.47	0.44
1:D:805:MET:HE1	1:D:819:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:901:COB:O7R	2:C:901:COB:H2B	2.18	0.43
1:F:416:TRP:HA	1:F:416:TRP:HE3	1.82	0.43
1:A:798:HIS:NE2	4:A:1001:HOH:O	2.36	0.43
1:A:839:LEU:HD23	1:A:839:LEU:HA	1.90	0.43
1:A:757:LYS:HG2	4:A:1009:HOH:O	2.18	0.43
1:C:365:GLU:CB	1:C:369:PHE:CD1	3.01	0.43
1:E:839:LEU:HD23	1:E:839:LEU:HA	1.92	0.43
1:F:576:PHE:HA	1:F:583:ARG:NH1	2.33	0.43
1:B:572:SER:HA	1:B:587:ASN:ND2	2.33	0.43
1:B:581:ARG:HD3	1:F:470:ASP:OD2	2.18	0.43
1:C:504:GLU:HG2	1:D:846:GLU:HG3	2.01	0.43
1:C:839:LEU:HB3	1:C:856:TYR:HE1	1.83	0.43
1:E:595:ARG:HA	1:E:599:LEU:HB3	1.99	0.43
1:B:834:LEU:HB3	1:B:839:LEU:HD11	2.01	0.43
1:E:805:MET:HE1	1:E:819:ASN:HB2	2.00	0.43
2:E:901:COB:H531	2:E:901:COB:C55	2.48	0.43
1:C:503:ARG:NH2	1:D:843:TYR:CZ	2.86	0.43
1:E:366:ALA:O	1:E:367:SER:C	2.61	0.43
1:B:721:PRO:O	1:B:725:GLN:HG2	2.18	0.43
1:D:786:VAL:HG12	1:D:791:ILE:HG13	2.01	0.43
1:E:633:GLU:CG	1:E:634:GLY:H	2.23	0.43
1:A:377:ALA:O	1:A:384:ARG:NH1	2.52	0.43
2:A:901:COB:H363	2:A:901:COB:H411	1.74	0.43
1:C:706:MET:CE	1:C:730:MET:HB2	2.49	0.43
1:C:839:LEU:HD23	1:C:839:LEU:HA	1.92	0.42
1:E:721:PRO:O	1:E:725:GLN:HG2	2.19	0.42
2:F:901:COB:N29	2:F:901:COB:H3	2.33	0.42
2:F:901:COB:H463	2:F:901:COB:C49	2.48	0.42
1:A:584:ARG:HG3	1:A:608:LYS:O	2.20	0.42
1:A:650:GLU:HG3	1:A:655:ARG:HH21	1.84	0.42
1:C:595:ARG:HA	1:C:599:LEU:HB3	2.01	0.42
1:E:368:LEU:HD21	1:E:591:LEU:HD11	2.01	0.42
1:E:556:GLU:OE1	1:E:597:ARG:NH1	2.52	0.42
2:B:901:COB:O28	2:B:901:COB:H3	2.19	0.42
1:D:738:GLU:N	1:D:739:PRO:CD	2.83	0.42
1:A:803:VAL:HG23	1:A:830:LEU:CD1	2.49	0.42
1:F:664:LEU:HD21	1:F:687:ALA:HB2	2.02	0.42
1:C:501:LYS:HD3	1:C:535:PHE:CE2	2.55	0.42
1:B:382:ARG:NH1	4:B:1003:HOH:O	2.53	0.42
1:B:665:LEU:N	1:B:665:LEU:HD22	2.34	0.42
1:C:365:GLU:HG2	1:C:366:ALA:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:901:COB:O28	2:D:901:COB:H3	2.19	0.42
2:B:901:COB:H531	2:B:901:COB:C55	2.50	0.41
1:C:556:GLU:OE1	1:C:597:ARG:NH1	2.53	0.41
1:D:839:LEU:HD23	1:D:839:LEU:HA	1.93	0.41
1:F:738:GLU:N	1:F:739:PRO:CD	2.83	0.41
1:B:803:VAL:HG23	1:B:830:LEU:HD11	2.02	0.41
1:E:851:TYR:O	1:E:854:VAL:HG23	2.20	0.41
2:B:901:COB:H363	2:B:901:COB:H411	1.76	0.41
1:E:398:LEU:O	1:E:402:GLN:HG3	2.20	0.41
1:A:714:GLY:HA2	2:A:901:COB:H292	1.84	0.41
1:A:805:MET:HE1	1:A:819:ASN:HB2	2.02	0.41
1:E:567:PHE:H	1:E:600:THR:HG22	1.86	0.41
1:B:595:ARG:HA	1:B:599:LEU:HB3	2.03	0.41
1:F:851:TYR:O	1:F:854:VAL:HG23	2.20	0.41
1:A:809:LEU:N	1:A:809:LEU:HD23	2.35	0.41
1:B:738:GLU:N	1:B:739:PRO:CD	2.83	0.41
1:C:366:ALA:O	1:C:367:SER:C	2.63	0.41
1:C:545:ARG:HB2	1:C:546:PRO:HD3	2.02	0.41
1:C:767:LEU:HD23	1:C:767:LEU:HA	1.90	0.41
1:D:795:VAL:HG11	1:D:830:LEU:HD21	2.03	0.41
1:F:377:ALA:O	1:F:384:ARG:NH1	2.53	0.41
1:A:398:LEU:O	1:A:402:GLN:HG3	2.20	0.41
1:B:848:ARG:HA	1:B:851:TYR:O	2.20	0.41
1:D:377:ALA:O	1:D:384:ARG:NH1	2.53	0.41
1:A:738:GLU:N	1:A:739:PRO:CD	2.84	0.41
1:A:762:ASP:HB2	1:A:765:LYS:HE3	2.03	0.41
1:B:556:GLU:OE1	1:B:597:ARG:NH1	2.54	0.41
1:A:462:LEU:HD12	1:A:462:LEU:N	2.36	0.41
1:B:377:ALA:O	1:B:384:ARG:NH1	2.54	0.41
1:B:632:LYS:HG2	1:B:633:GLU:N	2.36	0.41
2:C:901:COB:C61	2:C:901:COB:H551	2.51	0.41
3:C:903:GOL:C3	1:D:539:GLN:HA	2.51	0.41
1:A:752:VAL:HG23	1:A:800:PRO:HG3	2.04	0.40
1:B:809:LEU:N	1:B:809:LEU:HD23	2.36	0.40
1:C:377:ALA:O	1:C:384:ARG:NH1	2.55	0.40
1:F:474:ARG:O	1:F:474:ARG:HG2	2.20	0.40
1:E:532:LEU:CD1	1:E:532:LEU:N	2.85	0.40
1:E:738:GLU:N	1:E:739:PRO:CD	2.83	0.40
1:F:545:ARG:N	1:F:546:PRO:HD2	2.35	0.40
2:F:901:COB:H351	2:F:901:COB:C36	2.31	0.40
1:C:578:LEU:CD2	1:C:642:MET:HE3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:GLU:OE1	1:C:736:TYR:OH	2.39	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	508/511 (99%)	496 (98%)	12 (2%)	0	100	100
1	B	508/511 (99%)	493 (97%)	15 (3%)	0	100	100
1	C	508/511 (99%)	491 (97%)	17 (3%)	0	100	100
1	D	505/511 (99%)	495 (98%)	10 (2%)	0	100	100
1	E	507/511 (99%)	494 (97%)	12 (2%)	1 (0%)	44	72
1	F	508/511 (99%)	492 (97%)	15 (3%)	1 (0%)	44	72
All	All	3044/3066 (99%)	2961 (97%)	81 (3%)	2 (0%)	48	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	367	SER
1	F	367	SER

### 5.3.2 Protein sidechains [i](#)

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	414/414 (100%)	411 (99%)	3 (1%)	81	88
1	B	414/414 (100%)	410 (99%)	4 (1%)	73	84
1	C	414/414 (100%)	412 (100%)	2 (0%)	86	91
1	D	412/414 (100%)	405 (98%)	7 (2%)	56	75
1	E	413/414 (100%)	410 (99%)	3 (1%)	81	88
1	F	414/414 (100%)	407 (98%)	7 (2%)	56	75
All	All	2481/2484 (100%)	2455 (99%)	26 (1%)	73	84

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	580	PRO
1	A	678	GLN
1	A	809	LEU
1	B	448	GLU
1	B	580	PRO
1	B	809	LEU
1	B	811	LYS
1	C	580	PRO
1	C	724	LEU
1	D	448	GLU
1	D	455	LYS
1	D	572	SER
1	D	580	PRO
1	D	610	LEU
1	D	793	LYS
1	D	811	LYS
1	E	553	LEU
1	E	738	GLU
1	E	854	VAL
1	F	580	PRO
1	F	610	LEU
1	F	633	GLU
1	F	655	ARG
1	F	732	ARG
1	F	793	LYS
1	F	854	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	464	ASN
1	A	539	GLN
1	A	573	ASN
1	A	587	ASN
1	B	573	ASN
1	B	587	ASN
1	B	719	GLN
1	C	573	ASN
1	C	761	HIS
1	D	692	HIS
1	D	761	HIS
1	E	464	ASN
1	E	587	ASN
1	F	364	GLN
1	F	402	GLN
1	F	725	GLN
1	F	774	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands 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	COB	D	901	-	86,102,102	1.36	11 (12%)	128,170,170	1.93	28 (21%)
2	COB	B	901	1	86,102,102	1.33	9 (10%)	128,170,170	1.78	34 (26%)
3	GOL	C	903	-	5,5,5	0.20	0	5,5,5	0.55	0
3	GOL	F	902	-	5,5,5	0.33	0	5,5,5	1.01	0
2	COB	C	901	-	86,102,102	1.72	21 (24%)	128,170,170	2.29	36 (28%)
2	COB	E	901	1	86,102,102	1.42	10 (11%)	128,170,170	1.98	28 (21%)
3	GOL	A	902	-	5,5,5	0.73	0	5,5,5	1.11	0
3	GOL	E	902	-	5,5,5	0.47	0	5,5,5	1.58	1 (20%)
3	GOL	C	902	-	5,5,5	1.60	1 (20%)	5,5,5	0.90	0
2	COB	A	901	1	86,102,102	1.44	17 (19%)	128,170,170	2.05	31 (24%)
3	GOL	B	902	-	5,5,5	0.36	0	5,5,5	0.84	0
2	COB	F	901	1	86,102,102	1.34	11 (12%)	128,170,170	1.86	29 (22%)

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	COB	D	901	-	-	13/52/231/231	0/3/11/11
2	COB	B	901	1	-	13/52/231/231	0/3/11/11
3	GOL	C	903	-	-	0/4/4/4	-
3	GOL	F	902	-	-	2/4/4/4	-
2	COB	C	901	-	-	12/52/231/231	0/3/11/11
2	COB	E	901	1	-	9/52/231/231	0/3/11/11
3	GOL	A	902	-	-	2/4/4/4	-
3	GOL	E	902	-	-	2/4/4/4	-
3	GOL	C	902	-	-	1/4/4/4	-
2	COB	A	901	1	-	15/52/231/231	0/3/11/11
3	GOL	B	902	-	-	3/4/4/4	-
2	COB	F	901	1	-	13/52/231/231	0/3/11/11

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	901	COB	C36-C7	-6.13	1.44	1.54
2	C	901	COB	C1-C19	-4.92	1.45	1.51
2	C	901	COB	C8B-C9B	4.41	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	COB	C43-N45	4.30	1.46	1.32
2	A	901	COB	O6R-C1R	4.04	1.46	1.40
2	B	901	COB	C1-C19	-3.79	1.47	1.51
2	F	901	COB	C1-C19	-3.77	1.47	1.51
2	A	901	COB	C54-C17	-3.67	1.48	1.54
2	D	901	COB	C4B-C9B	-3.66	1.36	1.41
2	C	901	COB	C10-C11	-3.57	1.27	1.37
2	C	901	COB	O44-C43	3.51	1.34	1.23
2	A	901	COB	C8B-C9B	3.47	1.47	1.40
2	F	901	COB	C4B-C9B	-3.46	1.36	1.41
2	B	901	COB	C4B-C9B	-3.32	1.36	1.41
2	D	901	COB	C8B-C9B	3.28	1.47	1.40
2	F	901	COB	C36-C7	-3.28	1.49	1.54
2	B	901	COB	O6R-C1R	3.27	1.45	1.40
2	B	901	COB	C8B-C9B	3.21	1.47	1.40
2	E	901	COB	C4B-C9B	-3.20	1.37	1.41
2	C	901	COB	C4B-C9B	-3.20	1.37	1.41
2	C	901	COB	C47-C12	-3.16	1.47	1.54
2	C	901	COB	C43-N45	3.15	1.43	1.32
2	E	901	COB	O34-C32	-3.14	1.14	1.23
2	D	901	COB	O7R-C2R	3.09	1.50	1.43
2	E	901	COB	C10-C9	3.00	1.47	1.39
2	B	901	COB	C43-N45	2.97	1.42	1.32
2	D	901	COB	C36-C7	-2.91	1.49	1.54
2	E	901	COB	C8B-C9B	2.88	1.46	1.40
2	A	901	COB	O58-C57	2.87	1.28	1.23
2	A	901	COB	C4B-C5B	2.80	1.44	1.37
2	A	901	COB	O6R-C4R	-2.78	1.38	1.45
2	C	901	COB	C5R-C4R	2.78	1.61	1.51
2	C	901	COB	O63-C61	2.76	1.32	1.23
2	A	901	COB	C57-N59	2.75	1.39	1.33
2	B	901	COB	C6B-C5B	2.74	1.47	1.40
2	A	901	COB	O7R-C2R	2.71	1.49	1.43
2	F	901	COB	P-O2	2.65	1.67	1.59
2	C	901	COB	O34-C32	2.63	1.32	1.23
2	C	901	COB	C26-C2	-2.60	1.49	1.55
2	E	901	COB	C6B-C5B	2.59	1.47	1.40
2	B	901	COB	C10-C9	2.58	1.46	1.39
2	F	901	COB	O7R-C2R	2.53	1.49	1.43
2	C	901	COB	C8-C9	2.52	1.56	1.51
2	E	901	COB	O6R-C1R	2.49	1.44	1.40
2	C	901	COB	C36-C7	-2.49	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	COB	C47-C12	-2.48	1.49	1.54
2	F	901	COB	C10-C9	2.48	1.46	1.39
2	C	901	COB	C16-C15	-2.47	1.29	1.36
2	A	901	COB	C10-C9	2.45	1.46	1.39
2	A	901	COB	C4B-C9B	-2.45	1.38	1.41
2	F	901	COB	C1R-N1B	2.44	1.56	1.49
3	C	902	GOL	O2-C2	2.39	1.50	1.43
2	F	901	COB	C14-N23	-2.38	1.26	1.33
2	C	901	COB	C2-C3	-2.35	1.50	1.57
2	C	901	COB	C6B-C5B	2.33	1.46	1.40
2	D	901	COB	P-O5	2.32	1.66	1.55
2	E	901	COB	C14-N23	-2.24	1.26	1.33
2	D	901	COB	C10-C9	2.23	1.45	1.39
2	E	901	COB	CO-N24	-2.17	1.84	2.05
2	C	901	COB	C14-N23	-2.15	1.26	1.33
2	D	901	COB	O39-C38	2.14	1.30	1.23
2	A	901	COB	C43-N45	2.14	1.39	1.32
2	A	901	COB	C3R-C4R	2.13	1.58	1.52
2	C	901	COB	C12-C13	-2.13	1.49	1.55
2	A	901	COB	C1R-N1B	2.11	1.55	1.49
2	C	901	COB	C9B-N3B	-2.09	1.32	1.38
2	D	901	COB	C26-C2	-2.07	1.50	1.55
2	D	901	COB	C1-C19	-2.06	1.48	1.51
2	A	901	COB	C17-C18	-2.06	1.49	1.55
2	E	901	COB	C50-N52	2.05	1.39	1.32
2	B	901	COB	C4-C5	2.04	1.51	1.43
2	B	901	COB	C14-N23	-2.04	1.27	1.33
2	F	901	COB	C30-C3	2.04	1.59	1.54
2	C	901	COB	P-O5	2.03	1.64	1.55
2	C	901	COB	CO-N24	-2.03	1.85	2.05
2	D	901	COB	C17-C18	-2.01	1.50	1.55
2	A	901	COB	CO-N24	-2.01	1.86	2.05
2	F	901	COB	C37-C7	-2.01	1.50	1.56
2	F	901	COB	C41-C8	2.01	1.59	1.54
2	A	901	COB	C4-C5	2.00	1.51	1.43

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	COB	C20-C1-C19	-11.03	95.77	109.42
2	D	901	COB	C20-C1-C19	-7.66	99.93	109.42
2	E	901	COB	C20-C1-C19	-7.36	100.31	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	COB	C12-C11-C10	-6.94	117.31	123.54
2	B	901	COB	C20-C1-C19	-6.73	101.09	109.42
2	D	901	COB	O44-C43-C42	-6.68	100.87	121.04
2	C	901	COB	C41-C8-C9	6.53	122.58	111.19
2	E	901	COB	C41-C8-C9	6.47	122.48	111.19
2	F	901	COB	O6R-C1R-N1B	6.42	117.26	108.75
2	D	901	COB	O6R-C1R-N1B	6.42	117.25	108.75
2	A	901	COB	O58-C57-C56	-6.21	110.77	122.02
2	E	901	COB	C12-C11-C10	-6.12	118.04	123.54
2	A	901	COB	O6R-C1R-N1B	5.82	116.46	108.75
2	C	901	COB	C12-C11-C10	-5.76	118.37	123.54
2	A	901	COB	C20-C1-C19	-5.60	102.49	109.42
2	F	901	COB	C20-C1-C19	-5.52	102.59	109.42
2	E	901	COB	C31-C32-N33	5.45	133.97	116.49
2	A	901	COB	C2P-C1P-N59	5.32	120.75	112.92
2	A	901	COB	O58-C57-N59	5.28	133.40	123.03
2	C	901	COB	O44-C43-N45	5.07	136.07	122.53
2	E	901	COB	O6R-C1R-N1B	5.06	115.46	108.75
2	A	901	COB	C47-C12-C46	-5.04	101.05	109.41
2	C	901	COB	O2-P-O3	4.99	116.81	102.87
2	C	901	COB	C31-C32-N33	-4.79	101.15	116.49
2	D	901	COB	O3-C2P-C1P	4.78	116.40	106.94
2	B	901	COB	C12-C11-C10	-4.70	119.32	123.54
2	F	901	COB	C12-C11-C10	-4.67	119.34	123.54
2	D	901	COB	C60-C18-C19	4.65	121.44	112.39
2	C	901	COB	O34-C32-C31	4.53	134.72	121.04
2	B	901	COB	O6R-C1R-N1B	4.48	114.68	108.75
2	D	901	COB	O39-C38-C37	4.47	135.83	121.98
2	E	901	COB	O34-C32-N33	-4.47	110.59	122.53
2	C	901	COB	C12-C11-N23	4.41	116.21	111.49
2	F	901	COB	C41-C8-C9	4.36	118.79	111.19
2	F	901	COB	C49-C48-C13	4.36	127.00	114.65
2	B	901	COB	C42-C43-N45	4.32	130.33	116.49
2	F	901	COB	O34-C32-N33	-4.28	111.10	122.53
2	F	901	COB	C48-C13-C14	4.20	119.52	109.66
2	E	901	COB	C36-C7-C37	-4.05	103.86	110.74
2	C	901	COB	C55-C56-C57	4.02	120.21	111.25
2	A	901	COB	O44-C43-C42	-3.97	109.04	121.04
2	C	901	COB	C4B-C9B-C8B	-3.97	117.04	121.10
2	D	901	COB	C42-C43-N45	3.95	129.15	116.49
2	B	901	COB	O58-C57-N59	3.90	130.68	123.03
2	B	901	COB	C60-C18-C19	3.83	119.84	112.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	901	COB	O3-C2P-C1P	3.79	114.46	106.94
2	F	901	COB	C60-C18-C19	3.77	119.72	112.39
2	A	901	COB	C12-C11-N23	3.76	115.50	111.49
2	C	901	COB	O58-C57-N59	3.74	130.36	123.03
2	C	901	COB	C2-C3-C4	-3.73	97.44	101.64
2	D	901	COB	O51-C50-C49	-3.72	109.81	121.04
2	D	901	COB	C49-C50-N52	3.72	128.41	116.49
2	B	901	COB	C48-C49-C50	-3.70	99.97	112.55
2	F	901	COB	O58-C57-N59	3.63	130.15	123.03
2	A	901	COB	C25-C2-C26	-3.58	102.62	109.74
2	E	901	COB	O51-C50-C49	-3.58	110.25	121.04
2	C	901	COB	O8R-C5R-C4R	3.56	123.45	111.33
2	B	901	COB	O58-C57-C56	-3.55	115.58	122.02
2	A	901	COB	C55-C17-C18	-3.51	103.94	111.13
2	E	901	COB	C60-C18-C19	3.46	119.13	112.39
2	C	901	COB	O39-C38-N40	3.42	131.67	122.53
2	F	901	COB	C37-C38-N40	-3.39	106.00	116.49
2	E	901	COB	O58-C57-N59	3.38	129.66	123.03
2	C	901	COB	C4R-O6R-C1R	3.36	113.01	109.92
2	D	901	COB	C46-C12-C11	3.36	121.94	110.31
2	C	901	COB	O39-C38-C37	-3.29	111.78	121.98
2	C	901	COB	C46-C12-C11	3.26	121.59	110.31
2	F	901	COB	C8-C9-N22	3.26	117.21	110.77
2	D	901	COB	C47-C12-C11	-3.18	99.30	110.31
2	E	901	COB	C49-C50-N52	3.16	126.61	116.49
2	C	901	COB	C10-C9-N22	-3.14	122.16	125.74
2	F	901	COB	C7B-C8B-C9B	-3.14	117.44	120.54
2	C	901	COB	O2-P-O4	-3.12	99.84	109.81
2	E	901	COB	C13-C12-C11	-3.10	96.71	100.86
2	D	901	COB	C4B-C9B-C8B	-3.08	117.95	121.10
2	A	901	COB	C2-C26-C27	3.08	123.74	115.19
2	A	901	COB	C13-C12-C11	-3.06	96.75	100.86
2	C	901	COB	C56-C57-N59	-3.05	110.78	116.34
2	C	901	COB	C7-C8-C9	-3.05	97.03	100.89
2	D	901	COB	O2-P-O3	3.03	111.34	102.87
2	C	901	COB	P-O3-C2P	-2.99	110.88	121.10
2	F	901	COB	C56-C57-N59	-2.97	110.94	116.34
2	C	901	COB	C8-C9-N22	2.96	116.62	110.77
2	E	901	COB	C2-C1-N21	2.94	105.86	101.78
2	B	901	COB	O51-C50-C49	2.92	129.85	121.04
2	F	901	COB	O28-C27-C26	-2.91	112.97	121.98
2	B	901	COB	O34-C32-C31	2.91	129.82	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	COB	O63-C61-N62	2.91	130.30	122.53
2	A	901	COB	O3-C2P-C1P	2.90	112.69	106.94
2	C	901	COB	O3-C2P-C1P	2.89	112.67	106.94
2	E	901	COB	O58-C57-C56	-2.87	116.83	122.02
2	B	901	COB	O44-C43-N45	-2.86	114.89	122.53
3	E	902	GOL	O2-C2-C1	-2.86	97.35	109.18
2	E	901	COB	C35-C5-C6	-2.85	117.82	122.41
2	A	901	COB	O39-C38-C37	2.85	130.80	121.98
2	B	901	COB	C49-C50-N52	-2.84	107.39	116.49
2	A	901	COB	O34-C32-N33	-2.83	114.98	122.53
2	F	901	COB	C10-C9-N22	-2.83	122.52	125.74
2	F	901	COB	O51-C50-N52	2.82	130.06	122.53
2	D	901	COB	O44-C43-N45	2.78	129.97	122.53
2	A	901	COB	O28-C27-C26	2.78	130.58	121.98
2	A	901	COB	C42-C43-N45	2.75	125.32	116.49
2	A	901	COB	C60-C18-C19	2.75	117.74	112.39
2	B	901	COB	C4R-O6R-C1R	-2.75	107.41	109.92
2	D	901	COB	C37-C38-N40	-2.72	108.06	116.49
2	E	901	COB	O5-P-O4	2.69	124.97	112.44
2	A	901	COB	O5-P-O4	2.67	124.89	112.44
2	A	901	COB	C37-C38-N40	-2.67	108.24	116.49
2	B	901	COB	C55-C56-C57	2.64	117.15	111.25
2	E	901	COB	O2-P-O3	2.62	110.19	102.87
2	C	901	COB	C49-C50-N52	2.61	124.87	116.49
2	C	901	COB	C17-C16-N24	2.59	112.65	107.94
2	B	901	COB	C10-C9-N22	-2.59	122.79	125.74
2	A	901	COB	O2-P-O4	-2.56	101.61	109.81
2	F	901	COB	C2-C1-N21	2.55	105.33	101.78
2	C	901	COB	C60-C18-C19	2.55	117.35	112.39
2	C	901	COB	C60-C61-N62	-2.55	110.09	116.19
2	B	901	COB	C35-C5-C6	-2.52	118.34	122.41
2	F	901	COB	C7-C8-C9	-2.50	97.72	100.89
2	A	901	COB	C4B-C9B-C8B	-2.49	118.55	121.10
2	D	901	COB	C8-C7-C6	-2.48	96.71	100.92
2	C	901	COB	C47-C12-C46	-2.48	105.30	109.41
2	D	901	COB	O39-C38-N40	-2.45	115.98	122.53
2	D	901	COB	C35-C5-C6	-2.45	118.47	122.41
2	E	901	COB	C55-C56-C57	2.44	116.69	111.25
2	D	901	COB	O34-C32-C31	-2.43	113.70	121.04
2	E	901	COB	C17-C16-N24	2.42	112.35	107.94
2	B	901	COB	C8-C9-N22	2.41	115.53	110.77
2	E	901	COB	C12-C11-N23	2.40	114.06	111.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	901	COB	O2-P-O3	2.40	109.56	102.87
2	B	901	COB	O6R-C4R-C3R	2.39	109.97	104.92
2	B	901	COB	C46-C12-C11	2.38	118.56	110.31
2	A	901	COB	C35-C5-C6	-2.38	118.57	122.41
2	B	901	COB	C13-C12-C11	-2.38	97.67	100.86
2	A	901	COB	C46-C12-C11	2.37	118.51	110.31
2	F	901	COB	C41-C8-C7	2.37	120.70	114.19
2	C	901	COB	O44-C43-C42	-2.36	113.91	121.04
2	B	901	COB	C2-C1-N21	2.36	105.06	101.78
2	D	901	COB	C12-C11-C10	-2.35	121.43	123.54
2	A	901	COB	C8-C9-N22	2.33	115.37	110.77
2	D	901	COB	C17-C16-N24	2.31	112.14	107.94
2	C	901	COB	O5-P-O4	2.29	123.12	112.44
2	F	901	COB	O44-C43-C42	-2.29	114.12	121.04
2	D	901	COB	C55-C56-C57	2.29	116.35	111.25
2	C	901	COB	O58-C57-C56	-2.27	117.91	122.02
2	D	901	COB	C31-C32-N33	2.27	123.77	116.49
2	C	901	COB	C2-C1-N21	2.26	104.93	101.78
2	A	901	COB	C26-C2-C3	2.26	111.36	107.42
2	B	901	COB	C42-C41-C8	2.25	121.04	114.65
2	E	901	COB	C9-C10-C11	-2.25	122.53	125.84
2	B	901	COB	C2P-C1P-N59	2.23	116.21	112.92
2	B	901	COB	C12-C11-N23	2.23	113.87	111.49
2	B	901	COB	C31-C32-N33	-2.20	109.45	116.49
2	B	901	COB	C55-C17-C18	-2.19	106.64	111.13
2	B	901	COB	C30-C31-C32	-2.19	105.11	112.55
2	D	901	COB	C2-C1-N21	2.19	104.82	101.78
2	A	901	COB	C10-C9-N22	-2.19	123.24	125.74
2	F	901	COB	O39-C38-C37	2.18	128.72	121.98
2	F	901	COB	C55-C17-C16	2.17	120.83	116.59
2	F	901	COB	C17-C16-N24	2.17	111.88	107.94
2	F	901	COB	O28-C27-N29	2.16	128.30	122.53
2	F	901	COB	O44-C43-N45	2.15	128.28	122.53
2	B	901	COB	C31-C30-C3	2.15	120.74	114.65
2	E	901	COB	C41-C8-C7	2.15	120.09	114.19
2	C	901	COB	C13-C14-N23	2.14	113.95	109.39
2	E	901	COB	C5-C6-N22	-2.14	120.65	123.88
2	E	901	COB	C3R-C2R-C1R	2.13	104.58	99.89
2	B	901	COB	C17-C16-N24	2.13	111.81	107.94
2	D	901	COB	C37-C7-C8	2.13	113.99	108.37
2	D	901	COB	O2-P-O4	-2.13	103.01	109.81
2	F	901	COB	C13-C12-C11	-2.12	98.01	100.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	COB	O44-C43-C42	-2.12	114.63	121.04
2	F	901	COB	C31-C32-N33	2.12	123.27	116.49
2	A	901	COB	O7R-C2R-C3R	2.11	117.08	111.19
2	B	901	COB	O39-C38-C37	-2.09	115.51	121.98
2	E	901	COB	C46-C12-C11	2.08	117.50	110.31
2	A	901	COB	C12-C13-C14	2.07	104.57	101.86
2	D	901	COB	C41-C8-C9	-2.07	107.58	111.19
2	C	901	COB	O6R-C4R-C5R	2.07	113.59	109.22
2	A	901	COB	C55-C17-C16	2.06	120.63	116.59
2	F	901	COB	C1P-N59-C57	-2.06	118.27	122.69
2	E	901	COB	C7B-C8B-C9B	-2.03	118.53	120.54
2	B	901	COB	C60-C61-N62	-2.03	111.33	116.19
2	C	901	COB	C42-C43-N45	-2.02	110.00	116.49
2	B	901	COB	C26-C2-C3	-2.02	103.90	107.42
2	D	901	COB	O5-P-O4	2.02	121.83	112.44
2	E	901	COB	C55-C17-C16	2.00	120.51	116.59

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	COB	C1-C2-C26-C27
2	A	901	COB	C25-C2-C26-C27
2	A	901	COB	C3-C2-C26-C27
2	A	901	COB	C54-C17-C55-C56
2	A	901	COB	C18-C17-C55-C56
2	C	901	COB	C38-C37-C7-C36
2	D	901	COB	C42-C41-C8-C9
2	E	901	COB	C42-C41-C8-C9
3	A	902	GOL	O1-C1-C2-O2
3	A	902	GOL	O1-C1-C2-C3
2	A	901	COB	O6R-C4R-C5R-O8R
2	A	901	COB	C3R-C4R-C5R-O8R
2	D	901	COB	C42-C41-C8-C7
2	B	901	COB	C14-C13-C48-C49
2	D	901	COB	C3R-C4R-C5R-O8R
2	F	901	COB	O6R-C4R-C5R-O8R
2	B	901	COB	C12-C13-C48-C49
2	D	901	COB	O6R-C4R-C5R-O8R
2	C	901	COB	C3R-C4R-C5R-O8R
2	F	901	COB	C3R-C4R-C5R-O8R
2	A	901	COB	C42-C41-C8-C7

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Mol	Chain	Res	Type	Atoms
2	B	901	COB	C42-C41-C8-C7
2	F	901	COB	C12-C13-C48-C49
2	B	901	COB	C42-C41-C8-C9
2	B	901	COB	C7-C37-C38-N40
3	B	902	GOL	C1-C2-C3-O3
3	C	902	GOL	C1-C2-C3-O3
3	E	902	GOL	O1-C1-C2-C3
3	F	902	GOL	O1-C1-C2-C3
2	C	901	COB	O6R-C4R-C5R-O8R
3	B	902	GOL	O2-C2-C3-O3
3	E	902	GOL	O1-C1-C2-O2
3	F	902	GOL	O1-C1-C2-O2
2	A	901	COB	C42-C41-C8-C9
2	E	901	COB	C41-C42-C43-O44
2	A	901	COB	C55-C56-C57-N59
2	F	901	COB	C3P-C2P-O3-P
2	A	901	COB	C55-C56-C57-O58
2	B	901	COB	C7-C37-C38-O39
2	B	901	COB	C55-C56-C57-O58
2	F	901	COB	C42-C41-C8-C9
2	C	901	COB	C48-C49-C50-O51
2	C	901	COB	C48-C49-C50-N52
2	B	901	COB	C41-C42-C43-O44
2	B	901	COB	C41-C42-C43-N45
2	C	901	COB	C55-C56-C57-O58
2	E	901	COB	C55-C56-C57-O58
2	B	901	COB	C55-C56-C57-N59
2	C	901	COB	C3P-C2P-O3-P
2	D	901	COB	C3P-C2P-O3-P
2	F	901	COB	C1P-C2P-O3-P
2	A	901	COB	C41-C42-C43-N45
2	D	901	COB	C41-C42-C43-O44
2	E	901	COB	C41-C42-C43-N45
2	F	901	COB	C38-C37-C7-C36
2	D	901	COB	C48-C49-C50-O51
2	D	901	COB	C41-C42-C43-N45
2	F	901	COB	C2R-C3R-O2-P
2	B	901	COB	C17-C18-C60-C61
2	D	901	COB	C17-C18-C60-C61
2	E	901	COB	C30-C31-C32-O34
2	D	901	COB	C48-C49-C50-N52
2	E	901	COB	C48-C49-C50-N52

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Mol	Chain	Res	Type	Atoms
2	C	901	COB	C38-C37-C7-C8
2	F	901	COB	C38-C37-C7-C8
2	E	901	COB	C55-C56-C57-N59
2	C	901	COB	C55-C56-C57-N59
2	F	901	COB	C55-C56-C57-O58
2	E	901	COB	C48-C49-C50-O51
2	D	901	COB	C55-C56-C57-O58
2	A	901	COB	C16-C17-C55-C56
2	C	901	COB	C18-C60-C61-O63
3	B	902	GOL	O1-C1-C2-C3
2	A	901	COB	C41-C42-C43-O44
2	F	901	COB	C14-C13-C48-C49
2	D	901	COB	C55-C56-C57-N59
2	C	901	COB	C18-C60-C61-N62
2	B	901	COB	C2R-C3R-O2-P
2	A	901	COB	C3R-O2-P-O5
2	F	901	COB	C55-C56-C57-N59
2	B	901	COB	C19-C18-C60-C61
2	D	901	COB	C19-C18-C60-C61
2	C	901	COB	C1P-C2P-O3-P
2	E	901	COB	C1P-C2P-O3-P
2	F	901	COB	C41-C42-C43-N45

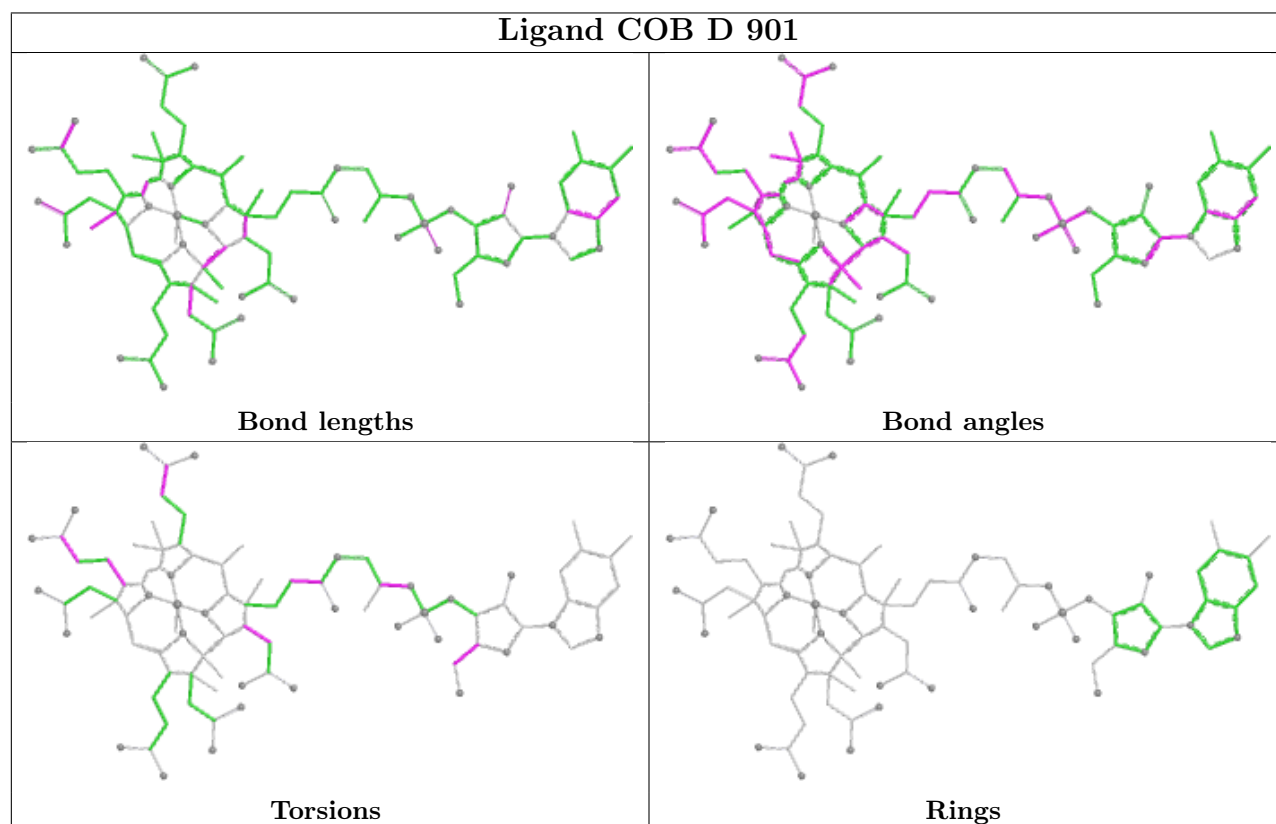
There are no ring outliers.

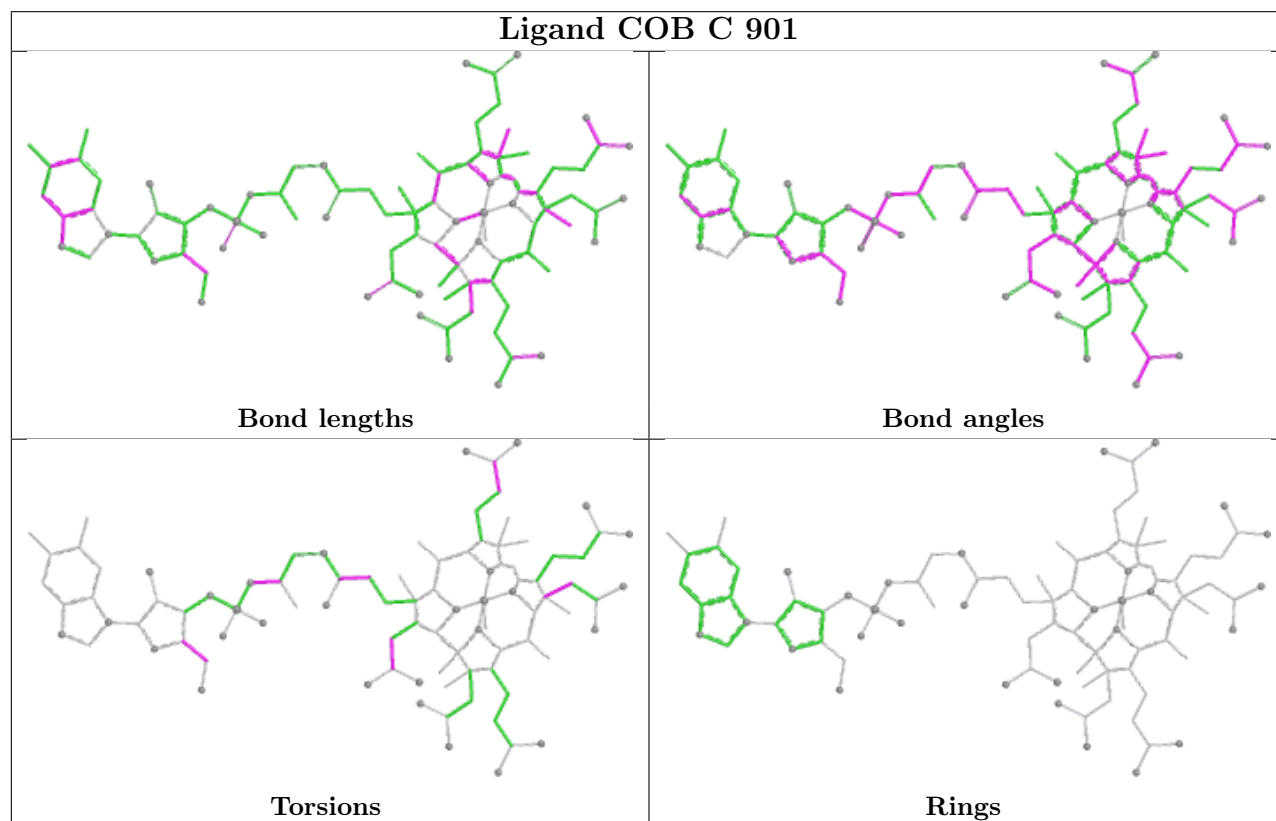
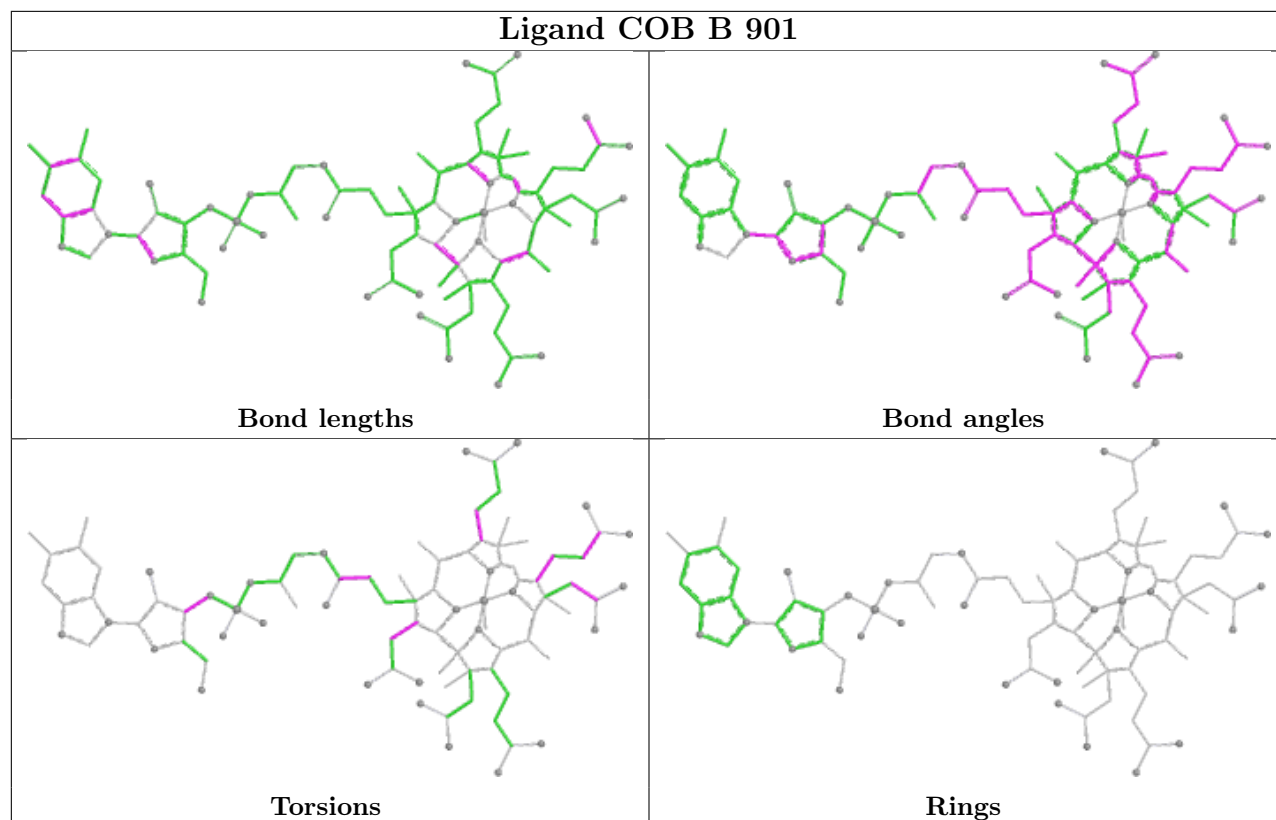
8 monomers are involved in 56 short contacts:

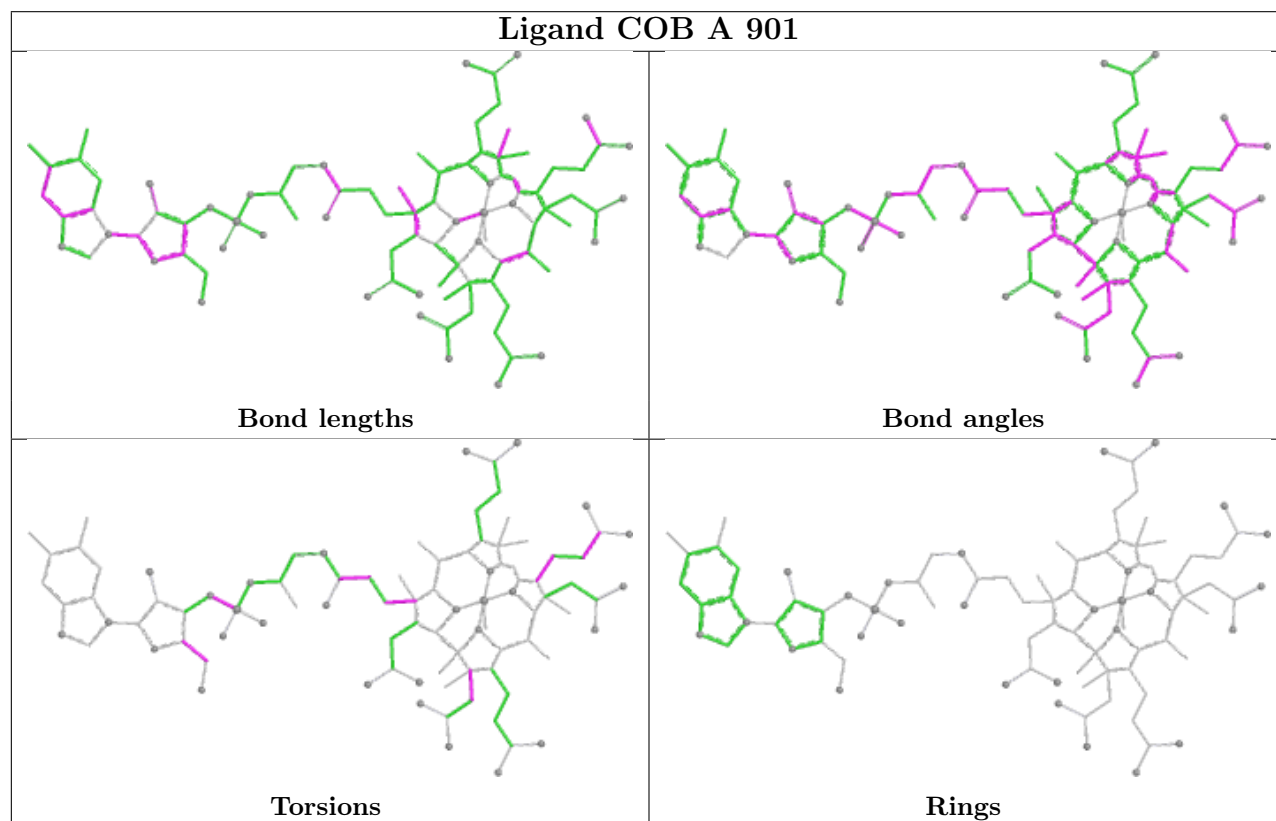
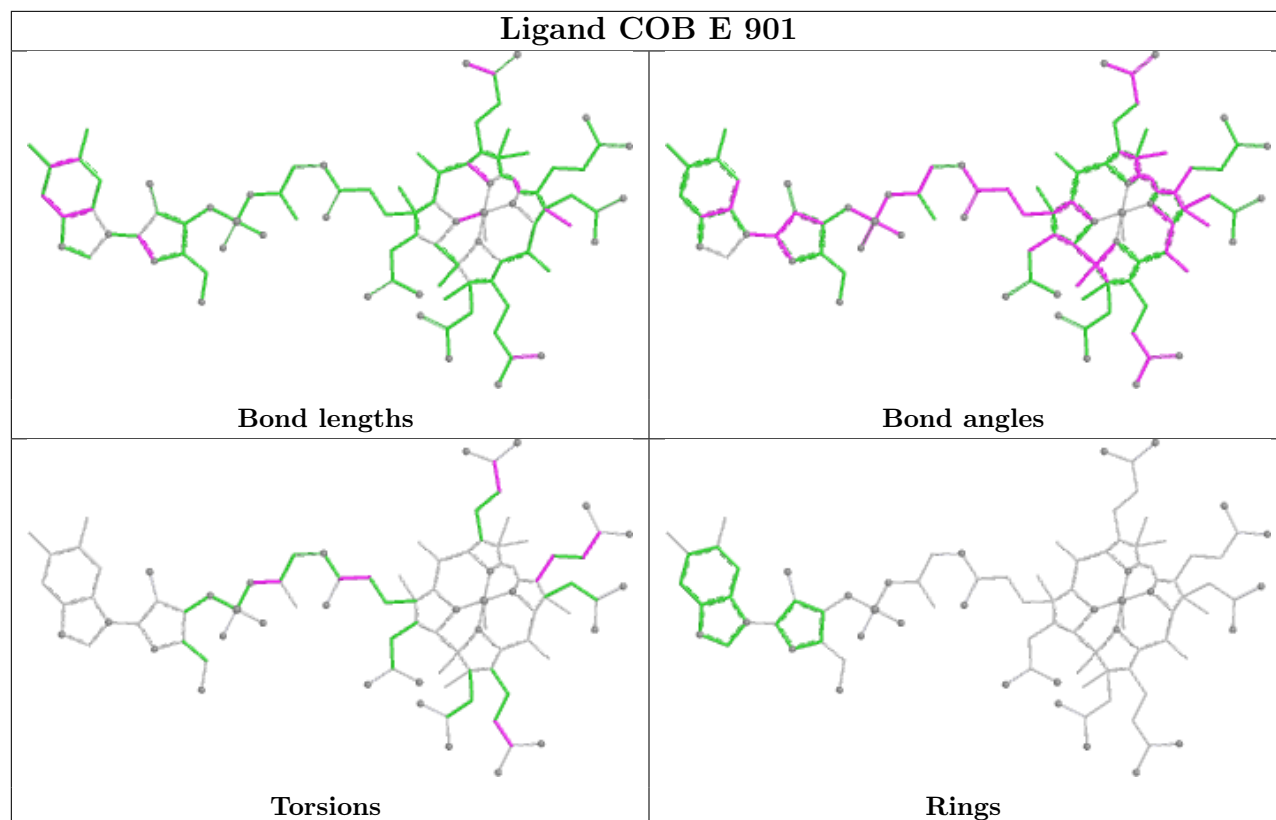
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	901	COB	8	0
2	B	901	COB	8	0
3	C	903	GOL	1	0
2	C	901	COB	11	0
2	E	901	COB	5	0
2	A	901	COB	13	0
3	B	902	GOL	1	0
2	F	901	COB	9	0

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

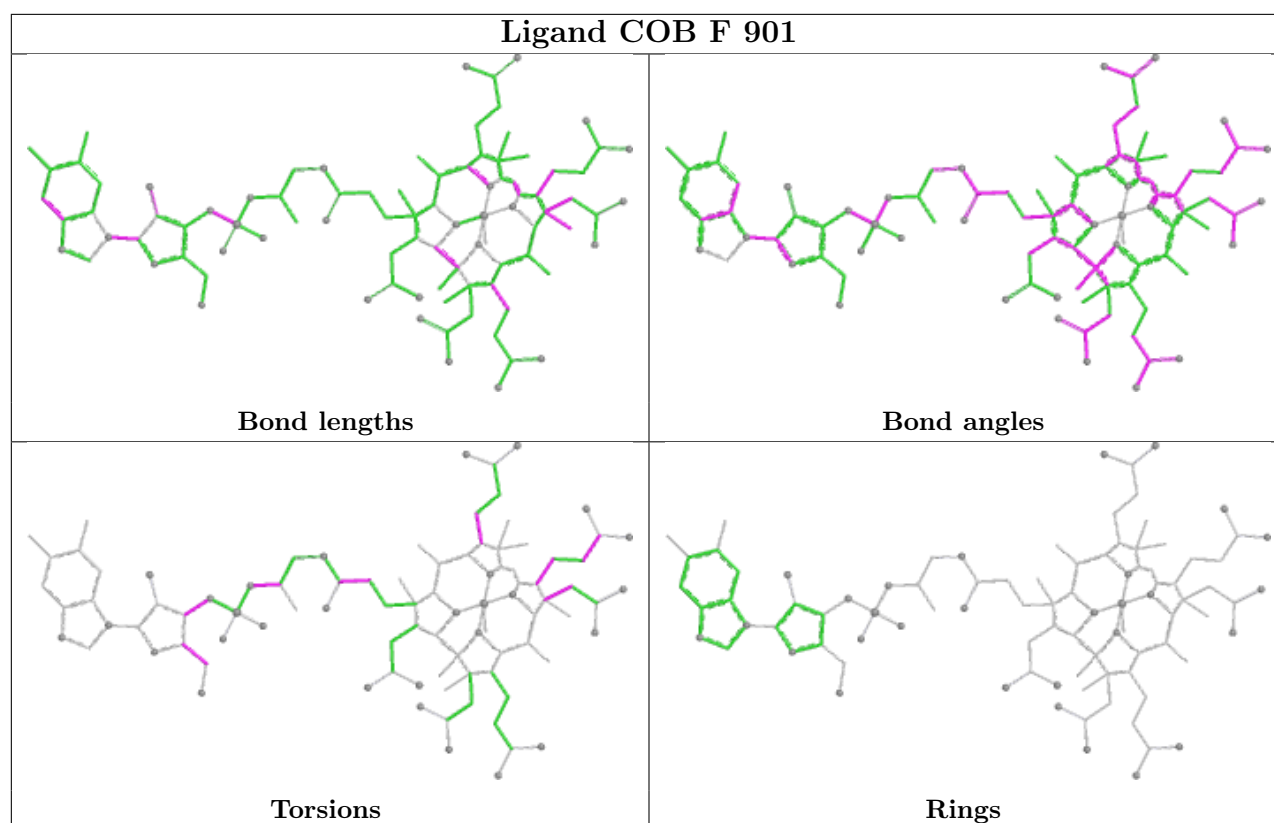
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.











## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	510/511 (99%)	-0.58	3 (0%) 85 79	65, 106, 183, 249	0
1	B	510/511 (99%)	-0.70	3 (0%) 85 79	73, 106, 169, 204	0
1	C	510/511 (99%)	-0.77	1 (0%) 92 90	68, 100, 154, 223	0
1	D	507/511 (99%)	-0.79	0 100 100	72, 107, 157, 188	0
1	E	509/511 (99%)	-0.61	2 (0%) 89 85	91, 146, 196, 233	0
1	F	510/511 (99%)	-0.74	0 100 100	80, 117, 160, 250	0
All	All	3056/3066 (99%)	-0.70	9 (0%) 90 87	65, 113, 179, 250	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	651	ASP	6.2
1	A	650	GLU	4.2
1	B	695	LEU	2.7
1	C	648	HIS	2.6
1	B	715	ALA	2.5
1	A	465	SER	2.4
1	E	647	ALA	2.3
1	B	465	SER	2.3
1	E	830	LEU	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands

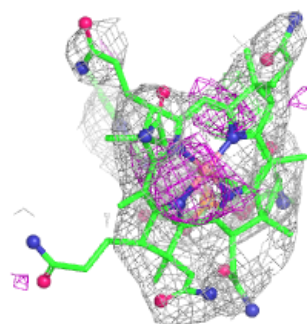
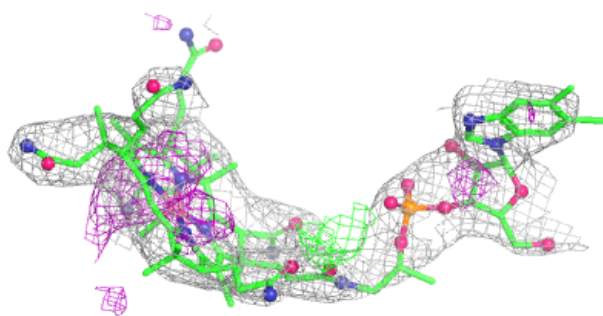
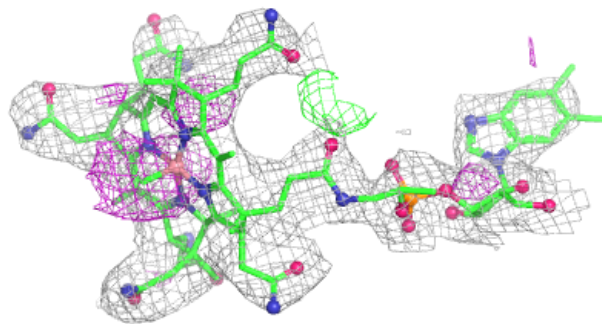
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	GOL	C	902	6/6	0.70	0.20	84,93,185,197	0
3	GOL	F	902	6/6	0.70	0.17	132,162,180,194	0
3	GOL	E	902	6/6	0.87	0.24	96,106,117,133	0
3	GOL	A	902	6/6	0.92	0.17	95,103,125,140	0
3	GOL	C	903	6/6	0.94	0.14	106,111,141,148	0
2	COB	A	901	92/92	0.95	0.10	88,132,171,185	0
3	GOL	B	902	6/6	0.95	0.10	76,97,131,158	0
2	COB	B	901	92/92	0.97	0.08	86,111,138,160	0
2	COB	E	901	92/92	0.98	0.07	82,104,131,144	0
2	COB	F	901	92/92	0.98	0.07	74,90,119,129	0
2	COB	C	901	92/92	0.98	0.07	60,75,95,101	0
2	COB	D	901	92/92	0.98	0.07	61,82,101,125	0

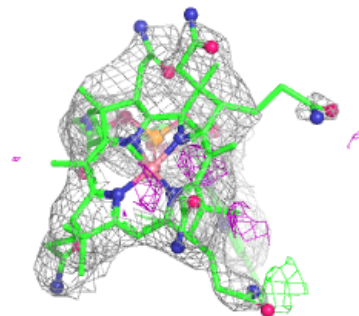
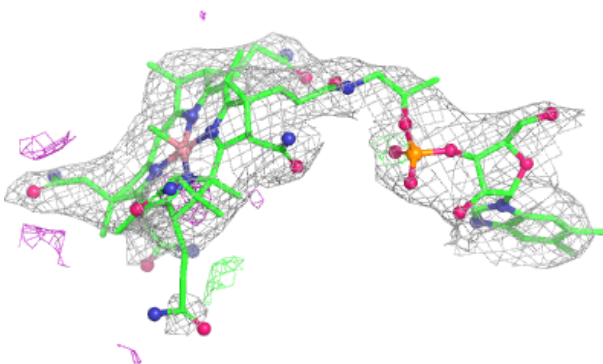
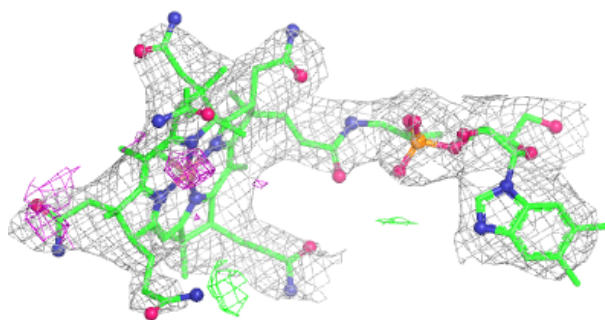
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around COB A 901:**

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

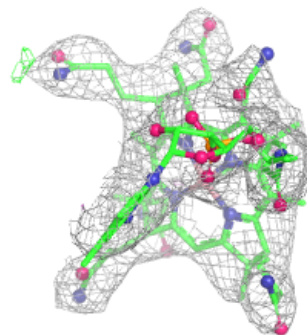
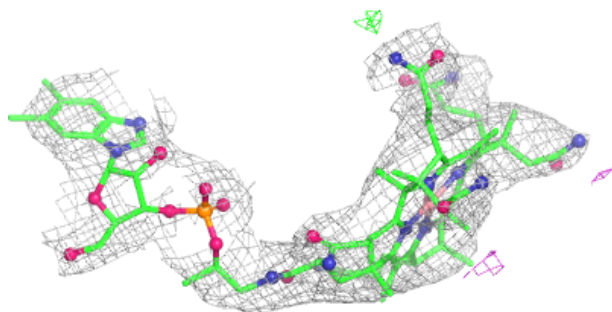
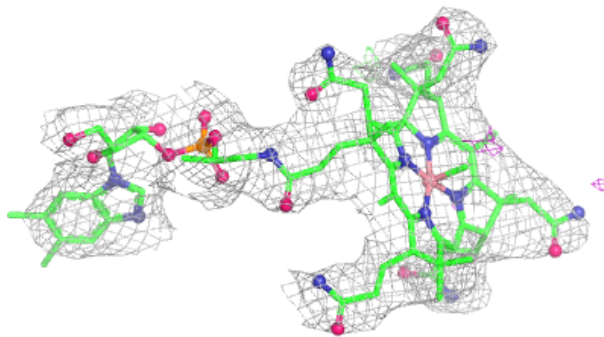
**Electron density around COB B 901:**

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

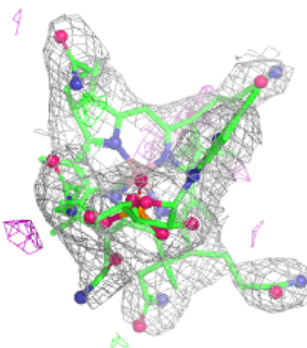
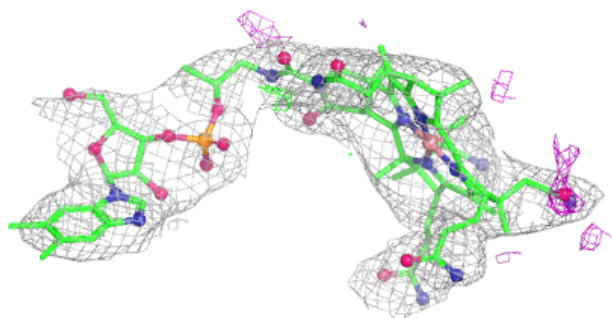
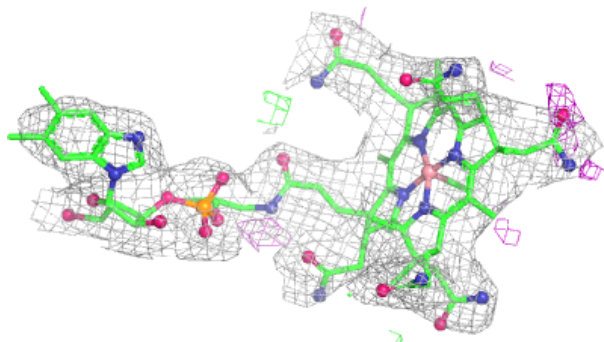


**Electron density around COB E 901:**

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

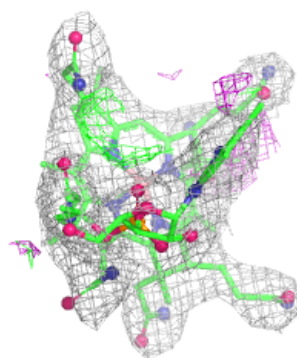
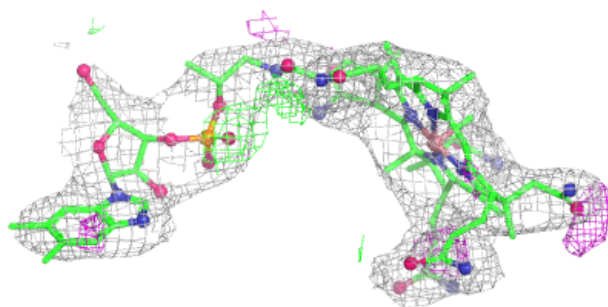
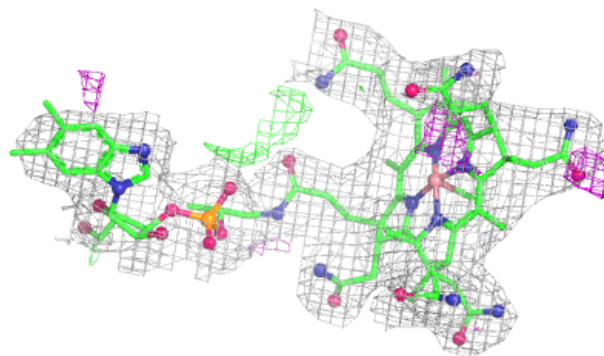
**Electron density around COB F 901:**

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

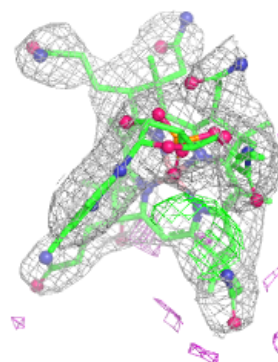
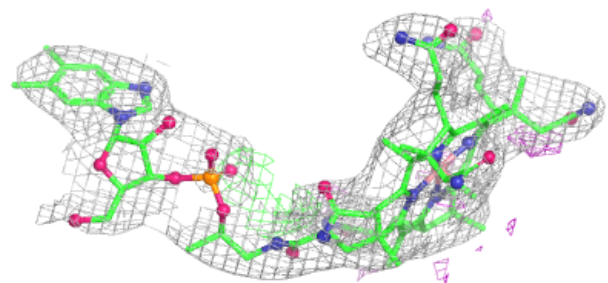
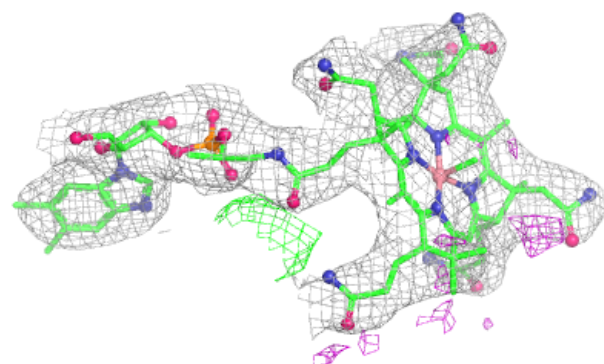


**Electron density around COB C 901:**

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

**Electron density around COB D 901:**

$2mF_o-DF_c$  (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.