



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:24 AM UTC

PDB ID : 6LFZ / pdb_00006lfz
Title : Crystal structure of SbCGTb in complex with UDPG
Authors : Gao, H.M.; Yun, C.H.
Deposited on : 2019-12-04
Resolution : 2.87 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

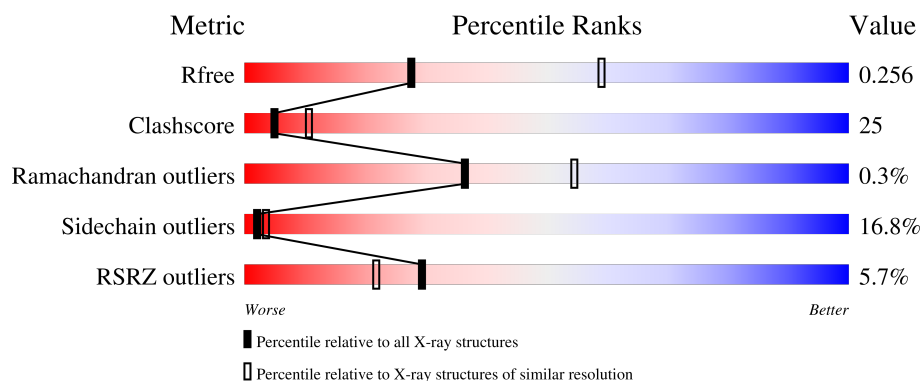
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	459	5% 57% 32% 5% 5%
1	B	459	6% 51% 34% 10% .

2 Entry composition [i](#)

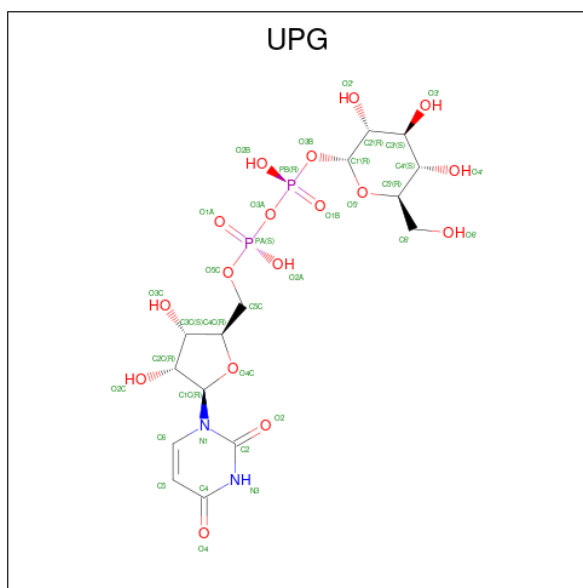
There are 3 unique types of molecules in this entry. The entry contains 6852 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SbCGTb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3333	2143	579	603	8			
1	B	439	Total	C	N	O	S	0	0	0
			3394	2180	596	609	9			

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

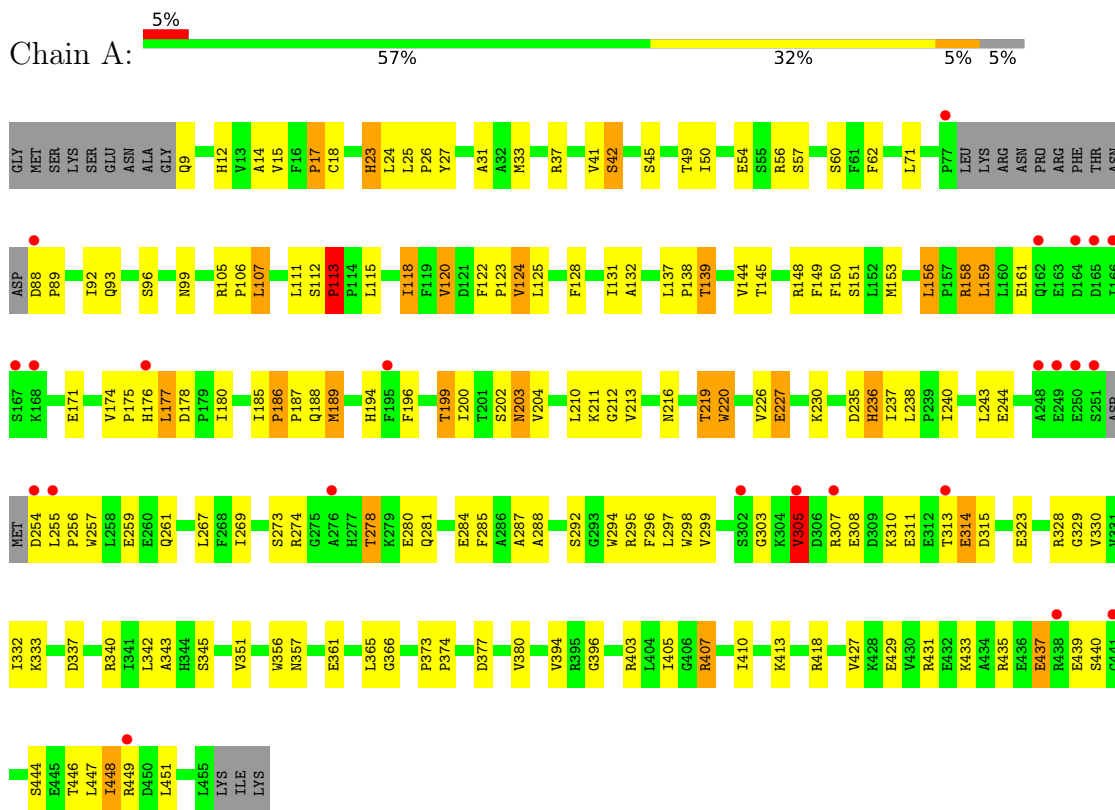
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total 34	O 34	0	0
3	B	19	Total 19	O 19	0	0

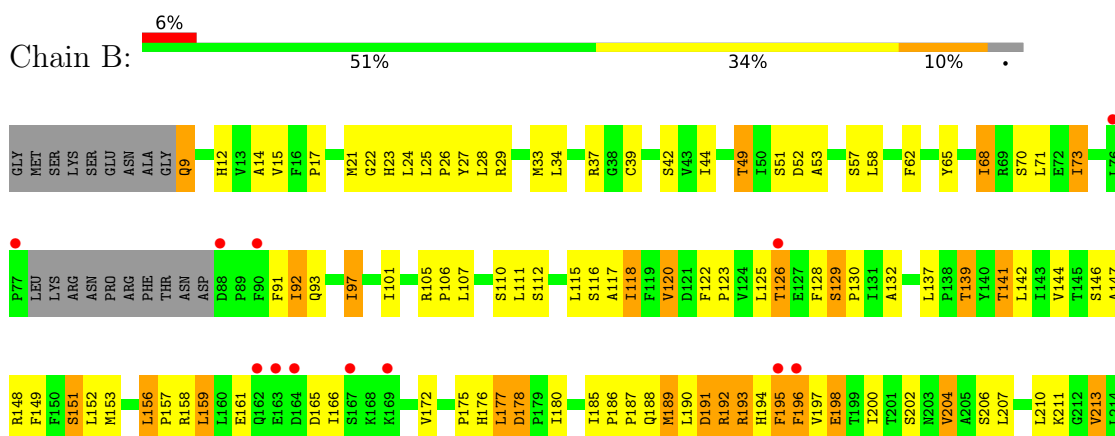
3 Residue-property plots

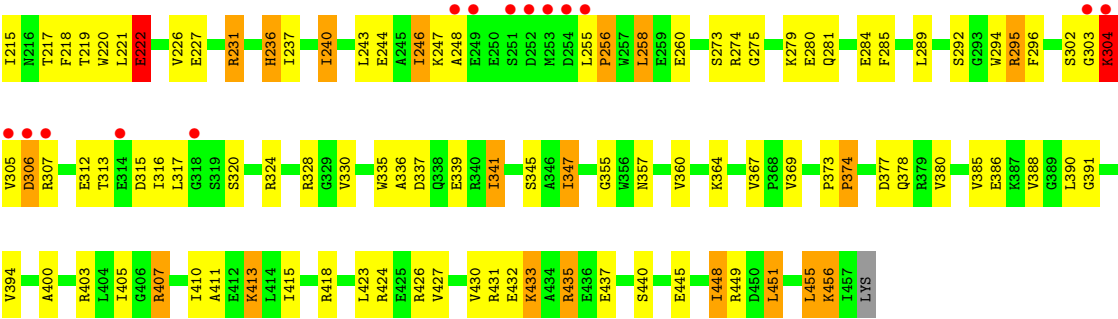
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: SbCGTb





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	107.29Å 216.95Å 104.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.16 – 2.87 36.16 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.3 (36.16-2.87) 99.2 (36.16-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.218 , 0.254 0.221 , 0.256	Depositor DCC
R_{free} test set	1337 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6852	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: UPG

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	1.16	6/3412 (0.2%)	1.34	14/4636 (0.3%)
1	B	1.01	2/3475 (0.1%)	1.17	18/4720 (0.4%)
All	All	1.09	8/6887 (0.1%)	1.26	32/9356 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	222	GLU	C-O	-6.17	1.16	1.23
1	A	238	LEU	C-O	-6.07	1.20	1.25
1	A	17	PRO	C-O	-5.68	1.17	1.23
1	B	373	PRO	C-O	-5.57	1.18	1.24
1	A	186	PRO	C-O	-5.57	1.18	1.24
1	A	175	PRO	C-O	-5.36	1.17	1.23
1	A	373	PRO	C-O	-5.30	1.18	1.24
1	A	113	PRO	C-O	-5.29	1.18	1.24

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	ASP	N-CA-C	-9.65	100.37	113.30
1	A	113	PRO	N-CA-C	-7.61	101.41	110.70
1	B	23	HIS	N-CA-C	7.58	119.62	111.36
1	B	126	THR	CB-CA-C	-7.24	99.80	110.96
1	A	305	VAL	N-CA-C	6.94	117.73	110.72
1	B	196	PHE	N-CA-C	-6.84	103.83	111.28
1	A	315	ASP	N-CA-C	-6.55	104.76	112.89
1	A	307	ARG	CB-CA-C	-6.36	100.81	110.92
1	B	456	LYS	N-CA-C	-6.20	104.69	112.93
1	B	248	ALA	CA-C-N	6.13	128.49	120.28
1	B	248	ALA	C-N-CA	6.13	128.49	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	296	PHE	N-CA-C	6.04	118.59	109.23
1	B	192	ARG	N-CA-C	5.85	117.74	111.36
1	A	23	HIS	N-CA-C	5.78	117.66	111.36
1	B	355	GLY	N-CA-C	-5.72	104.77	112.14
1	B	256	PRO	N-CA-C	5.50	121.18	113.53
1	B	304	LYS	N-CA-C	-5.44	99.22	110.80
1	A	315	ASP	CA-C-N	5.35	128.01	120.42
1	A	315	ASP	C-N-CA	5.35	128.01	120.42
1	B	306	ASP	N-CA-C	5.30	118.05	109.40
1	A	305	VAL	CA-C-N	-5.30	115.51	122.99
1	A	305	VAL	C-N-CA	-5.30	115.51	122.99
1	B	206	SER	N-CA-C	-5.22	106.97	113.19
1	B	92	ILE	CB-CA-C	-5.19	105.13	112.14
1	A	176	HIS	CB-CA-C	5.18	120.25	110.35
1	A	62	PHE	CB-CA-C	5.16	119.35	110.79
1	B	204	VAL	CA-C-O	-5.13	115.71	121.05
1	B	222	GLU	CA-C-O	-5.10	116.08	121.29
1	A	42	SER	CA-C-N	-5.10	116.51	122.93
1	A	42	SER	C-N-CA	-5.10	116.51	122.93
1	B	178	ASP	N-CA-C	-5.09	103.18	109.64
1	A	203	ASN	CB-CA-C	5.07	120.01	110.63

There are no chirality outliers.

There are no planarity outliers.

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	3333	0	3267	140	0
1	B	3394	0	3358	200	0
2	A	36	0	22	1	0
2	B	36	0	22	4	0
3	A	34	0	0	6	0
3	B	19	0	0	5	0
All	All	6852	0	6669	338	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 25.

All (338) 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:112:SER:OG	1:A:113:PRO:HD3	1.17	1.27
1:B:193:ARG:HG3	1:B:193:ARG:HH11	1.04	1.15
1:B:295:ARG:HH21	1:B:295:ARG:CG	1.68	1.06
1:B:166:ILE:CB	1:B:190:LEU:HD22	1.88	1.04
1:B:117:ALA:HB2	1:B:455:LEU:HD21	1.42	1.01
1:B:295:ARG:HH21	1:B:295:ARG:HG2	0.87	1.00
1:A:112:SER:OG	1:A:113:PRO:CD	2.09	1.00
1:B:374:PRO:HD2	1:B:378:GLN:OE1	1.59	1.00
1:B:295:ARG:HG2	1:B:295:ARG:NH2	1.70	0.99
1:B:193:ARG:HG3	1:B:193:ARG:NH1	1.74	0.97
1:A:37:ARG:HG3	1:A:37:ARG:HH11	1.31	0.93
1:B:186:PRO:HD2	1:B:189:MET:HE3	1.48	0.92
1:A:185:ILE:HG23	1:A:189:MET:HE3	1.54	0.88
1:A:437:GLU:HG2	1:A:444:SER:OG	1.74	0.87
1:A:274:ARG:HD2	1:A:305:VAL:HA	1.55	0.87
1:B:149:PHE:CD1	1:B:377:ASP:HB2	2.10	0.87
1:B:213:VAL:HG22	1:B:237:ILE:HD12	1.55	0.86
1:A:49:THR:HG21	1:A:54:GLU:HB2	1.55	0.86
1:A:105:ARG:HB2	1:A:106:PRO:HD3	1.57	0.86
1:B:191:ASP:OD1	1:B:194:HIS:HB2	1.76	0.85
1:B:407:ARG:HG2	1:B:407:ARG:HH11	1.40	0.85
1:A:357:ASN:O	1:A:361:GLU:HG3	1.77	0.84
1:B:29:ARG:HG2	1:B:244:GLU:O	1.78	0.84
1:B:204:VAL:O	1:B:207:LEU:HB2	1.77	0.84
1:A:112:SER:CB	1:A:113:PRO:HD3	2.07	0.83
1:B:33:MET:HE1	1:B:243:LEU:HD23	1.59	0.83
1:B:407:ARG:HG2	1:B:407:ARG:NH1	1.94	0.83
1:A:150:PHE:HA	1:A:153:MET:HE3	1.61	0.82
1:B:73:ILE:HD11	1:B:107:LEU:HD22	1.62	0.82
1:A:112:SER:HG	1:A:113:PRO:HD3	1.04	0.81
1:B:394:VAL:CG2	1:B:413:LYS:HE3	2.10	0.81
1:B:220:TRP:CE2	1:B:433:LYS:HG2	2.16	0.81
1:B:21:MET:HE1	1:B:57:SER:OG	1.82	0.80
1:A:356:TRP:HD1	3:A:622:HOH:O	1.64	0.79
1:B:200:ILE:O	1:B:204:VAL:HG23	1.82	0.79
1:B:49:THR:CG2	1:B:51:SER:O	2.30	0.79
1:A:174:VAL:HB	1:A:177:LEU:HD11	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:SER:CB	1:B:312:GLU:OE2	2.32	0.78
1:A:18:CYS:SG	1:A:124:VAL:HG22	2.23	0.77
1:B:407:ARG:HH11	1:B:407:ARG:CG	1.97	0.77
1:B:426:ARG:HD2	3:B:612:HOH:O	1.85	0.77
1:B:149:PHE:CG	1:B:377:ASP:HB2	2.20	0.76
1:B:426:ARG:O	1:B:430:VAL:HG23	1.84	0.76
1:A:33:MET:HE1	1:A:243:LEU:HD23	1.69	0.75
1:A:278:THR:HG22	1:A:281:GLN:H	1.50	0.74
1:B:316:ILE:HG22	1:B:317:LEU:HD23	1.70	0.74
1:B:374:PRO:CB	1:B:400:ALA:HB2	2.18	0.73
1:B:426:ARG:CD	3:B:612:HOH:O	2.37	0.73
1:B:159:LEU:HD23	1:B:159:LEU:O	1.89	0.72
1:B:451:LEU:HD12	1:B:451:LEU:C	2.13	0.72
1:B:148:ARG:HG2	1:B:380:VAL:CG1	2.20	0.72
1:B:105:ARG:HB2	1:B:106:PRO:HD3	1.69	0.72
1:B:144:VAL:HG23	2:B:500:UPG:O6'	1.90	0.72
1:B:148:ARG:NH1	1:B:178:ASP:HB3	2.05	0.72
1:B:394:VAL:HG22	1:B:413:LYS:HE3	1.70	0.72
1:A:255:LEU:N	1:A:256:PRO:HD2	2.05	0.71
1:B:33:MET:HE1	1:B:243:LEU:CD2	2.21	0.71
1:B:374:PRO:HB2	1:B:400:ALA:HB2	1.70	0.71
1:B:451:LEU:O	1:B:455:LEU:HB2	1.91	0.71
1:A:88:ASP:N	1:A:89:PRO:CD	2.53	0.71
1:B:9:GLN:N	1:B:9:GLN:CD	2.48	0.70
1:A:18:CYS:SG	1:A:124:VAL:CG2	2.79	0.70
1:A:227:GLU:CG	3:A:602:HOH:O	2.40	0.70
1:A:216:ASN:HB3	3:A:622:HOH:O	1.92	0.70
1:B:159:LEU:O	1:B:159:LEU:CD2	2.40	0.69
1:A:148:ARG:HD3	1:A:380:VAL:HG13	1.72	0.69
1:A:149:PHE:CG	1:A:377:ASP:HB2	2.27	0.69
1:A:213:VAL:HG23	1:A:237:ILE:HD12	1.74	0.69
1:B:280:GLU:O	1:B:284:GLU:HG2	1.93	0.69
1:B:33:MET:CE	1:B:243:LEU:CD2	2.71	0.68
1:B:33:MET:CE	1:B:243:LEU:HD22	2.24	0.68
1:B:33:MET:HE2	1:B:243:LEU:HD22	1.75	0.68
1:B:149:PHE:CZ	1:B:189:MET:CE	2.77	0.68
1:A:37:ARG:HG3	1:A:37:ARG:NH1	2.03	0.68
1:B:159:LEU:CD2	1:B:159:LEU:C	2.66	0.67
1:A:159:LEU:O	1:A:159:LEU:HD22	1.95	0.67
1:A:188:GLN:CD	1:A:188:GLN:H	2.02	0.67
1:B:49:THR:HG22	1:B:51:SER:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:TRP:CD1	3:A:622:HOH:O	2.42	0.67
1:B:149:PHE:HZ	1:B:189:MET:HE2	1.60	0.67
1:A:88:ASP:N	1:A:89:PRO:HD3	2.10	0.66
1:A:227:GLU:HG2	3:A:602:HOH:O	1.94	0.66
1:A:303:GLY:HA3	1:A:310:LYS:HB2	1.78	0.66
1:A:33:MET:HE1	1:A:243:LEU:CD2	2.25	0.66
1:A:278:THR:CG2	1:A:281:GLN:H	2.08	0.66
1:B:117:ALA:CB	1:B:455:LEU:HD21	2.23	0.66
1:B:12:HIS:ND1	1:B:115:LEU:HD23	2.10	0.66
1:B:25:LEU:N	1:B:26:PRO:HD2	2.11	0.65
1:B:116:SER:HB2	1:B:455:LEU:HD11	1.78	0.65
1:A:49:THR:CG2	1:A:54:GLU:HB2	2.26	0.65
1:B:193:ARG:HH11	1:B:193:ARG:CG	1.91	0.64
1:B:423:LEU:O	1:B:427:VAL:HG23	1.96	0.64
1:A:138:PRO:HB3	1:A:211:LYS:HD3	1.79	0.64
1:B:53:ALA:H	1:B:307:ARG:CD	2.11	0.64
1:B:191:ASP:HB2	1:B:193:ARG:HH21	1.62	0.64
1:B:220:TRP:CD2	1:B:433:LYS:HG2	2.33	0.64
1:B:195:PHE:H	1:B:195:PHE:HD1	1.44	0.63
1:B:188:GLN:OE1	1:B:188:GLN:N	2.29	0.63
1:B:255:LEU:N	1:B:256:PRO:HD2	2.14	0.63
1:B:149:PHE:CZ	1:B:189:MET:HE1	2.34	0.63
1:A:145:THR:HG21	1:A:153:MET:HE1	1.80	0.63
1:B:116:SER:HB2	1:B:455:LEU:CD1	2.30	0.62
1:B:189:MET:HG3	1:B:196:PHE:HE2	1.64	0.62
1:A:161:GLU:CB	3:A:618:HOH:O	2.48	0.62
1:B:122:PHE:N	1:B:123:PRO:HD2	2.15	0.62
1:A:257:TRP:O	1:A:261:GLN:HG2	2.00	0.62
1:B:193:ARG:NH1	1:B:193:ARG:H	1.98	0.62
1:A:200:ILE:O	1:A:204:VAL:HG23	2.00	0.61
1:B:451:LEU:HD12	1:B:451:LEU:O	2.01	0.61
1:B:149:PHE:CZ	1:B:189:MET:HE2	2.36	0.61
1:B:191:ASP:CB	1:B:193:ARG:NH2	2.63	0.61
1:B:213:VAL:CG2	1:B:237:ILE:HD12	2.30	0.60
1:B:118:ILE:HD13	1:B:120:VAL:HG12	1.84	0.60
1:B:411:ALA:O	1:B:415:ILE:HG13	2.02	0.60
1:A:199:THR:O	1:A:203:ASN:ND2	2.35	0.59
1:B:73:ILE:CD1	1:B:107:LEU:HD22	2.31	0.59
1:A:311:GLU:OE2	1:A:311:GLU:HA	2.03	0.59
1:B:153:MET:HG2	1:B:200:ILE:HD12	1.85	0.59
1:A:33:MET:HE2	1:A:243:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ARG:NH1	1:B:193:ARG:CG	2.56	0.59
1:B:156:LEU:HB3	1:B:157:PRO:HD3	1.85	0.58
1:B:149:PHE:CZ	1:B:377:ASP:HB3	2.38	0.58
1:A:50:ILE:HD11	1:A:93:GLN:HB2	1.83	0.58
1:A:33:MET:CE	1:A:243:LEU:CD2	2.81	0.58
1:B:195:PHE:CD1	1:B:195:PHE:N	2.58	0.58
1:B:360:VAL:O	1:B:364:LYS:HB3	2.03	0.57
1:B:279:LYS:HD3	1:B:316:ILE:HA	1.87	0.57
1:A:149:PHE:CD1	1:A:377:ASP:HB2	2.39	0.57
1:A:396:GLY:O	1:A:403:ARG:NH2	2.38	0.57
1:B:120:VAL:CG2	1:B:125:LEU:HD23	2.35	0.57
1:A:14:ALA:HB3	1:A:118:ILE:HG13	1.86	0.57
1:A:178:ASP:N	1:A:178:ASP:OD1	2.36	0.57
1:B:128:PHE:CD1	1:B:128:PHE:O	2.56	0.57
1:A:285:PHE:O	1:A:288:ALA:HB3	2.05	0.57
1:B:148:ARG:HH11	1:B:178:ASP:HB3	1.68	0.57
1:A:137:LEU:O	1:A:139:THR:HG22	2.04	0.56
1:B:21:MET:HE1	1:B:57:SER:HG	1.68	0.56
1:B:295:ARG:CG	1:B:295:ARG:NH2	2.38	0.56
1:A:120:VAL:HG22	1:A:125:LEU:HD23	1.85	0.56
1:B:195:PHE:O	1:B:198:GLU:N	2.38	0.56
1:A:88:ASP:O	1:A:92:ILE:HG13	2.06	0.56
1:A:25:LEU:N	1:A:26:PRO:HD2	2.20	0.56
1:A:437:GLU:HG3	1:A:444:SER:H	1.70	0.56
1:B:141:THR:OG1	1:B:210:LEU:HD13	2.06	0.56
1:A:297:LEU:HD11	1:A:332:ILE:HG13	1.87	0.55
1:A:437:GLU:CG	1:A:444:SER:OG	2.53	0.55
1:A:254:ASP:OD2	1:B:435:ARG:HD3	2.06	0.55
1:A:255:LEU:N	1:A:256:PRO:CD	2.69	0.55
1:A:194:HIS:HD2	1:A:196:PHE:H	1.54	0.55
1:A:149:PHE:CE2	1:A:377:ASP:HB3	2.41	0.54
1:A:122:PHE:N	1:A:123:PRO:HD2	2.23	0.54
1:A:159:LEU:HD22	1:A:159:LEU:C	2.32	0.54
1:A:213:VAL:HG23	1:A:213:VAL:O	2.07	0.54
1:B:149:PHE:CE2	1:B:377:ASP:HB3	2.42	0.54
1:B:149:PHE:CE1	1:B:377:ASP:CB	2.90	0.54
1:B:258:LEU:HD11	1:B:341:ILE:HG23	1.90	0.54
1:A:149:PHE:CD2	1:A:153:MET:HE2	2.43	0.54
1:B:149:PHE:CD1	1:B:377:ASP:CB	2.87	0.54
1:B:149:PHE:CE1	1:B:189:MET:HE1	2.42	0.53
1:A:37:ARG:NH1	1:A:37:ARG:CG	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PHE:HD2	1:A:153:MET:HE2	1.74	0.53
1:B:28:LEU:HB3	1:B:246:ILE:HD11	1.90	0.53
1:B:122:PHE:HB3	1:B:123:PRO:HD3	1.91	0.53
1:B:126:THR:O	1:B:129:SER:HB2	2.08	0.53
1:A:17:PRO:HG3	1:A:27:TYR:CB	2.38	0.53
1:B:378:GLN:HG3	2:B:500:UPG:O3'	2.09	0.53
1:B:120:VAL:O	1:B:141:THR:HG23	2.08	0.53
1:B:159:LEU:C	1:B:159:LEU:HD22	2.34	0.53
1:A:278:THR:HG23	1:A:280:GLU:H	1.73	0.53
1:A:33:MET:CE	1:A:243:LEU:HD22	2.39	0.52
1:A:71:LEU:HB3	1:A:107:LEU:HD21	1.91	0.52
1:B:191:ASP:O	1:B:197:VAL:HG21	2.09	0.52
1:B:305:VAL:C	1:B:306:ASP:OD1	2.53	0.52
1:B:29:ARG:O	1:B:33:MET:HG3	2.09	0.52
1:A:429:GLU:O	1:A:433:LYS:HG2	2.09	0.52
1:B:148:ARG:HG2	1:B:380:VAL:HG12	1.90	0.52
1:B:65:TYR:OH	1:B:247:LYS:HB2	2.09	0.52
1:B:207:LEU:HB2	3:B:604:HOH:O	2.09	0.52
1:A:278:THR:HG23	1:A:280:GLU:N	2.25	0.52
1:A:314:GLU:N	1:A:314:GLU:OE1	2.43	0.52
1:A:405:ILE:HG22	1:A:410:ILE:HG13	1.91	0.52
1:A:56:ARG:HG2	1:B:449:ARG:NH2	2.24	0.52
1:B:189:MET:HG3	1:B:196:PHE:CE2	2.42	0.52
1:B:191:ASP:HB2	1:B:193:ARG:NH2	2.25	0.52
1:A:118:ILE:HD13	1:A:120:VAL:HG12	1.92	0.52
1:A:303:GLY:HA3	1:A:310:LYS:CB	2.40	0.52
1:A:292:SER:O	1:A:418:ARG:NH1	2.43	0.52
1:B:116:SER:CB	1:B:455:LEU:CD1	2.88	0.51
1:A:37:ARG:NH2	1:A:244:GLU:OE2	2.42	0.51
1:B:129:SER:HB3	1:B:130:PRO:HD3	1.92	0.51
1:B:191:ASP:CB	1:B:193:ARG:HH21	2.24	0.51
1:A:394:VAL:CG2	1:A:413:LYS:HE2	2.41	0.51
1:B:337:ASP:O	1:B:341:ILE:HG13	2.10	0.51
1:A:177:LEU:CD1	1:A:177:LEU:C	2.84	0.51
1:A:227:GLU:HA	1:A:230:LYS:HE2	1.92	0.51
1:B:129:SER:N	1:B:130:PRO:CD	2.73	0.51
1:A:144:VAL:HG23	2:A:500:UPG:O6'	2.11	0.50
1:B:65:TYR:HB3	1:B:68:ILE:HG13	1.94	0.50
1:A:177:LEU:C	1:A:177:LEU:HD12	2.37	0.50
1:A:366:GLY:O	1:A:427:VAL:HG11	2.11	0.50
1:B:191:ASP:OD1	1:B:191:ASP:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:VAL:HG23	2:B:500:UPG:C6'	2.42	0.50
1:B:159:LEU:O	1:B:159:LEU:HD22	2.12	0.49
1:B:122:PHE:N	1:B:123:PRO:CD	2.76	0.49
1:B:191:ASP:OD2	1:B:193:ARG:NE	2.46	0.49
1:B:24:LEU:HD11	1:B:58:LEU:HD21	1.93	0.49
1:B:65:TYR:CZ	1:B:247:LYS:HB2	2.47	0.49
1:B:191:ASP:OD1	1:B:191:ASP:C	2.55	0.49
1:A:254:ASP:OD1	1:A:254:ASP:O	2.30	0.49
1:A:23:HIS:O	1:A:26:PRO:HG2	2.13	0.48
1:A:303:GLY:HA3	1:A:310:LYS:CG	2.43	0.48
1:A:212:GLY:HA2	1:A:236:HIS:HB2	1.95	0.48
1:B:292:SER:O	1:B:418:ARG:NH1	2.46	0.48
1:A:281:GLN:O	1:A:284:GLU:HB2	2.14	0.48
1:B:313:THR:O	1:B:313:THR:OG1	2.21	0.48
1:B:215:ILE:HG23	1:B:217:THR:HG22	1.94	0.48
1:A:269:ILE:HG23	1:A:351:VAL:HB	1.95	0.48
1:A:50:ILE:HD11	1:A:89:PRO:O	2.14	0.48
1:B:116:SER:HB3	1:B:455:LEU:HD13	1.95	0.48
1:B:195:PHE:O	1:B:196:PHE:C	2.57	0.48
1:B:156:LEU:N	1:B:157:PRO:CD	2.77	0.48
1:A:112:SER:HG	1:A:113:PRO:CD	1.98	0.47
1:A:255:LEU:O	1:A:259:GLU:N	2.40	0.47
1:A:177:LEU:HD12	1:A:177:LEU:O	2.15	0.47
1:B:147:ALA:O	1:B:151:SER:OG	2.32	0.47
1:A:313:THR:HG23	1:A:313:THR:O	2.14	0.47
1:B:175:PRO:O	1:B:176:HIS:HB2	2.15	0.47
1:A:105:ARG:HB2	1:A:106:PRO:CD	2.38	0.47
1:B:220:TRP:CD2	1:B:433:LYS:CG	2.98	0.47
1:A:138:PRO:HB3	1:A:211:LYS:CD	2.44	0.47
1:A:149:PHE:CZ	1:A:377:ASP:HB3	2.50	0.47
1:A:12:HIS:O	1:A:115:LEU:HA	2.15	0.47
1:A:18:CYS:SG	1:A:124:VAL:HG21	2.54	0.46
1:B:448:ILE:CG2	1:B:449:ARG:N	2.78	0.46
1:B:25:LEU:N	1:B:26:PRO:CD	2.79	0.46
1:B:213:VAL:HG22	1:B:237:ILE:CD1	2.36	0.46
1:A:366:GLY:O	1:A:427:VAL:CG1	2.63	0.46
1:B:390:LEU:HD12	1:B:427:VAL:HG13	1.97	0.46
1:A:287:ALA:HB3	1:A:407:ARG:HG2	1.98	0.46
1:A:237:ILE:O	1:A:237:ILE:HG23	2.15	0.46
1:A:366:GLY:C	1:A:427:VAL:CG1	2.89	0.46
1:B:14:ALA:HB3	1:B:118:ILE:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:CD1	1:A:115:LEU:HD21	2.46	0.45
1:B:22:GLY:O	1:B:26:PRO:HG3	2.17	0.45
1:B:128:PHE:CE1	1:B:132:ALA:HB2	2.51	0.45
1:B:62:PHE:CE2	1:B:70:SER:HB2	2.51	0.45
1:B:451:LEU:C	1:B:451:LEU:CD1	2.86	0.45
1:A:267:LEU:HB2	1:A:294:TRP:CE3	2.52	0.45
1:B:186:PRO:HA	1:B:187:PRO:HD3	1.85	0.45
1:A:297:LEU:HD13	1:A:330:VAL:HB	1.98	0.45
1:B:25:LEU:HB2	1:B:26:PRO:CD	2.47	0.45
1:B:445:GLU:O	1:B:448:ILE:HG22	2.16	0.45
1:A:24:LEU:HD22	1:A:54:GLU:HB3	1.99	0.44
1:A:296:PHE:CZ	1:A:329:GLY:HA3	2.52	0.44
1:A:343:ALA:HA	1:A:365:LEU:HD22	1.99	0.44
1:B:149:PHE:O	1:B:152:LEU:HB3	2.17	0.44
1:B:22:GLY:O	1:B:357:ASN:ND2	2.48	0.44
1:B:218:PHE:CB	1:B:437:GLU:HG3	2.47	0.44
1:A:219:THR:CG2	1:A:226:VAL:HG11	2.47	0.44
1:B:307:ARG:H	1:B:307:ARG:HG2	1.50	0.44
1:B:27:TYR:CZ	1:B:142:LEU:HB3	2.52	0.44
1:B:156:LEU:N	1:B:157:PRO:HD2	2.32	0.44
1:A:148:ARG:NH2	1:A:180:ILE:HG12	2.33	0.44
1:A:274:ARG:NE	1:A:305:VAL:HG12	2.33	0.44
1:B:22:GLY:O	1:B:26:PRO:CG	2.65	0.44
1:B:191:ASP:CA	1:B:193:ARG:NH2	2.81	0.44
1:B:222:GLU:O	1:B:226:VAL:HG23	2.18	0.44
1:A:111:LEU:HD13	1:A:115:LEU:HD21	1.99	0.43
1:A:158:ARG:HA	1:A:158:ARG:HD3	1.34	0.43
1:A:337:ASP:CG	1:A:340:ARG:HB3	2.43	0.43
1:A:448:ILE:CG2	1:A:449:ARG:N	2.81	0.43
1:B:191:ASP:CG	1:B:193:ARG:NH2	2.76	0.43
1:B:156:LEU:CB	1:B:157:PRO:HD3	2.48	0.43
1:A:125:LEU:HD13	1:A:210:LEU:HD11	2.00	0.43
1:A:186:PRO:HD2	1:A:189:MET:CE	2.49	0.43
1:A:236:HIS:ND1	1:A:236:HIS:N	2.59	0.43
1:B:191:ASP:HA	1:B:193:ARG:HH22	1.82	0.43
1:A:159:LEU:C	1:A:159:LEU:CD2	2.91	0.43
1:B:105:ARG:N	1:B:106:PRO:CD	2.82	0.43
1:B:275:GLY:HA3	1:B:303:GLY:HA3	2.01	0.43
1:A:125:LEU:CD1	1:A:210:LEU:HD11	2.49	0.43
1:B:341:ILE:O	1:B:347:ILE:HG12	2.19	0.43
1:A:448:ILE:HG22	1:A:449:ARG:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ILE:HA	1:B:186:PRO:HD3	1.89	0.42
1:B:347:ILE:HD13	1:B:347:ILE:N	2.34	0.42
1:B:320:SER:OG	1:B:324:ARG:NH2	2.52	0.42
1:A:128:PHE:O	1:A:128:PHE:CG	2.72	0.42
1:A:132:ALA:CB	1:A:139:THR:HG21	2.50	0.42
1:B:137:LEU:O	1:B:139:THR:HG22	2.19	0.42
1:A:31:ALA:HB1	1:A:41:VAL:HG11	2.01	0.42
1:B:17:PRO:HD2	1:B:44:ILE:O	2.20	0.42
1:A:105:ARG:CB	1:A:106:PRO:HD3	2.39	0.42
1:A:33:MET:CE	1:A:243:LEU:HD23	2.42	0.42
1:A:220:TRP:CE2	1:A:433:LYS:HG3	2.55	0.42
1:B:149:PHE:CE1	1:B:377:ASP:HA	2.55	0.42
1:B:204:VAL:O	1:B:207:LEU:CB	2.58	0.42
1:B:207:LEU:HD23	1:B:207:LEU:HA	1.85	0.42
1:B:221:LEU:HD12	1:B:388:VAL:HG21	2.02	0.42
1:B:12:HIS:CE1	1:B:115:LEU:HD23	2.54	0.42
1:B:227:GLU:O	1:B:231:ARG:HG3	2.20	0.41
1:B:122:PHE:HB3	1:B:123:PRO:CD	2.48	0.41
1:B:158:ARG:O	1:B:161:GLU:HB2	2.20	0.41
1:B:37:ARG:HG2	1:B:449:ARG:CZ	2.50	0.41
1:B:304:LYS:HD3	1:B:304:LYS:HA	1.54	0.41
1:B:306:ASP:OD1	1:B:306:ASP:N	2.50	0.41
1:B:407:ARG:H	1:B:407:ARG:HG3	1.49	0.41
1:B:28:LEU:HD23	1:B:28:LEU:HA	1.85	0.41
1:B:34:LEU:O	1:B:39:CYS:HB2	2.20	0.41
1:B:116:SER:CB	1:B:455:LEU:HD11	2.50	0.41
1:B:149:PHE:CG	1:B:377:ASP:CB	3.00	0.41
1:B:294:TRP:CE2	1:B:418:ARG:HG3	2.55	0.41
1:A:413:LYS:HD2	1:A:413:LYS:HA	1.61	0.41
1:A:447:LEU:HA	1:A:447:LEU:HD23	1.82	0.41
1:B:177:LEU:HD23	1:B:177:LEU:HA	1.72	0.41
1:B:284:GLU:OE2	1:B:407:ARG:NH1	2.54	0.41
1:A:213:VAL:CG2	1:A:237:ILE:HA	2.51	0.41
1:A:298:TRP:C	1:A:298:TRP:CD1	2.99	0.41
1:B:21:MET:HG3	1:B:335:TRP:CH2	2.56	0.41
1:B:42:SER:HB3	1:B:71:LEU:CD1	2.51	0.41
1:B:129:SER:CB	1:B:130:PRO:HD3	2.51	0.41
1:B:255:LEU:N	1:B:256:PRO:CD	2.83	0.41
1:B:285:PHE:HD1	1:B:410:ILE:HG21	1.86	0.41
1:B:369:VAL:O	1:B:391:GLY:HA2	2.21	0.41
1:B:93:GLN:O	1:B:97:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:VAL:O	1:B:237:ILE:HA	2.20	0.41
1:A:342:LEU:HB3	1:A:365:LEU:HD13	2.02	0.41
1:A:186:PRO:HA	1:A:187:PRO:HD3	1.97	0.41
1:B:374:PRO:HB2	1:B:400:ALA:CB	2.46	0.41
1:B:236:HIS:ND1	1:B:236:HIS:N	2.64	0.41
1:B:240:ILE:O	1:B:240:ILE:HG23	2.20	0.41
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.77	0.40
1:A:298:TRP:HD1	1:A:299:VAL:N	2.19	0.40
1:A:213:VAL:O	1:A:213:VAL:CG2	2.70	0.40
1:B:111:LEU:HD23	1:B:111:LEU:HA	1.89	0.40
1:B:281:GLN:O	1:B:284:GLU:HB2	2.22	0.40
1:B:336:ALA:O	2:B:500:UPG:N3	2.36	0.40
1:B:339:GLU:N	3:B:602:HOH:O	2.35	0.40
1:B:426:ARG:HB3	3:B:608:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/459 (94%)	420 (98%)	7 (2%)	2 (0%)	24	42
1	B	435/459 (95%)	428 (98%)	6 (1%)	1 (0%)	43	62
All	All	864/918 (94%)	848 (98%)	13 (2%)	3 (0%)	36	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	PRO
1	B	374	PRO
1	A	113	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	343/396 (87%)	295 (86%)	48 (14%)	3	6
1	B	355/396 (90%)	286 (81%)	69 (19%)	1	2
All	All	698/792 (88%)	581 (83%)	117 (17%)	2	3

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	15	VAL
1	A	42	SER
1	A	45	SER
1	A	57	SER
1	A	60	SER
1	A	96	SER
1	A	99	ASN
1	A	107	LEU
1	A	118	ILE
1	A	120	VAL
1	A	124	VAL
1	A	131	ILE
1	A	139	THR
1	A	151	SER
1	A	156	LEU
1	A	158	ARG
1	A	159	LEU
1	A	171	GLU
1	A	177	LEU
1	A	189	MET
1	A	199	THR
1	A	202	SER
1	A	219	THR
1	A	220	TRP
1	A	227	GLU
1	A	235	ASP

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Mol	Chain	Res	Type
1	A	236	HIS
1	A	240	ILE
1	A	273	SER
1	A	278	THR
1	A	295	ARG
1	A	305	VAL
1	A	308	GLU
1	A	314	GLU
1	A	323	GLU
1	A	328	ARG
1	A	333	LYS
1	A	345	SER
1	A	407	ARG
1	A	431	ARG
1	A	435	ARG
1	A	437	GLU
1	A	439	GLU
1	A	440	SER
1	A	446	THR
1	A	448	ILE
1	A	451	LEU
1	B	9	GLN
1	B	15	VAL
1	B	49	THR
1	B	52	ASP
1	B	68	ILE
1	B	73	ILE
1	B	91	PHE
1	B	92	ILE
1	B	97	ILE
1	B	101	ILE
1	B	110	SER
1	B	112	SER
1	B	118	ILE
1	B	120	VAL
1	B	129	SER
1	B	139	THR
1	B	141	THR
1	B	146	SER
1	B	151	SER
1	B	156	LEU
1	B	159	LEU

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Mol	Chain	Res	Type
1	B	165	ASP
1	B	172	VAL
1	B	177	LEU
1	B	180	ILE
1	B	189	MET
1	B	191	ASP
1	B	192	ARG
1	B	193	ARG
1	B	195	PHE
1	B	198	GLU
1	B	202	SER
1	B	211	LYS
1	B	213	VAL
1	B	219	THR
1	B	222	GLU
1	B	231	ARG
1	B	236	HIS
1	B	240	ILE
1	B	246	ILE
1	B	258	LEU
1	B	260	GLU
1	B	273	SER
1	B	274	ARG
1	B	289	LEU
1	B	295	ARG
1	B	304	LYS
1	B	328	ARG
1	B	330	VAL
1	B	341	ILE
1	B	345	SER
1	B	347	ILE
1	B	367	VAL
1	B	385	VAL
1	B	386	GLU
1	B	403	ARG
1	B	405	ILE
1	B	407	ARG
1	B	413	LYS
1	B	424	ARG
1	B	431	ARG
1	B	432	GLU
1	B	433	LYS

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Mol	Chain	Res	Type
1	B	435	ARG
1	B	440	SER
1	B	448	ILE
1	B	451	LEU
1	B	455	LEU
1	B	456	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	A	194	HIS
1	A	375	HIS
1	B	9	GLN
1	B	176	HIS
1	B	261	GLN
1	B	277	HIS
1	B	338	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 ⓘ

2 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	UPG	A	500	-	37,38,38	1.34	5 (13%)	55,58,58	1.73	12 (21%)
2	UPG	B	500	-	37,38,38	0.47	0	55,58,58	0.55	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	UPG	A	500	-	-	7/23/59/59	0/3/3/3
2	UPG	B	500	-	-	2/23/59/59	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	UPG	C4-N3	-3.83	1.32	1.38
2	A	500	UPG	C2-N3	-3.38	1.32	1.38
2	A	500	UPG	PB-O3A	2.70	1.62	1.59
2	A	500	UPG	C5-C4	-2.70	1.37	1.43
2	A	500	UPG	C6-N1	-2.69	1.31	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	UPG	C4-N3-C2	-5.95	119.23	126.61
2	A	500	UPG	N3-C2-N1	5.23	121.70	114.89
2	A	500	UPG	C5-C4-N3	4.02	120.43	114.80
2	A	500	UPG	O4-C4-C5	-3.02	119.96	125.16
2	A	500	UPG	O2-C2-N1	-2.96	118.95	122.80
2	A	500	UPG	O6'-C6'-C5'	-2.60	102.48	111.33
2	A	500	UPG	C6'-C5'-C4'	-2.39	107.16	113.02
2	A	500	UPG	C5C-C4C-C3C	-2.29	106.97	115.21
2	A	500	UPG	C5-C6-N1	-2.24	118.20	121.84
2	A	500	UPG	O2A-PA-O3A	2.20	113.22	107.27
2	A	500	UPG	C2C-C1C-N1	-2.06	107.51	113.25
2	A	500	UPG	O5'-C1'-C2'	-2.02	106.22	110.37

There are no chirality outliers.

All (9) torsion outliers are listed below:

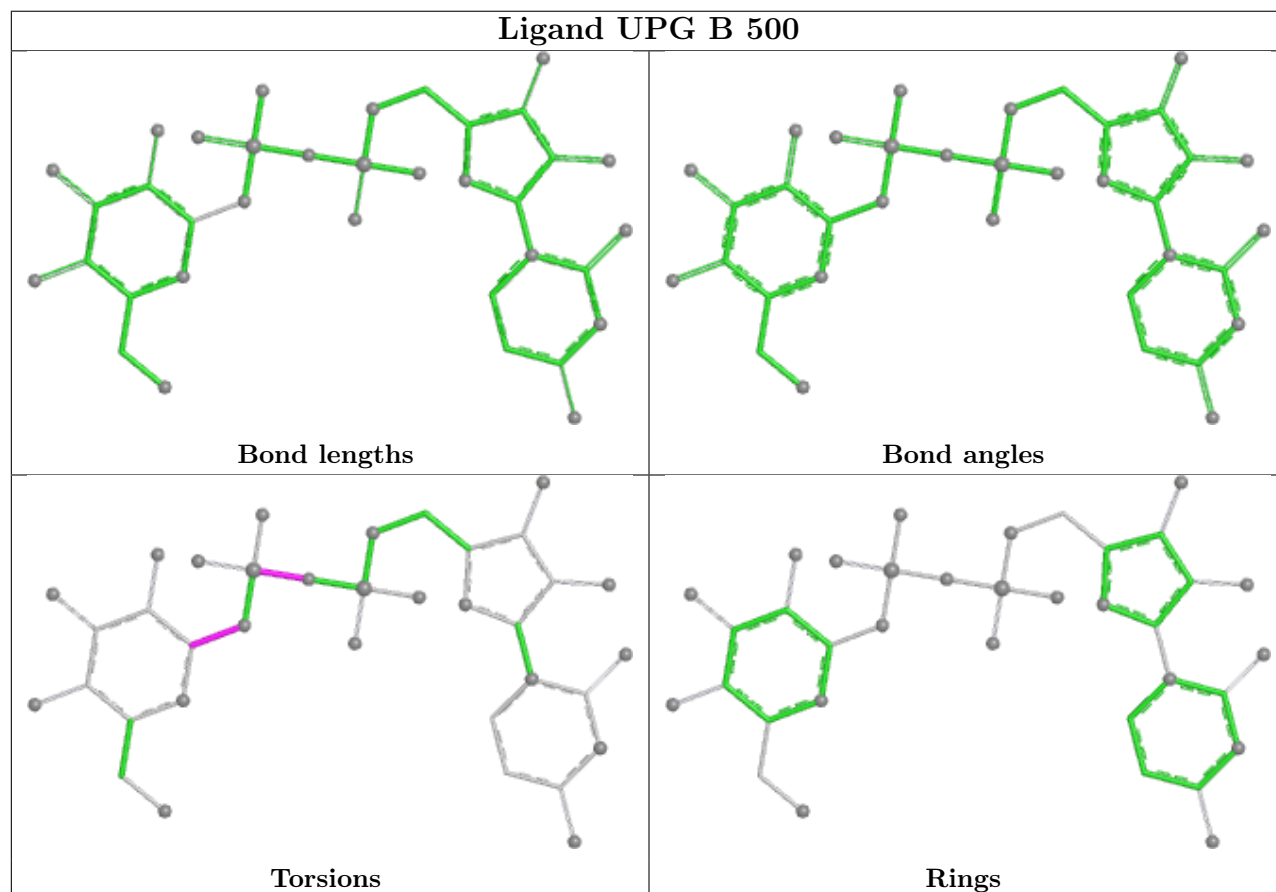
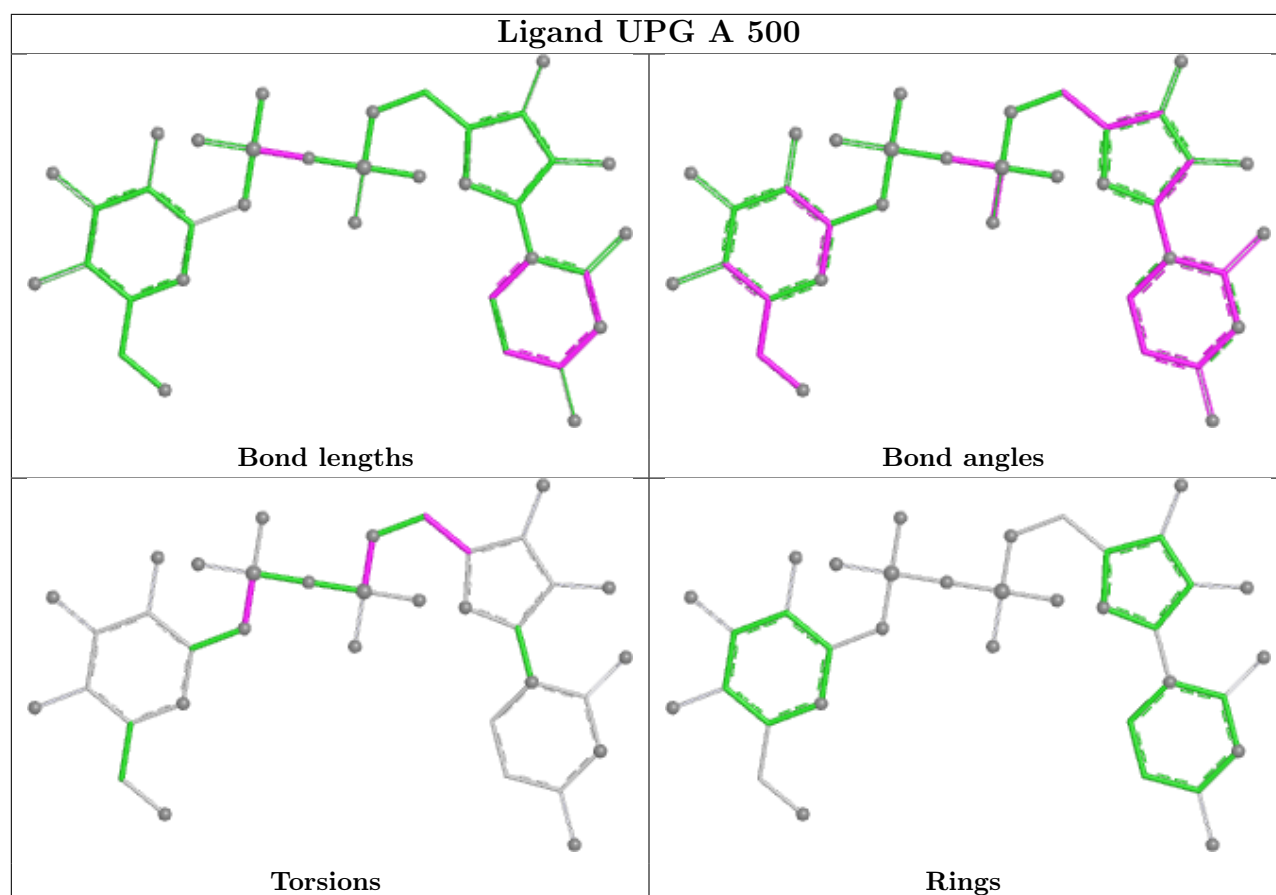
Mol	Chain	Res	Type	Atoms
2	A	500	UPG	C5C-O5C-PA-O1A
2	A	500	UPG	C5C-O5C-PA-O3A
2	A	500	UPG	C1'-O3B-PB-O3A
2	B	500	UPG	PA-O3A-PB-O3B
2	B	500	UPG	O5'-C1'-O3B-PB
2	A	500	UPG	C3C-C4C-C5C-O5C
2	A	500	UPG	O4C-C4C-C5C-O5C
2	A	500	UPG	C1'-O3B-PB-O2B
2	A	500	UPG	C5C-O5C-PA-O2A

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	UPG	1	0
2	B	500	UPG	4	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 ⓘ

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	435/459 (94%)	0.22	24 (5%) 30 23	22, 34, 61, 103	0
1	B	439/459 (95%)	0.31	26 (5%) 28 21	21, 39, 72, 106	0
All	All	874/918 (95%)	0.27	50 (5%) 29 22	21, 37, 69, 106	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	ASP	8.0
1	A	167	SER	7.1
1	A	165	ASP	6.9
1	A	254	ASP	6.6
1	A	251	SER	6.5
1	A	168	LYS	6.4
1	B	251	SER	5.6
1	B	252	ASP	4.8
1	B	77	PRO	4.8
1	A	302	SER	4.3
1	B	306	ASP	4.2
1	A	88	ASP	4.2
1	B	305	VAL	4.1
1	B	164	ASP	3.9
1	A	166	ILE	3.9
1	A	248	ALA	3.8
1	B	318	GLY	3.7
1	A	250	GLU	3.6
1	B	167	SER	3.6
1	A	249	GLU	3.6
1	B	163	GLU	3.5
1	A	162	GLN	3.4
1	A	255	LEU	3.2
1	A	77	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	254	ASP	3.1
1	B	303	GLY	3.1
1	A	313	THR	3.0
1	B	249	GLU	3.0
1	A	438	ARG	3.0
1	B	253	MET	2.9
1	B	88	ASP	2.8
1	B	248	ALA	2.8
1	A	307	ARG	2.7
1	B	314	GLU	2.7
1	A	276	ALA	2.7
1	B	304	LYS	2.6
1	A	176	HIS	2.5
1	B	195	PHE	2.5
1	A	195	PHE	2.4
1	B	162	GLN	2.4
1	B	90	PHE	2.4
1	A	449	ARG	2.3
1	B	76	LEU	2.3
1	A	441	GLY	2.3
1	B	126	THR	2.2
1	B	307	ARG	2.2
1	B	196	PHE	2.2
1	A	305	VAL	2.1
1	B	255	LEU	2.1
1	B	169	LYS	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](#)

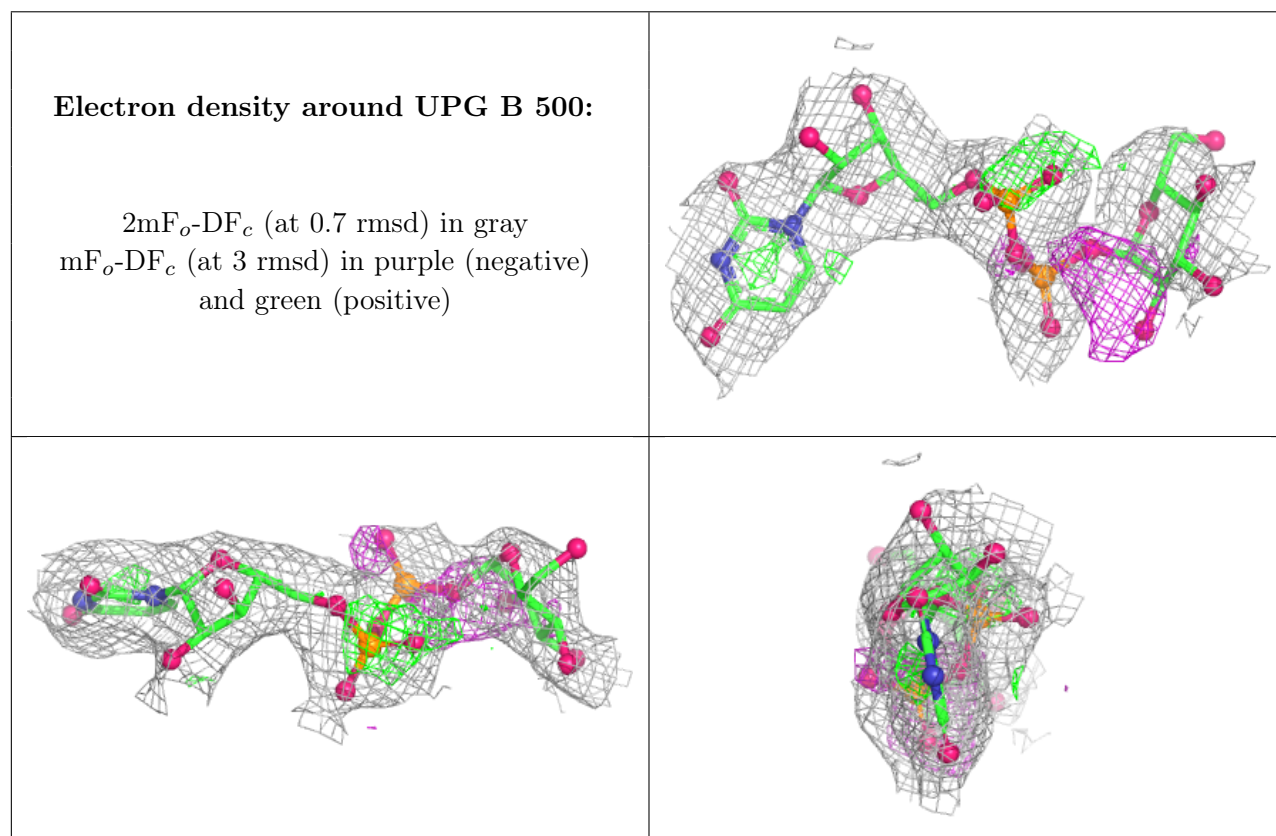
There are no oligosaccharides in this entry.

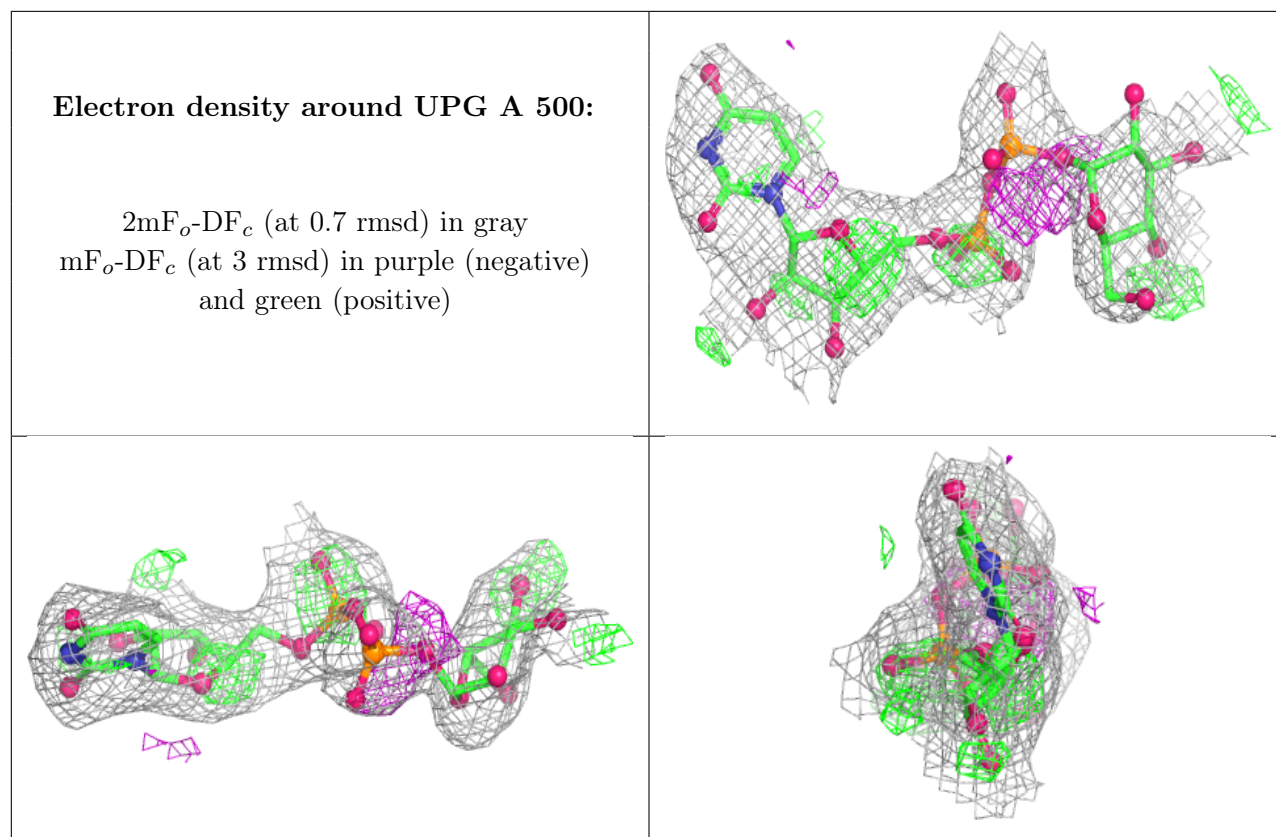
6.4 Ligands [i](#)

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
2	UPG	B	500	36/36	0.86	0.19	55,55,68,69	0
2	UPG	A	500	36/36	0.87	0.19	55,55,59,69	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.