



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 10:22 PM EDT

PDB ID : 3QS1
Title : Crystal structure of KNI-10006 complex of Plasmepsin I (PMI) from Plasmodium falciparum
Authors : Bhaumik, P.; Gustchina, A.; Wlodawer, A.
Deposited on : 2011-02-19
Resolution : 3.10 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

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>.

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

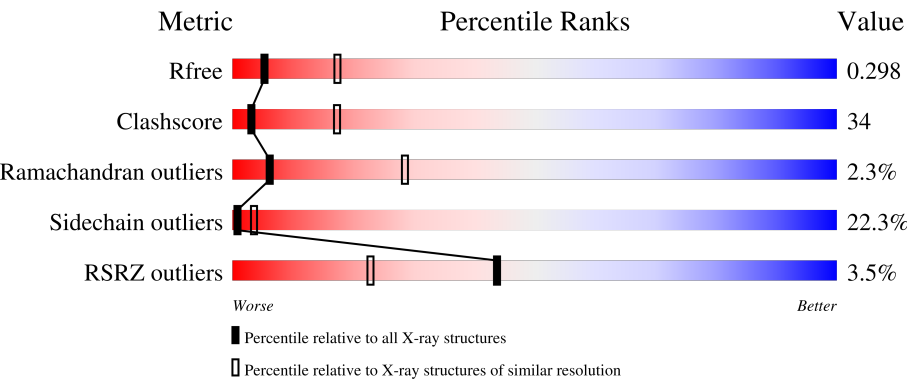
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 ≥ 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	336	<div><div>2%</div><div>45%39%12%..</div></div>
1	B	336	<div><div>%</div><div>46%36%13%..</div></div>
1	C	336	<div><div>2%</div><div>36%49%12%..</div></div>
1	D	336	<div><div>9%</div><div>35%49%11%..</div></div>

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
3	GOL	A	331	-	-	X	-
3	GOL	C	331	-	-	X	X
3	GOL	C	333	-	-	X	-
3	GOL	D	331	-	-	X	-
3	GOL	D	332	-	-	-	X

2 Entry composition [i](#)

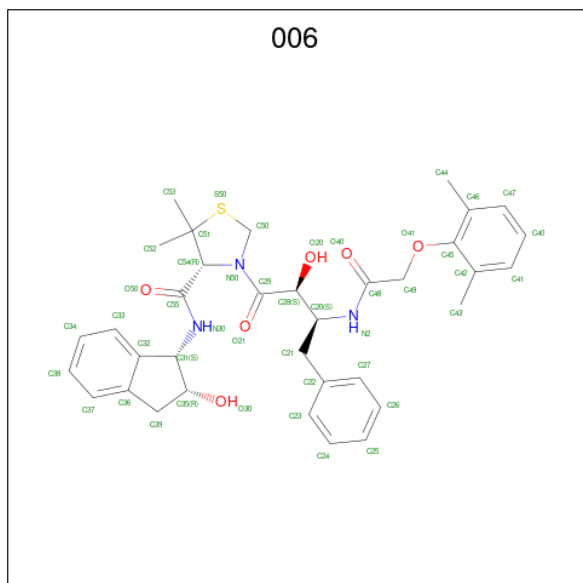
There are 3 unique types of molecules in this entry. The entry contains 10646 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Plasmepsin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2604	1693	403	500	8			
1	B	327	Total	C	N	O	S	0	0	0
			2604	1693	403	500	8			
1	C	326	Total	C	N	O	S	0	0	0
			2599	1690	402	499	8			
1	D	326	Total	C	N	O	S	0	0	0
			2599	1690	402	499	8			

- Molecule 2 is (4R)-3-[(2S,3S)-3-[[[(2,6-dimethylphenoxy)acetyl]amino}-2-hydroxy-4-phenylbutanoyl]-N-[(1S,2R)-2-hydroxy-2,3-dihydro-1H-inden-1-yl]-5,5-dimethyl-1,3-thiazolidine-4-carboxamide (three-letter code: 006) (formula: C₃₅H₄₁N₃O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			45	35	3	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			45	35	3	6	1		
2	C	1	Total	C	N	O	S	0	0
			45	35	3	6	1		
2	D	1	Total	C	N	O	S	0	0
			45	35	3	6	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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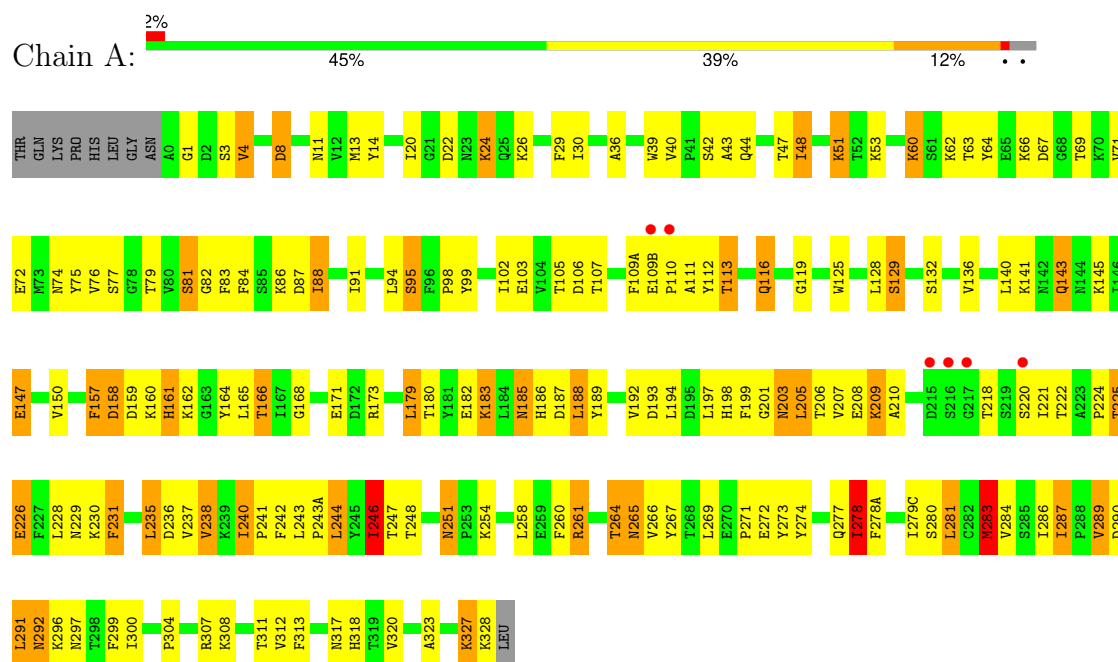
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

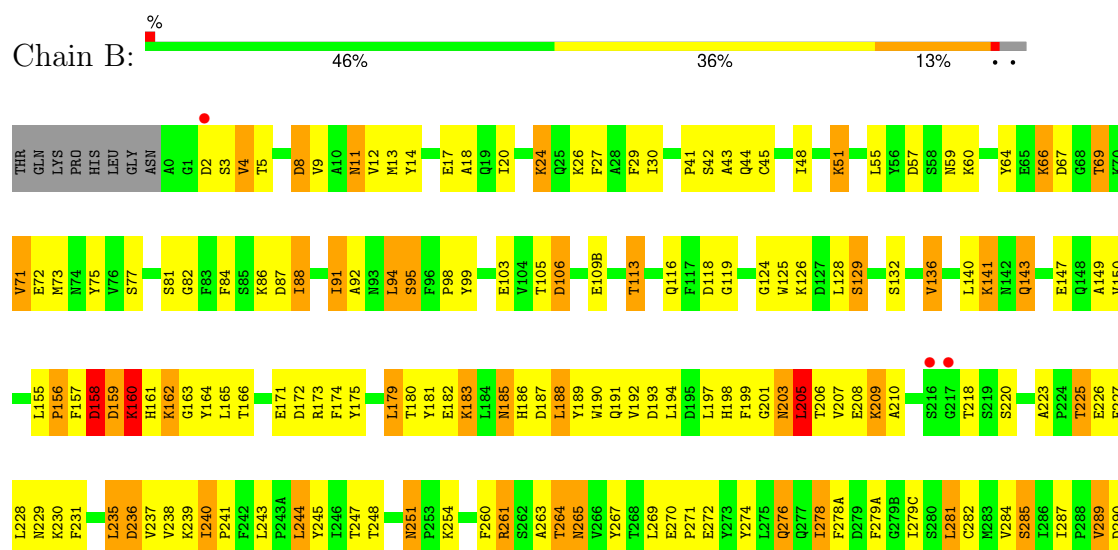
3 Residue-property plots

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: Plasmepsin-1

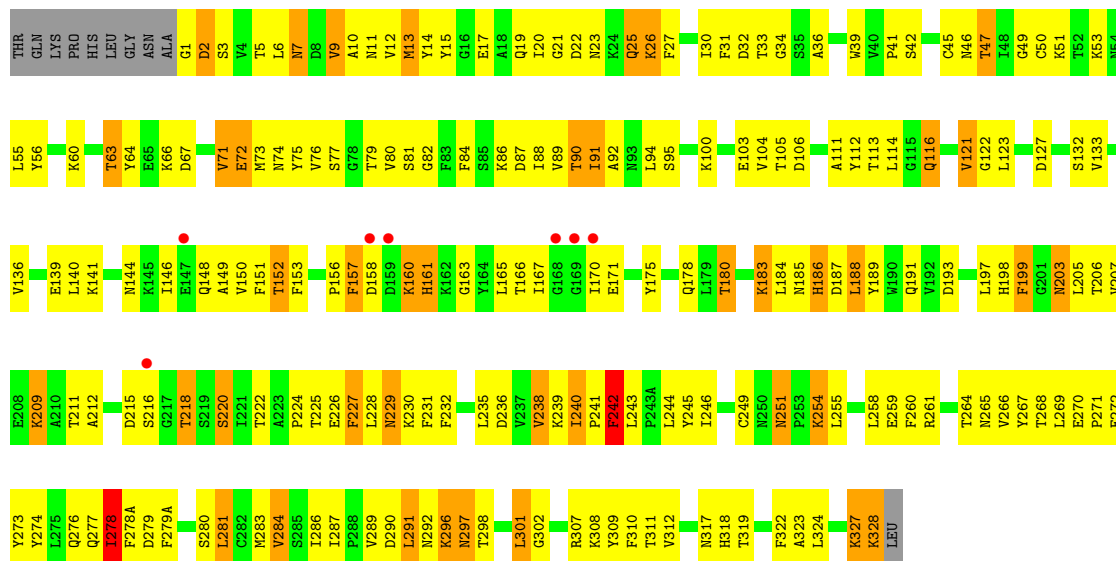


• Molecule 1: Plasmepsin-1

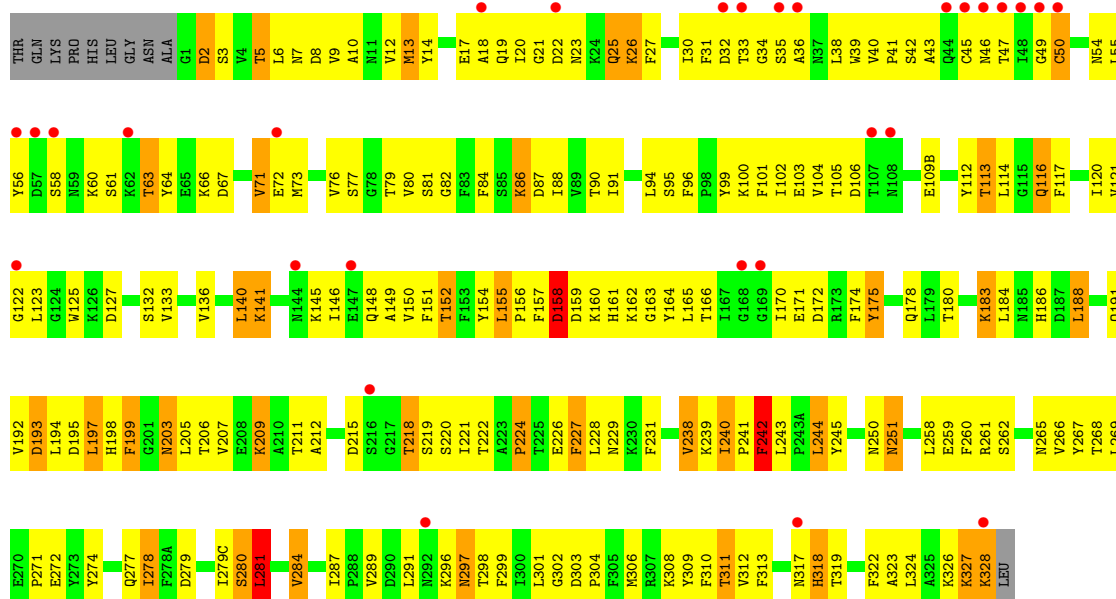




● Molecule 1: Plasmepsin-1



● Molecule 1: Plasmepsin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	93.69Å 93.69Å 160.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 29.63 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.10) 99.1 (29.63-3.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.5.0104	Depositor
R, R_{free}	0.211 , 0.300 0.210 , 0.298	Depositor DCC
R_{free} test set	1240 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10646	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 006, 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	1.03	3/2670 (0.1%)	1.06	4/3627 (0.1%)
1	B	0.97	2/2670 (0.1%)	1.01	2/3627 (0.1%)
1	C	0.97	2/2665 (0.1%)	0.99	2/3620 (0.1%)
1	D	0.97	0/2665	0.98	3/3620 (0.1%)
All	All	0.98	7/10670 (0.1%)	1.01	11/14494 (0.1%)

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	1
1	B	0	4
1	C	0	2
1	D	0	1
All	All	0	8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	GLU	CB-CG	6.42	1.64	1.52
1	A	226	GLU	CG-CD	6.05	1.61	1.51
1	C	72	GLU	CG-CD	5.36	1.59	1.51
1	B	9	VAL	CB-CG1	-5.12	1.42	1.52
1	B	158	ASP	CB-CG	5.12	1.62	1.51
1	A	147	GLU	CG-CD	5.08	1.59	1.51
1	C	209	LYS	CD-CE	5.03	1.63	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	LEU	CB-CG-CD2	-12.98	88.94	111.00
1	A	205	LEU	CB-CG-CD2	-10.89	92.49	111.00
1	A	283	MET	CG-SD-CE	-9.83	84.47	100.20
1	A	205	LEU	CB-CG-CD1	8.76	125.89	111.00
1	D	209	LYS	CD-CE-NZ	-7.20	95.14	111.70
1	B	106	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	246	ILE	CG1-CB-CG2	-5.49	99.33	111.40
1	C	207	VAL	CB-CA-C	5.38	121.62	111.40
1	C	278	ILE	CG1-CB-CG2	-5.33	99.68	111.40
1	D	207	VAL	CB-CA-C	5.06	121.01	111.40
1	D	281	LEU	CB-CG-CD1	-5.02	102.46	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	LYS	Peptide
1	B	157	PHE	Peptide
1	B	158	ASP	Peptide
1	B	160	LYS	Peptide
1	B	296	LYS	Peptide
1	C	160	LYS	Peptide
1	C	296	LYS	Peptide
1	D	296	LYS	Peptide

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	2604	0	2535	161	0
1	B	2604	0	2535	149	0
1	C	2599	0	2530	196	0
1	D	2599	0	2530	234	0
2	A	45	0	41	6	0
2	B	45	0	41	3	0
2	C	45	0	41	5	0
2	D	45	0	41	1	0
3	A	18	0	24	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	16	1	0
3	C	18	0	24	23	0
3	D	12	0	16	20	0
All	All	10646	0	10374	711	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 34.

All (711) 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:A:292:ASN:CB	3:A:331:GOL:H32	1.72	1.17
1:A:292:ASN:HB3	3:A:331:GOL:H32	1.16	1.14
1:D:20:ILE:HD11	1:D:87:ASP:HB3	1.32	1.11
3:C:331:GOL:C1	1:D:242:PHE:HA	1.80	1.10
1:B:240:ILE:HD11	1:B:243:LEU:HD12	1.28	1.09
1:D:155:LEU:HD12	1:D:306:MET:HB3	1.36	1.06
1:A:328:LYS:HA	1:A:328:LYS:NZ	1.72	1.05
1:C:327:LYS:H	1:C:327:LYS:HD3	1.23	1.04
1:D:194:LEU:HA	3:D:331:GOL:H12	1.37	1.04
1:D:155:LEU:CD1	1:D:306:MET:HB3	1.88	1.03
1:D:327:LYS:H	1:D:327:LYS:HD3	1.22	1.03
1:C:114:LEU:HD23	3:C:331:GOL:H32	1.03	1.03
1:C:114:LEU:CD2	3:C:331:GOL:H32	1.88	1.01
3:C:331:GOL:O2	1:D:239:LYS:HE2	1.59	1.01
1:D:195:ASP:N	3:D:331:GOL:O1	1.94	1.00
1:A:240:ILE:HD11	1:A:243:LEU:HD12	1.43	0.99
1:D:262:SER:HA	3:D:331:GOL:H31	1.46	0.98
3:C:331:GOL:H12	1:D:242:PHE:HA	1.42	0.98
1:C:114:LEU:HD23	3:C:331:GOL:C3	1.94	0.97
1:D:180:THR:CG2	1:D:267:TYR:OH	2.13	0.97
1:B:218:THR:HG22	1:B:220:SER:H	1.27	0.95
1:A:225:THR:HG22	1:A:290:ASP:OD2	1.65	0.95
1:D:81:SER:HB2	1:D:106:ASP:HB3	1.47	0.95
1:D:261:ARG:O	3:D:331:GOL:O1	1.84	0.93
1:C:198:HIS:HB2	1:C:261:ARG:HH12	1.34	0.92
1:C:20:ILE:HD11	1:C:87:ASP:HB3	1.52	0.92
1:A:75:TYR:HA	2:A:330:006:H49A	1.49	0.91
1:C:180:THR:CG2	1:C:267:TYR:OH	2.19	0.91
1:D:194:LEU:HA	3:D:331:GOL:C1	2.00	0.90
1:B:182:GLU:CB	1:B:192:VAL:HG21	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:331:GOL:H11	1:D:242:PHE:HA	1.55	0.89
1:A:197:LEU:CD1	1:A:210:ALA:HB3	2.03	0.89
1:C:198:HIS:CB	1:C:261:ARG:HH12	1.85	0.88
1:A:328:LYS:HA	1:A:328:LYS:HZ3	1.34	0.88
1:A:182:GLU:CB	1:A:192:VAL:HG21	2.05	0.87
1:B:205:LEU:N	1:B:205:LEU:HD23	1.86	0.87
1:A:238:VAL:CG1	1:D:279(C):ILE:HG12	2.04	0.87
1:D:6:LEU:N	1:D:163:GLY:O	2.09	0.86
1:D:327:LYS:H	1:D:327:LYS:CD	1.87	0.86
1:C:111:ALA:HA	3:C:331:GOL:O1	1.75	0.86
1:D:198:HIS:HB2	1:D:261:ARG:HH12	1.38	0.86
1:D:198:HIS:CD2	1:D:206:THR:HG22	2.10	0.86
1:A:218:THR:HG22	1:A:220:SER:H	1.38	0.85
1:D:5:THR:HG23	1:D:164:TYR:HE1	1.40	0.85
1:C:183:LYS:H	1:C:183:LYS:HD2	1.42	0.84
1:B:199:PHE:HB3	1:B:231:PHE:CE2	2.13	0.84
1:D:180:THR:HG21	1:D:267:TYR:OH	1.77	0.84
1:D:262:SER:CA	3:D:331:GOL:H31	2.08	0.83
1:D:157:PHE:O	1:D:158:ASP:HB3	1.80	0.82
1:C:327:LYS:H	1:C:327:LYS:CD	1.92	0.82
1:D:268:THR:O	1:D:308:LYS:NZ	2.13	0.82
1:B:182:GLU:HB2	1:B:192:VAL:HG21	1.61	0.82
1:C:22:ASP:HB2	1:C:63:THR:OG1	1.80	0.81
1:B:199:PHE:HB3	1:B:231:PHE:HE2	1.45	0.81
1:A:292:ASN:HB2	3:A:331:GOL:H32	1.62	0.81
1:B:160:LYS:HE2	1:B:162:LYS:NZ	1.96	0.81
1:D:180:THR:HG22	1:D:267:TYR:OH	1.80	0.81
1:D:195:ASP:H	3:D:331:GOL:C1	1.93	0.80
1:D:39:TRP:CE3	1:D:104:VAL:HG21	2.16	0.80
1:A:182:GLU:HB2	1:A:192:VAL:HG21	1.63	0.80
1:D:262:SER:HA	3:D:331:GOL:H11	1.62	0.80
1:C:180:THR:HG22	1:C:267:TYR:OH	1.82	0.79
1:A:3:SER:OG	1:A:166:THR:HG23	1.83	0.79
1:B:261:ARG:HH11	1:B:261:ARG:HB2	1.45	0.79
1:C:198:HIS:HB2	1:C:261:ARG:NH1	1.96	0.79
1:B:225:THR:HG22	1:B:290:ASP:OD2	1.83	0.78
3:C:331:GOL:H11	1:D:242:PHE:CA	2.12	0.78
1:B:182:GLU:HB3	1:B:192:VAL:HG21	1.66	0.78
1:D:22:ASP:HB2	1:D:63:THR:OG1	1.84	0.78
1:B:197:LEU:CD1	1:B:210:ALA:HB3	2.13	0.77
1:A:238:VAL:HG11	1:D:279(C):ILE:HG12	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLY:C	1:B:164:TYR:CD2	2.59	0.76
1:C:278:ILE:HD11	1:C:283:MET:SD	2.25	0.76
1:D:152:THR:HB	1:D:310:PHE:CZ	2.21	0.76
3:C:331:GOL:H31	1:D:242:PHE:H	1.51	0.75
1:D:198:HIS:CB	1:D:261:ARG:HH12	1.98	0.75
1:C:39:TRP:CE3	1:C:104:VAL:HG21	2.21	0.75
1:D:155:LEU:CD1	1:D:306:MET:CB	2.63	0.75
1:D:258:LEU:O	1:D:268:THR:HA	1.86	0.75
1:A:243:LEU:HD11	1:B:244:LEU:CD1	2.17	0.74
1:A:261:ARG:HH11	1:A:261:ARG:HB2	1.52	0.74
1:D:198:HIS:HB2	1:D:261:ARG:NH1	2.02	0.74
1:C:180:THR:HG21	1:C:267:TYR:OH	1.86	0.74
1:A:243:LEU:CD1	1:B:244:LEU:CD1	2.66	0.73
1:C:158:ASP:HB2	1:C:161:HIS:HD2	1.53	0.73
1:A:205:LEU:HD12	1:A:230:LYS:HB3	1.70	0.73
1:D:45:CYS:HB2	1:D:104:VAL:O	1.88	0.73
1:D:245:TYR:HB2	1:D:284:VAL:HG13	1.70	0.73
1:B:51:LYS:NZ	1:B:51:LYS:HB3	2.03	0.73
1:C:183:LYS:HD2	1:C:183:LYS:N	2.03	0.73
1:B:205:LEU:HD11	1:B:230:LYS:HB3	1.69	0.73
1:B:271:PRO:HA	1:B:274:TYR:CE2	2.23	0.73
1:C:327:LYS:O	1:C:328:LYS:HB2	1.87	0.73
1:C:191:GLN:NE2	3:C:333:GOL:O3	2.22	0.73
1:C:73:MET:HB3	1:C:80:VAL:CG2	2.19	0.73
1:A:51:LYS:NZ	1:A:51:LYS:HB3	2.04	0.72
1:A:199:PHE:HB3	1:A:231:PHE:CE2	2.25	0.72
1:D:6:LEU:HB2	1:D:163:GLY:O	1.88	0.72
1:A:221:ILE:HD11	1:A:304:PRO:HB2	1.72	0.72
1:A:182:GLU:HB3	1:A:192:VAL:HG21	1.70	0.71
1:C:170:ILE:HD12	1:C:170:ILE:H	1.54	0.71
1:C:228:LEU:O	1:C:231:PHE:N	2.23	0.71
1:C:81:SER:HB2	1:C:106:ASP:HB3	1.71	0.71
1:A:62:LYS:O	1:A:62:LYS:HD3	1.90	0.71
1:B:41:PRO:HB2	1:B:55:LEU:HD23	1.73	0.71
1:A:328:LYS:HA	1:A:328:LYS:HZ2	1.56	0.71
1:D:327:LYS:O	1:D:328:LYS:HB2	1.89	0.71
1:B:237:VAL:HG22	1:B:247:THR:HB	1.73	0.70
1:D:19:GLN:HE21	1:D:26:LYS:CD	2.04	0.70
1:D:41:PRO:HB2	1:D:55:LEU:HD22	1.74	0.70
1:A:243:LEU:HD13	1:B:244:LEU:HD13	1.73	0.69
1:A:98:PRO:HD2	1:A:143:GLN:HE22	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:LEU:HD22	3:C:333:GOL:O1	1.92	0.69
1:B:77:SER:OG	2:B:330:006:O50	2.11	0.69
2:C:330:006:H35	1:D:242:PHE:CD1	2.27	0.69
1:D:6:LEU:HB2	1:D:163:GLY:C	2.13	0.69
1:B:279(C):ILE:HG12	1:C:238:VAL:HG11	1.73	0.69
1:C:279:ASP:OD1	1:C:280:SER:HB2	1.93	0.69
1:D:262:SER:HA	3:D:331:GOL:C3	2.20	0.69
1:D:5:THR:HG23	1:D:164:TYR:CE1	2.26	0.68
1:D:199:PHE:HD1	1:D:231:PHE:CZ	2.11	0.68
1:C:184:LEU:HG	1:C:318:HIS:O	1.92	0.68
1:B:99:TYR:CZ	1:B:136:VAL:HG12	2.29	0.68
1:A:67:ASP:HB3	1:A:84:PHE:O	1.94	0.68
1:A:199:PHE:HB3	1:A:231:PHE:HE2	1.59	0.67
1:B:261:ARG:HB2	1:B:261:ARG:NH1	2.09	0.67
1:D:199:PHE:CD1	1:D:231:PHE:CZ	2.83	0.67
1:B:264:THR:OG1	1:B:265:ASN:HB2	1.93	0.67
1:B:192:VAL:HG13	1:B:193:ASP:N	2.08	0.67
1:C:308:LYS:HD3	1:C:309:TYR:CE2	2.30	0.67
1:C:17:GLU:HA	1:C:27:PHE:O	1.95	0.67
1:B:163:GLY:C	1:B:164:TYR:HD2	1.97	0.66
1:B:279(C):ILE:CG1	1:C:238:VAL:HG11	2.24	0.66
1:A:77:SER:OG	2:A:330:006:O50	2.12	0.66
1:A:261:ARG:HB2	1:A:261:ARG:NH1	2.09	0.66
1:B:278:ILE:HG22	1:B:281:LEU:O	1.96	0.66
1:C:73:MET:HB3	1:C:80:VAL:HG23	1.77	0.66
1:D:47:THR:O	1:D:50:CYS:HB2	1.95	0.66
1:A:87:ASP:OD1	1:A:88:ILE:N	2.25	0.65
1:B:192:VAL:HG13	1:B:193:ASP:H	1.61	0.65
1:D:45:CYS:HA	1:D:105:THR:HA	1.78	0.65
1:A:289:VAL:O	1:A:289:VAL:CG1	2.45	0.65
1:A:246:ILE:HG23	1:D:279(C):ILE:HG13	1.78	0.65
1:A:125:TRP:CE3	1:A:187:ASP:HB3	2.31	0.65
1:B:260:PHE:HB2	1:B:267:TYR:HB2	1.79	0.65
1:D:261:ARG:HA	1:D:266:VAL:HA	1.77	0.65
1:A:8:ASP:HB2	1:A:14:TYR:CE1	2.31	0.65
1:B:287:ILE:HD11	2:B:330:006:H37	1.78	0.65
1:A:289:VAL:O	1:A:289:VAL:HG12	1.97	0.65
1:A:205:LEU:CD1	1:A:230:LYS:HB3	2.26	0.65
1:D:73:MET:HB3	1:D:80:VAL:CG2	2.26	0.65
1:D:227:PHE:CD1	1:D:227:PHE:C	2.71	0.64
1:A:197:LEU:HD11	1:A:210:ALA:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ILE:CD1	1:A:243:LEU:HD12	2.24	0.64
1:D:262:SER:HA	3:D:331:GOL:C1	2.28	0.64
1:D:17:GLU:HA	1:D:27:PHE:O	1.98	0.64
1:C:19:GLN:HE21	1:C:26:LYS:CD	2.11	0.63
1:C:41:PRO:HB2	1:C:55:LEU:HD22	1.80	0.63
1:C:271:PRO:HA	1:C:274:TYR:CE2	2.33	0.63
1:C:75:TYR:HA	2:C:330:006:H49A	1.80	0.63
1:B:279(C):ILE:CG1	1:C:238:VAL:CG1	2.77	0.63
1:D:5:THR:CG2	1:D:164:TYR:HE1	2.11	0.63
1:D:14:TYR:CE1	1:D:156:PRO:HD2	2.34	0.63
1:D:6:LEU:CB	1:D:163:GLY:O	2.46	0.62
1:A:110:PRO:HA	1:A:113:THR:OG1	1.99	0.62
1:C:141:LYS:HG3	1:C:149:ALA:HB2	1.81	0.62
1:D:194:LEU:HD23	3:D:331:GOL:O1	2.00	0.62
1:A:224:PRO:HD3	1:A:299:PHE:CE2	2.35	0.62
1:D:170:ILE:HD12	1:D:170:ILE:H	1.64	0.62
1:A:4:VAL:HG23	1:A:165:LEU:HB3	1.81	0.62
1:B:125:TRP:CE3	1:B:187:ASP:HB3	2.34	0.62
1:C:222:THR:HB	1:C:289:VAL:CG1	2.30	0.62
1:A:42:SER:C	1:A:44:GLN:H	2.03	0.62
1:A:171:GLU:OE1	1:A:173:ARG:NH1	2.32	0.62
1:B:225:THR:CG2	1:B:290:ASP:OD2	2.48	0.62
1:C:90:THR:HA	1:C:94:LEU:O	2.00	0.62
1:D:186:HIS:HB2	1:D:191:GLN:OE1	2.00	0.61
1:B:150:VAL:HG23	1:B:313:PHE:O	2.00	0.61
1:D:327:LYS:HD3	1:D:327:LYS:N	2.07	0.61
1:C:199:PHE:HD1	1:C:231:PHE:CZ	2.17	0.61
1:B:18:ALA:HB3	1:B:29:PHE:CE1	2.36	0.61
1:C:19:GLN:HE21	1:C:26:LYS:HD3	1.64	0.61
1:D:19:GLN:HE21	1:D:26:LYS:HD3	1.64	0.61
1:B:42:SER:C	1:B:44:GLN:H	2.04	0.61
1:D:8:ASP:HB3	1:D:159:ASP:O	2.01	0.61
1:C:111:ALA:CA	3:C:331:GOL:O1	2.49	0.61
1:C:198:HIS:CD2	1:C:206:THR:HG22	2.36	0.61
1:A:264:THR:OG1	1:A:265:ASN:HB2	2.02	0.60
1:B:14:TYR:HE1	1:B:156:PRO:HD2	1.66	0.60
1:B:183:LYS:CD	1:B:183:LYS:H	2.14	0.60
1:B:328:LYS:NZ	1:B:328:LYS:HA	2.16	0.60
1:C:199:PHE:CD1	1:C:231:PHE:CZ	2.89	0.60
1:D:198:HIS:CG	1:D:206:THR:HG22	2.37	0.60
1:A:244:LEU:HD21	1:A:283:MET:HE1	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:PHE:CD2	1:D:121:VAL:CG2	2.83	0.60
1:D:222:THR:HB	1:D:289:VAL:HG12	1.83	0.60
1:C:152:THR:HB	1:C:310:PHE:CZ	2.36	0.60
1:D:222:THR:HB	1:D:289:VAL:CG1	2.31	0.60
1:D:13:MET:HG3	1:D:30:ILE:HD13	1.83	0.60
1:A:278(A):PHE:HB3	1:A:281:LEU:HB2	1.81	0.60
1:C:148:GLN:HB2	1:C:150:VAL:HG12	1.83	0.60
1:A:279(C):ILE:HG21	1:D:281:LEU:HD22	1.84	0.59
1:D:262:SER:CA	3:D:331:GOL:H11	2.30	0.59
1:C:261:ARG:HA	1:C:266:VAL:HA	1.84	0.59
1:A:243:LEU:HD11	1:B:244:LEU:HD11	1.84	0.59
1:A:225:THR:CG2	1:A:290:ASP:OD2	2.45	0.59
1:B:160:LYS:HE2	1:B:162:LYS:HZ3	1.67	0.59
1:C:47:THR:O	1:C:50:CYS:HB2	2.01	0.59
1:D:262:SER:N	1:D:265:ASN:O	2.29	0.59
1:A:260:PHE:HB2	1:A:267:TYR:HB2	1.84	0.59
1:C:122:GLY:O	1:C:123:LEU:HD23	2.01	0.59
1:A:76:VAL:HG21	2:A:330:006:H26	1.85	0.59
1:B:75:TYR:HA	2:B:330:006:H49	1.85	0.59
1:B:98:PRO:HD2	1:B:143:GLN:HE22	1.69	0.58
1:C:222:THR:HB	1:C:289:VAL:HG12	1.85	0.58
1:A:271:PRO:HA	1:A:274:TYR:CE2	2.39	0.58
1:B:279(C):ILE:HG13	1:C:238:VAL:CG1	2.33	0.58
1:D:31:PHE:CD2	1:D:121:VAL:HG22	2.38	0.58
1:A:240:ILE:HD11	1:A:243:LEU:CD1	2.28	0.58
1:A:244:LEU:HD21	1:A:283:MET:CE	2.33	0.58
1:D:19:GLN:HE21	1:D:26:LYS:HD2	1.68	0.58
1:B:182:GLU:HB3	1:B:192:VAL:CG2	2.34	0.58
1:D:198:HIS:CD2	1:D:206:THR:CG2	2.85	0.58
1:B:87:ASP:OD1	1:B:88:ILE:N	2.34	0.57
1:D:308:LYS:HD3	1:D:309:TYR:CE2	2.39	0.57
1:D:73:MET:HB3	1:D:80:VAL:HG23	1.86	0.57
1:B:125:TRP:CD2	1:B:187:ASP:HB3	2.40	0.57
1:C:187:ASP:OD2	1:C:318:HIS:CE1	2.58	0.57
1:D:73:MET:O	1:D:79:THR:HG23	2.03	0.57
1:D:166:THR:OG1	1:D:174:PHE:CE2	2.57	0.57
1:D:23:ASN:ND2	1:D:60:LYS:HB2	2.19	0.57
1:A:278:ILE:HD11	1:C:279(A):PHE:CD1	2.39	0.57
1:B:109(B):GLU:HB3	1:B:113:THR:OG1	2.04	0.57
1:C:261:ARG:HB3	1:C:266:VAL:HG23	1.85	0.57
1:C:251:ASN:HD21	1:C:254:LYS:HG3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LYS:HB2	1:B:149:ALA:HB2	1.87	0.57
1:D:170:ILE:HG13	1:D:312:VAL:HG21	1.86	0.57
1:A:205:LEU:CD1	1:A:230:LYS:HD3	2.35	0.56
1:B:180:THR:HG21	1:B:265:ASN:HB2	1.87	0.56
1:B:197:LEU:HD13	1:B:210:ALA:HB3	1.87	0.56
1:C:6:LEU:N	1:C:163:GLY:O	2.25	0.56
1:A:150:VAL:HG23	1:A:313:PHE:O	2.04	0.56
1:C:6:LEU:HB2	1:C:163:GLY:CA	2.35	0.56
1:D:197:LEU:HD22	1:D:299:PHE:CE2	2.41	0.56
1:C:31:PHE:CD2	1:C:121:VAL:HG22	2.41	0.56
1:A:240:ILE:HD12	1:A:240:ILE:C	2.25	0.56
1:B:8:ASP:HB2	1:B:14:TYR:CE1	2.41	0.56
1:D:17:GLU:HG2	1:D:27:PHE:O	2.05	0.56
1:B:198:HIS:HA	1:B:206:THR:HG22	1.86	0.56
1:D:184:LEU:HG	1:D:318:HIS:O	2.05	0.56
1:A:51:LYS:HB3	1:A:51:LYS:HZ3	1.70	0.56
1:A:279(C):ILE:HG21	1:D:281:LEU:CD2	2.36	0.56
1:A:48:ILE:HD13	1:A:109(B):GLU:OE1	2.06	0.56
1:A:225:THR:HG22	1:A:290:ASP:CG	2.26	0.56
1:B:274:TYR:O	1:B:285:SER:HB2	2.06	0.56
1:A:125:TRP:CD2	1:A:187:ASP:HB3	2.41	0.56
1:C:56:TYR:OH	1:C:87:ASP:OD2	2.19	0.56
1:D:56:TYR:OH	1:D:87:ASP:OD2	2.23	0.56
1:A:42:SER:C	1:A:44:GLN:N	2.59	0.56
1:A:327:LYS:O	1:A:328:LYS:HD2	2.06	0.56
1:B:94:LEU:HD22	1:B:140:LEU:HD22	1.87	0.56
1:C:49:GLY:HA2	1:C:113:THR:HG23	1.88	0.55
1:B:42:SER:C	1:B:44:GLN:N	2.57	0.55
1:A:53:LYS:HG3	1:A:112:TYR:OH	2.06	0.55
1:C:170:ILE:HG13	1:C:312:VAL:HG21	1.88	0.55
1:D:31:PHE:HD2	1:D:121:VAL:CG2	2.19	0.55
1:D:154:TYR:OH	1:D:326:LYS:O	2.20	0.55
1:D:228:LEU:O	1:D:231:PHE:N	2.38	0.55
1:D:161:HIS:ND1	1:D:328:LYS:HE3	2.22	0.55
1:D:260:PHE:HB2	1:D:267:TYR:HB2	1.88	0.55
1:C:13:MET:HG3	1:C:30:ILE:HD13	1.89	0.55
1:C:23:ASN:ND2	1:C:60:LYS:HB2	2.22	0.55
1:C:42:SER:HB2	1:C:103:GLU:HB3	1.88	0.55
3:C:331:GOL:C1	1:D:242:PHE:CA	2.66	0.55
1:D:114:LEU:HD12	1:D:114:LEU:O	2.07	0.55
1:B:198:HIS:CB	1:B:206:THR:HG22	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:VAL:HG21	2:C:330:006:C26	2.36	0.55
1:C:258:LEU:O	1:C:268:THR:HA	2.07	0.55
1:D:41:PRO:HG2	1:D:54:ASN:O	2.07	0.55
1:A:246:ILE:CG2	1:D:279(C):ILE:HG13	2.36	0.55
1:D:261:ARG:O	3:D:331:GOL:C1	2.55	0.54
1:D:174:PHE:HB3	1:D:310:PHE:CE1	2.41	0.54
1:C:45:CYS:HA	1:C:105:THR:HA	1.88	0.54
1:A:39:TRP:HB3	1:A:102:ILE:HB	1.90	0.54
1:A:242:PHE:HE1	1:B:12:VAL:HG13	1.72	0.54
1:D:5:THR:CG2	1:D:164:TYR:CE1	2.89	0.54
1:D:9:VAL:HG21	1:D:116:GLN:NE2	2.22	0.54
1:B:158:ASP:CG	1:B:159:ASP:H	2.10	0.54
1:D:3:SER:HA	1:D:165:LEU:O	2.08	0.54
1:D:158:ASP:C	1:D:158:ASP:OD2	2.45	0.54
1:D:10:ALA:HB3	1:D:12:VAL:HG12	1.90	0.54
1:A:44:GLN:HB3	1:A:105:THR:HG22	1.89	0.54
1:B:4:VAL:HG23	1:B:165:LEU:HB3	1.89	0.54
1:C:236:ASP:OD2	1:C:254:LYS:HE3	2.07	0.54
1:A:292:ASN:CB	3:A:331:GOL:C3	2.66	0.53
1:C:268:THR:O	1:C:308:LYS:NZ	2.38	0.53
1:C:228:LEU:HD21	1:C:286:ILE:HG22	1.89	0.53
1:A:231:PHE:HE1	1:A:235:LEU:HD11	1.71	0.53
1:C:327:LYS:HD3	1:C:327:LYS:N	2.07	0.53
1:D:5:THR:HA	1:D:164:TYR:CE1	2.43	0.53
1:C:17:GLU:HG2	1:C:27:PHE:O	2.08	0.53
1:D:90:THR:HA	1:D:94:LEU:O	2.09	0.53
1:A:109(A):PHE:O	1:A:111:ALA:HB3	2.09	0.53
1:D:148:GLN:HB2	1:D:150:VAL:HG12	1.90	0.53
1:D:260:PHE:O	1:D:267:TYR:N	2.34	0.53
1:C:243:LEU:O	1:C:244:LEU:N	2.41	0.53
1:D:14:TYR:HE1	1:D:156:PRO:HD2	1.73	0.53
1:D:71:VAL:HG11	1:D:102:ILE:HG12	1.90	0.53
1:C:67:ASP:OD1	1:C:67:ASP:C	2.47	0.53
1:C:114:LEU:O	1:C:114:LEU:HD12	2.08	0.53
1:C:198:HIS:HB2	1:C:261:ARG:HH22	1.74	0.53
1:A:180:THR:HG21	1:A:265:ASN:HB2	1.91	0.53
1:C:227:PHE:CD1	1:C:227:PHE:C	2.82	0.53
1:D:194:LEU:HA	3:D:331:GOL:O1	2.08	0.53
1:A:29:PHE:HA	1:A:119:GLY:O	2.09	0.53
1:B:271:PRO:HA	1:B:274:TYR:CD2	2.43	0.53
1:C:36:ALA:HA	1:C:122:GLY:HA3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:LEU:HB3	1:D:151:PHE:CZ	2.44	0.53
1:B:197:LEU:HD11	1:B:210:ALA:HB3	1.91	0.52
1:A:292:ASN:HB2	3:A:331:GOL:C3	2.37	0.52
1:C:14:TYR:CE1	1:C:156:PRO:HD2	2.45	0.52
1:C:240:ILE:HD11	1:C:243:LEU:HD12	1.91	0.52
1:A:128:LEU:HB2	1:A:188:LEU:HD22	1.91	0.52
1:D:194:LEU:HD23	3:D:331:GOL:C1	2.40	0.52
1:D:32:ASP:C	1:D:34:GLY:H	2.13	0.52
1:B:279(C):ILE:HG12	1:C:238:VAL:CG1	2.37	0.52
1:D:31:PHE:CD2	1:D:121:VAL:HG21	2.44	0.52
1:A:150:VAL:O	1:A:168:GLY:N	2.39	0.52
1:B:158:ASP:O	1:B:161:HIS:HB2	2.10	0.52
1:C:53:LYS:NZ	1:C:112:TYR:O	2.43	0.52
1:C:73:MET:HB3	1:C:80:VAL:HG22	1.90	0.52
1:D:183:LYS:H	1:D:183:LYS:HD2	1.74	0.52
1:D:259:GLU:HG3	1:D:268:THR:HG22	1.91	0.52
1:B:41:PRO:HB2	1:B:55:LEU:CD2	2.39	0.52
1:A:76:VAL:HG21	2:A:330:006:C26	2.40	0.52
1:C:198:HIS:HB2	1:C:261:ARG:CZ	2.40	0.52
1:A:205:LEU:HD11	1:A:230:LYS:HD3	1.92	0.51
1:C:199:PHE:O	1:C:231:PHE:HE2	1.93	0.51
1:D:180:THR:CG2	1:D:267:TYR:HH	2.22	0.51
1:C:111:ALA:HA	3:C:331:GOL:C1	2.40	0.51
1:C:232:PHE:O	1:C:235:LEU:HB2	2.10	0.51
1:C:235:LEU:HD13	1:C:255:LEU:HD23	1.92	0.51
1:A:74:ASN:ND2	1:A:79:THR:HG23	2.25	0.51
1:A:222:THR:OG1	1:A:300:ILE:HB	2.10	0.51
1:B:91:ILE:O	1:B:92:ALA:HB3	2.11	0.51
1:A:317:ASN:O	1:A:318:HIS:HB2	2.10	0.51
1:B:163:GLY:O	1:B:164:TYR:CD2	2.63	0.51
1:B:278:ILE:HG22	1:B:281:LEU:C	2.30	0.51
1:C:198:HIS:HB2	1:C:261:ARG:NH2	2.25	0.51
1:D:240:ILE:HD11	1:D:243:LEU:HD12	1.92	0.51
1:B:311:THR:HB	1:B:313:PHE:CE1	2.46	0.51
1:C:292:ASN:OD1	3:C:333:GOL:H12	2.11	0.51
1:A:83:PHE:N	1:A:83:PHE:CD2	2.77	0.51
1:D:100:LYS:HD2	1:D:133:VAL:HG22	1.92	0.50
1:D:175:TYR:O	1:D:326:LYS:HE3	2.10	0.50
1:D:193:ASP:OD1	1:D:209:LYS:HG2	2.11	0.50
1:D:271:PRO:HA	1:D:274:TYR:CE2	2.46	0.50
1:B:171:GLU:OE1	1:B:173:ARG:NH1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ILE:CG2	1:C:167:ILE:HD11	2.41	0.50
1:D:218:THR:HG22	1:D:220:SER:H	1.75	0.50
1:C:25:GLN:OE1	1:C:56:TYR:HA	2.10	0.50
1:D:183:LYS:HD2	1:D:183:LYS:N	2.27	0.50
1:A:179:LEU:CD1	1:A:323:ALA:HB2	2.42	0.50
1:A:238:VAL:HG13	1:A:246:ILE:HG22	1.94	0.50
1:D:141:LYS:HG3	1:D:149:ALA:HB2	1.93	0.50
1:A:279(C):ILE:HG12	1:D:238:VAL:CG1	2.42	0.50
1:B:88:ILE:HD11	1:B:95:SER:HB3	1.93	0.50
1:B:199:PHE:O	1:B:203:ASN:N	2.45	0.50
1:C:14:TYR:HE1	1:C:156:PRO:HD2	1.76	0.50
1:C:183:LYS:N	1:C:183:LYS:CD	2.71	0.50
1:D:224:PRO:HB2	1:D:227:PHE:HB3	1.94	0.50
1:A:48:ILE:HD11	1:A:113:THR:HG21	1.94	0.50
1:A:182:GLU:HB3	1:A:192:VAL:CG2	2.39	0.50
1:C:73:MET:CB	1:C:80:VAL:HG23	2.39	0.50
3:C:331:GOL:O2	1:D:239:LYS:CE	2.48	0.50
1:A:231:PHE:C	1:A:231:PHE:CD1	2.85	0.50
1:A:240:ILE:HD12	1:A:241:PRO:N	2.27	0.50
1:B:205:LEU:HD23	1:B:205:LEU:H	1.74	0.50
3:C:331:GOL:H11	1:D:242:PHE:CB	2.41	0.50
1:D:42:SER:O	1:D:55:LEU:HD13	2.11	0.50
1:D:49:GLY:HA2	1:D:113:THR:HG23	1.93	0.50
1:C:12:VAL:HG11	1:D:241:PRO:HG3	1.94	0.49
1:C:224:PRO:HA	1:C:290:ASP:OD1	2.10	0.49
1:D:73:MET:CB	1:D:80:VAL:HG23	2.42	0.49
1:B:126:LYS:O	1:B:129:SER:HB3	2.11	0.49
1:C:34:GLY:HA3	2:C:330:006:O20	2.12	0.49
1:C:10:ALA:HB3	1:C:12:VAL:HG12	1.94	0.49
1:D:125:TRP:HB2	1:D:188:LEU:O	2.12	0.49
1:A:197:LEU:HD13	1:A:210:ALA:HB3	1.92	0.49
1:A:228:LEU:O	1:A:231:PHE:N	2.45	0.49
1:D:31:PHE:HD2	1:D:121:VAL:HG21	1.77	0.49
1:B:71:VAL:O	1:B:81:SER:HA	2.11	0.49
1:C:251:ASN:HD21	1:C:254:LYS:CG	2.26	0.49
1:C:278(A):PHE:HB3	1:C:281:LEU:HD12	1.94	0.49
1:D:96:PHE:CD1	1:D:140:LEU:HD21	2.48	0.49
1:A:157:PHE:CE2	1:A:307:ARG:HD2	2.48	0.49
1:A:279(C):ILE:HG22	1:A:280:SER:N	2.28	0.49
1:B:71:VAL:HG11	1:B:84:PHE:CE2	2.48	0.49
1:C:31:PHE:O	1:C:216:SER:OG	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ILE:CG1	1:C:312:VAL:HG21	2.42	0.49
1:D:73:MET:HB3	1:D:80:VAL:HG22	1.94	0.49
1:A:246:ILE:HD12	1:A:283:MET:SD	2.53	0.49
1:C:45:CYS:HB2	1:C:104:VAL:O	2.12	0.49
1:D:33:THR:OG1	1:D:215:ASP:HA	2.13	0.49
1:B:189:TYR:H	1:B:191:GLN:HE21	1.59	0.49
1:D:12:VAL:O	1:D:219:SER:HB2	2.12	0.49
1:A:231:PHE:CE1	1:A:235:LEU:HD11	2.47	0.49
1:B:327:LYS:O	1:B:328:LYS:HD2	2.13	0.49
1:A:8:ASP:HB2	1:A:14:TYR:CD1	2.47	0.49
1:A:157:PHE:CD2	1:A:307:ARG:HD2	2.47	0.49
1:C:73:MET:O	1:C:79:THR:HG23	2.12	0.49
1:C:82:GLY:HA3	1:C:103:GLU:O	2.13	0.49
1:D:166:THR:HG21	1:D:171:GLU:HG3	1.94	0.48
1:D:265:ASN:CG	1:D:266:VAL:H	2.16	0.48
1:B:279(C):ILE:HG13	1:C:238:VAL:HG11	1.94	0.48
1:C:6:LEU:HB2	1:C:163:GLY:HA3	1.93	0.48
1:C:9:VAL:HG21	1:C:116:GLN:NE2	2.28	0.48
1:D:151:PHE:HB2	1:D:166:THR:O	2.13	0.48
1:D:279:ASP:OD1	1:D:280:SER:HB2	2.12	0.48
1:D:279(C):ILE:HG22	1:D:280:SER:N	2.28	0.48
1:A:183:LYS:CD	1:A:183:LYS:H	2.26	0.48
1:D:262:SER:HA	3:D:331:GOL:C2	2.44	0.48
1:A:94:LEU:HD22	1:A:140:LEU:HD22	1.94	0.48
1:B:281:LEU:HD23	1:C:278(A):PHE:CE1	2.49	0.48
1:C:278:ILE:HG13	1:C:283:MET:HB2	1.95	0.48
1:D:3:SER:OG	1:D:166:THR:HG23	2.14	0.48
1:D:327:LYS:CD	1:D:327:LYS:N	2.67	0.48
1:A:243:LEU:CD1	1:B:244:LEU:HD11	2.42	0.48
1:B:51:LYS:HB3	1:B:51:LYS:HZ3	1.75	0.48
1:B:194:LEU:HD13	1:B:260:PHE:HB3	1.96	0.48
1:B:205:LEU:CD1	1:B:230:LYS:HD3	2.43	0.48
1:B:3:SER:OG	1:B:166:THR:HG23	2.13	0.48
1:D:23:ASN:OD1	1:D:61:SER:HB2	2.13	0.48
1:B:225:THR:HG22	1:B:290:ASP:CG	2.34	0.48
1:B:328:LYS:HA	1:B:328:LYS:HZ3	1.77	0.48
1:B:71:VAL:HG11	1:B:84:PHE:HE2	1.77	0.48
1:A:287:ILE:HD11	2:A:330:006:H37	1.95	0.47
1:C:2:ASP:OD2	1:C:92:ALA:HB3	2.14	0.47
1:C:32:ASP:C	1:C:34:GLY:H	2.17	0.47
1:C:111:ALA:HA	3:C:331:GOL:H2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:GLN:H	1:D:116:GLN:HG3	1.62	0.47
1:A:81:SER:HB3	1:A:106:ASP:HB3	1.95	0.47
1:B:189:TYR:CE2	3:B:331:GOL:H31	2.49	0.47
1:A:161:HIS:CE1	1:A:328:LYS:HE2	2.49	0.47
1:B:194:LEU:O	1:B:210:ALA:N	2.36	0.47
1:B:239:LYS:HD2	1:B:245:TYR:CE2	2.50	0.47
1:C:94:LEU:HD13	1:C:140:LEU:CD1	2.44	0.47
1:B:317:ASN:O	1:B:318:HIS:HB2	2.14	0.47
1:D:218:THR:HG22	1:D:220:SER:O	2.14	0.47
1:D:218:THR:HG22	1:D:302:GLY:HA3	1.96	0.47
1:A:269:LEU:HD12	1:A:269:LEU:HA	1.78	0.47
1:B:82:GLY:HA3	1:B:103:GLU:O	2.14	0.47
1:B:180:THR:HG21	1:B:265:ASN:CB	2.45	0.47
1:C:6:LEU:HB2	1:C:163:GLY:C	2.34	0.47
1:C:94:LEU:HD23	1:C:94:LEU:HA	1.63	0.47
1:C:212:ALA:HB1	1:C:301:LEU:HD22	1.96	0.47
1:C:317:ASN:O	1:C:319:THR:HG23	2.13	0.47
1:D:310:PHE:CE2	1:D:312:VAL:HG23	2.50	0.47
1:A:291:LEU:HD11	2:A:330:006:H24	1.95	0.47
1:B:185:ASN:O	1:B:186:HIS:CD2	2.68	0.47
1:C:20:ILE:HD12	1:C:21:GLY:N	2.30	0.47
1:C:151:PHE:HB2	1:C:166:THR:O	2.15	0.47
1:C:211:THR:O	1:C:298:THR:HA	2.15	0.47
1:A:109(B):GLU:HB3	1:A:113:THR:OG1	2.14	0.47
1:D:195:ASP:H	3:D:331:GOL:C2	2.28	0.47
1:A:292:ASN:HB2	3:A:331:GOL:H12	1.96	0.47
1:B:289:VAL:O	1:B:289:VAL:CG1	2.63	0.47
1:A:185:ASN:O	1:A:186:HIS:CD2	2.68	0.46
1:A:292:ASN:HB3	3:A:331:GOL:C3	2.11	0.46
1:B:14:TYR:CE1	1:B:156:PRO:HD2	2.48	0.46
1:B:73:MET:HB2	1:B:73:MET:HE2	1.88	0.46
1:D:203:ASN:N	1:D:203:ASN:ND2	2.61	0.46
1:D:309:TYR:HA	1:D:323:ALA:O	2.15	0.46
1:A:241:PRO:O	1:A:242:PHE:HB2	2.16	0.46
1:C:218:THR:HG22	1:C:302:GLY:HA3	1.97	0.46
1:D:20:ILE:HD12	1:D:21:GLY:H	1.79	0.46
1:D:170:ILE:CG1	1:D:312:VAL:HG21	2.45	0.46
1:B:179:LEU:HB3	1:B:181:TYR:CE1	2.51	0.46
1:C:161:HIS:ND1	1:C:328:LYS:HE3	2.31	0.46
1:C:185:ASN:O	1:C:186:HIS:ND1	2.48	0.46
1:A:237:VAL:HG22	1:A:247:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:VAL:HG21	1:B:165:LEU:HD23	1.98	0.46
1:B:29:PHE:HA	1:B:119:GLY:O	2.16	0.46
1:C:1:GLY:O	1:C:2:ASP:CB	2.63	0.46
1:C:11:ASN:OD1	1:C:157:PHE:O	2.34	0.46
1:D:197:LEU:O	1:D:206:THR:HA	2.15	0.46
1:D:265:ASN:OD1	1:D:266:VAL:N	2.45	0.46
1:A:60:LYS:HZ2	1:A:60:LYS:HB3	1.80	0.46
1:B:231:PHE:CD1	1:B:231:PHE:C	2.89	0.46
1:C:20:ILE:HD12	1:C:21:GLY:H	1.80	0.46
1:C:264:THR:OG1	1:C:265:ASN:N	2.48	0.46
1:D:87:ASP:OD1	1:D:88:ILE:N	2.44	0.46
1:C:87:ASP:OD1	1:C:88:ILE:N	2.44	0.46
1:C:242:PHE:HZ	1:D:13:MET:HB3	1.81	0.46
1:B:199:PHE:N	1:B:199:PHE:CD2	2.83	0.46
1:C:158:ASP:HB2	1:C:161:HIS:CD2	2.41	0.46
1:C:225:THR:O	1:C:229:ASN:HB3	2.15	0.46
1:D:30:ILE:HG13	1:D:117:PHE:CD1	2.50	0.46
1:D:58:SER:HB2	1:D:64:TYR:CD2	2.51	0.46
1:B:327:LYS:HB2	1:B:327:LYS:HE3	1.75	0.46
1:C:64:TYR:CZ	1:C:66:LYS:HA	2.51	0.46
1:C:198:HIS:HB3	1:C:261:ARG:HH12	1.77	0.46
1:A:238:VAL:CG1	1:D:279(C):ILE:CG1	2.86	0.46
1:B:155:LEU:HA	1:B:156:PRO:HD3	1.79	0.46
1:C:7:ASN:HB2	1:C:15:TYR:O	2.15	0.46
1:D:25:GLN:HB2	1:D:27:PHE:HE1	1.81	0.46
1:D:100:LYS:HG2	1:D:101:PHE:N	2.31	0.46
1:D:218:THR:CG2	1:D:220:SER:O	2.63	0.46
1:C:309:TYR:HA	1:C:323:ALA:O	2.16	0.45
1:D:109(B):GLU:HG2	1:D:112:TYR:HB3	1.99	0.45
1:A:161:HIS:CE1	1:A:328:LYS:CE	3.00	0.45
1:B:124:GLY:HA2	1:B:190:TRP:HE1	1.81	0.45
1:B:166:THR:HG1	1:B:174:PHE:HE2	1.63	0.45
1:B:188:LEU:HD23	1:B:188:LEU:HA	1.80	0.45
1:C:260:PHE:HB2	1:C:267:TYR:HB2	1.97	0.45
1:C:270:GLU:HB2	1:C:273:TYR:HD2	1.81	0.45
1:C:328:LYS:HD2	1:C:328:LYS:HA	1.67	0.45
1:D:20:ILE:CD1	1:D:87:ASP:HB3	2.24	0.45
1:D:239:LYS:NZ	1:D:243:LEU:O	2.40	0.45
1:C:240:ILE:HD12	1:C:241:PRO:HD2	1.99	0.45
1:A:199:PHE:O	1:A:203:ASN:N	2.50	0.45
1:B:44:GLN:HB3	1:B:105:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:VAL:HG13	1:A:193:ASP:N	2.32	0.45
1:D:311:THR:HB	1:D:313:PHE:CE1	2.52	0.45
1:B:269:LEU:HD12	1:B:269:LEU:HA	1.78	0.45
1:D:258:LEU:O	1:D:268:THR:CA	2.61	0.45
1:A:88:ILE:HD11	1:A:95:SER:HB3	1.98	0.45
1:B:198:HIS:HB2	1:B:206:THR:HG22	1.98	0.45
1:C:19:GLN:HE21	1:C:26:LYS:HD2	1.81	0.45
1:C:31:PHE:CD2	1:C:121:VAL:CG2	3.00	0.45
1:C:249:CYS:SG	1:C:280:SER:OG	2.74	0.45
1:B:251:ASN:HD21	1:B:254:LYS:HB2	1.82	0.45
1:A:260:PHE:O	1:A:267:TYR:N	2.43	0.45
1:B:66:LYS:HB2	1:B:66:LYS:HE3	1.50	0.45
1:C:291:LEU:HD22	3:C:333:GOL:C1	2.46	0.45
1:C:291:LEU:HB3	1:C:292:ASN:H	1.56	0.45
2:D:330:006:H50A	2:D:330:006:H28	1.64	0.45
1:A:228:LEU:HD21	1:A:286:ILE:HG22	1.99	0.44
1:A:243(A):PRO:HG2	1:B:243:LEU:HD21	1.98	0.44
1:C:220:SER:OG	1:C:287:ILE:HG12	2.17	0.44
1:C:259:GLU:HG3	1:C:268:THR:HG22	1.98	0.44
1:D:45:CYS:CA	1:D:105:THR:HA	2.46	0.44
1:D:269:LEU:HD12	1:D:269:LEU:HA	1.49	0.44
1:A:47:THR:HG21	1:A:107:THR:H	1.82	0.44
1:A:327:LYS:HE3	1:A:327:LYS:HB2	1.64	0.44
1:A:199:PHE:N	1:A:199:PHE:CD2	2.85	0.44
1:C:203:ASN:N	1:C:203:ASN:ND2	2.61	0.44
1:A:188:LEU:HD13	1:A:189:TYR:CD2	2.53	0.44
1:B:223:ALA:HA	1:B:299:PHE:CD2	2.53	0.44
1:C:33:THR:OG1	1:C:215:ASP:HA	2.18	0.44
1:C:100:LYS:HD2	1:C:133:VAL:HG22	1.99	0.44
1:C:166:THR:HG21	1:C:171:GLU:HG3	2.00	0.44
1:A:251:ASN:HD21	1:A:254:LYS:HB2	1.82	0.44
1:D:19:GLN:HG3	1:D:26:LYS:HD3	2.00	0.44
1:A:261:ARG:NH1	1:A:266:VAL:HG23	2.32	0.44
1:A:273:TYR:CE2	1:A:308:LYS:HG3	2.52	0.44
1:C:64:TYR:OH	1:C:66:LYS:HD2	2.17	0.44
1:D:67:ASP:C	1:D:67:ASP:OD1	2.56	0.44
1:D:76:VAL:HG23	3:D:332:GOL:H11	2.00	0.44
1:A:82:GLY:HA3	1:A:103:GLU:O	2.18	0.44
1:A:228:LEU:O	1:A:229:ASN:C	2.56	0.44
1:D:86:LYS:HG2	1:D:99:TYR:O	2.18	0.44
1:D:194:LEU:CD2	3:D:331:GOL:O1	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:ILE:HG21	1:D:278:ILE:HD13	1.57	0.44
1:B:313:PHE:CD1	1:B:313:PHE:N	2.85	0.44
1:C:3:SER:HA	1:C:165:LEU:O	2.18	0.44
1:C:66:LYS:HG3	1:C:67:ASP:N	2.32	0.44
1:D:12:VAL:O	1:D:219:SER:CB	2.66	0.44
1:C:20:ILE:HD13	1:C:89:VAL:HG22	2.00	0.43
1:C:11:ASN:ND2	1:C:307:ARG:HD3	2.33	0.43
1:B:41:PRO:HD3	1:B:118:ASP:O	2.18	0.43
1:B:199:PHE:N	1:B:199:PHE:HD2	2.16	0.43
1:D:240:ILE:HD12	1:D:241:PRO:HD2	1.99	0.43
1:A:271:PRO:HA	1:A:274:TYR:CD2	2.53	0.43
1:B:11:ASN:HD22	1:B:11:ASN:HA	1.63	0.43
1:C:114:LEU:CG	3:C:331:GOL:H32	2.47	0.43
1:D:20:ILE:HD12	1:D:21:GLY:N	2.33	0.43
1:D:258:LEU:N	1:D:258:LEU:HD23	2.33	0.43
1:A:22:ASP:HB3	1:A:63:THR:OG1	2.19	0.43
1:A:197:LEU:CD1	1:A:210:ALA:CB	2.87	0.43
1:B:67:ASP:HB3	1:B:84:PHE:O	2.19	0.43
1:B:328:LYS:HG2	1:D:328:LYS:HB3	2.01	0.43
1:C:94:LEU:HD13	1:C:140:LEU:HD13	2.00	0.43
1:C:170:ILE:HG13	1:C:312:VAL:CG2	2.48	0.43
1:D:159:ASP:OD1	1:D:160:LYS:N	2.51	0.43
1:D:166:THR:OG1	1:D:174:PHE:HE2	1.99	0.43
1:A:228:LEU:HD12	1:A:228:LEU:HA	1.73	0.43
1:C:199:PHE:CE1	1:C:258:LEU:HD22	2.53	0.43
1:D:262:SER:C	3:D:331:GOL:H31	2.38	0.43
1:A:94:LEU:CD2	1:A:145:LYS:HB3	2.49	0.43
1:D:84:PHE:CD1	1:D:100:LYS:HD3	2.53	0.43
1:D:199:PHE:CE1	1:D:258:LEU:HD22	2.53	0.43
1:D:250:ASN:O	1:D:251:ASN:C	2.57	0.43
1:A:24:LYS:HB3	1:A:24:LYS:HE2	1.61	0.43
1:B:240:ILE:HD12	1:B:241:PRO:N	2.34	0.43
1:C:243:LEU:HD11	1:D:244:LEU:HD11	2.01	0.43
1:D:43:ALA:HA	1:D:55:LEU:CD1	2.48	0.43
1:D:148:GLN:HE21	1:D:148:GLN:HB3	1.62	0.43
1:B:8:ASP:OD1	1:B:11:ASN:HA	2.18	0.43
1:D:94:LEU:HD13	1:D:140:LEU:CD1	2.49	0.43
1:A:157:PHE:HD2	1:A:157:PHE:HA	1.71	0.42
1:C:23:ASN:ND2	1:C:60:LYS:CB	2.81	0.42
1:C:123:LEU:HB3	1:C:151:PHE:CZ	2.53	0.42
1:D:194:LEU:HD12	1:D:212:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:THR:O	1:D:298:THR:HA	2.18	0.42
1:A:42:SER:OG	1:A:44:GLN:HB2	2.19	0.42
1:B:67:ASP:OD1	1:B:69:THR:OG1	2.36	0.42
1:C:148:GLN:HE21	1:C:148:GLN:HB3	1.59	0.42
1:D:317:ASN:O	1:D:319:THR:HG23	2.19	0.42
1:A:180:THR:HG21	1:A:265:ASN:CB	2.49	0.42
1:B:235:LEU:O	1:B:236:ASP:C	2.57	0.42
1:B:278(A):PHE:CZ	1:B:279(A):PHE:HB3	2.53	0.42
1:C:260:PHE:O	1:C:267:TYR:N	2.48	0.42
1:C:74:ASN:ND2	1:C:79:THR:CG2	2.82	0.42
1:A:74:ASN:ND2	1:A:79:THR:OG1	2.51	0.42
1:B:228:LEU:HD12	1:B:228:LEU:HA	1.84	0.42
3:C:331:GOL:H11	1:D:242:PHE:N	2.35	0.42
1:D:238:VAL:CG2	1:D:239:LYS:N	2.81	0.42
1:B:81:SER:HB3	1:B:106:ASP:HB3	2.00	0.42
1:B:172:ASP:HA	1:B:175:TYR:CE1	2.55	0.42
1:C:269:LEU:HA	1:C:269:LEU:HD12	1.59	0.42
1:D:6:LEU:CA	1:D:163:GLY:O	2.68	0.42
1:D:215:ASP:C	1:D:215:ASP:OD1	2.54	0.42
1:D:303:ASP:N	1:D:304:PRO:CD	2.83	0.42
1:A:36:ALA:O	1:A:129:SER:HB2	2.20	0.42
1:A:192:VAL:HG22	1:A:193:ASP:H	1.85	0.42
1:B:278:ILE:HD13	1:B:278:ILE:HG21	1.72	0.42
1:D:9:VAL:HG21	1:D:116:GLN:HE22	1.84	0.42
1:D:261:ARG:HB3	1:D:266:VAL:HG23	2.01	0.42
1:C:11:ASN:ND2	1:C:14:TYR:OH	2.53	0.42
3:C:331:GOL:H11	1:D:242:PHE:CD2	2.55	0.42
1:D:35:SER:O	1:D:122:GLY:CA	2.67	0.42
1:A:198:HIS:HA	1:A:206:THR:HG22	2.01	0.42
1:A:231:PHE:C	1:A:231:PHE:HD1	2.23	0.42
1:A:312:VAL:O	1:A:320:VAL:HA	2.20	0.42
1:C:199:PHE:CE2	1:C:258:LEU:HD13	2.55	0.42
1:A:197:LEU:HD13	1:A:210:ALA:CB	2.49	0.42
1:B:8:ASP:OD2	1:B:158:ASP:HA	2.20	0.42
1:B:278(A):PHE:HB3	1:B:281:LEU:HB2	2.02	0.42
1:A:194:LEU:O	1:A:210:ALA:N	2.41	0.41
1:B:270:GLU:OE1	1:B:270:GLU:N	2.40	0.41
1:B:281:LEU:HA	1:B:281:LEU:HD12	1.81	0.41
1:C:116:GLN:H	1:C:116:GLN:HG3	1.59	0.41
1:C:244:LEU:CD1	1:D:243:LEU:HD11	2.50	0.41
1:D:40:VAL:HB	1:D:41:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:VAL:HG11	1:D:241:PRO:CG	2.51	0.41
1:C:139:GLU:O	1:C:140:LEU:C	2.56	0.41
1:C:153:PHE:CZ	1:C:165:LEU:HD13	2.55	0.41
1:D:39:TRP:CZ2	1:D:120:ILE:HD12	2.56	0.41
1:D:222:THR:HG22	1:D:287:ILE:HG13	2.03	0.41
1:A:279(C):ILE:CG2	1:A:280:SER:N	2.83	0.41
1:C:55:LEU:HD23	1:C:55:LEU:N	2.34	0.41
1:C:71:VAL:HG21	1:C:84:PHE:CE2	2.55	0.41
1:D:64:TYR:CZ	1:D:66:LYS:HA	2.55	0.41
1:D:172:ASP:HA	1:D:175:TYR:HE1	1.86	0.41
1:C:74:ASN:ND2	1:C:79:THR:HG21	2.35	0.41
1:D:82:GLY:HA3	1:D:103:GLU:O	2.21	0.41
1:A:296:LYS:HG3	1:A:297:ASN:N	2.34	0.41
1:B:45:CYS:HB2	1:B:105:THR:HA	2.01	0.41
1:B:276:GLN:O	1:B:282:CYS:HA	2.20	0.41
1:C:25:GLN:HB2	1:C:27:PHE:CE1	2.55	0.41
1:C:148:GLN:HB2	1:C:150:VAL:CG1	2.48	0.41
1:C:245:TYR:HB2	1:C:284:VAL:HG13	2.02	0.41
1:D:140:LEU:O	1:D:145:LYS:HB2	2.20	0.41
1:D:174:PHE:HB3	1:D:310:PHE:CD1	2.56	0.41
1:A:283:MET:HE1	1:C:279(A):PHE:CE1	2.55	0.41
1:B:291:LEU:O	1:B:292:ASN:C	2.59	0.41
1:C:188:LEU:HB3	1:C:189:TYR:H	1.64	0.41
1:C:279:ASP:HA	1:C:280:SER:HA	2.02	0.41
1:D:99:TYR:CZ	1:D:133:VAL:HG12	2.56	0.41
1:D:279(C):ILE:HG22	1:D:280:SER:H	1.85	0.41
1:B:18:ALA:HB3	1:B:29:PHE:HE1	1.84	0.41
1:B:24:LYS:HB3	1:B:24:LYS:HE2	1.69	0.41
1:D:94:LEU:HD23	1:D:94:LEU:HA	1.67	0.41
1:A:74:ASN:HD21	1:A:79:THR:HG23	1.85	0.41
1:A:199:PHE:CD2	1:A:258:LEU:HD22	2.55	0.41
1:B:4:VAL:CG2	1:B:165:LEU:HD23	2.51	0.41
1:B:17:GLU:HA	1:B:27:PHE:O	2.21	0.41
1:B:57:ASP:C	1:B:59:ASN:H	2.24	0.41
1:B:128:LEU:HB2	1:B:188:LEU:HD22	2.03	0.41
1:B:188:LEU:HB3	1:B:189:TYR:H	1.66	0.41
1:C:199:PHE:O	1:C:231:PHE:CE2	2.72	0.41
1:C:310:PHE:CE2	1:C:312:VAL:HG23	2.56	0.41
1:D:42:SER:HB2	1:D:103:GLU:HB3	2.03	0.41
1:D:175:TYR:H	1:D:175:TYR:HD1	1.69	0.41
1:C:33:THR:HG22	1:C:123:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:MET:HG3	1:D:30:ILE:CD1	2.49	0.41
1:A:116:GLN:HE21	1:A:116:GLN:HB2	1.64	0.40
1:A:198:HIS:C	1:A:199:PHE:HD2	2.24	0.40
1:D:23:ASN:ND2	1:D:60:LYS:CB	2.83	0.40
1:A:205:LEU:HA	1:A:205:LEU:HD23	1.16	0.40
1:B:199:PHE:CD1	1:B:227:PHE:HE1	2.39	0.40
1:C:235:LEU:HD23	1:C:235:LEU:HA	1.84	0.40
1:D:18:ALA:HB1	1:D:91:ILE:HG13	2.04	0.40
1:D:218:THR:CG2	1:D:220:SER:H	2.34	0.40
1:C:13:MET:HG2	1:C:14:TYR:N	2.37	0.40
1:C:123:LEU:HD23	1:C:123:LEU:HA	1.76	0.40
1:C:238:VAL:CG2	1:C:239:LYS:N	2.84	0.40
1:D:203:ASN:N	1:D:203:ASN:HD22	2.20	0.40
1:A:185:ASN:HD22	1:A:185:ASN:C	2.25	0.40
1:A:271:PRO:C	1:A:273:TYR:N	2.75	0.40
1:C:205:LEU:HD11	1:C:230:LYS:HE2	2.04	0.40
1:D:35:SER:O	1:D:122:GLY:HA2	2.21	0.40
1:D:36:ALA:HA	1:D:122:GLY:HA3	2.03	0.40
1:D:221:ILE:HG22	1:D:222:THR:N	2.35	0.40
1:A:125:TRP:HB2	1:A:188:LEU:O	2.21	0.40
1:B:260:PHE:O	1:B:267:TYR:N	2.43	0.40
1:C:76:VAL:HG13	2:C:330:006:H49	2.02	0.40
1:C:170:ILE:H	1:C:170:ILE:CD1	2.29	0.40
1:D:64:TYR:OH	1:D:66:LYS:HD2	2.21	0.40
1:D:328:LYS:HD2	1:D:328:LYS:HA	1.77	0.40

There are no symmetry-related clashes.

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	325/336 (97%)	286 (88%)	31 (10%)	8 (2%)	5 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	325/336 (97%)	286 (88%)	31 (10%)	8 (2%)	5	27
1	C	324/336 (96%)	273 (84%)	45 (14%)	6 (2%)	8	33
1	D	324/336 (96%)	261 (81%)	55 (17%)	8 (2%)	5	27
All	All	1298/1344 (97%)	1106 (85%)	162 (12%)	30 (2%)	6	28

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASP
1	A	201	GLY
1	B	158	ASP
1	C	2	ASP
1	C	161	HIS
1	D	2	ASP
1	D	158	ASP
1	D	242	PHE
1	A	278	ILE
1	B	43	ALA
1	B	201	GLY
1	B	292	ASN
1	C	242	PHE
1	D	297	ASN
1	A	11	ASN
1	A	43	ALA
1	B	11	ASN
1	B	156	PRO
1	B	209	LYS
1	C	144	ASN
1	C	297	ASN
1	A	1	GLY
1	B	263	ALA
1	D	178	GLN
1	D	205	LEU
1	D	318	HIS
1	A	161	HIS
1	A	209	LYS
1	C	178	GLN
1	D	224	PRO

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	288/296 (97%)	218 (76%)	70 (24%)	0	2
1	B	288/296 (97%)	221 (77%)	67 (23%)	1	3
1	C	288/296 (97%)	226 (78%)	62 (22%)	1	4
1	D	288/296 (97%)	230 (80%)	58 (20%)	1	5
All	All	1152/1184 (97%)	895 (78%)	257 (22%)	1	3

All (257) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	8	ASP
1	A	13	MET
1	A	20	ILE
1	A	24	LYS
1	A	26	LYS
1	A	30	ILE
1	A	40	VAL
1	A	48	ILE
1	A	51	LYS
1	A	60	LYS
1	A	64	TYR
1	A	66	LYS
1	A	69	THR
1	A	71	VAL
1	A	72	GLU
1	A	81	SER
1	A	86	LYS
1	A	88	ILE
1	A	91	ILE
1	A	95	SER
1	A	99	TYR
1	A	113	THR
1	A	116	GLN

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Mol	Chain	Res	Type
1	A	129	SER
1	A	132	SER
1	A	136	VAL
1	A	141	LYS
1	A	143	GLN
1	A	147	GLU
1	A	157	PHE
1	A	158	ASP
1	A	159	ASP
1	A	162	LYS
1	A	164	TYR
1	A	166	THR
1	A	179	LEU
1	A	183	LYS
1	A	185	ASN
1	A	188	LEU
1	A	203	ASN
1	A	207	VAL
1	A	208	GLU
1	A	209	LYS
1	A	225	THR
1	A	226	GLU
1	A	231	PHE
1	A	235	LEU
1	A	236	ASP
1	A	238	VAL
1	A	240	ILE
1	A	244	LEU
1	A	246	ILE
1	A	248	THR
1	A	251	ASN
1	A	261	ARG
1	A	264	THR
1	A	265	ASN
1	A	272	GLU
1	A	277	GLN
1	A	278	ILE
1	A	281	LEU
1	A	283	MET
1	A	284	VAL
1	A	287	ILE
1	A	289	VAL

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Mol	Chain	Res	Type
1	A	291	LEU
1	A	292	ASN
1	A	311	THR
1	A	327	LYS
1	B	2	ASP
1	B	4	VAL
1	B	5	THR
1	B	8	ASP
1	B	13	MET
1	B	20	ILE
1	B	24	LYS
1	B	26	LYS
1	B	30	ILE
1	B	48	ILE
1	B	51	LYS
1	B	60	LYS
1	B	64	TYR
1	B	66	LYS
1	B	69	THR
1	B	71	VAL
1	B	72	GLU
1	B	86	LYS
1	B	88	ILE
1	B	91	ILE
1	B	94	LEU
1	B	95	SER
1	B	113	THR
1	B	116	GLN
1	B	129	SER
1	B	132	SER
1	B	136	VAL
1	B	141	LYS
1	B	143	GLN
1	B	147	GLU
1	B	159	ASP
1	B	160	LYS
1	B	162	LYS
1	B	179	LEU
1	B	183	LYS
1	B	185	ASN
1	B	188	LEU
1	B	203	ASN

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Mol	Chain	Res	Type
1	B	205	LEU
1	B	207	VAL
1	B	208	GLU
1	B	209	LYS
1	B	225	THR
1	B	226	GLU
1	B	229	ASN
1	B	235	LEU
1	B	236	ASP
1	B	238	VAL
1	B	240	ILE
1	B	244	LEU
1	B	248	THR
1	B	251	ASN
1	B	261	ARG
1	B	264	THR
1	B	265	ASN
1	B	272	GLU
1	B	276	GLN
1	B	278	ILE
1	B	281	LEU
1	B	284	VAL
1	B	285	SER
1	B	289	VAL
1	B	291	LEU
1	B	292	ASN
1	B	311	THR
1	B	327	LYS
1	B	328	LYS
1	C	5	THR
1	C	7	ASN
1	C	9	VAL
1	C	13	MET
1	C	25	GLN
1	C	26	LYS
1	C	46	ASN
1	C	47	THR
1	C	51	LYS
1	C	63	THR
1	C	71	VAL
1	C	72	GLU
1	C	77	SER

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Mol	Chain	Res	Type
1	C	86	LYS
1	C	90	THR
1	C	91	ILE
1	C	95	SER
1	C	116	GLN
1	C	121	VAL
1	C	127	ASP
1	C	132	SER
1	C	136	VAL
1	C	146	ILE
1	C	152	THR
1	C	157	PHE
1	C	160	LYS
1	C	175	TYR
1	C	180	THR
1	C	183	LYS
1	C	186	HIS
1	C	188	LEU
1	C	193	ASP
1	C	197	LEU
1	C	199	PHE
1	C	203	ASN
1	C	209	LYS
1	C	218	THR
1	C	220	SER
1	C	226	GLU
1	C	227	PHE
1	C	229	ASN
1	C	238	VAL
1	C	240	ILE
1	C	242	PHE
1	C	246	ILE
1	C	251	ASN
1	C	254	LYS
1	C	272	GLU
1	C	276	GLN
1	C	277	GLN
1	C	278	ILE
1	C	281	LEU
1	C	284	VAL
1	C	291	LEU
1	C	296	LYS

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Mol	Chain	Res	Type
1	C	297	ASN
1	C	301	LEU
1	C	311	THR
1	C	322	PHE
1	C	324	LEU
1	C	327	LYS
1	C	328	LYS
1	D	2	ASP
1	D	5	THR
1	D	7	ASN
1	D	13	MET
1	D	25	GLN
1	D	26	LYS
1	D	38	LEU
1	D	46	ASN
1	D	50	CYS
1	D	63	THR
1	D	71	VAL
1	D	72	GLU
1	D	77	SER
1	D	86	LYS
1	D	95	SER
1	D	113	THR
1	D	116	GLN
1	D	127	ASP
1	D	132	SER
1	D	136	VAL
1	D	140	LEU
1	D	141	LYS
1	D	146	ILE
1	D	152	THR
1	D	155	LEU
1	D	158	ASP
1	D	162	LYS
1	D	175	TYR
1	D	183	LYS
1	D	188	LEU
1	D	192	VAL
1	D	193	ASP
1	D	197	LEU
1	D	199	PHE
1	D	203	ASN

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Mol	Chain	Res	Type
1	D	218	THR
1	D	226	GLU
1	D	227	PHE
1	D	229	ASN
1	D	238	VAL
1	D	240	ILE
1	D	242	PHE
1	D	244	LEU
1	D	251	ASN
1	D	272	GLU
1	D	277	GLN
1	D	278	ILE
1	D	280	SER
1	D	281	LEU
1	D	284	VAL
1	D	291	LEU
1	D	297	ASN
1	D	301	LEU
1	D	311	THR
1	D	322	PHE
1	D	324	LEU
1	D	327	LYS
1	D	328	LYS

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	11	ASN
1	A	74	ASN
1	A	116	GLN
1	A	143	GLN
1	A	185	ASN
1	A	186	HIS
1	A	191	GLN
1	A	203	ASN
1	A	229	ASN
1	A	251	ASN
1	A	292	ASN
1	B	11	ASN
1	B	74	ASN
1	B	108	ASN
1	B	116	GLN

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Mol	Chain	Res	Type
1	B	143	GLN
1	B	185	ASN
1	B	186	HIS
1	B	191	GLN
1	B	203	ASN
1	B	251	ASN
1	B	292	ASN
1	C	7	ASN
1	C	11	ASN
1	C	19	GLN
1	C	74	ASN
1	C	116	GLN
1	C	148	GLN
1	C	161	HIS
1	C	185	ASN
1	C	191	GLN
1	C	198	HIS
1	C	203	ASN
1	C	251	ASN
1	C	277	GLN
1	C	318	HIS
1	D	7	ASN
1	D	11	ASN
1	D	19	GLN
1	D	23	ASN
1	D	74	ASN
1	D	116	GLN
1	D	148	GLN
1	D	203	ASN
1	D	251	ASN
1	D	292	ASN
1	D	318	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	006	B	330	-	49,49,49	1.47	6 (12%)	62,71,71	1.80	18 (29%)
2	006	A	330	-	49,49,49	1.72	8 (16%)	62,71,71	2.35	24 (38%)
3	GOL	D	331	-	5,5,5	0.53	0	5,5,5	0.66	0
3	GOL	A	332	-	5,5,5	0.52	0	5,5,5	0.81	0
3	GOL	B	332	-	5,5,5	0.46	0	5,5,5	0.43	0
3	GOL	D	332	-	5,5,5	0.57	0	5,5,5	0.53	0
2	006	C	330	-	49,49,49	1.50	5 (10%)	62,71,71	2.15	21 (33%)
3	GOL	A	333	-	5,5,5	0.40	0	5,5,5	0.90	0
3	GOL	C	333	-	5,5,5	0.32	0	5,5,5	0.76	0
3	GOL	B	331	-	5,5,5	0.39	0	5,5,5	0.94	0
2	006	D	330	-	49,49,49	1.45	5 (10%)	62,71,71	1.48	9 (14%)
3	GOL	C	331	-	5,5,5	0.47	0	5,5,5	0.80	0
3	GOL	C	332	-	5,5,5	0.52	0	5,5,5	1.07	0
3	GOL	A	331	-	5,5,5	0.56	0	5,5,5	0.80	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
2	006	B	330	-	-	8/33/61/61	0/5/5/5
2	006	A	330	-	-	4/33/61/61	0/5/5/5
3	GOL	D	331	-	-	2/4/4/4	-
3	GOL	A	332	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	332	-	-	3/4/4/4	-
3	GOL	D	332	-	-	4/4/4/4	-
2	006	C	330	-	-	5/33/61/61	0/5/5/5
3	GOL	A	333	-	-	4/4/4/4	-
3	GOL	C	333	-	-	0/4/4/4	-
3	GOL	B	331	-	-	4/4/4/4	-
2	006	D	330	-	-	3/33/61/61	0/5/5/5
3	GOL	C	331	-	-	4/4/4/4	-
3	GOL	C	332	-	-	2/4/4/4	-
3	GOL	A	331	-	-	0/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	330	006	C28-C29	-5.86	1.47	1.53
2	B	330	006	C51-S50	-5.60	1.74	1.85
2	A	330	006	C28-C29	-5.31	1.48	1.53
2	D	330	006	C51-S50	-5.24	1.75	1.85
2	D	330	006	C28-C29	-4.62	1.49	1.53
2	C	330	006	C51-S50	-4.56	1.76	1.85
2	A	330	006	C51-S50	-4.39	1.76	1.85
2	A	330	006	C28-C20	-4.32	1.49	1.54
2	A	330	006	C50-S50	-4.14	1.73	1.83
2	D	330	006	C50-S50	-3.61	1.74	1.83
2	B	330	006	C50-S50	-3.59	1.74	1.83
2	C	330	006	C50-S50	-3.59	1.74	1.83
2	B	330	006	C28-C29	-3.55	1.50	1.53
2	D	330	006	C54-N50	3.48	1.49	1.46
2	C	330	006	C28-C20	-3.09	1.50	1.54
2	A	330	006	C35-C31	-2.88	1.52	1.55
2	B	330	006	C36-C32	-2.84	1.34	1.39
2	A	330	006	O50-C55	-2.78	1.18	1.23
2	A	330	006	C54-C55	-2.61	1.49	1.53
2	C	330	006	C54-N50	2.48	1.48	1.46
2	B	330	006	C35-C31	-2.47	1.52	1.55
2	A	330	006	C49-C48	2.26	1.55	1.51
2	B	330	006	C54-C55	-2.24	1.49	1.53
2	D	330	006	C36-C32	-2.04	1.36	1.39

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	330	006	C39-C35-C31	6.97	110.27	103.70
2	B	330	006	C36-C39-C35	-6.60	97.40	103.43
2	A	330	006	C21-C20-N2	-6.26	101.19	110.08
2	C	330	006	C20-N2-C48	-6.09	113.26	123.40
2	C	330	006	C39-C35-C31	5.79	109.16	103.70
2	A	330	006	C36-C39-C35	-5.31	98.57	103.43
2	D	330	006	C39-C35-C31	4.95	108.36	103.70
2	C	330	006	C36-C39-C35	-4.71	99.12	103.43
2	B	330	006	C32-C31-C35	-4.40	99.27	102.48
2	C	330	006	C49-C48-N2	4.22	123.71	116.41
2	A	330	006	C22-C21-C20	-4.08	106.48	113.40
2	D	330	006	C21-C20-N2	-4.07	104.30	110.08
2	C	330	006	C34-C33-C32	-3.91	116.30	120.99
2	A	330	006	C52-C51-C54	3.90	120.01	111.61
2	A	330	006	C43-C42-C41	-3.55	113.44	120.28
2	A	330	006	C46-C45-C42	-3.45	114.83	122.07
2	A	330	006	C49-O41-C45	3.41	124.73	114.78
2	A	330	006	C41-C42-C45	3.38	123.14	117.75
2	C	330	006	C28-C20-N2	-3.32	103.75	109.93
2	A	330	006	C20-N2-C48	-3.21	118.04	123.40
2	D	330	006	C28-C20-N2	-3.15	104.07	109.93
2	A	330	006	O41-C49-C48	3.12	119.40	110.80
2	C	330	006	C38-C37-C36	-3.12	116.31	120.88
2	B	330	006	O41-C49-C48	3.09	119.32	110.80
2	C	330	006	O20-C28-C29	-3.07	103.90	108.54
2	C	330	006	O41-C45-C42	3.04	124.52	118.90
2	C	330	006	O40-C48-N2	-3.02	117.83	122.95
2	B	330	006	C44-C46-C47	-2.93	114.63	120.28
2	B	330	006	C22-C21-C20	-2.92	108.45	113.40
2	C	330	006	C43-C42-C41	-2.83	114.83	120.28
2	A	330	006	O40-C48-N2	-2.82	118.18	122.95
2	C	330	006	C47-C46-C45	2.81	122.23	117.75
2	C	330	006	C46-C45-C42	-2.79	116.21	122.07
2	A	330	006	C32-C31-C35	-2.74	100.48	102.48
2	A	330	006	O20-C28-C29	-2.72	104.42	108.54
2	C	330	006	C49-O41-C45	2.66	122.55	114.78
2	B	330	006	C25-C26-C27	-2.55	117.09	120.24
2	C	330	006	C32-C31-C35	-2.55	100.62	102.48
2	B	330	006	C43-C42-C45	2.53	124.86	120.80
2	C	330	006	O41-C49-C48	2.51	117.72	110.80
2	B	330	006	C34-C33-C32	-2.48	118.02	120.99
2	B	330	006	O30-C35-C39	-2.47	105.24	110.81
2	B	330	006	C53-C51-S50	-2.47	105.21	109.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	330	006	C43-C42-C45	2.43	124.70	120.80
2	C	330	006	C39-C36-C37	-2.38	124.71	129.17
2	D	330	006	O20-C28-C29	-2.37	104.95	108.54
2	D	330	006	O21-C29-N50	2.37	125.64	121.38
2	B	330	006	C38-C37-C36	-2.36	117.43	120.88
2	A	330	006	O41-C45-C42	2.34	123.23	118.90
2	A	330	006	O30-C35-C31	-2.32	103.37	110.00
2	A	330	006	C24-C23-C22	-2.32	117.35	120.61
2	A	330	006	C53-C51-C54	-2.31	106.63	111.61
2	B	330	006	C44-C46-C45	2.30	124.49	120.80
2	B	330	006	C27-C22-C23	2.29	121.63	118.23
2	A	330	006	C51-C54-N50	-2.25	103.18	106.43
2	D	330	006	C52-C51-S50	-2.25	105.57	109.19
2	A	330	006	C54-C51-S50	-2.25	100.50	104.12
2	D	330	006	C52-C51-C54	2.24	116.43	111.61
2	A	330	006	C53-C51-C52	-2.23	107.07	110.70
2	C	330	006	O21-C29-N50	2.19	125.31	121.38
2	A	330	006	C44-C46-C47	-2.17	116.10	120.28
2	B	330	006	C21-C20-N2	-2.15	107.02	110.08
2	C	330	006	C51-C54-N50	2.12	109.49	106.43
2	D	330	006	O50-C55-C54	-2.12	116.63	121.49
2	B	330	006	C43-C42-C41	-2.11	116.20	120.28
2	D	330	006	C36-C39-C35	-2.10	101.51	103.43
2	A	330	006	C38-C34-C33	-2.08	117.68	120.24
2	B	330	006	O20-C28-C20	2.07	114.26	108.43
2	B	330	006	O20-C28-C29	-2.06	105.43	108.54
2	A	330	006	C47-C46-C45	2.05	121.01	117.75
2	C	330	006	C47-C40-C41	-2.05	117.61	120.24
2	B	330	006	C52-C51-C54	2.02	115.97	111.61

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	330	006	N2-C20-C28-O20
2	A	330	006	C21-C20-C28-O20
2	A	330	006	C21-C20-C28-C29
2	B	330	006	N2-C20-C28-O20
2	B	330	006	C21-C20-C28-O20
2	B	330	006	C21-C20-C28-C29
2	C	330	006	C21-C20-C28-O20
2	C	330	006	C32-C31-N30-C55

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Mol	Chain	Res	Type	Atoms
2	D	330	006	C32-C31-N30-C55
3	A	332	GOL	C1-C2-C3-O3
3	A	333	GOL	O1-C1-C2-C3
3	A	333	GOL	C1-C2-C3-O3
3	B	331	GOL	C1-C2-C3-O3
3	B	332	GOL	C1-C2-C3-O3
3	C	331	GOL	O1-C1-C2-C3
3	C	332	GOL	C1-C2-C3-O3
3	D	332	GOL	O1-C1-C2-C3
3	C	331	GOL	C1-C2-C3-O3
3	D	331	GOL	O1-C1-C2-C3
3	D	332	GOL	C1-C2-C3-O3
3	A	332	GOL	O2-C2-C3-O3
3	A	333	GOL	O1-C1-C2-O2
3	A	333	GOL	O2-C2-C3-O3
3	B	331	GOL	O2-C2-C3-O3
3	B	332	GOL	O2-C2-C3-O3
3	C	331	GOL	O1-C1-C2-O2
3	C	331	GOL	O2-C2-C3-O3
2	B	330	006	O40-C48-C49-O41
2	B	330	006	N2-C48-C49-O41
3	C	332	GOL	O2-C2-C3-O3
3	D	332	GOL	O1-C1-C2-O2
2	B	330	006	N2-C20-C28-C29
3	B	332	GOL	O1-C1-C2-C3
3	A	332	GOL	O1-C1-C2-O2
3	D	331	GOL	O1-C1-C2-O2
2	C	330	006	N2-C20-C28-O20
3	B	331	GOL	O1-C1-C2-O2
2	B	330	006	C35-C31-N30-C55
2	C	330	006	C35-C31-N30-C55
2	A	330	006	N2-C20-C28-C29
2	C	330	006	N2-C20-C28-C29
3	B	331	GOL	O1-C1-C2-C3
3	D	332	GOL	O2-C2-C3-O3
2	B	330	006	N2-C20-C21-C22
2	D	330	006	N2-C48-C49-O41
2	D	330	006	O20-C28-C29-O21

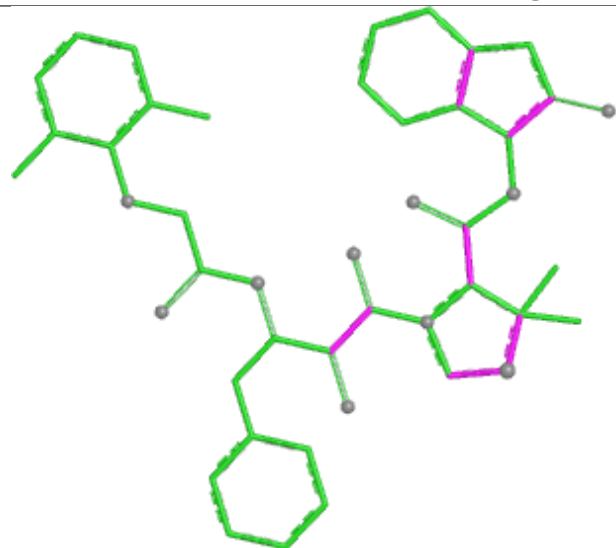
There are no ring outliers.

10 monomers are involved in 66 short contacts:

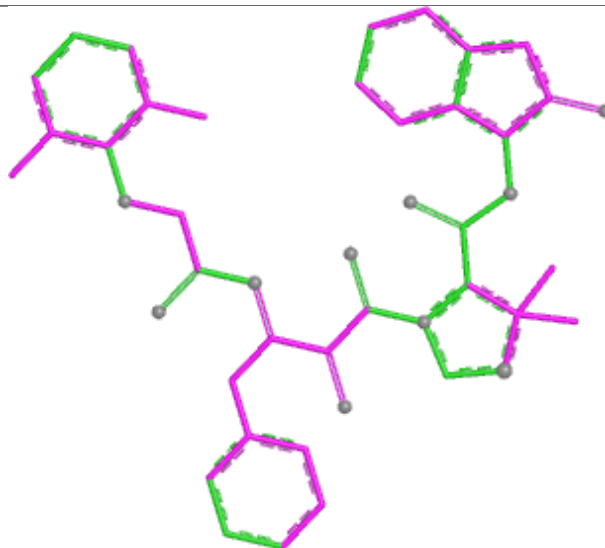
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	330	006	3	0
2	A	330	006	6	0
3	D	331	GOL	19	0
3	D	332	GOL	1	0
2	C	330	006	5	0
3	C	333	GOL	4	0
3	B	331	GOL	1	0
2	D	330	006	1	0
3	C	331	GOL	19	0
3	A	331	GOL	7	0

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.

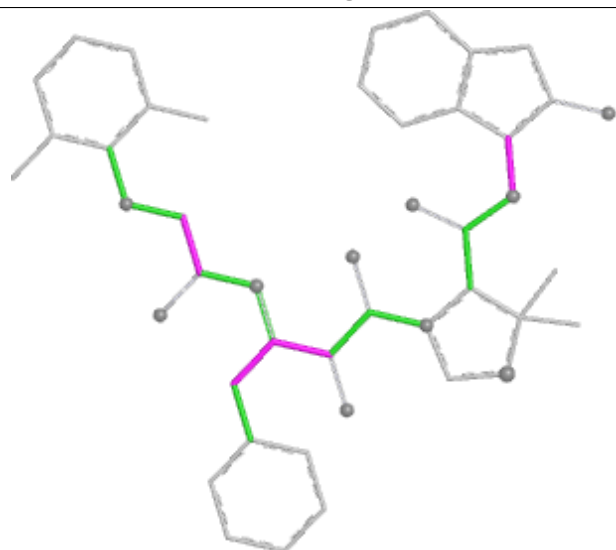
Ligand 006 B 330



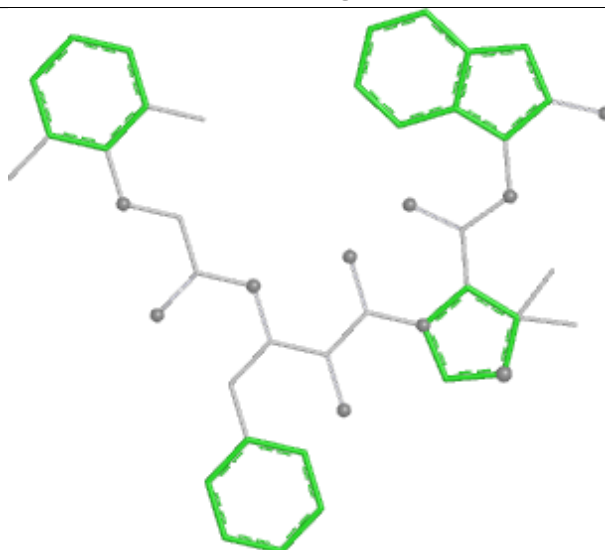
Bond lengths



Bond angles

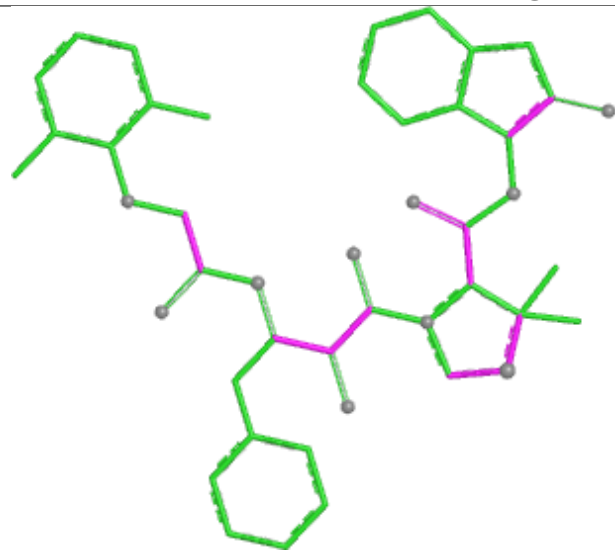


Torsions

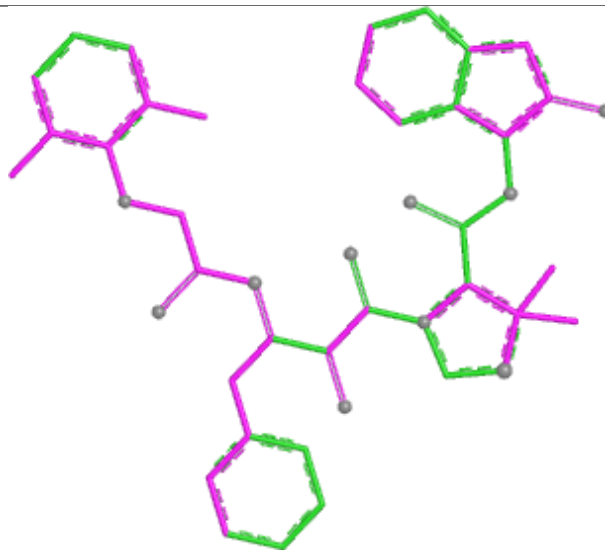


Rings

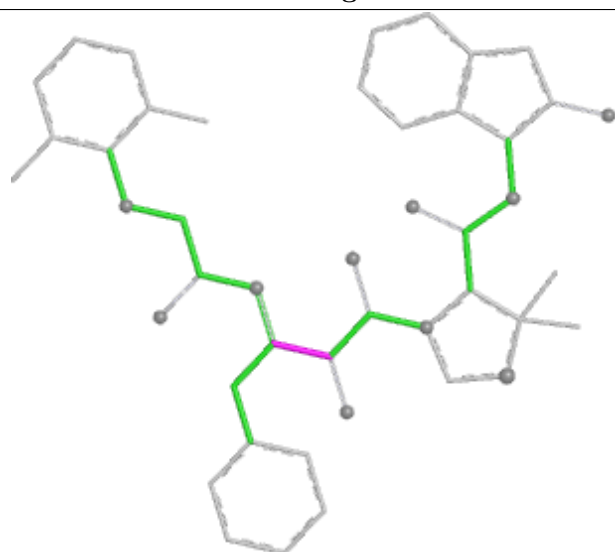
Ligand 006 A 330



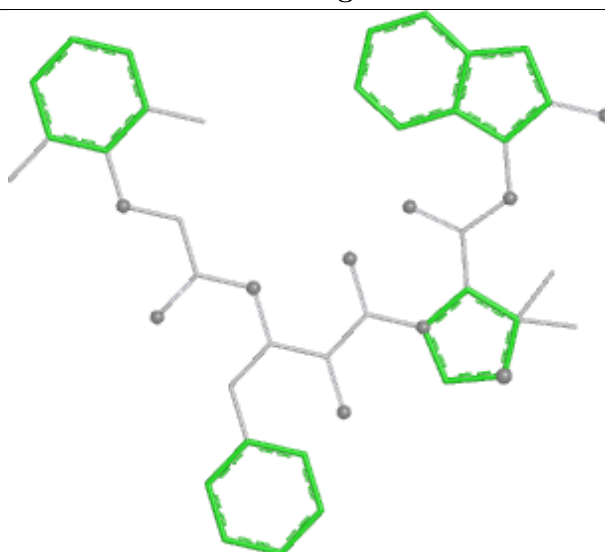
Bond lengths



Bond angles

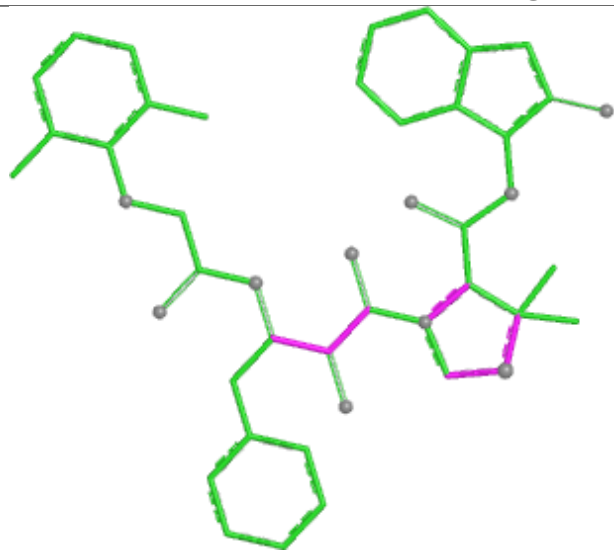


Torsions

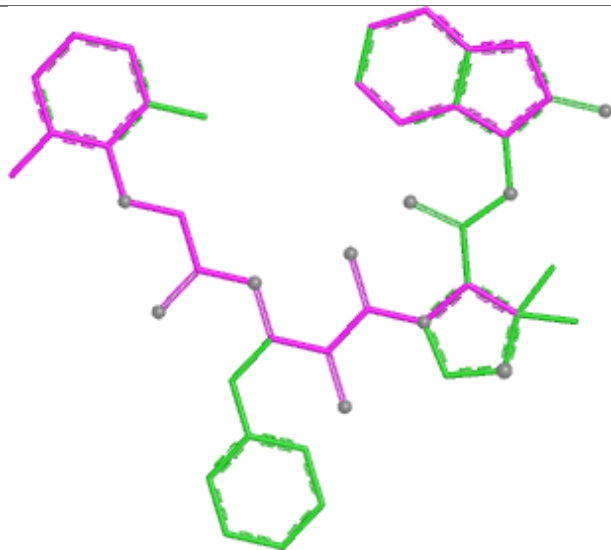


Rings

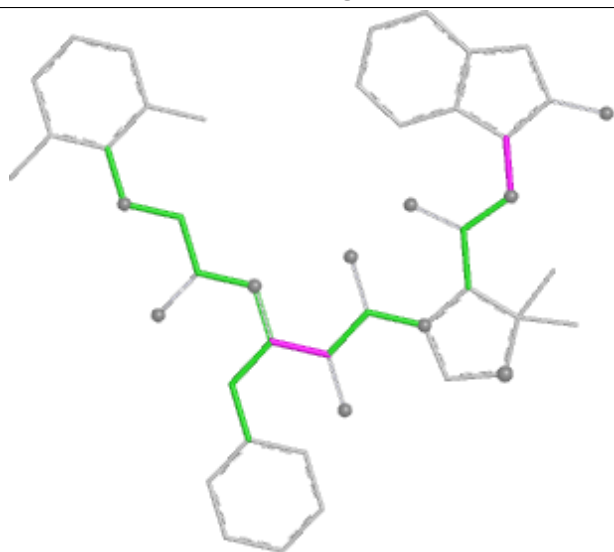
Ligand 006 C 330



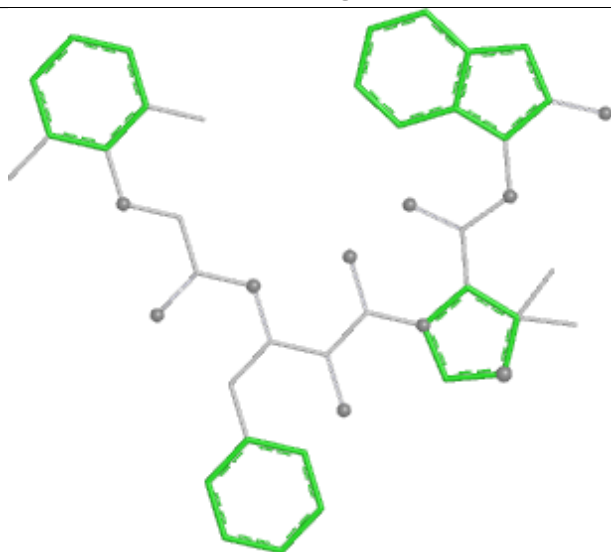
Bond lengths



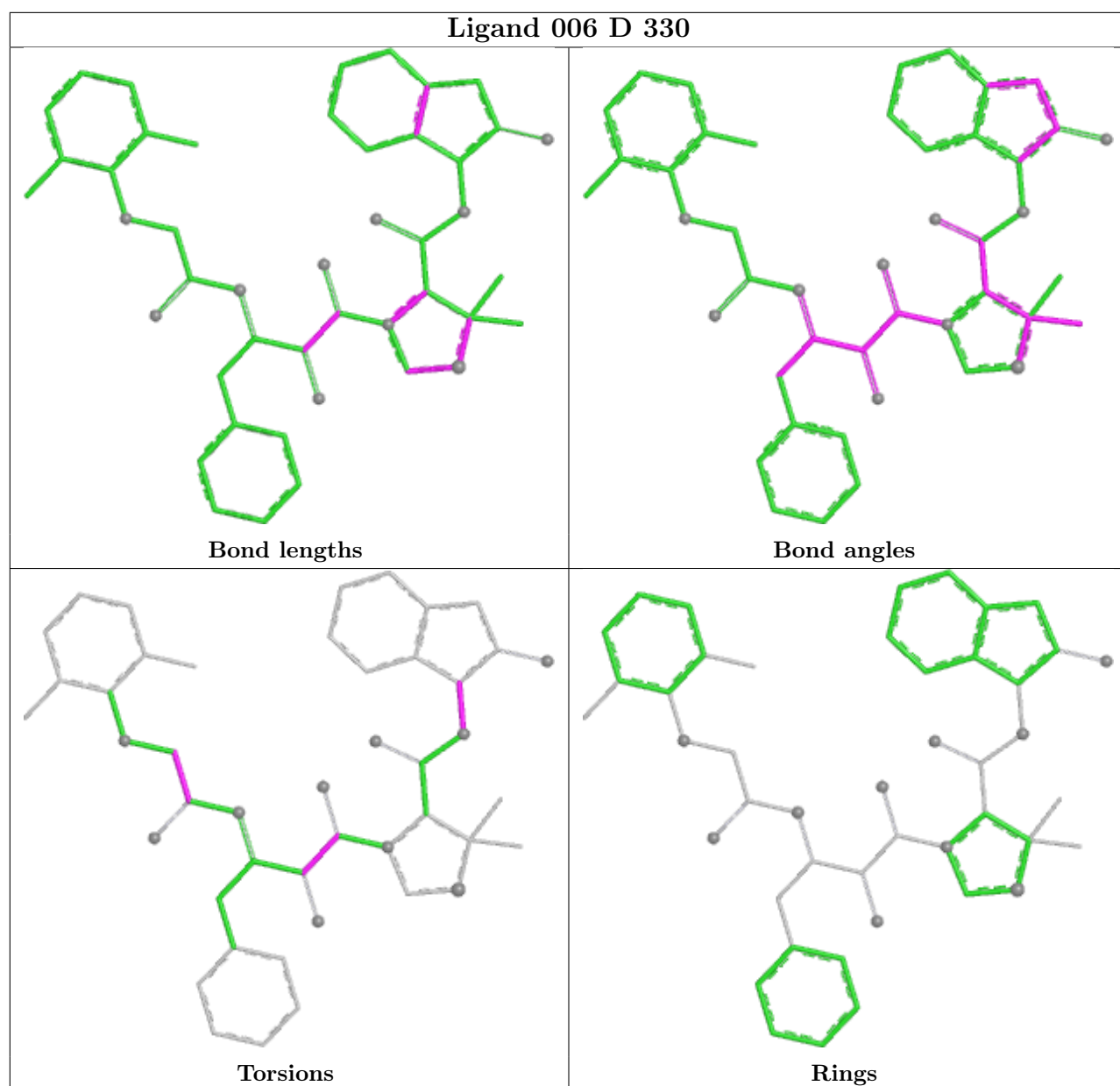
Bond angles



Torsions



Rings



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, 95th 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 ²)	Q<0.9
1	A	327/336 (97%)	-0.22	6 (1%) 68 47	56, 72, 96, 163	0
1	B	327/336 (97%)	-0.20	4 (1%) 79 61	56, 78, 102, 158	0
1	C	326/336 (97%)	-0.06	7 (2%) 63 43	63, 85, 109, 154	0
1	D	326/336 (97%)	0.36	29 (8%) 9 3	56, 101, 121, 307	0
All	All	1306/1344 (97%)	-0.03	46 (3%) 44 23	56, 83, 115, 307	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	46	ASN	4.9
1	D	169	GLY	4.4
1	D	57	ASP	4.2
1	B	216	SER	4.1
1	D	58	SER	3.4
1	A	216	SER	3.3
1	D	107	THR	3.3
1	D	18	ALA	3.2
1	D	216	SER	3.0
1	D	32	ASP	3.0
1	D	328	LYS	2.9
1	D	45	CYS	2.9
1	D	33	THR	2.7
1	D	47	THR	2.7
1	B	328	LYS	2.7
1	C	158	ASP	2.7
1	A	217	GLY	2.6
1	C	159	ASP	2.6
1	C	216	SER	2.6
1	D	108	ASN	2.5
1	D	292	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	168	GLY	2.5
1	D	122	GLY	2.5
1	A	109(B)	GLU	2.5
1	D	147	GLU	2.4
1	D	56	TYR	2.4
1	D	36	ALA	2.4
1	B	217	GLY	2.4
1	C	147	GLU	2.2
1	A	215	ASP	2.2
1	D	317	ASN	2.2
1	A	110	PRO	2.2
1	C	169	GLY	2.2
1	B	2	ASP	2.2
1	D	48	ILE	2.2
1	D	22	ASP	2.2
1	D	44	GLN	2.1
1	D	50	CYS	2.1
1	D	35	SER	2.1
1	D	72	GLU	2.1
1	D	49	GLY	2.1
1	A	220	SER	2.0
1	D	168	GLY	2.0
1	C	170	ILE	2.0
1	D	62	LYS	2.0
1	D	144	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

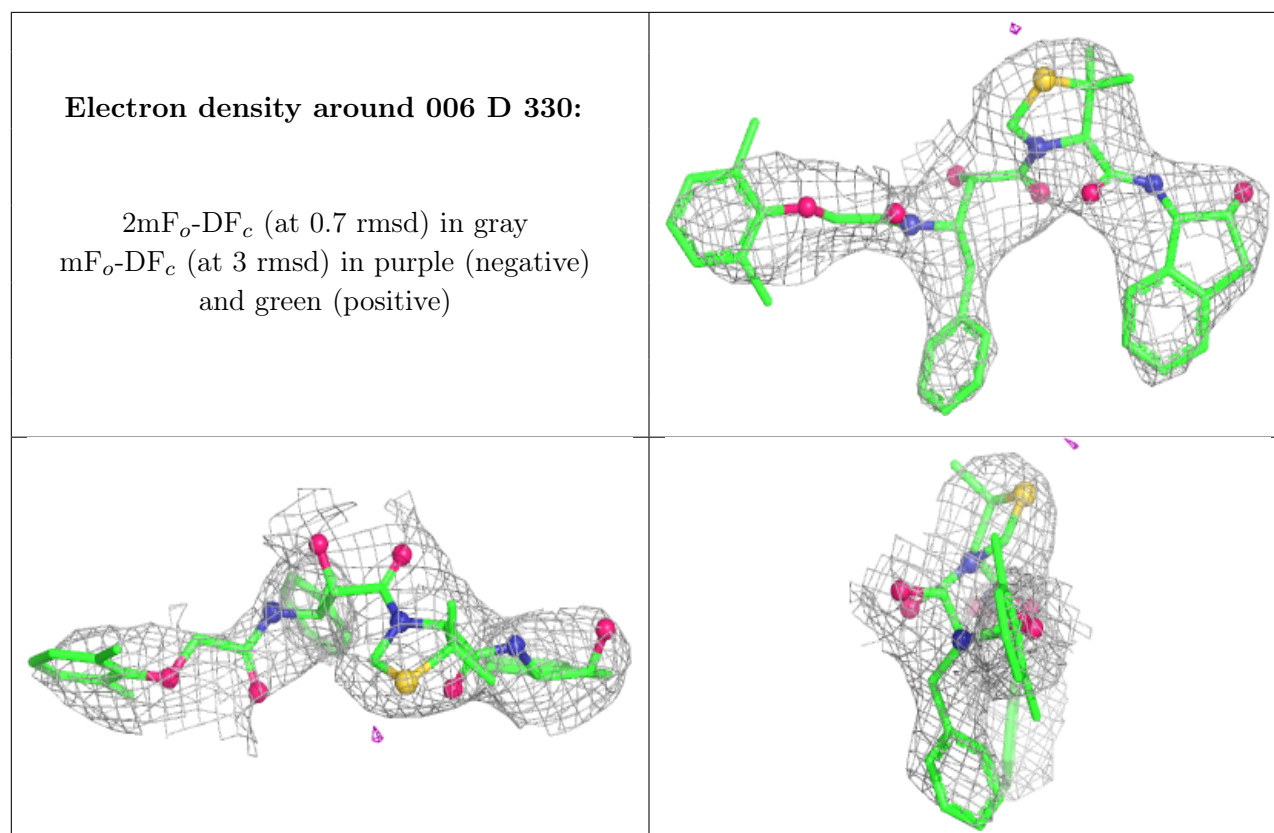
There are no monosaccharides in this entry.

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, 95th 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.

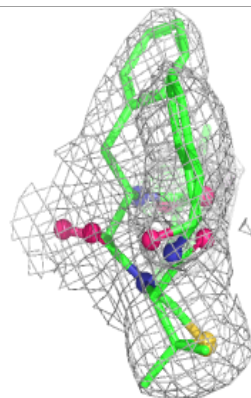
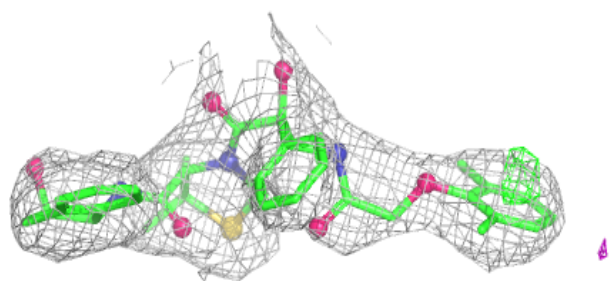
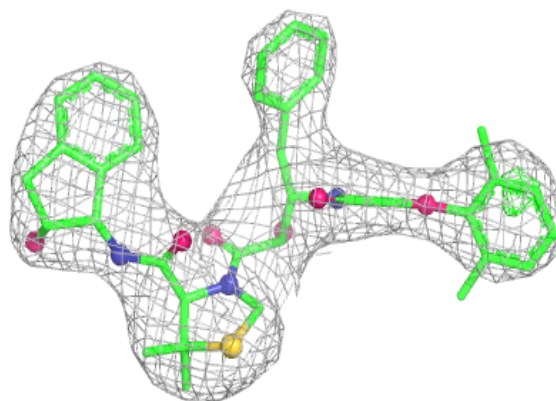
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	332	6/6	0.75	0.34	77,85,88,91	0
3	GOL	D	332	6/6	0.78	0.62	86,89,90,91	0
3	GOL	C	331	6/6	0.80	0.74	94,96,100,103	0
3	GOL	A	331	6/6	0.81	0.27	86,92,92,92	0
3	GOL	C	332	6/6	0.82	0.26	83,85,86,86	0
3	GOL	D	331	6/6	0.85	0.21	87,90,90,90	0
2	006	D	330	45/45	0.86	0.26	102,107,125,126	0
3	GOL	B	331	6/6	0.86	0.28	81,82,84,84	0
3	GOL	B	332	6/6	0.87	0.41	88,89,91,93	0
3	GOL	C	333	6/6	0.87	0.43	97,97,98,98	0
3	GOL	A	333	6/6	0.88	0.19	88,88,90,90	0
2	006	C	330	45/45	0.92	0.25	64,69,84,87	0
2	006	A	330	45/45	0.93	0.24	58,64,88,92	0
2	006	B	330	45/45	0.93	0.23	61,74,90,91	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.

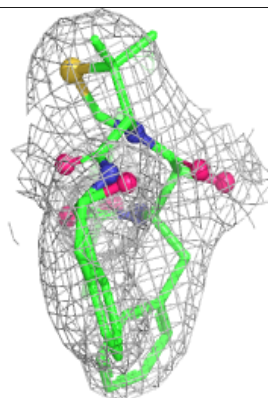
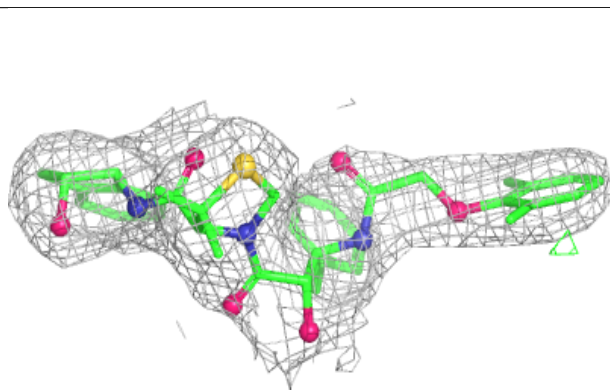
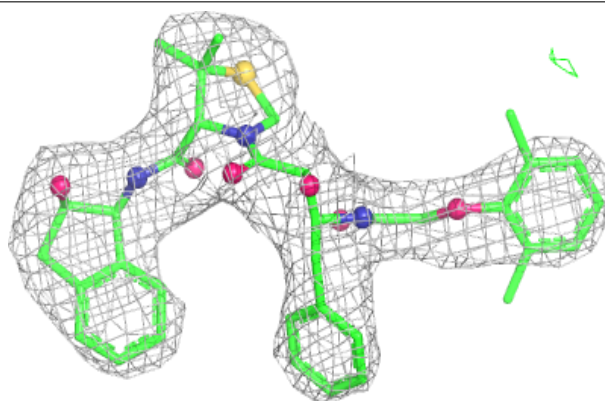


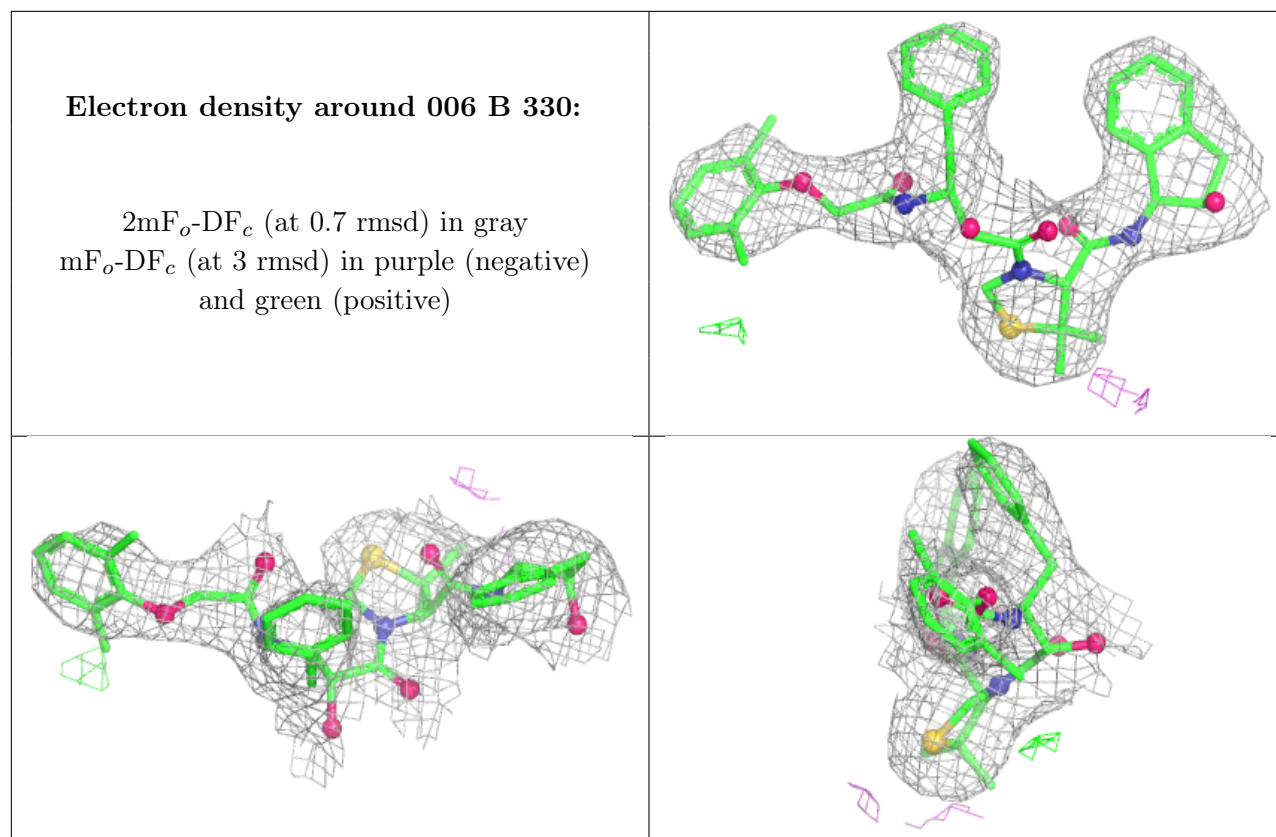
Electron density around 006 C 330:

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

**Electron density around 006 A 330:**

$2mF_o-DF_c$ (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.