



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:58 PM UTC

PDB ID : 5L6J / pdb_00005l6j
Title : Uba1 in complex with Ub-MLN7243 covalent adduct
Authors : Misra, M.; Schindelin, H.
Deposited on : 2016-05-30
Resolution : 2.68 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

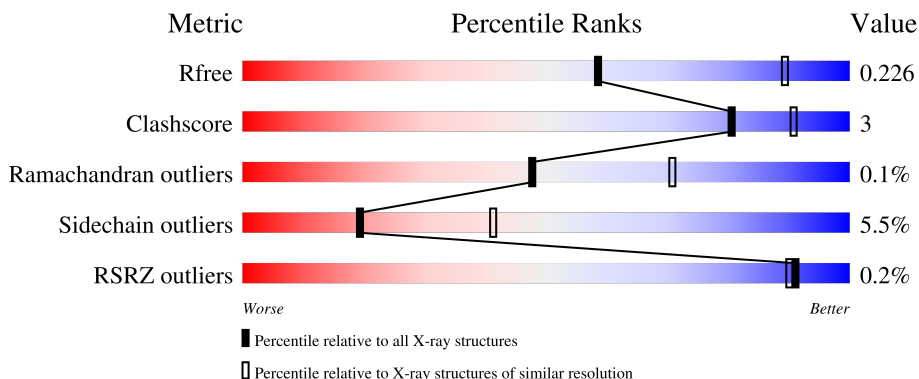
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	1024	88% 9% ..
1	C	1024	87% 10% ..
2	B	76	91% 9%
2	D	76	91% 8% .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17935 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 Ubiquitin-activating enzyme E1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1006	Total	C	N	O	S	0	0	0
			7945	5062	1312	1548	23			
1	C	1003	Total	C	N	O	S	0	1	0
			7927	5053	1310	1541	23			

- Molecule 2 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	1	0
			608	380	108	119	1			
2	D	76	Total	C	N	O	S	0	1	0
			608	380	108	119	1			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	C	2	Total Cl 2 2	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



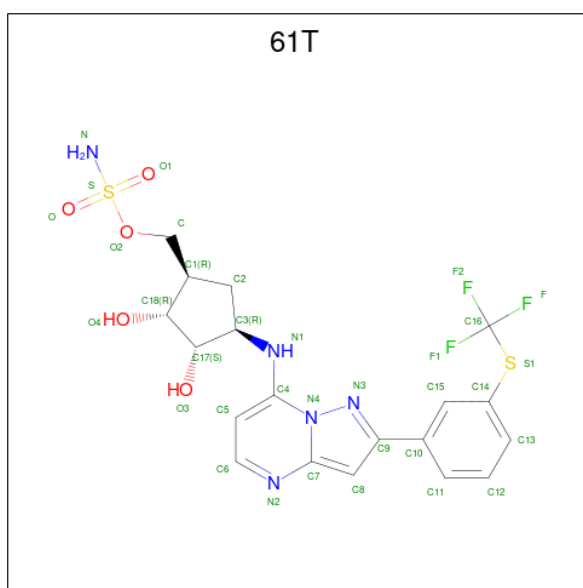
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

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

- Molecule 6 is [(1 {R},2 {R},3 {S},4 {R})-2,3-bis(oxidanyl)-4-[[2-[3-(trifluoromethylsulfanyl)phenyl]pyrazolo[1,5-a]pyrimidin-7-yl]amino]cyclopentyl]methyl sulfamate (CCD ID: 61T) (formula: C₁₉H₂₀F₃N₅O₅S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	F	N	O	S	0	0
			34	19	3	5	5	2		
6	D	1	Total	C	F	N	O	S	0	0
			34	19	3	5	5	2		

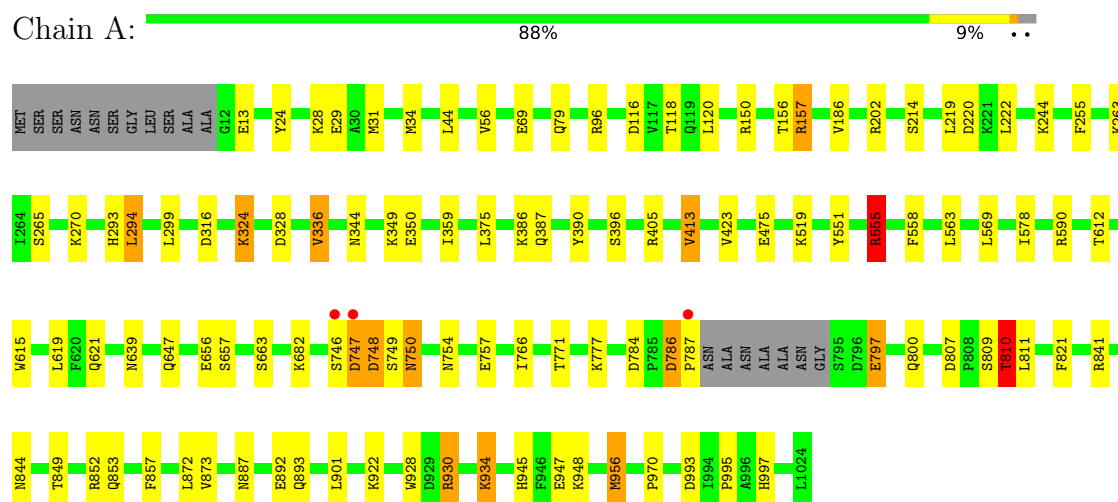
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	331	Total	O	0	0
			331	331		
7	B	18	Total	O	0	0
			18	18		
7	C	302	Total	O	0	0
			302	302		
7	D	13	Total	O	0	0
			13	13		

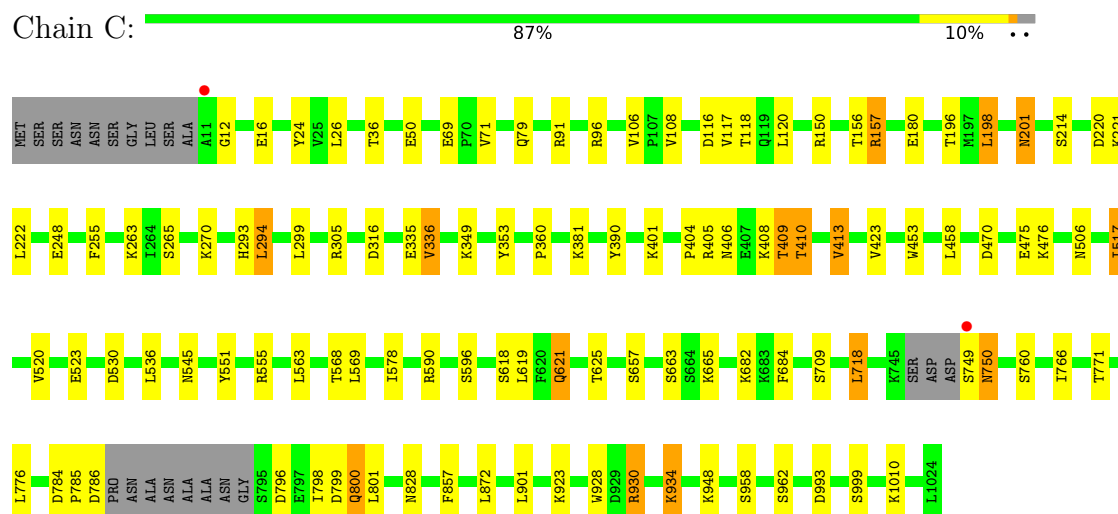
3 Residue-property plots

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: Ubiquitin-activating enzyme E1 1

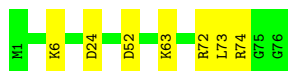


• Molecule 1: Ubiquitin-activating enzyme E1 1



• Molecule 2: Ubiquitin-40S ribosomal protein S31





- Molecule 2: Ubiquitin-40S ribosomal protein S31

Chain D:
91% 8% •



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	72.48Å 193.92Å 230.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.68 20.00 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.68) 99.1 (20.00-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.171 , 0.224 0.177 , 0.226	Depositor DCC
R_{free} test set	4511 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17935	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, SO4, 61T

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	1.21	8/8110 (0.1%)	1.17	13/10975 (0.1%)
1	C	1.20	12/8093 (0.1%)	1.16	12/10949 (0.1%)
2	B	1.17	0/616	1.18	0/826
2	D	1.11	0/616	1.18	1/826 (0.1%)
All	All	1.20	20/17435 (0.1%)	1.17	26/23576 (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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1010	LYS	C-O	-6.62	1.15	1.24
1	C	750	ASN	CA-C	6.52	1.61	1.52
1	C	506	ASN	C-O	-6.40	1.18	1.24
1	C	108	VAL	C-O	-6.40	1.17	1.24
1	C	106	VAL	CA-C	-6.35	1.46	1.52
1	C	36	THR	C-O	-6.07	1.16	1.24
1	A	970	PRO	CA-C	5.80	1.57	1.52
1	A	892	GLU	C-O	-5.65	1.16	1.24
1	C	180	GLU	CA-C	-5.58	1.46	1.53
1	A	821	PHE	C-O	-5.58	1.17	1.23
1	A	849	THR	C-O	-5.55	1.16	1.23
1	C	568	THR	C-O	-5.42	1.17	1.23
1	A	747	ASP	CA-C	5.33	1.59	1.52
1	A	893	GLN	CD-NE2	-5.33	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	934	LYS	CA-CB	5.32	1.60	1.53
1	C	536	LEU	C-O	-5.24	1.17	1.23
1	A	56	VAL	C-O	-5.20	1.18	1.24
1	A	873	VAL	C-O	-5.11	1.18	1.24
1	C	517	ILE	CA-CB	5.11	1.60	1.54
1	C	106	VAL	C-O	-5.11	1.18	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ASP	N-CA-C	7.39	119.42	111.36
1	C	316	ASP	N-CA-C	7.27	119.29	111.36
1	C	410	THR	N-CA-CB	-7.14	99.83	110.61
1	C	413	VAL	N-CA-CB	-6.67	103.48	112.16
1	C	618	SER	CB-CA-C	-6.61	100.46	110.90
1	A	349	LYS	CG-CD-CE	6.51	126.27	111.30
1	C	150	ARG	NE-CZ-NH2	6.38	124.94	119.20
1	C	517	ILE	N-CA-CB	-6.34	103.92	112.16
1	A	413	VAL	N-CA-CB	-6.29	103.99	112.16
1	A	555	ARG	CG-CD-NE	6.18	125.61	112.00
1	A	150	ARG	NE-CZ-NH2	6.12	124.71	119.20
1	A	797	GLU	N-CA-CB	6.06	119.68	110.28
1	C	265	SER	CA-CB-OG	-5.93	99.24	111.10
1	A	13	GLU	N-CA-C	5.90	118.03	108.41
1	A	359	ILE	N-CA-C	5.74	114.82	108.05
1	A	265	SER	CA-CB-OG	-5.67	99.75	111.10
1	C	305	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	A	810	THR	CA-CB-CG2	5.42	119.71	110.50
2	D	54	ARG	N-CA-C	5.40	118.73	110.36
1	C	517	ILE	CA-CB-CG2	5.33	119.57	110.50
1	A	777	LYS	N-CA-C	-5.32	100.74	109.40
1	C	545	ASN	N-CA-C	5.30	116.86	108.96
1	C	476	LYS	N-CA-C	5.29	117.46	111.11
1	A	934	LYS	CB-CG-CD	5.15	123.14	111.30
1	A	396	SER	N-CA-C	5.13	118.64	112.38
1	C	117	VAL	CB-CA-C	-5.03	104.70	112.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	LEU	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	7945	0	7846	47	0
1	C	7927	0	7838	37	0
2	B	608	0	638	3	0
2	D	608	0	638	3	0
3	A	10	0	0	0	0
3	C	5	0	0	0	0
4	A	2	0	0	1	0
4	C	2	0	0	0	0
5	A	42	0	56	1	0
5	C	54	0	72	1	0
6	B	34	0	0	0	0
6	D	34	0	0	1	0
7	A	331	0	0	9	0
7	B	18	0	0	0	0
7	C	302	0	0	2	0
7	D	13	0	0	0	0
All	All	17935	0	17088	89	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 3.

All (89) 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:810:THR:HG22	1:A:811:LEU:HG	1.66	0.76
1:A:294:LEU:HD13	1:A:336:VAL:HG21	1.68	0.76
1:C:294:LEU:HD13	1:C:336:VAL:HG21	1.67	0.75
1:C:798:ILE:O	1:C:799:ASP:C	2.28	0.73
1:C:116:ASP:OD1	1:C:118:THR:HB	1.89	0.72
1:C:569:LEU:HB3	2:D:73:LEU:HD22	1.71	0.71
1:A:116:ASP:OD1	1:A:118:THR:HB	1.91	0.69
1:A:555:ARG:HH21	1:A:555:ARG:HG2	1.58	0.68
4:A:1104:CL:CL	7:A:1483:HOH:O	2.50	0.66
1:C:349:LYS:HD3	1:C:353:TYR:CE2	2.31	0.65
1:A:569:LEU:HB3	2:B:73:LEU:HD22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:TRP:O	1:A:930:ARG:NH2	2.25	0.62
1:C:404:PRO:O	1:C:409:THR:HG21	1.99	0.62
1:C:928:TRP:O	1:C:930:ARG:NH1	2.31	0.61
1:A:69:GLU:HG3	7:A:1297:HOH:O	2.01	0.60
1:A:157:ARG:HD3	1:A:299:LEU:HD13	1.84	0.60
1:C:798:ILE:O	1:C:800:GLN:N	2.35	0.60
1:C:406:ASN:H	1:C:409:THR:HG22	1.71	0.55
7:A:1482:HOH:O	1:C:12:GLY:HA3	2.06	0.55
1:C:872:LEU:HD13	1:C:901:LEU:HD21	1.89	0.55
1:A:748:ASP:N	1:A:748:ASP:OD1	2.40	0.54
1:C:198:LEU:O	1:C:201:ASN:ND2	2.41	0.54
1:C:405:ARG:HD2	1:C:423:VAL:O	2.08	0.54
1:C:201:ASN:HD22	1:C:201:ASN:N	2.06	0.54
1:A:656:GLU:HG2	7:A:1501:HOH:O	2.07	0.54
2:B:24:ASP:OD2	2:B:52:ASP:O	2.26	0.53
1:C:157:ARG:HD3	1:C:299:LEU:HD13	1.90	0.53
1:A:405:ARG:HD2	1:A:423:VAL:O	2.08	0.53
1:A:872:LEU:HD13	1:A:901:LEU:HD21	1.92	0.52
1:C:470:ASP:OD2	6:D:101:61T:O4	2.28	0.52
1:A:841:ARG:NH2	7:A:1203:HOH:O	2.45	0.50
1:A:615:TRP:CE3	1:A:841:ARG:HD2	2.46	0.50
1:C:26:LEU:O	1:C:381:LYS:HE2	2.12	0.50
2:D:72:ARG:C	2:D:73:LEU:HG	2.37	0.49
1:A:344:ASN:HD21	5:A:1110:GOL:H32	1.78	0.48
1:C:201:ASN:HD22	1:C:201:ASN:H	1.60	0.48
1:A:807:ASP:O	1:A:810:THR:HB	2.14	0.48
1:A:255:PHE:C	1:A:255:PHE:CD1	2.91	0.48
1:A:746:SER:CB	1:A:749:SER:HB3	2.44	0.48
2:B:72:ARG:C	2:B:73:LEU:HG	2.39	0.47
1:C:255:PHE:CD1	1:C:255:PHE:C	2.92	0.47
1:C:785:PRO:O	1:C:786:ASP:C	2.57	0.47
1:A:551:TYR:CZ	1:A:555:ARG:HD2	2.49	0.47
1:C:349:LYS:HD3	1:C:353:TYR:CZ	2.49	0.47
1:A:157:ARG:HD3	1:A:299:LEU:CD1	2.45	0.47
1:A:887:ASN:HB3	7:A:1224:HOH:O	2.13	0.47
1:C:293:HIS:HA	1:C:390:TYR:CZ	2.49	0.46
1:C:24:TYR:CE1	1:C:857:PHE:HB2	2.51	0.46
1:C:157:ARG:HD3	1:C:299:LEU:CD1	2.46	0.46
1:A:324:LYS:HE2	1:A:328:ASP:OD2	2.15	0.46
1:A:551:TYR:OH	1:A:555:ARG:HD2	2.16	0.46
1:A:24:TYR:CE1	1:A:857:PHE:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:SER:HB2	1:A:749:SER:HB3	1.99	0.45
1:A:350:GLU:OE1	1:A:405:ARG:NH2	2.49	0.45
1:C:798:ILE:O	1:C:801:LEU:N	2.50	0.45
1:A:558:PHE:O	1:A:930:ARG:NH1	2.51	0.44
1:A:612:THR:HG22	1:A:841:ARG:HG2	1.99	0.44
1:A:750:ASN:OD1	1:A:750:ASN:N	2.51	0.43
1:A:810:THR:HG22	1:A:811:LEU:CG	2.43	0.43
1:C:71:VAL:HG22	1:C:91:ARG:HG2	2.00	0.43
1:A:852:ARG:HD3	7:A:1494:HOH:O	2.18	0.43
1:C:684:PHE:HB3	1:C:718:LEU:HD22	2.00	0.43
1:C:530:ASP:OD2	1:C:999:SER:OG	2.35	0.43
1:A:293:HIS:HA	1:A:390:TYR:CZ	2.54	0.43
1:C:69:GLU:HG3	7:C:1227:HOH:O	2.19	0.43
1:C:453:TRP:CD2	1:C:458:LEU:HD23	2.53	0.43
1:A:995:PRO:HB2	1:A:997:HIS:CE1	2.53	0.42
1:C:930:ARG:HD2	7:C:1419:HOH:O	2.19	0.42
1:A:639:ASN:OD1	1:A:639:ASN:N	2.41	0.42
2:D:1:MET:HE2	2:D:63:LYS:HB3	2.02	0.42
1:C:563:LEU:HB3	1:C:578:ILE:HB	2.03	0.41
1:C:828:ASN:HB2	5:C:1107:GOL:H2	2.02	0.41
1:A:34:MET:HE3	1:A:375:LEU:HD22	2.03	0.41
1:A:750:ASN:HA	7:A:1460:HOH:O	2.21	0.41
1:C:201:ASN:ND2	1:C:201:ASN:N	2.68	0.41
1:A:31:MET:HE2	1:A:31:MET:HB3	1.92	0.41
1:C:551:TYR:OH	1:C:555:ARG:HD2	2.21	0.41
1:A:807:ASP:OD2	1:A:809:SER:OG	2.38	0.41
1:C:621[B]:GLN:NE2	1:C:625:THR:HB	2.35	0.41
1:A:841:ARG:O	1:A:844:ASN:HB2	2.21	0.41
1:A:956:MET:HE3	1:A:956:MET:HB2	1.99	0.41
1:A:386:LYS:HA	1:A:387:GLN:HA	1.87	0.40
1:A:754:ASN:OD1	1:A:757:GLU:HG3	2.20	0.40
1:A:786:ASP:CG	1:A:787:PRO:HD2	2.46	0.40
1:C:156:THR:C	1:C:157:ARG:HG2	2.45	0.40
1:A:156:THR:C	1:A:157:ARG:HG2	2.46	0.40
1:A:945:HIS:HB2	7:A:1516:HOH:O	2.21	0.40
1:A:563:LEU:HB3	1:A:578:ILE:HB	2.03	0.40
1:A:810:THR:HG22	1:A:811:LEU:CD2	2.51	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	1002/1024 (98%)	970 (97%)	31 (3%)	1 (0%)	48	71
1	C	998/1024 (98%)	966 (97%)	31 (3%)	1 (0%)	48	71
2	B	75/76 (99%)	74 (99%)	1 (1%)	0	100	100
2	D	75/76 (99%)	73 (97%)	2 (3%)	0	100	100
All	All	2150/2200 (98%)	2083 (97%)	65 (3%)	2 (0%)	48	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	747	ASP
1	C	796	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	889/900 (99%)	843 (95%)	46 (5%)	21	43
1	C	886/900 (98%)	831 (94%)	55 (6%)	16	36
2	B	70/69 (101%)	66 (94%)	4 (6%)	18	40
2	D	70/69 (101%)	67 (96%)	3 (4%)	26	51
All	All	1915/1938 (99%)	1807 (94%)	108 (6%)	19	40

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	29	GLU
1	A	44	LEU
1	A	79	GLN
1	A	96	ARG
1	A	120	LEU
1	A	157	ARG
1	A	186	VAL
1	A	202	ARG
1	A	214	SER
1	A	220	ASP
1	A	222	LEU
1	A	244	LYS
1	A	263	LYS
1	A	270	LYS
1	A	294	LEU
1	A	324	LYS
1	A	336	VAL
1	A	413	VAL
1	A	475	GLU
1	A	519	LYS
1	A	555	ARG
1	A	590	ARG
1	A	619	LEU
1	A	621	GLN
1	A	647	GLN
1	A	657	SER
1	A	663	SER
1	A	682	LYS
1	A	748	ASP
1	A	750	ASN
1	A	766	ILE
1	A	771	THR
1	A	784	ASP
1	A	786	ASP
1	A	797	GLU
1	A	800	GLN
1	A	810	THR
1	A	853	GLN
1	A	922	LYS
1	A	930	ARG
1	A	934	LYS
1	A	947	GLU

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Mol	Chain	Res	Type
1	A	948	LYS
1	A	956	MET
1	A	993	ASP
2	B	6	LYS
2	B	63	LYS
2	B	74[A]	ARG
2	B	74[B]	ARG
1	C	16	GLU
1	C	50	GLU
1	C	79	GLN
1	C	96	ARG
1	C	120	LEU
1	C	157	ARG
1	C	196	THR
1	C	198	LEU
1	C	201	ASN
1	C	214	SER
1	C	220	ASP
1	C	221	LYS
1	C	222	LEU
1	C	248	GLU
1	C	263	LYS
1	C	270	LYS
1	C	294	LEU
1	C	335	GLU
1	C	336	VAL
1	C	360	PRO
1	C	401	LYS
1	C	408	LYS
1	C	409	THR
1	C	410	THR
1	C	413	VAL
1	C	475	GLU
1	C	517	ILE
1	C	520	VAL
1	C	523	GLU
1	C	590	ARG
1	C	596	SER
1	C	619	LEU
1	C	621[A]	GLN
1	C	621[B]	GLN
1	C	657	SER

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Mol	Chain	Res	Type
1	C	663	SER
1	C	665	LYS
1	C	682	LYS
1	C	709	SER
1	C	718	LEU
1	C	749	SER
1	C	750	ASN
1	C	760	SER
1	C	766	ILE
1	C	771	THR
1	C	776	LEU
1	C	784	ASP
1	C	800	GLN
1	C	923	LYS
1	C	930	ARG
1	C	934	LYS
1	C	948	LYS
1	C	958	SER
1	C	962	SER
1	C	993	ASP
2	D	28	SER
2	D	54	ARG
2	D	64	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	A	333	GLN
1	A	372	GLN
1	A	429	GLN
1	A	545	ASN
1	A	647	GLN
1	A	878	ASN
1	A	984	GLN
1	A	997	HIS
2	B	62	GLN
1	C	38	ASN
1	C	201	ASN
1	C	209	ASN
1	C	297	GLN
1	C	301	GLN

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Mol	Chain	Res	Type
1	C	333	GLN
1	C	429	GLN
1	C	750	ASN
1	C	997	HIS
2	D	60	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 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	$\# Z > 2$
5	GOL	A	1108	-	5,5,5	0.83	0	5,5,5	0.58	0
3	SO4	C	1101	-	4,4,4	0.70	0	6,6,6	1.31	1 (16%)
5	GOL	A	1109	-	5,5,5	0.86	0	5,5,5	0.68	0
5	GOL	A	1107	-	5,5,5	0.78	0	5,5,5	0.79	0
6	61T	D	101	2	35,37,37	2.44	9 (25%)	50,56,56	2.98	20 (40%)
5	GOL	A	1105	-	5,5,5	0.77	0	5,5,5	1.34	1 (20%)
3	SO4	A	1102	-	4,4,4	0.47	0	6,6,6	0.21	0
5	GOL	A	1110	-	5,5,5	0.66	0	5,5,5	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	C	1112	-	5,5,5	0.45	0	5,5,5	0.49	0
5	GOL	C	1105	-	5,5,5	0.95	0	5,5,5	0.75	0
5	GOL	C	1110	-	5,5,5	0.63	0	5,5,5	0.56	0
5	GOL	C	1106	-	5,5,5	0.74	0	5,5,5	0.42	0
5	GOL	C	1107	-	5,5,5	0.64	0	5,5,5	0.76	0
5	GOL	C	1111	-	5,5,5	0.56	0	5,5,5	0.84	0
5	GOL	C	1104	-	5,5,5	0.57	0	5,5,5	0.58	0
5	GOL	C	1108	-	5,5,5	1.13	0	5,5,5	1.21	0
5	GOL	C	1109	-	5,5,5	0.80	0	5,5,5	0.75	0
5	GOL	A	1106	-	5,5,5	0.88	0	5,5,5	0.76	0
5	GOL	A	1111	-	5,5,5	0.80	0	5,5,5	0.81	0
3	SO4	A	1101	-	4,4,4	0.58	0	6,6,6	0.74	0
6	61T	B	101	2	35,37,37	2.24	11 (31%)	50,56,56	2.64	17 (34%)

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
5	GOL	C	1107	-	-	0/4/4/4	-
5	GOL	A	1108	-	-	2/4/4/4	-
5	GOL	C	1111	-	-	2/4/4/4	-
5	GOL	A	1106	-	-	3/4/4/4	-
5	GOL	A	1111	-	-	0/4/4/4	-
5	GOL	C	1105	-	-	3/4/4/4	-
5	GOL	C	1112	-	-	0/4/4/4	-
5	GOL	A	1109	-	-	2/4/4/4	-
5	GOL	C	1104	-	-	1/4/4/4	-
6	61T	B	101	2	-	0/18/35/35	0/4/4/4
5	GOL	A	1107	-	-	1/4/4/4	-
5	GOL	C	1110	-	-	0/4/4/4	-
6	61T	D	101	2	-	4/18/35/35	0/4/4/4
5	GOL	A	1105	-	-	1/4/4/4	-
5	GOL	A	1110	-	-	2/4/4/4	-
5	GOL	C	1106	-	-	2/4/4/4	-
5	GOL	C	1108	-	-	2/4/4/4	-
5	GOL	C	1109	-	-	2/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	101	61T	C4-N4	-6.96	1.30	1.37
6	B	101	61T	C14-S1	-6.31	1.68	1.78
6	D	101	61T	C7-N4	-5.29	1.31	1.39
6	D	101	61T	C8-C7	-4.68	1.33	1.38
6	B	101	61T	C5-C6	4.67	1.51	1.39
6	D	101	61T	C14-S1	-4.64	1.71	1.78
6	B	101	61T	C17-C3	-4.56	1.48	1.53
6	D	101	61T	C5-C6	4.43	1.50	1.39
6	D	101	61T	C17-C3	-4.43	1.49	1.53
6	B	101	61T	C8-C9	4.09	1.47	1.40
6	B	101	61T	C4-N4	-3.81	1.33	1.37
6	B	101	61T	C7-N4	-3.58	1.34	1.39
6	B	101	61T	C2-C3	-3.51	1.48	1.54
6	D	101	61T	C8-C9	3.42	1.46	1.40
6	D	101	61T	C2-C3	-3.06	1.48	1.54
6	B	101	61T	C8-C7	-2.95	1.35	1.38
6	B	101	61T	C7-N2	-2.55	1.34	1.36
6	B	101	61T	S-N	2.30	1.61	1.58
6	B	101	61T	C9-N3	2.26	1.37	1.34
6	D	101	61T	C3-N1	-2.04	1.42	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	101	61T	O-S-O1	-10.35	109.41	119.94
6	D	101	61T	O-S-O1	-9.64	110.12	119.94
6	D	101	61T	C9-C8-C7	7.37	109.36	105.56
6	D	101	61T	C2-C3-C17	6.78	113.92	103.17
6	B	101	61T	C2-C3-C17	6.38	113.28	103.17
6	D	101	61T	C5-C6-N2	-6.02	119.98	124.75
6	D	101	61T	C2-C1-C	-5.43	102.02	112.78
6	B	101	61T	C16-S1-C14	5.11	111.69	99.30
6	D	101	61T	N4-C7-N2	5.07	125.09	121.61
6	B	101	61T	C9-C8-C7	4.89	108.08	105.56
6	D	101	61T	C8-C9-N3	-4.76	105.88	111.11
6	B	101	61T	C8-C9-N3	-3.99	106.73	111.11
6	B	101	61T	C17-C3-N1	3.90	120.07	112.24
6	D	101	61T	O2-C-C1	3.78	116.05	108.24
6	D	101	61T	C10-C9-N3	3.77	125.45	120.49
6	B	101	61T	C5-C6-N2	-3.61	121.90	124.75
6	D	101	61T	C8-C7-N2	-3.54	129.72	132.87
6	D	101	61T	C16-S1-C14	3.46	107.69	99.30
6	D	101	61T	C2-C1-C18	3.44	111.61	102.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	101	61T	C-O2-S	3.41	121.65	117.29
6	D	101	61T	C17-C3-N1	2.99	118.24	112.24
6	B	101	61T	C8-C7-N2	-2.95	130.25	132.87
6	B	101	61T	C2-C1-C18	2.83	110.08	102.89
6	B	101	61T	O1-S-N	-2.80	105.08	109.13
6	D	101	61T	O1-S-N	-2.63	105.33	109.13
6	D	101	61T	O4-C18-C17	2.51	119.87	111.82
6	B	101	61T	C10-C9-N3	2.47	123.75	120.49
6	B	101	61T	N4-C7-N2	2.46	123.30	121.61
6	D	101	61T	C2-C3-N1	2.44	117.36	112.27
6	B	101	61T	O4-C18-C1	-2.35	106.43	112.56
3	C	1101	SO4	O3-S-O1	2.32	121.69	109.56
6	D	101	61T	C7-N4-N3	2.30	115.24	111.96
6	D	101	61T	C-O2-S	2.28	120.20	117.29
6	D	101	61T	C1-C2-C3	-2.20	100.47	103.55
6	B	101	61T	O4-C18-C17	2.12	118.61	111.82
5	A	1105	GOL	O1-C1-C2	2.11	119.88	110.38
6	D	101	61T	C5-C4-N4	2.07	117.66	114.70
6	B	101	61T	F1-C16-F	2.06	111.85	106.52
6	B	101	61T	O-S-N	2.01	112.04	109.13

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1106	GOL	O1-C1-C2-C3
5	A	1109	GOL	C1-C2-C3-O3
5	A	1110	GOL	O1-C1-C2-C3
5	C	1105	GOL	O1-C1-C2-O2
5	C	1105	GOL	O1-C1-C2-C3
5	C	1106	GOL	C1-C2-C3-O3
5	C	1106	GOL	O2-C2-C3-O3
6	D	101	61T	C-O2-S-O
6	D	101	61T	O2-C-C1-C18
6	D	101	61T	O2-C-C1-C2
5	C	1111	GOL	O1-C1-C2-O2
5	A	1108	GOL	O1-C1-C2-C3
5	C	1108	GOL	C1-C2-C3-O3
5	C	1109	GOL	O1-C1-C2-C3
5	C	1111	GOL	O1-C1-C2-C3
5	A	1106	GOL	O1-C1-C2-O2
5	A	1109	GOL	O2-C2-C3-O3

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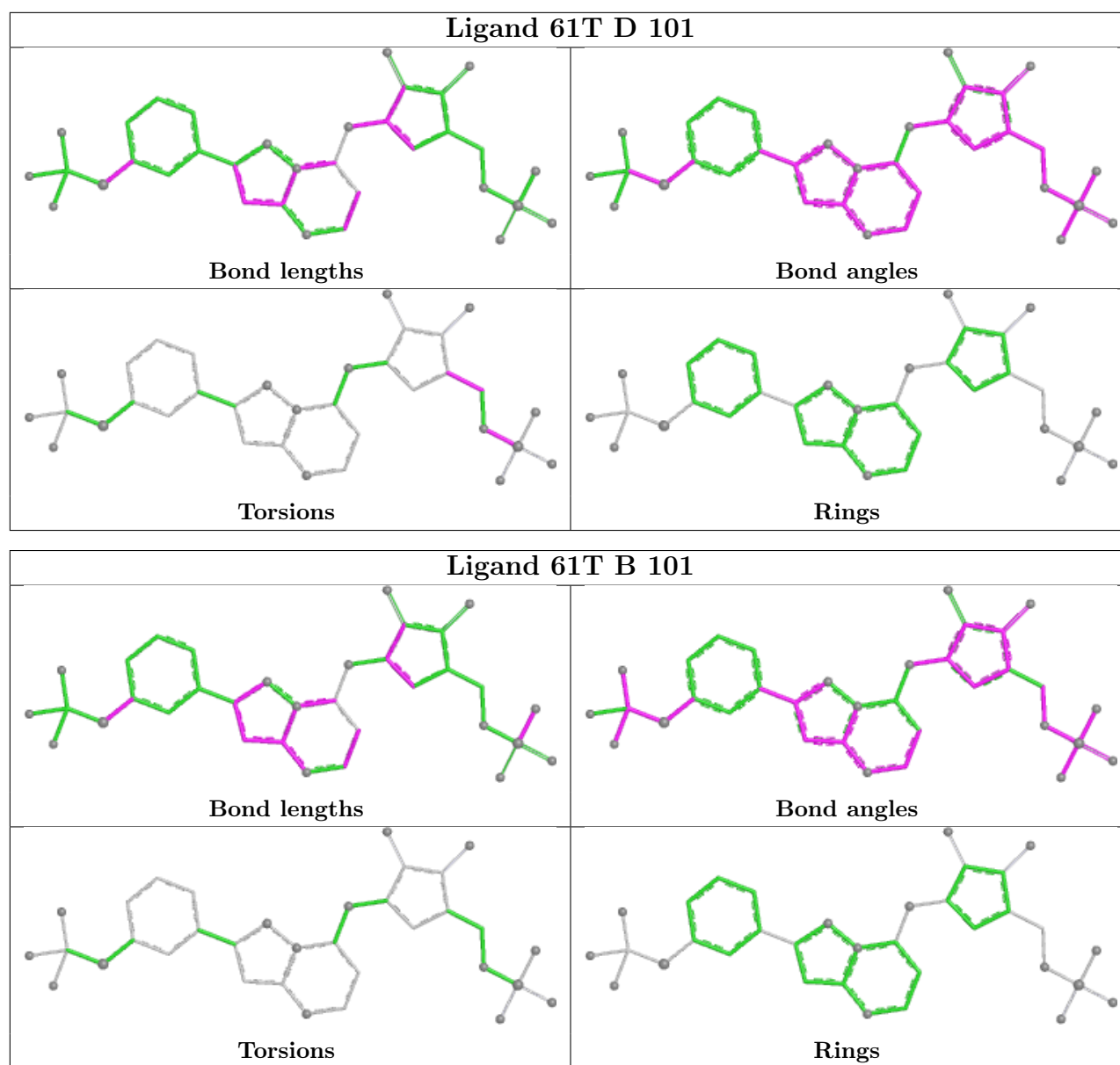
Mol	Chain	Res	Type	Atoms
5	A	1110	GOL	O1-C1-C2-O2
5	C	1109	GOL	O1-C1-C2-O2
5	A	1106	GOL	O2-C2-C3-O3
5	A	1108	GOL	O1-C1-C2-O2
5	A	1107	GOL	O1-C1-C2-O2
5	C	1105	GOL	O2-C2-C3-O3
5	A	1105	GOL	O1-C1-C2-C3
6	D	101	61T	C-O2-S-O1
5	C	1104	GOL	O2-C2-C3-O3
5	C	1108	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	101	61T	1	0
5	A	1110	GOL	1	0
5	C	1107	GOL	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	1006/1024 (98%)	-0.68	3 (0%) 90 89	26, 44, 90, 150	0
1	C	1003/1024 (97%)	-0.64	2 (0%) 91 90	26, 45, 91, 141	1 (0%)
2	B	76/76 (100%)	-0.68	0 100 100	20, 50, 75, 88	1 (1%)
2	D	76/76 (100%)	-0.49	0 100 100	26, 57, 84, 89	1 (1%)
All	All	2161/2200 (98%)	-0.66	5 (0%) 91 90	20, 45, 89, 150	3 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	11	ALA	3.4
1	A	787	PRO	2.6
1	A	746	SER	2.6
1	A	747	ASP	2.4
1	C	749	SER	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,

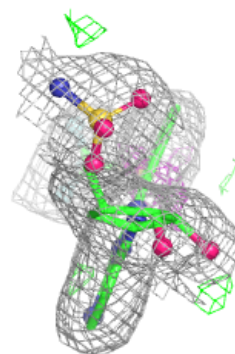
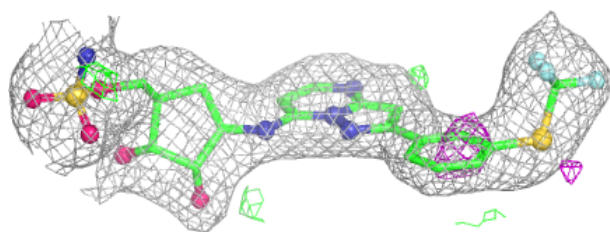
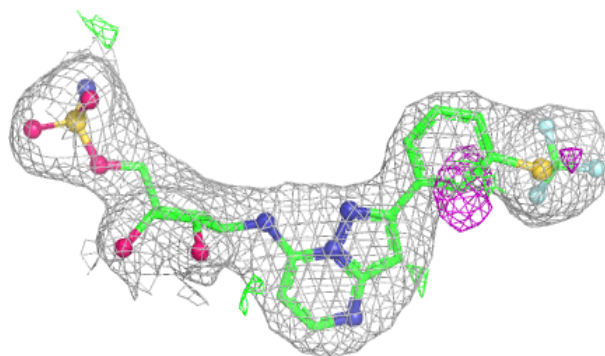
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	1106	6/6	0.73	0.21	71,86,89,90	0
5	GOL	C	1105	6/6	0.73	0.18	56,72,77,77	0
5	GOL	C	1104	6/6	0.79	0.14	64,68,71,72	0
5	GOL	A	1108	6/6	0.83	0.12	60,63,66,67	0
5	GOL	A	1109	6/6	0.85	0.14	62,70,75,80	0
5	GOL	C	1108	6/6	0.85	0.14	57,63,67,69	0
5	GOL	C	1110	6/6	0.85	0.13	76,83,85,87	0
5	GOL	C	1111	6/6	0.87	0.14	51,60,69,75	0
3	SO4	A	1102	5/5	0.88	0.14	99,101,110,110	0
5	GOL	A	1105	6/6	0.90	0.14	47,52,56,58	0
5	GOL	A	1111	6/6	0.90	0.14	57,63,66,67	0
5	GOL	C	1107	6/6	0.90	0.13	60,66,67,67	0
5	GOL	A	1110	6/6	0.91	0.09	50,56,59,66	0
4	CL	C	1103	1/1	0.92	0.07	64,64,64,64	0
5	GOL	C	1109	6/6	0.93	0.09	52,63,64,66	0
4	CL	C	1102	1/1	0.93	0.08	62,62,62,62	0
5	GOL	C	1106	6/6	0.93	0.09	38,42,44,47	0
4	CL	A	1104	1/1	0.95	0.06	59,59,59,59	0
4	CL	A	1103	1/1	0.97	0.05	56,56,56,56	0
5	GOL	A	1107	6/6	0.97	0.07	37,51,54,55	0
5	GOL	C	1112	6/6	0.97	0.07	42,46,46,49	0
6	61T	B	101	34/34	0.97	0.07	26,35,54,57	0
6	61T	D	101	34/34	0.97	0.08	26,49,79,82	0
3	SO4	A	1101	5/5	0.99	0.06	28,29,32,33	0
3	SO4	C	1101	5/5	0.99	0.08	26,27,31,33	0

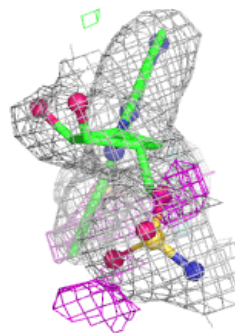
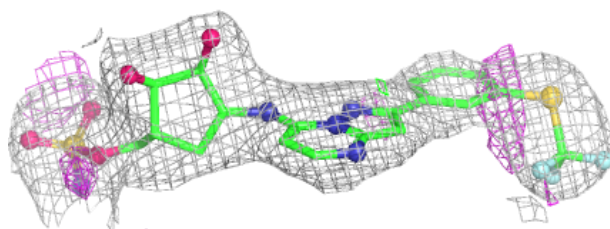
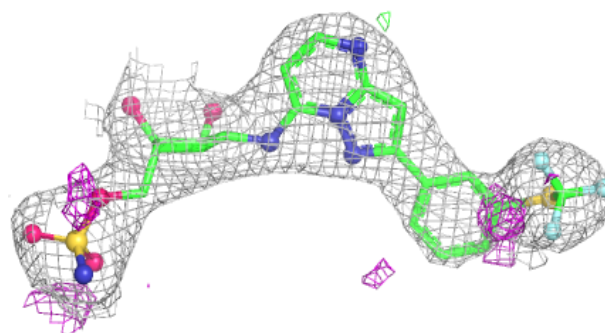
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 61T B 101:

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

**Electron density around 61T D 101:**

$2mF_o-DF_c$ (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.