



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:38 AM UTC

PDB ID : 2EWG / pdb_00002ewg
Title : T. brucei Farnesyl Diphosphate Synthase Complexed with Minodronate
Authors : Cao, R.; Mao, J.; Gao, Y.; Robinson, H.; Odeh, S.; Goddard, A.; Oldfield, E.
Deposited on : 2005-11-03
Resolution : 2.48 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

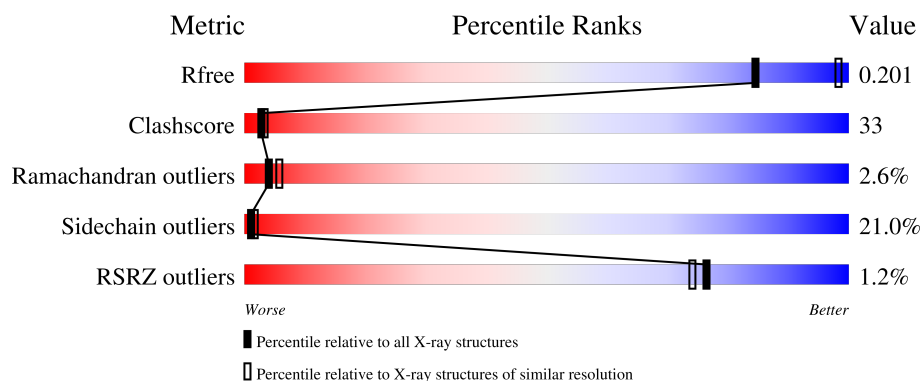
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	390	
1	B	390	

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
4	PGO	A	5002	-	X	-	-
4	PGO	A	5003	-	X	-	-
4	PGO	B	5001	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6275 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 farnesyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	1	0
			2942	1867	486	561	28			
1	B	367	Total	C	N	O	S	0	1	0
			2942	1868	486	560	28			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	cloning artifact	UNP Q86C09
A	-21	GLY	-	cloning artifact	UNP Q86C09
A	-20	SER	-	cloning artifact	UNP Q86C09
A	-19	SER	-	cloning artifact	UNP Q86C09
A	-18	HIS	-	expression tag	UNP Q86C09
A	-17	HIS	-	expression tag	UNP Q86C09
A	-16	HIS	-	expression tag	UNP Q86C09
A	-15	HIS	-	expression tag	UNP Q86C09
A	-14	HIS	-	expression tag	UNP Q86C09
A	-13	HIS	-	expression tag	UNP Q86C09
A	-12	SER	-	cloning artifact	UNP Q86C09
A	-11	SER	-	cloning artifact	UNP Q86C09
A	-10	GLY	-	cloning artifact	UNP Q86C09
A	-9	LEU	-	cloning artifact	UNP Q86C09
A	-8	VAL	-	cloning artifact	UNP Q86C09
A	-7	PRO	-	cloning artifact	UNP Q86C09
A	-6	ARG	-	cloning artifact	UNP Q86C09
A	-5	GLY	-	cloning artifact	UNP Q86C09
A	-4	SER	-	cloning artifact	UNP Q86C09
A	-3	HIS	-	cloning artifact	UNP Q86C09
A	-2	MET	-	cloning artifact	UNP Q86C09
A	-1	ALA	-	cloning artifact	UNP Q86C09
A	0	SER	-	cloning artifact	UNP Q86C09
B	-22	MET	-	cloning artifact	UNP Q86C09
B	-21	GLY	-	cloning artifact	UNP Q86C09

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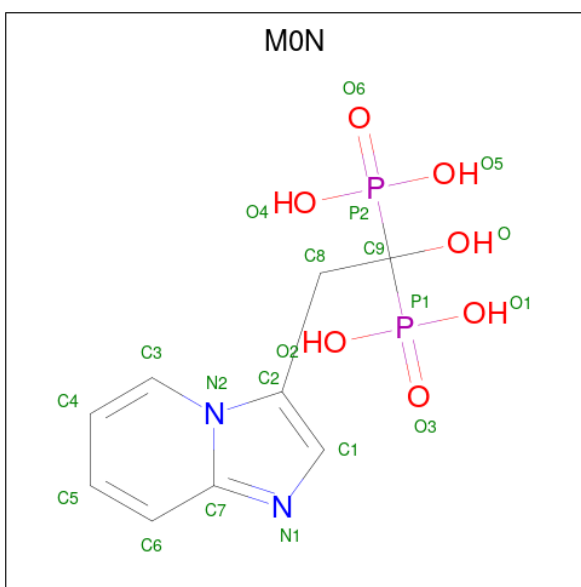
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	cloning artifact	UNP Q86C09
B	-19	SER	-	cloning artifact	UNP Q86C09
B	-18	HIS	-	expression tag	UNP Q86C09
B	-17	HIS	-	expression tag	UNP Q86C09
B	-16	HIS	-	expression tag	UNP Q86C09
B	-15	HIS	-	expression tag	UNP Q86C09
B	-14	HIS	-	expression tag	UNP Q86C09
B	-13	HIS	-	expression tag	UNP Q86C09
B	-12	SER	-	cloning artifact	UNP Q86C09
B	-11	SER	-	cloning artifact	UNP Q86C09
B	-10	GLY	-	cloning artifact	UNP Q86C09
B	-9	LEU	-	cloning artifact	UNP Q86C09
B	-8	VAL	-	cloning artifact	UNP Q86C09
B	-7	PRO	-	cloning artifact	UNP Q86C09
B	-6	ARG	-	cloning artifact	UNP Q86C09
B	-5	GLY	-	cloning artifact	UNP Q86C09
B	-4	SER	-	cloning artifact	UNP Q86C09
B	-3	HIS	-	cloning artifact	UNP Q86C09
B	-2	MET	-	cloning artifact	UNP Q86C09
B	-1	ALA	-	cloning artifact	UNP Q86C09
B	0	SER	-	cloning artifact	UNP Q86C09

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

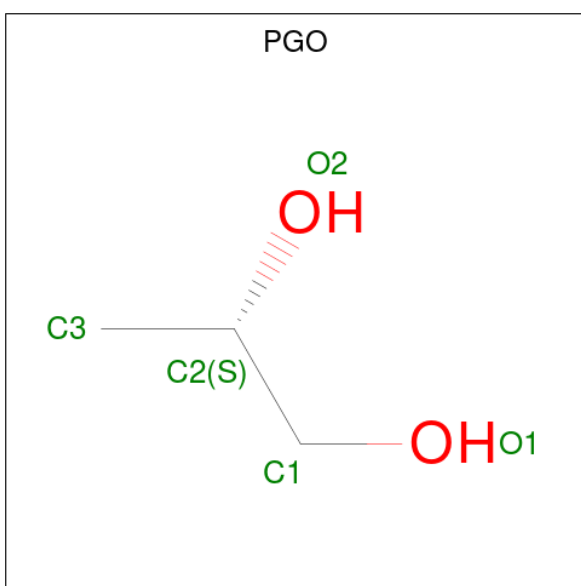
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Mg 3 3	0	0
2	B	3	Total Mg 3 3	0	0

- Molecule 3 is (1-HYDROXY-2-IMIDAZO[1,2-A]PYRIDIN-3-YLETHANE-1,1-DIYL)BIS(P HOSPHONIC ACID) (CCD ID: M0N) (formula: C₉H₁₂N₂O₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			20	9	2	7	2		
3	B	1	Total	C	N	O	P	0	0
			20	9	2	7	2		

- Molecule 4 is S-1,2-PROPANEDIOL (CCD ID: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0
			5	3	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			5	3	2		

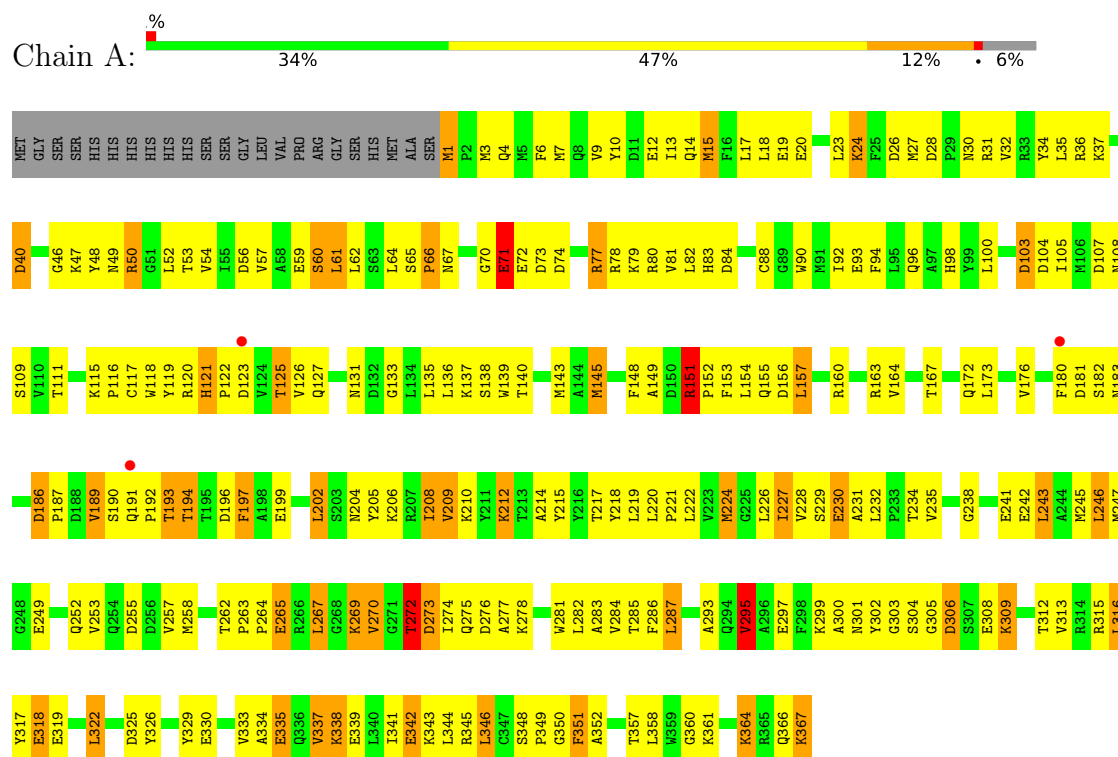
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	173	Total	O	0	0
			173	173		
5	B	157	Total	O	0	0
			157	157		

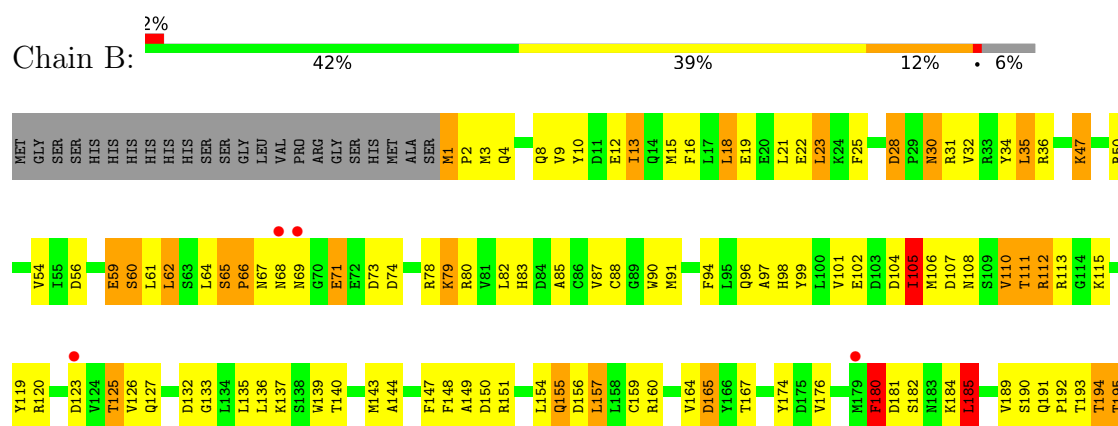
3 Residue-property plots

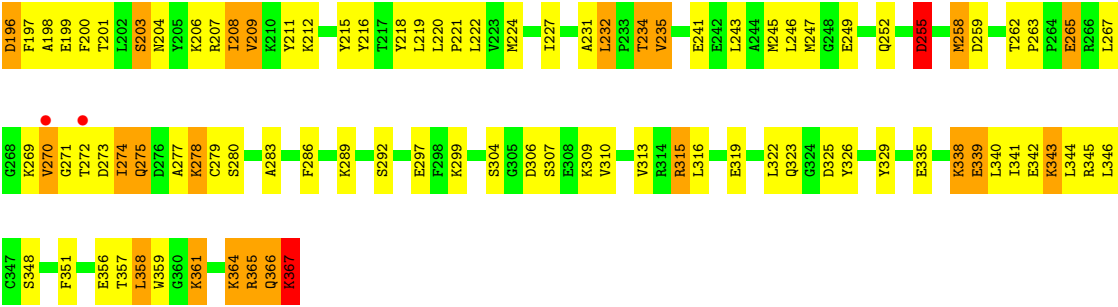
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: farnesyl pyrophosphate synthase



- Molecule 1: farnesyl pyrophosphate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.98Å 118.10Å 63.25Å 90.00° 112.48° 90.00°	Depositor
Resolution (Å)	30.00 – 2.48 30.00 – 2.48	Depositor EDS
% Data completeness (in resolution range)	90.7 (30.00-2.48) 91.0 (30.00-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.48Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.241 , 0.260 (Not available) , 0.201	Depositor DCC
R_{free} test set	1447 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 107.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6275	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.16% 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: PGO, MG, M0N

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	0.41	1/3007 (0.0%)	1.22	16/4068 (0.4%)
1	B	0.40	1/3008 (0.0%)	1.25	14/4068 (0.3%)
All	All	0.40	2/6015 (0.0%)	1.24	30/8136 (0.4%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	LYS	C-OXT	10.96	1.45	1.23
1	B	367	LYS	C-OXT	10.28	1.44	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	ASP	CA-CB-CG	8.11	120.71	112.60
1	B	65	SER	O-C-N	8.08	125.25	121.53
1	A	272	THR	CA-C-N	7.25	135.40	121.54
1	A	272	THR	C-N-CA	7.25	135.40	121.54
1	B	343	LYS	CA-C-N	6.83	129.92	120.63
1	B	343	LYS	C-N-CA	6.83	129.92	120.63
1	A	151	ARG	O-C-N	6.72	126.71	121.47
1	A	40	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	207	ARG	CA-C-N	-5.66	112.39	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	ARG	C-N-CA	-5.66	112.39	120.42
1	A	153	PHE	CA-CB-CG	5.65	119.45	113.80
1	A	295	VAL	CA-C-N	5.59	127.77	120.28
1	A	295	VAL	C-N-CA	5.59	127.77	120.28
1	A	151	ARG	CA-C-N	5.50	125.21	119.82
1	A	151	ARG	C-N-CA	5.50	125.21	119.82
1	A	196	ASP	CA-CB-CG	5.49	118.09	112.60
1	B	105	ILE	CA-C-N	5.46	127.54	120.44
1	B	105	ILE	C-N-CA	5.46	127.54	120.44
1	B	366	GLN	N-CA-C	-5.40	107.71	114.56
1	A	351	PHE	CA-CB-CG	5.29	119.09	113.80
1	B	165	ASP	CA-C-N	5.28	127.35	120.28
1	B	165	ASP	C-N-CA	5.28	127.35	120.28
1	B	180	PHE	CA-CB-CG	5.25	119.05	113.80
1	A	121	HIS	CA-C-N	5.23	126.38	119.84
1	A	121	HIS	C-N-CA	5.23	126.38	119.84
1	B	274	ILE	CA-C-N	5.21	127.52	120.38
1	B	274	ILE	C-N-CA	5.21	127.52	120.38
1	A	121	HIS	O-C-N	5.19	126.36	121.38
1	A	335	GLU	CA-C-N	5.08	127.05	120.44
1	A	335	GLU	C-N-CA	5.08	127.05	120.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ASP	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2942	0	2884	206	0
1	B	2942	0	2891	180	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	20	0	8	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	8	4	0
4	A	10	0	16	0	0
4	B	5	0	8	1	0
5	A	173	0	0	32	0
5	B	157	0	0	27	0
All	All	6275	0	5815	387	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 33.

All (387) 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:262:THR:HB	1:A:267:LEU:HD22	1.40	1.03
1:B:18:LEU:HD11	1:B:36:ARG:HB2	1.40	0.98
1:B:361:LYS:HA	1:B:364:LYS:HE2	1.45	0.98
1:B:174:TYR:HB3	1:B:208:ILE:HG22	1.55	0.86
1:B:274:ILE:HD12	1:B:310:VAL:HG13	1.60	0.83
1:A:209:VAL:HG22	1:A:252:GLN:HG2	1.61	0.83
1:B:111:THR:HG22	1:B:269:LYS:HA	1.60	0.81
1:B:364:LYS:HD3	5:B:6182:HOH:O	1.84	0.78
1:A:164:VAL:O	1:A:167:THR:HG22	1.83	0.77
1:A:77:ARG:O	1:A:81:VAL:HG23	1.84	0.77
1:B:231:ALA:O	1:B:234:THR:HB	1.86	0.76
1:B:28:ASP:O	1:B:32:VAL:HG23	1.85	0.76
1:A:125:THR:HG21	1:A:127:GLN:HE21	1.49	0.75
1:A:226:LEU:HD13	1:A:232:LEU:HA	1.70	0.74
1:B:96:GLN:HB2	1:B:216:TYR:HE1	1.51	0.74
1:A:20:GLU:O	1:A:24:LYS:HB2	1.87	0.74
1:A:342:GLU:HA	1:A:345:ARG:HB3	1.70	0.72
1:B:338:LYS:O	1:B:342:GLU:HG2	1.89	0.72
1:B:105:ILE:HD13	1:B:126:VAL:HG13	1.70	0.72
1:B:110:VAL:HB	1:B:120:ARG:NH1	2.04	0.72
1:A:1:MET:HE2	5:A:6098:HOH:O	1.88	0.72
1:A:71:GLU:HG2	1:A:77:ARG:NH2	2.06	0.71
1:A:71:GLU:OE1	1:A:74:ASP:HB3	1.90	0.71
1:A:215:TYR:HB2	5:A:6208:HOH:O	1.89	0.70
1:A:364:LYS:HA	5:A:6263:HOH:O	1.91	0.70
1:B:150:ASP:HB2	5:B:6033:HOH:O	1.92	0.70
1:A:145:MET:HE1	5:A:6307:HOH:O	1.92	0.69
1:A:312:THR:HG23	1:A:315:ARG:NH2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LYS:HE3	5:A:6120:HOH:O	1.91	0.69
1:B:255:ASP:O	1:B:259:ASP:HB2	1.93	0.69
1:B:271:GLY:HA2	5:B:6231:HOH:O	1.92	0.69
1:A:230:GLU:HA	5:A:6287:HOH:O	1.92	0.69
1:A:269:LYS:HD3	1:A:270:VAL:O	1.93	0.68
1:B:102:GLU:O	1:B:106:MET:HG3	1.92	0.68
1:B:278:LYS:HD3	1:B:279:CYS:H	1.58	0.68
1:A:241:GLU:O	1:A:245:MET:HG2	1.93	0.68
1:A:344:LEU:HD23	1:A:352:ALA:HA	1.75	0.68
1:B:227:ILE:HG13	1:B:232:LEU:HD13	1.76	0.68
1:A:88:CYS:SG	1:A:224:MET:HG2	2.34	0.67
1:B:335:GLU:O	1:B:339:GLU:HG2	1.94	0.67
1:A:125:THR:HG22	5:A:6168:HOH:O	1.93	0.67
1:B:98:HIS:O	1:B:102:GLU:HG2	1.93	0.67
1:B:243:LEU:O	1:B:247:MET:HG3	1.93	0.67
1:B:241:GLU:O	1:B:245:MET:HG2	1.95	0.67
1:B:189:VAL:HG11	5:B:6181:HOH:O	1.94	0.66
1:B:262:THR:HB	1:B:267:LEU:HD13	1.78	0.66
1:A:243:LEU:O	1:A:247:MET:HG3	1.96	0.66
1:A:344:LEU:HD11	1:A:351:PHE:HD2	1.60	0.66
1:B:306:ASP:HB3	1:B:309:LYS:HG3	1.77	0.66
1:A:118:TRP:O	1:A:121:HIS:HB2	1.97	0.65
1:B:364:LYS:HG3	1:B:365:ARG:H	1.60	0.65
1:A:131:ASN:HB3	5:A:6174:HOH:O	1.95	0.65
1:B:201:THR:HG22	1:B:203:SER:H	1.60	0.65
1:A:360:GLY:O	1:A:364:LYS:HE3	1.97	0.65
1:B:323:GLN:HG3	5:B:6226:HOH:O	1.95	0.65
1:B:258:MET:HB3	1:B:267:LEU:HD11	1.79	0.65
1:A:313:VAL:HA	1:A:316:LEU:HD11	1.78	0.65
1:A:277:ALA:HB2	1:A:303:GLY:HA3	1.78	0.64
1:B:182:SER:O	1:B:185:LEU:HB2	1.97	0.64
1:B:62:LEU:HD21	1:B:78:ARG:HA	1.78	0.64
1:A:208:ILE:O	1:A:212:LYS:HB3	1.98	0.63
1:A:193:THR:HB	5:A:6133:HOH:O	1.97	0.63
1:A:78:ARG:HB2	5:A:6323:HOH:O	1.97	0.63
1:A:78:ARG:HG2	5:A:6292:HOH:O	1.96	0.63
1:A:202:LEU:HA	1:A:284:VAL:HG11	1.81	0.63
1:A:160:ARG:HD2	1:A:227:ILE:HD11	1.81	0.63
1:A:263:PRO:HB2	1:A:265:GLU:OE1	1.98	0.62
1:A:301:ASN:HD22	1:A:309:LYS:HA	1.64	0.62
1:B:197:PHE:O	1:B:200:PHE:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ALA:O	1:A:287:LEU:HB2	1.98	0.62
1:A:238:GLY:O	1:A:242:GLU:HG3	2.00	0.62
1:A:9:VAL:O	1:A:13:ILE:HG12	1.98	0.62
1:B:286:PHE:CZ	1:B:316:LEU:HB3	2.35	0.61
1:B:319:GLU:HG3	5:B:6225:HOH:O	1.99	0.61
1:A:17:LEU:HD22	1:A:139:TRP:CD1	2.34	0.61
1:B:56:ASP:O	1:B:60:SER:HB3	1.99	0.61
1:A:62:LEU:O	1:A:66:PRO:HB3	2.01	0.61
1:A:270:VAL:HG13	5:A:6069:HOH:O	2.01	0.61
1:B:247:MET:HE3	1:B:359:TRP:HE3	1.65	0.60
1:B:235:VAL:HG21	1:B:351:PHE:CD2	2.36	0.60
1:A:318:GLU:HG2	1:A:319:GLU:N	2.17	0.60
1:B:272:THR:HB	1:B:275:GLN:HG3	1.84	0.60
1:A:181:ASP:OD2	1:A:183:ASN:HB2	2.01	0.60
1:A:54:VAL:HG22	1:A:221:PRO:O	2.01	0.60
1:A:1:MET:O	1:A:4:GLN:HB3	2.02	0.59
1:B:59:GLU:HG3	1:B:59:GLU:O	2.02	0.59
1:A:274:ILE:O	1:A:303:GLY:HA2	2.02	0.59
1:A:274:ILE:HG23	1:A:302:TYR:CD1	2.38	0.59
1:A:15:MET:O	1:A:19:GLU:HG3	2.02	0.59
1:A:337:VAL:O	1:A:341:ILE:HG13	2.03	0.58
1:B:326:TYR:O	1:B:329:TYR:HB3	2.03	0.58
1:A:197:PHE:CE2	1:A:299:LYS:HG3	2.38	0.58
1:B:148:PHE:O	1:B:154:LEU:HD22	2.04	0.58
1:A:277:ALA:HB2	1:A:303:GLY:CA	2.34	0.58
1:B:164:VAL:HG11	1:B:220:LEU:HD22	1.84	0.58
1:B:9:VAL:HG12	1:B:13:ILE:HD12	1.85	0.58
1:A:3:MET:HE1	5:A:6084:HOH:O	2.03	0.58
1:A:78:ARG:O	1:A:82:LEU:HG	2.05	0.57
1:A:88:CYS:SG	1:A:157:LEU:HD11	2.44	0.57
1:B:209:VAL:HG22	1:B:252:GLN:HG2	1.85	0.57
1:A:10:TYR:HB2	1:A:90:TRP:CZ2	2.40	0.57
1:A:148:PHE:O	1:A:151:ARG:HB2	2.04	0.57
1:A:28:ASP:OD2	1:A:30:ASN:HB2	2.05	0.56
1:B:140:THR:HA	1:B:143:MET:HE3	1.87	0.56
1:B:21:LEU:O	1:B:25:PHE:HB2	2.05	0.56
1:A:103:ASP:OD1	3:A:3001:M0N:H82	2.06	0.56
1:A:349:PRO:O	1:A:352:ALA:HB3	2.06	0.56
1:A:12:GLU:OE2	1:A:83:HIS:HE1	1.89	0.55
1:A:48:TYR:HA	1:A:93:GLU:OE2	2.07	0.55
1:B:15:MET:O	1:B:19:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ARG:HG3	5:B:6109:HOH:O	2.05	0.55
1:A:48:TYR:O	1:A:52:LEU:HG	2.06	0.55
1:A:209:VAL:CG1	1:A:249:GLU:HA	2.37	0.55
4:B:5001:PGO:H31	5:B:6289:HOH:O	2.07	0.55
1:A:357:THR:HG23	5:A:6016:HOH:O	2.06	0.55
1:A:264:PRO:HB3	1:A:269:LYS:O	2.07	0.55
1:A:301:ASN:ND2	1:A:309:LYS:HA	2.21	0.55
1:A:19:GLU:O	1:A:23:LEU:HD12	2.07	0.55
1:A:305:GLY:O	1:A:306:ASP:HB2	2.07	0.55
1:A:160:ARG:CD	1:A:227:ILE:HD11	2.37	0.55
1:B:10:TYR:HB2	1:B:90:TRP:CZ2	2.41	0.55
1:A:190:SER:O	1:A:192:PRO:HD3	2.08	0.54
1:A:309:LYS:O	1:A:313:VAL:HG23	2.08	0.54
1:B:110:VAL:HA	1:B:120:ARG:HD2	1.88	0.54
1:A:286:PHE:HB2	1:A:322:LEU:HD11	1.88	0.54
1:B:181:ASP:HB3	1:B:184:LYS:HD2	1.88	0.54
1:B:197:PHE:H	1:B:299:LYS:NZ	2.05	0.54
1:A:111:THR:HB	1:A:115:LYS:O	2.08	0.54
1:B:119:TYR:HD2	1:B:126:VAL:HG22	1.73	0.54
1:B:270:VAL:O	1:B:272:THR:HG23	2.07	0.53
1:B:278:LYS:HD3	1:B:279:CYS:N	2.22	0.53
1:A:172:GLN:HA	1:A:172:GLN:NE2	2.22	0.53
1:B:357:THR:O	1:B:361:LYS:HE2	2.08	0.53
1:A:36:ARG:HD3	1:A:37:LYS:HZ2	1.74	0.53
1:B:209:VAL:HG11	1:B:249:GLU:HG3	1.90	0.53
1:A:257:VAL:HG22	1:A:282:LEU:HD21	1.91	0.53
1:A:269:LYS:HE3	5:A:6217:HOH:O	2.08	0.53
1:B:125:THR:HB	1:B:127:GLN:HG2	1.91	0.52
1:B:345:ARG:HG3	1:B:345:ARG:HH11	1.74	0.52
1:A:186:ASP:OD2	1:A:189:VAL:HG22	2.10	0.52
1:B:34:TYR:HD1	1:B:35:LEU:HD13	1.74	0.52
1:A:157:LEU:HD21	1:A:224:MET:HG3	1.91	0.52
1:B:91:MET:SD	1:B:144:ALA:HB2	2.49	0.52
1:B:148:PHE:C	1:B:154:LEU:HD22	2.34	0.52
1:A:98:HIS:HD2	1:A:133:GLY:O	1.91	0.52
1:A:317:TYR:HA	1:A:322:LEU:HD12	1.91	0.52
1:A:317:TYR:O	1:A:322:LEU:HB2	2.10	0.52
1:A:318:GLU:HA	5:A:6251:HOH:O	2.10	0.52
1:B:18:LEU:HD22	1:B:32:VAL:HG13	1.91	0.52
1:A:334:ALA:O	1:A:338:LYS:HG3	2.10	0.52
1:B:245:MET:HE2	1:B:245:MET:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LYS:O	3:A:3001:M0N:H6	2.10	0.51
1:A:344:LEU:HD11	1:A:351:PHE:CD2	2.42	0.51
1:B:47:LYS:HZ1	1:B:367:LYS:NZ	2.08	0.51
1:A:138:SER:HA	5:A:6147:HOH:O	2.11	0.51
1:B:94:PHE:HB2	1:B:140:THR:HG22	1.93	0.51
1:B:83:HIS:HD2	5:B:6230:HOH:O	1.94	0.50
1:A:252:GLN:O	1:A:255:ASP:HB3	2.11	0.50
1:B:18:LEU:HD13	1:B:32:VAL:HG12	1.93	0.50
1:B:125:THR:HG21	1:B:127:GLN:NE2	2.25	0.50
1:A:62:LEU:C	1:A:66:PRO:HB3	2.36	0.50
1:A:71:GLU:CD	1:A:74:ASP:HB3	2.36	0.50
1:A:317:TYR:O	1:A:322:LEU:HD12	2.12	0.50
1:B:125:THR:CG2	1:B:127:GLN:HG2	2.42	0.50
1:A:90:TRP:O	1:A:94:PHE:HB2	2.11	0.50
1:A:220:LEU:HB3	1:A:221:PRO:HD3	1.94	0.50
1:A:297:GLU:O	1:A:300:ALA:HB3	2.12	0.50
1:A:326:TYR:O	1:A:329:TYR:HB3	2.12	0.50
1:B:180:PHE:HD2	1:B:192:PRO:O	1.95	0.49
1:A:232:LEU:HD23	1:A:232:LEU:H	1.77	0.49
1:A:245:MET:N	1:A:245:MET:HE2	2.27	0.49
1:B:19:GLU:O	1:B:23:LEU:HG	2.12	0.49
1:B:272:THR:CA	1:B:275:GLN:HG3	2.42	0.49
1:A:31:ARG:HG3	1:A:31:ARG:HH11	1.76	0.49
1:B:50:ARG:NH1	1:B:96:GLN:HE22	2.10	0.49
1:B:208:ILE:O	1:B:212:LYS:HG2	2.13	0.49
1:B:96:GLN:HB2	1:B:216:TYR:CE1	2.40	0.49
1:A:94:PHE:HB3	1:A:140:THR:HG22	1.93	0.49
1:A:217:THR:O	1:A:221:PRO:HG2	2.13	0.49
1:B:107:ASP:HB2	5:B:6004:HOH:O	2.12	0.49
1:B:194:THR:O	1:B:195:THR:O	2.30	0.49
1:B:99:TYR:HB3	3:B:4001:M0N:C4	2.43	0.49
1:A:231:ALA:O	1:A:234:THR:HG23	2.13	0.48
1:B:275:GLN:H	1:B:275:GLN:HG2	1.27	0.48
1:A:125:THR:HB	1:A:127:GLN:HG3	1.94	0.48
1:A:366:GLN:O	1:A:367:LYS:O	2.31	0.48
1:B:36:ARG:HH11	1:B:36:ARG:HG2	1.78	0.48
1:B:201:THR:HG22	1:B:203:SER:N	2.26	0.48
1:A:258:MET:HE1	1:A:367:LYS:HG2	1.95	0.48
1:B:194:THR:HB	5:B:6019:HOH:O	2.14	0.47
1:B:272:THR:O	1:B:275:GLN:HG3	2.14	0.47
1:A:57:VAL:O	1:A:61:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:THR:HA	1:A:143:MET:HE3	1.96	0.47
1:A:303:GLY:N	5:A:6224:HOH:O	2.47	0.47
1:B:149:ALA:HA	1:B:154:LEU:CD2	2.44	0.47
1:B:278:LYS:HG2	5:B:6040:HOH:O	2.13	0.47
1:B:148:PHE:CB	1:B:154:LEU:HD13	2.44	0.47
1:A:360:GLY:C	1:A:361:LYS:HD3	2.39	0.47
1:B:1:MET:HE1	5:B:6294:HOH:O	2.15	0.47
1:A:62:LEU:CD2	1:A:82:LEU:HD21	2.45	0.47
1:A:309:LYS:HB3	1:A:309:LYS:HE3	1.50	0.47
1:B:125:THR:HG21	1:B:127:GLN:HE21	1.79	0.47
1:A:156:ASP:HB2	5:A:6311:HOH:O	2.15	0.47
1:A:204:ASN:O	1:A:208:ILE:HG23	2.14	0.47
1:A:226:LEU:HD11	1:A:235:VAL:HG21	1.96	0.47
1:A:274:ILE:HG13	5:A:6258:HOH:O	2.14	0.46
1:B:255:ASP:HA	1:B:258:MET:HE2	1.98	0.46
1:B:215:TYR:CD2	1:B:219:LEU:HD23	2.51	0.46
1:B:88:CYS:SG	1:B:224:MET:HE2	2.55	0.46
1:B:112:ARG:O	1:B:113:ARG:HB2	2.15	0.46
1:B:200:PHE:CE1	1:B:279:CYS:HA	2.50	0.46
1:A:145:MET:SD	1:A:154:LEU:HD21	2.55	0.46
1:A:194:THR:HA	5:A:6037:HOH:O	2.16	0.46
1:A:301:ASN:HB3	1:A:309:LYS:O	2.15	0.46
1:A:361:LYS:HD2	5:A:6078:HOH:O	2.16	0.46
1:A:59:GLU:O	1:A:62:LEU:HG	2.15	0.46
1:A:117:CYS:HB3	5:A:6057:HOH:O	2.15	0.46
1:A:194:THR:HG23	1:A:197:PHE:H	1.81	0.46
1:B:157:LEU:HD11	1:B:224:MET:HE3	1.96	0.46
1:A:36:ARG:NH1	1:A:36:ARG:HG3	2.30	0.46
1:A:335:GLU:OE2	5:A:6329:HOH:O	2.20	0.46
1:B:112:ARG:NH2	3:B:4001:M0N:O6	2.49	0.46
1:A:117:CYS:O	1:A:120:ARG:HB2	2.16	0.46
1:B:315:ARG:HE	1:B:315:ARG:HB3	1.64	0.46
1:A:258:MET:CE	1:A:367:LYS:O	2.64	0.46
1:B:345:ARG:HG3	1:B:345:ARG:NH1	2.31	0.46
1:B:160:ARG:HD2	1:B:227:ILE:HD11	1.99	0.45
1:B:209:VAL:HG22	1:B:252:GLN:CG	2.46	0.45
1:A:226:LEU:HD21	1:A:351:PHE:CD1	2.51	0.45
1:A:82:LEU:N	1:A:82:LEU:HD23	2.31	0.45
1:A:265:GLU:H	1:A:265:GLU:CD	2.23	0.45
1:B:104:ASP:O	1:B:108:ASN:N	2.49	0.45
1:B:198:ALA:HB3	5:B:6121:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:GLU:HA	1:B:204:ASN:OD1	2.15	0.45
1:B:220:LEU:HB3	1:B:221:PRO:HD3	1.98	0.45
1:A:31:ARG:O	1:A:34:TYR:N	2.50	0.45
1:A:111:THR:HA	1:A:116:PRO:HA	1.98	0.45
1:A:313:VAL:O	1:A:316:LEU:HD12	2.16	0.45
1:A:70:GLY:HA2	1:A:77:ARG:HD3	1.99	0.45
1:A:167:THR:HG21	1:A:215:TYR:HB3	1.96	0.45
1:A:342:GLU:OE1	1:A:345:ARG:NH1	2.50	0.45
1:B:289:LYS:NZ	1:B:325:ASP:OD2	2.50	0.45
1:A:269:LYS:NZ	5:A:6229:HOH:O	2.50	0.45
1:B:155:GLN:H	1:B:155:GLN:HG3	1.48	0.45
1:A:14:GLN:HG3	1:A:18:LEU:CD1	2.47	0.45
1:A:301:ASN:HA	1:A:309:LYS:HE3	1.97	0.45
1:B:9:VAL:HG12	1:B:13:ILE:CD1	2.47	0.45
1:B:80:ARG:HG2	1:B:80:ARG:HH11	1.82	0.45
1:A:218:TYR:CD2	1:A:358:LEU:HD21	2.52	0.45
1:A:264:PRO:HD2	1:A:265:GLU:OE1	2.17	0.45
1:B:69:ASN:ND2	5:B:6018:HOH:O	2.50	0.45
1:A:35:LEU:HD21	1:A:135:LEU:HD13	1.98	0.45
1:A:103:ASP:CB	3:A:3001:M0N:H3	2.48	0.45
1:A:151:ARG:HA	1:A:152:PRO:HD3	1.69	0.45
1:B:79:LYS:HB2	1:B:79:LYS:HE2	1.47	0.45
1:B:252:GLN:NE2	1:B:255:ASP:OD2	2.50	0.45
1:B:345:ARG:NH2	1:B:356:GLU:OE2	2.50	0.45
1:A:53:THR:O	1:A:56:ASP:N	2.50	0.44
1:A:304:SER:CB	1:A:309:LYS:HE2	2.47	0.44
1:A:304:SER:N	5:A:6224:HOH:O	2.50	0.44
1:B:271:GLY:N	5:B:6236:HOH:O	2.49	0.44
1:B:357:THR:HG22	1:B:361:LYS:HE2	1.99	0.44
1:A:172:GLN:O	1:A:176:VAL:HG23	2.17	0.44
1:A:194:THR:HG21	1:A:197:PHE:HA	1.98	0.44
1:A:312:THR:O	1:A:315:ARG:N	2.50	0.44
1:B:113:ARG:NH2	5:B:6189:HOH:O	2.50	0.44
1:B:190:SER:O	1:B:192:PRO:HD3	2.18	0.44
1:A:109:SER:O	1:A:119:TYR:OH	2.30	0.44
1:B:111:THR:CG2	1:B:269:LYS:HA	2.40	0.44
1:B:65:SER:O	1:B:67:ASN:N	2.50	0.44
1:A:210:LYS:O	1:A:214:ALA:HB3	2.17	0.44
1:A:272:THR:HB	5:A:6330:HOH:O	2.16	0.44
1:A:287:LEU:HD12	1:A:295:VAL:HG22	2.00	0.44
1:A:293:ALA:HB2	5:A:6210:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:HG2	1:A:77:ARG:CZ	2.47	0.44
1:B:12:GLU:OE1	1:B:83:HIS:HE1	2.00	0.44
1:A:36:ARG:HD3	1:A:37:LYS:NZ	2.31	0.44
1:A:36:ARG:NH2	5:A:6091:HOH:O	2.50	0.44
1:A:84:ASP:OD2	1:A:151:ARG:NH2	2.50	0.44
1:A:115:LYS:HB3	1:A:116:PRO:HD2	1.99	0.44
1:A:272:THR:OG1	1:A:273:ASP:N	2.50	0.44
1:B:28:ASP:OD2	1:B:31:ARG:HG3	2.18	0.44
1:B:36:ARG:HG2	1:B:36:ARG:NH1	2.31	0.44
1:B:83:HIS:O	1:B:87:VAL:HG23	2.17	0.44
1:B:278:LYS:HD3	1:B:278:LYS:HA	1.55	0.43
1:B:306:ASP:HB3	1:B:309:LYS:CG	2.46	0.43
1:A:31:ARG:HG3	1:A:31:ARG:NH1	2.31	0.43
1:B:1:MET:O	1:B:4:GLN:HB3	2.18	0.43
1:B:206:LYS:NZ	5:B:6137:HOH:O	2.51	0.43
1:A:295:VAL:O	1:A:299:LYS:HD3	2.19	0.43
1:A:350:GLY:N	5:A:6288:HOH:O	2.50	0.43
1:B:82:LEU:HA	1:B:85:ALA:HB3	2.01	0.43
1:B:280:SER:O	1:B:283:ALA:HB3	2.19	0.43
1:A:182:SER:OG	1:A:199:GLU:OE1	2.37	0.43
1:B:136:LEU:HD23	1:B:139:TRP:HE3	1.83	0.43
1:A:88:CYS:O	1:A:92:ILE:HG13	2.19	0.43
1:B:143:MET:O	1:B:147:PHE:HD1	2.02	0.43
1:A:6:PHE:CE2	1:A:48:TYR:HB3	2.53	0.43
1:A:302:TYR:HD1	1:A:313:VAL:HG11	1.83	0.43
1:B:112:ARG:HH22	3:B:4001:M0N:P2	2.42	0.43
1:B:1:MET:HB3	1:B:2:PRO:HD3	2.01	0.43
1:B:258:MET:HG2	5:B:6266:HOH:O	2.18	0.43
1:A:133:GLY:O	1:A:136:LEU:HB2	2.19	0.42
1:A:317:TYR:CA	1:A:322:LEU:HD12	2.49	0.42
1:B:132:ASP:O	1:B:135:LEU:HB2	2.19	0.42
1:B:167:THR:HG23	1:B:211:TYR:HD2	1.83	0.42
1:A:205:TYR:HB2	1:A:284:VAL:HG21	2.00	0.42
1:A:243:LEU:HA	1:A:246:LEU:HB2	1.99	0.42
1:B:136:LEU:HD23	1:B:139:TRP:CE3	2.54	0.42
1:B:315:ARG:HD2	5:B:6225:HOH:O	2.18	0.42
1:A:56:ASP:O	1:A:60:SER:OG	2.30	0.42
1:B:148:PHE:HB3	1:B:154:LEU:HD13	1.99	0.42
1:B:310:VAL:O	1:B:313:VAL:N	2.53	0.42
1:B:358:LEU:HD23	1:B:358:LEU:HA	1.87	0.42
1:A:3:MET:O	1:A:7:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TYR:O	1:A:222:LEU:HG	2.19	0.42
1:B:149:ALA:HA	1:B:154:LEU:HD22	2.02	0.42
1:A:281:TRP:CE3	1:A:282:LEU:HD23	2.54	0.42
1:B:47:LYS:NZ	1:B:367:LYS:NZ	2.67	0.42
1:B:151:ARG:NH1	5:B:6033:HOH:O	2.52	0.42
1:B:263:PRO:HB3	1:B:265:GLU:OE1	2.20	0.42
1:A:157:LEU:HD23	1:A:157:LEU:HA	1.83	0.42
1:B:155:GLN:NE2	1:B:156:ASP:H	2.18	0.42
1:B:47:LYS:NZ	1:B:367:LYS:HZ2	2.18	0.42
1:B:309:LYS:HZ2	1:B:309:LYS:HG2	1.74	0.42
1:A:49:ASN:HD22	1:A:49:ASN:HA	1.58	0.42
1:A:253:VAL:HG22	1:A:281:TRP:CD1	2.54	0.42
1:B:194:THR:O	1:B:194:THR:OG1	2.30	0.42
1:A:232:LEU:HD23	1:A:232:LEU:N	2.34	0.42
1:B:125:THR:CB	1:B:127:GLN:HG2	2.49	0.42
1:A:36:ARG:HG3	1:A:36:ARG:HH11	1.85	0.42
1:A:50:ARG:HH11	1:A:50:ARG:HD3	1.67	0.42
1:A:92:ILE:HG23	1:A:220:LEU:HD23	2.01	0.42
1:A:164:VAL:HA	1:A:167:THR:CG2	2.50	0.42
1:A:272:THR:HG21	5:A:6217:HOH:O	2.19	0.42
1:B:137:LYS:NZ	1:B:165:ASP:OD2	2.52	0.42
1:B:195:THR:HG22	1:B:196:ASP:N	2.35	0.42
1:A:329:TYR:O	1:A:333:VAL:HG23	2.20	0.41
1:B:71:GLU:OE2	1:B:74:ASP:OD1	2.38	0.41
1:A:98:HIS:CE1	1:A:137:LYS:HE3	2.54	0.41
1:A:103:ASP:CG	3:A:3001:M0N:H3	2.44	0.41
1:B:35:LEU:HD12	1:B:35:LEU:HA	1.78	0.41
1:B:101:VAL:O	1:B:105:ILE:HG13	2.20	0.41
1:B:249:GLU:O	1:B:249:GLU:HG2	2.20	0.41
1:A:253:VAL:HG11	1:A:329:TYR:CE2	2.55	0.41
1:A:312:THR:HG23	1:A:315:ARG:CZ	2.49	0.41
1:A:349:PRO:O	1:A:352:ALA:N	2.53	0.41
1:B:151:ARG:NH2	5:B:6289:HOH:O	2.53	0.41
1:B:338:LYS:HB2	1:B:338:LYS:HE3	1.19	0.41
1:A:9:VAL:HG12	1:A:13:ILE:HD11	2.02	0.41
1:A:148:PHE:HB2	1:A:154:LEU:HD13	2.02	0.41
1:B:247:MET:HE2	1:B:247:MET:HB3	1.90	0.41
1:A:94:PHE:CB	1:A:140:THR:HG22	2.50	0.41
1:A:117:CYS:HB2	1:A:119:TYR:CE1	2.55	0.41
1:A:334:ALA:O	1:A:338:LYS:HB2	2.20	0.41
5:A:6321:HOH:O	1:B:364:LYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ASN:HD22	1:B:30:ASN:HA	1.68	0.41
1:B:208:ILE:HD12	1:B:208:ILE:HG21	1.78	0.41
1:B:274:ILE:O	1:B:277:ALA:N	2.49	0.41
1:B:91:MET:HE2	1:B:91:MET:HB3	1.89	0.41
1:B:184:LYS:HB3	5:B:6181:HOH:O	2.19	0.41
1:B:272:THR:CB	1:B:275:GLN:HG3	2.47	0.41
1:A:96:GLN:O	1:A:100:LEU:HG	2.21	0.41
1:B:16:PHE:HE1	5:B:6092:HOH:O	2.02	0.41
1:B:50:ARG:NH2	1:B:96:GLN:OE1	2.54	0.41
1:A:10:TYR:OH	1:A:40:ASP:HA	2.21	0.41
1:B:98:HIS:HD2	1:B:133:GLY:O	2.03	0.41
1:B:204:ASN:O	1:B:208:ILE:HG23	2.20	0.41
1:A:27:MET:HG2	1:A:32:VAL:HG23	2.03	0.41
1:B:36:ARG:HD3	5:B:6243:HOH:O	2.19	0.41
1:B:99:TYR:HB3	3:B:4001:M0N:H4	2.02	0.41
1:A:104:ASP:O	1:A:108:ASN:N	2.54	0.41
1:A:123:ASP:OD1	1:A:123:ASP:O	2.39	0.41
1:A:252:GLN:O	1:A:255:ASP:N	2.53	0.41
1:A:335:GLU:O	1:A:338:LYS:HB2	2.20	0.41
1:A:361:LYS:HD3	1:A:361:LYS:N	2.35	0.41
1:B:110:VAL:HB	1:B:120:ARG:HH11	1.83	0.40
1:B:94:PHE:O	1:B:97:ALA:HB3	2.21	0.40
1:B:104:ASP:HA	5:B:6004:HOH:O	2.19	0.40
1:B:151:ARG:HH11	1:B:151:ARG:HG2	1.86	0.40
1:B:274:ILE:HD13	1:B:313:VAL:CG1	2.50	0.40
1:A:79:LYS:H	1:A:79:LYS:HG2	1.72	0.40
1:B:83:HIS:CD2	5:B:6230:HOH:O	2.72	0.40
1:A:62:LEU:HD23	1:A:82:LEU:HD21	2.04	0.40
1:B:54:VAL:HG22	1:B:221:PRO:O	2.21	0.40
1:B:65:SER:N	1:B:66:PRO:HD3	2.35	0.40
1:B:218:TYR:O	1:B:222:LEU:HD12	2.22	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	366/390 (94%)	322 (88%)	33 (9%)	11 (3%)	3	4
1	B	366/390 (94%)	322 (88%)	36 (10%)	8 (2%)	5	8
All	All	732/780 (94%)	644 (88%)	69 (9%)	19 (3%)	4	6

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	ASP
1	A	306	ASP
1	B	185	LEU
1	B	195	THR
1	B	364	LYS
1	A	46	GLY
1	A	346	LEU
1	B	365	ARG
1	A	265	GLU
1	B	68	ASN
1	B	191	GLN
1	A	149	ALA
1	B	73	ASP
1	A	71	GLU
1	B	66	PRO
1	A	187	PRO
1	A	122	PRO
1	A	66	PRO
1	A	348	SER

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	322/340 (95%)	253 (79%)	69 (21%)	1	1
1	B	322/340 (95%)	256 (80%)	66 (20%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	644/680 (95%)	509 (79%)	135 (21%)	1 2

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	15	MET
1	A	24	LYS
1	A	26	ASP
1	A	47	LYS
1	A	50	ARG
1	A	60	SER
1	A	61	LEU
1	A	64	LEU
1	A	65	SER
1	A	67	ASN
1	A	71	GLU
1	A	72	GLU
1	A	73	ASP
1	A	77	ARG
1	A	80	ARG
1	A	105	ILE
1	A	107	ASP
1	A	125	THR
1	A	126	VAL
1	A	145	MET
1	A	151	ARG
1	A	155	GLN
1	A	157	LEU
1	A	163	ARG
1	A	173	LEU
1	A	180	PHE
1	A	186	ASP
1	A	189	VAL
1	A	191	GLN
1	A	193	THR
1	A	194	THR
1	A	197	PHE
1	A	202	LEU
1	A	208	ILE
1	A	209	VAL
1	A	212	LYS

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Mol	Chain	Res	Type
1	A	219	LEU
1	A	224	MET
1	A	227	ILE
1	A	228	VAL
1	A	229	SER
1	A	230	GLU
1	A	243	LEU
1	A	246	LEU
1	A	267	LEU
1	A	269	LYS
1	A	270	VAL
1	A	272	THR
1	A	275	GLN
1	A	276	ASP
1	A	278	LYS
1	A	285	THR
1	A	287	LEU
1	A	295	VAL
1	A	308	GLU
1	A	309	LYS
1	A	316	LEU
1	A	318	GLU
1	A	322	LEU
1	A	325	ASP
1	A	330	GLU
1	A	337	VAL
1	A	338	LYS
1	A	339	GLU
1	A	342	GLU
1	A	343	LYS
1	A	346	LEU
1	A	364	LYS
1	B	1	MET
1	B	3	MET
1	B	8	GLN
1	B	13	ILE
1	B	18	LEU
1	B	22	GLU
1	B	23	LEU
1	B	28	ASP
1	B	30	ASN
1	B	35	LEU

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Mol	Chain	Res	Type
1	B	47	LYS
1	B	59	GLU
1	B	60	SER
1	B	61	LEU
1	B	62	LEU
1	B	64	LEU
1	B	71	GLU
1	B	79	LYS
1	B	105	ILE
1	B	110	VAL
1	B	111	THR
1	B	112	ARG
1	B	115	LYS
1	B	123	ASP
1	B	125	THR
1	B	155	GLN
1	B	157	LEU
1	B	159	CYS
1	B	176	VAL
1	B	180	PHE
1	B	185	LEU
1	B	193	THR
1	B	194	THR
1	B	196	ASP
1	B	203	SER
1	B	208	ILE
1	B	209	VAL
1	B	232	LEU
1	B	234	THR
1	B	235	VAL
1	B	246	LEU
1	B	255	ASP
1	B	258	MET
1	B	265	GLU
1	B	270	VAL
1	B	273	ASP
1	B	275	GLN
1	B	278	LYS
1	B	292	SER
1	B	297	GLU
1	B	304	SER
1	B	307	SER

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Mol	Chain	Res	Type
1	B	315	ARG
1	B	322	LEU
1	B	338	LYS
1	B	339	GLU
1	B	340	LEU
1	B	341	ILE
1	B	343	LYS
1	B	344	LEU
1	B	346	LEU
1	B	348	SER
1	B	358	LEU
1	B	361	LYS
1	B	366	GLN
1	B	367	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	67	ASN
1	A	83	HIS
1	A	98	HIS
1	A	121	HIS
1	A	127	GLN
1	A	183	ASN
1	A	191	GLN
1	A	204	ASN
1	A	301	ASN
1	B	4	GLN
1	B	30	ASN
1	B	83	HIS
1	B	98	HIS
1	B	108	ASN
1	B	127	GLN
1	B	131	ASN
1	B	155	GLN
1	B	162	ASN
1	B	254	GLN
1	B	323	GLN
1	B	366	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	M0N	A	3001	2	20,21,21	3.43	8 (40%)	30,34,34	2.72	13 (43%)
4	PGO	A	5002	-	4,4,4	1.31	1 (25%)	4,4,4	2.08	1 (25%)
3	M0N	B	4001	2	20,21,21	3.34	9 (45%)	30,34,34	2.63	11 (36%)
4	PGO	A	5003	-	4,4,4	1.33	1 (25%)	4,4,4	2.04	1 (25%)
4	PGO	B	5001	-	4,4,4	1.33	1 (25%)	4,4,4	2.15	1 (25%)

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
3	M0N	A	3001	2	-	5/23/23/23	0/2/2/2
4	PGO	A	5002	-	-	2/2/2/2	-
3	M0N	B	4001	2	-	5/23/23/23	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGO	A	5003	-	-	2/2/2/2	-
4	PGO	B	5001	-	-	2/2/2/2	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3001	M0N	C8-C9	-10.09	1.36	1.55
3	B	4001	M0N	C8-C9	-9.64	1.37	1.55
3	B	4001	M0N	P1-C9	-6.63	1.80	1.85
3	A	3001	M0N	P1-C9	-6.23	1.80	1.85
3	A	3001	M0N	P2-C9	-5.16	1.81	1.85
3	B	4001	M0N	C2-N2	4.17	1.44	1.39
3	B	4001	M0N	P2-O6	4.11	1.57	1.50
3	B	4001	M0N	P1-O3	4.09	1.57	1.50
3	A	3001	M0N	P2-O6	4.08	1.57	1.50
3	A	3001	M0N	P1-O3	3.76	1.56	1.50
3	A	3001	M0N	C2-N2	3.45	1.43	1.39
3	B	4001	M0N	P2-C9	-3.28	1.82	1.85
3	A	3001	M0N	C7-N1	2.65	1.37	1.33
3	B	4001	M0N	C7-N1	2.53	1.37	1.33
3	B	4001	M0N	P1-O2	-2.45	1.48	1.54
4	B	5001	PGO	C1-C2	2.43	1.59	1.46
4	A	5003	PGO	C1-C2	2.40	1.59	1.46
4	A	5002	PGO	C1-C2	2.37	1.58	1.46
3	A	3001	M0N	P1-O2	-2.26	1.49	1.54
3	B	4001	M0N	C7-N2	2.02	1.42	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3001	M0N	O1-P1-O2	6.06	125.33	108.24
3	B	4001	M0N	C1-N1-C7	5.85	109.01	105.11
3	A	3001	M0N	C1-N1-C7	5.82	108.99	105.11
3	B	4001	M0N	N2-C7-N1	-5.38	106.92	111.02
3	A	3001	M0N	N2-C7-N1	-5.16	107.09	111.02
3	A	3001	M0N	O2-P1-O3	-4.81	101.18	112.96
3	B	4001	M0N	C3-N2-C7	-4.56	117.27	121.97
3	B	4001	M0N	C3-N2-C2	4.01	134.90	130.09
3	B	4001	M0N	O1-P1-O3	-4.00	103.16	112.96
3	B	4001	M0N	O3-P1-C9	-3.84	99.98	109.82
3	A	3001	M0N	C3-N2-C7	-3.53	118.34	121.97
3	B	4001	M0N	C6-C7-N2	3.50	121.72	118.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3001	M0N	O1-P1-C9	-3.43	98.63	106.19
3	A	3001	M0N	O2-P1-C9	3.42	113.70	106.19
3	A	3001	M0N	C3-N2-C2	3.34	134.09	130.09
3	B	4001	M0N	O6-P2-C9	-3.27	101.44	109.82
3	A	3001	M0N	C6-C7-N2	3.26	121.49	118.41
3	B	4001	M0N	O5-P2-C9	3.22	113.28	106.19
3	B	4001	M0N	O-C9-C8	3.06	117.86	110.56
4	B	5001	PGO	O2-C2-C1	-2.92	100.68	114.99
3	A	3001	M0N	O5-P2-C9	2.92	112.61	106.19
4	A	5002	PGO	O2-C2-C1	-2.84	101.07	114.99
4	A	5003	PGO	O2-C2-C1	-2.84	101.08	114.99
3	A	3001	M0N	O6-P2-C9	-2.80	102.64	109.82
3	A	3001	M0N	P1-C9-O	-2.64	101.37	107.42
3	B	4001	M0N	O2-P1-C9	2.48	111.64	106.19
3	A	3001	M0N	O-C9-C8	2.13	115.64	110.56

There are no chirality outliers.

All (16) torsion outliers are listed below:

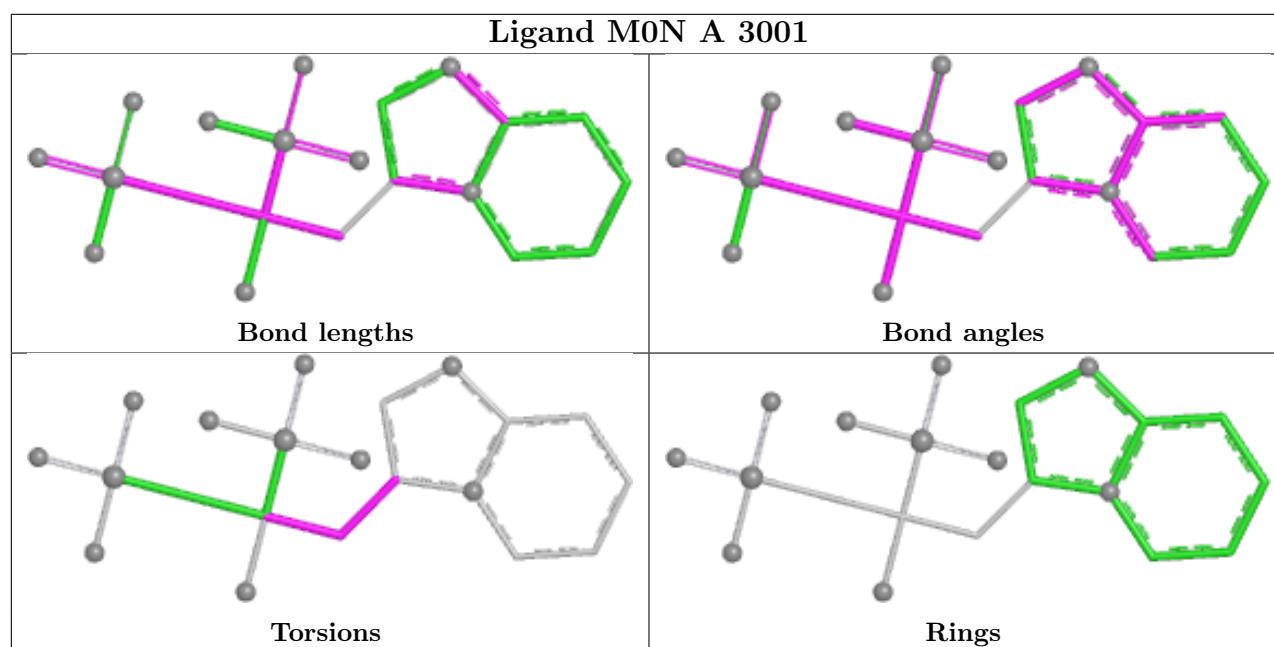
Mol	Chain	Res	Type	Atoms
3	A	3001	M0N	C2-C8-C9-O
3	A	3001	M0N	C1-C2-C8-C9
3	A	3001	M0N	N2-C2-C8-C9
3	B	4001	M0N	O-C9-P1-O3
3	B	4001	M0N	C1-C2-C8-C9
3	B	4001	M0N	N2-C2-C8-C9
4	A	5002	PGO	O1-C1-C2-O2
4	A	5003	PGO	O1-C1-C2-C3
4	A	5003	PGO	O1-C1-C2-O2
4	B	5001	PGO	O1-C1-C2-O2
4	A	5002	PGO	O1-C1-C2-C3
4	B	5001	PGO	O1-C1-C2-C3
3	A	3001	M0N	C2-C8-C9-P2
3	A	3001	M0N	C2-C8-C9-P1
3	B	4001	M0N	C8-C9-P1-O3
3	B	4001	M0N	P2-C9-P1-O3

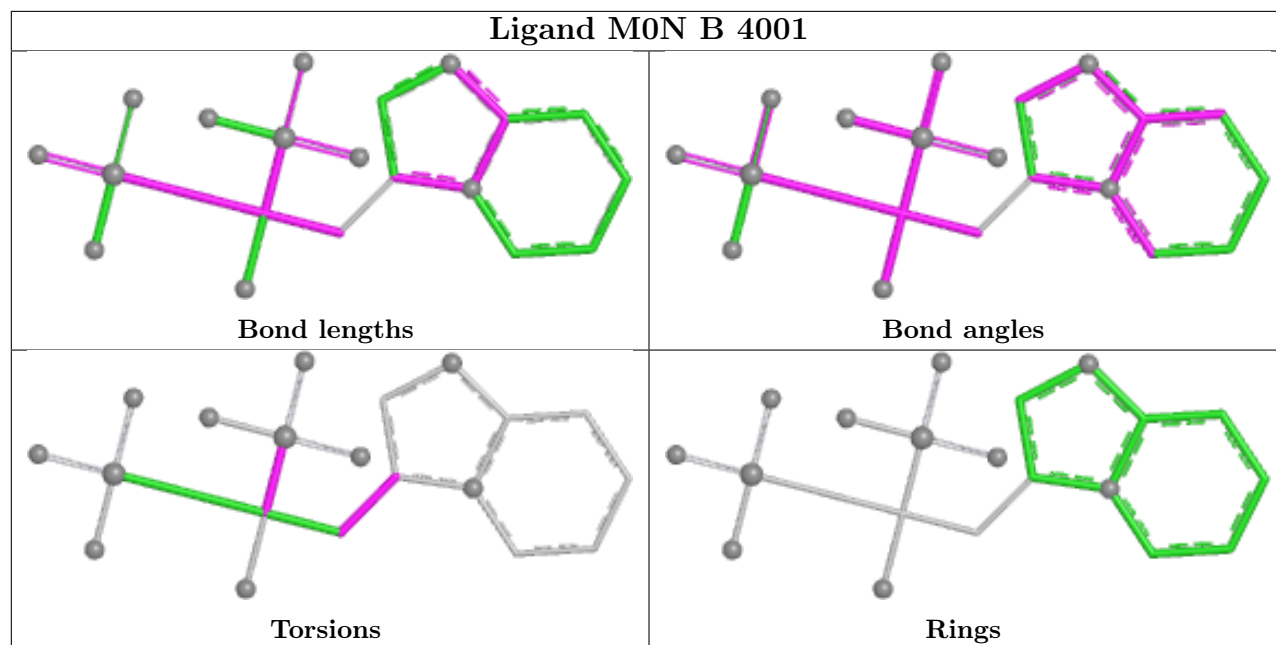
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	M0N	4	0
3	B	4001	M0N	4	0
4	B	5001	PGO	1	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, 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	367/390 (94%)	-0.02	3 (0%) 82 80	13, 34, 67, 94	1 (0%)
1	B	367/390 (94%)	-0.06	6 (1%) 70 68	12, 31, 64, 92	1 (0%)
All	All	734/780 (94%)	-0.04	9 (1%) 76 74	12, 32, 66, 94	2 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	123	ASP	3.4
1	B	272	THR	2.9
1	A	123	ASP	2.8
1	B	68	ASN	2.4
1	B	69	ASN	2.3
1	A	180	PHE	2.3
1	B	270	VAL	2.1
1	A	191	GLN	2.0
1	B	179	MET	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

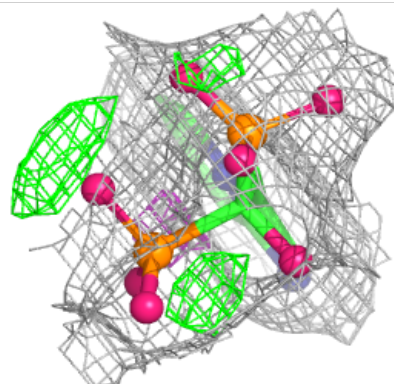
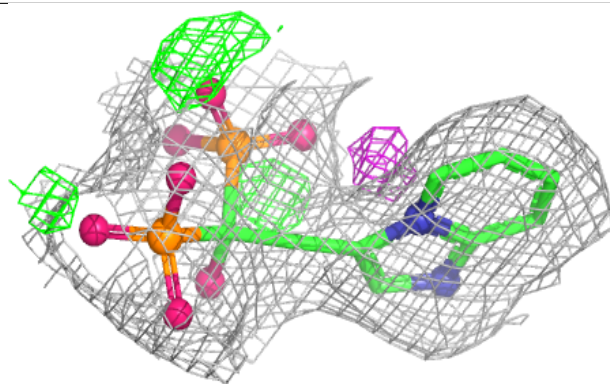
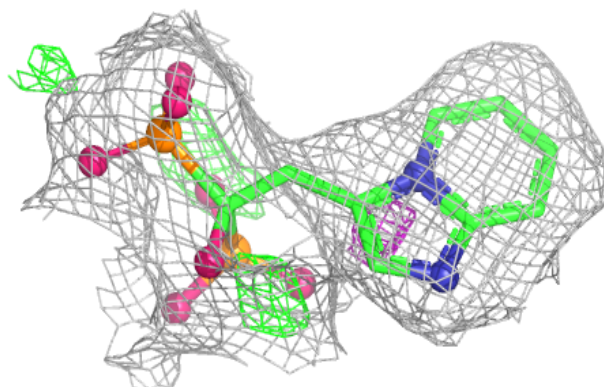
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

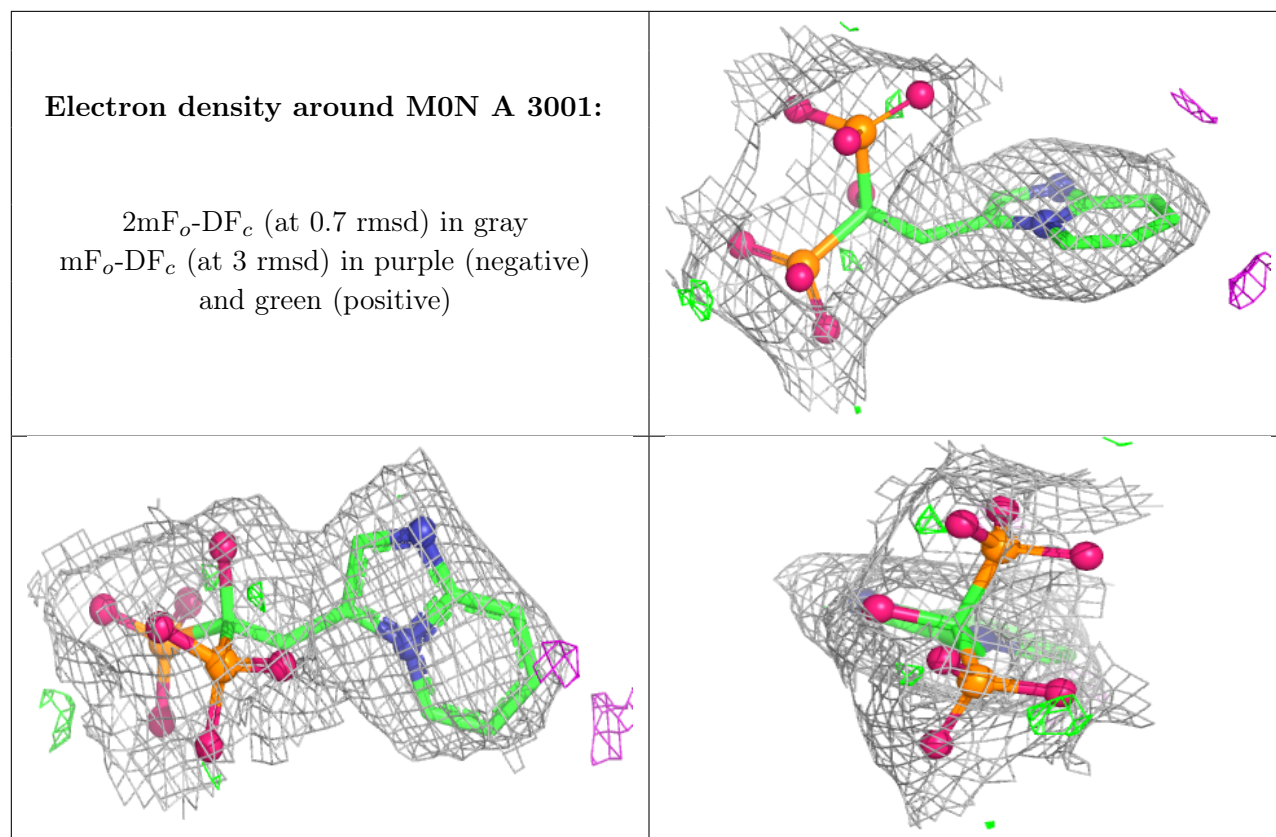
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PGO	A	5002	5/5	0.54	0.14	59,67,73,83	0
4	PGO	A	5003	5/5	0.66	0.13	58,60,64,65	0
4	PGO	B	5001	5/5	0.79	0.25	16,23,28,32	5
2	MG	A	3004	1/1	0.90	0.04	21,21,21,21	0
2	MG	A	3003	1/1	0.93	0.05	19,19,19,19	0
3	M0N	B	4001	20/20	0.94	0.08	24,30,37,40	0
2	MG	B	4004	1/1	0.95	0.08	11,11,11,11	0
3	M0N	A	3001	20/20	0.95	0.09	29,35,38,39	0
2	MG	B	4002	1/1	0.97	0.11	35,35,35,35	0
2	MG	B	4003	1/1	0.98	0.09	19,19,19,19	0
2	MG	A	3002	1/1	0.99	0.03	17,17,17,17	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 M0N B 4001:

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.