Full wwPDB X-ray Structure Validation Report (i)

Feb 23, 2023 – 03:34 pm GMT

PDB ID	:	5L6J
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 (i) 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 (i)) were used in the production of this report:

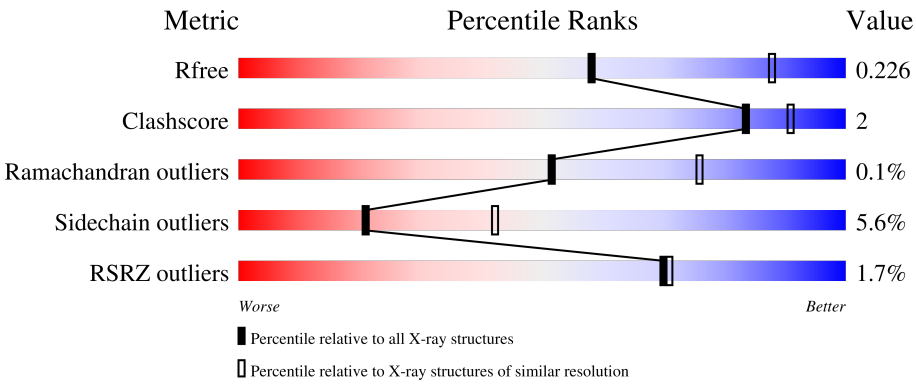
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (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 <=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	2% 87% 9% • •
1	C	1024	% 87% 10% • •
2	B	76	89% 8% •
2	D	76	% 92% 5% •

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.

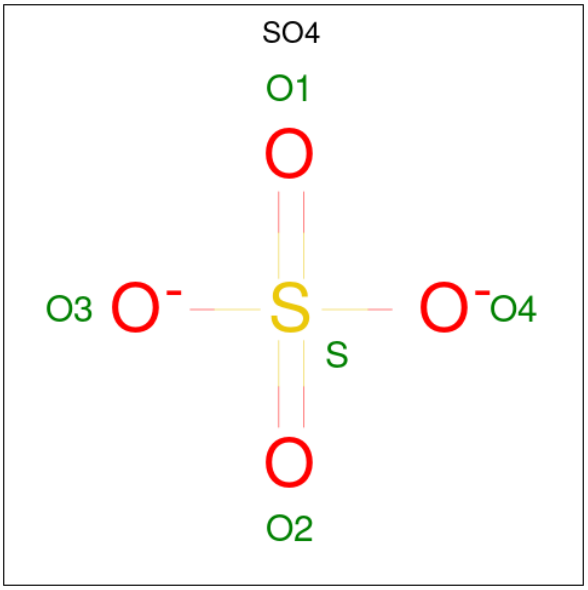
- Molecule 1 is a protein called Ubiquitin-activating enzyme E1 1.

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

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

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

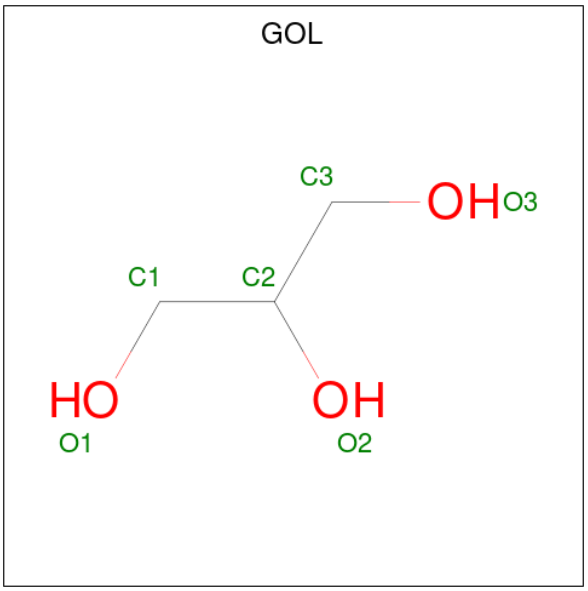


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: 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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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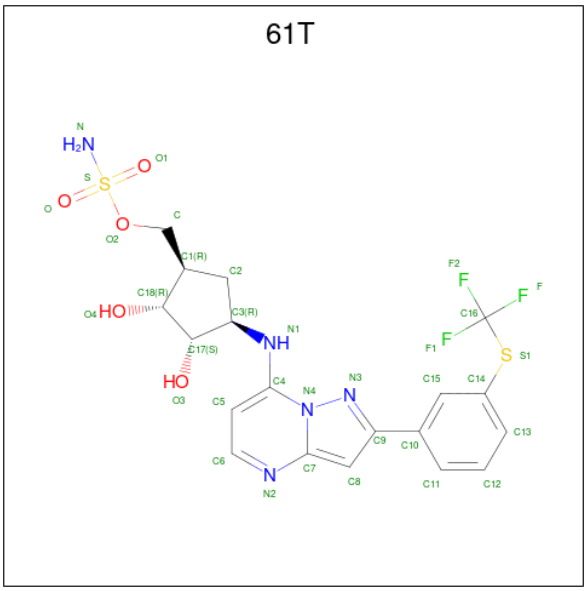
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	A	1	6	3	3		0	0
			Total	C	O			
5	A	1	6	3	3		0	0
			Total	C	O			
5	C	1	6	3	3		0	0
			Total	C	O			
5	C	1	6	3	3		0	0
			Total	C	O			
5	C	1	6	3	3		0	0
			Total	C	O			
5	C	1	6	3	3		0	0
			Total	C	O			
5	C	1	6	3	3		0	0
			Total	C	O			
5	C	1	6	3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

- 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 (three-letter code: 61T) (formula: $C_{19}H_{20}F_3N_5O_5S_2$).



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

- Molecule 7 is water.

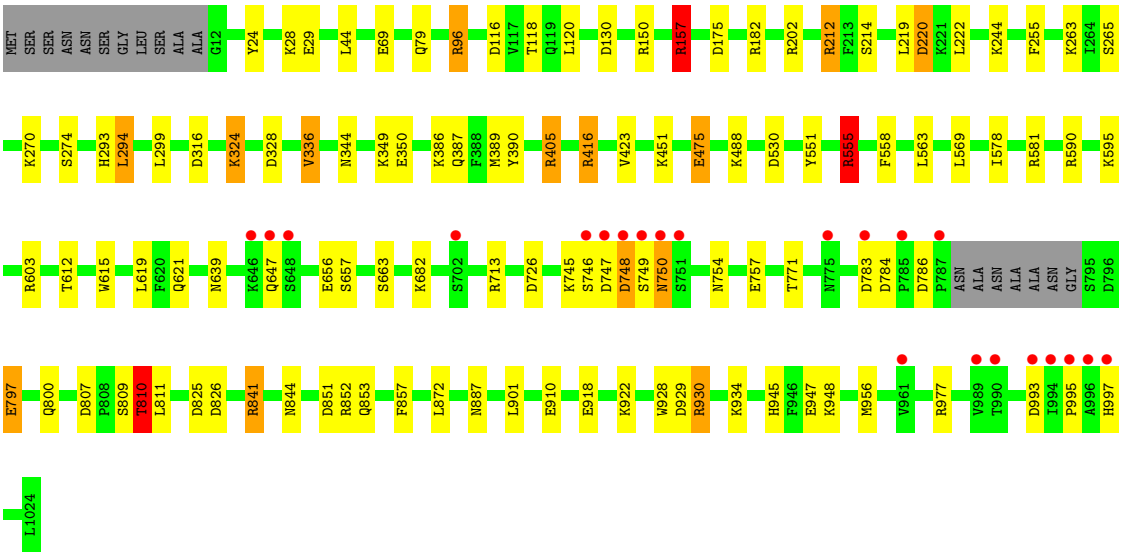
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	331	331	331	0	0
			Total	O		
7	B	18	18	18	0	0
			Total	O		
7	C	302	302	302	0	0
			Total	O		
7	D	13	13	13	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

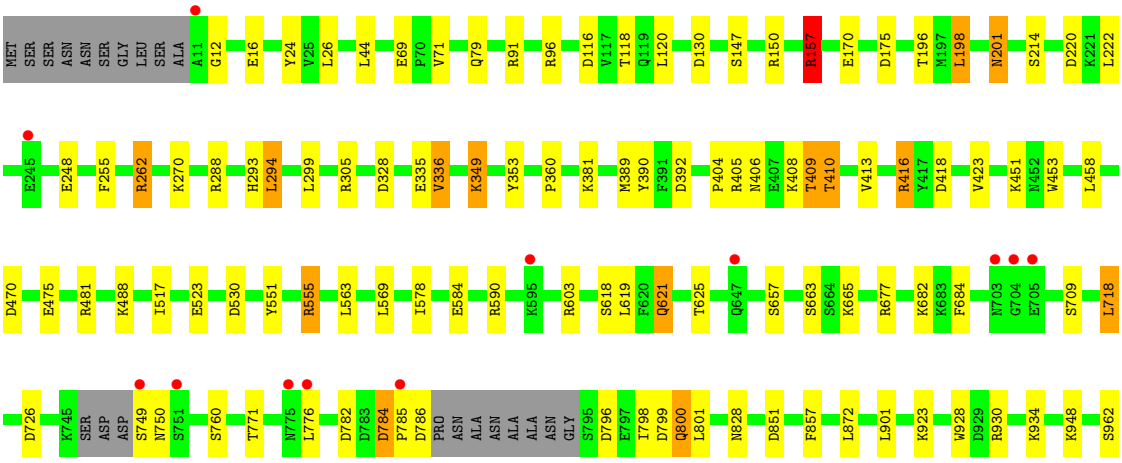
• Molecule 1: Ubiquitin-activating enzyme E1 1

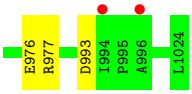
Chain A:



• Molecule 1: Ubiquitin-activating enzyme E1 1

Chain C:



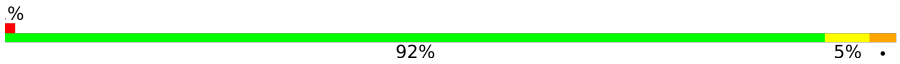


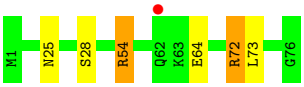
• Molecule 2: Ubiquitin-40S ribosomal protein S31

Chain B:

• Molecule 2: Ubiquitin-40S ribosomal protein S31

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	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 48.48 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.68) 99.3 (48.48-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [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 (4.93%)	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 , 33.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, CL, 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	0.93	4/8110 (0.0%)	1.04	36/10975 (0.3%)
1	C	0.93	4/8093 (0.0%)	1.02	29/10949 (0.3%)
2	B	0.92	0/616	1.17	5/826 (0.6%)
2	D	0.82	0/616	1.08	2/826 (0.2%)
All	All	0.93	8/17435 (0.0%)	1.04	72/23576 (0.3%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	584	GLU	CD-OE1	7.09	1.33	1.25
1	C	147	SER	CB-OG	-6.46	1.33	1.42
1	A	274	SER	CB-OG	-5.53	1.35	1.42
1	A	475	GLU	CD-OE1	5.34	1.31	1.25
1	C	170	GLU	CD-OE1	5.31	1.31	1.25
1	A	265	SER	CB-OG	-5.28	1.35	1.42
1	C	976	GLU	CD-OE1	5.16	1.31	1.25
1	A	910	GLU	CD-OE1	5.12	1.31	1.25

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	841	ARG	NE-CZ-NH2	-10.46	115.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	416	ARG	NE-CZ-NH2	-10.27	115.16	120.30
1	C	150	ARG	NE-CZ-NH2	9.29	124.94	120.30
1	A	130	ASP	CB-CG-OD1	9.22	126.60	118.30
1	A	726	ASP	CB-CG-OD1	9.20	126.58	118.30
1	C	851	ASP	CB-CG-OD1	9.20	126.58	118.30
1	A	212	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	A	150	ARG	NE-CZ-NH2	8.81	124.71	120.30
1	A	851	ASP	CB-CG-OD1	8.73	126.16	118.30
1	A	841	ARG	NE-CZ-NH1	8.49	124.55	120.30
2	D	54	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	157	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	A	96	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	C	305	ARG	NE-CZ-NH2	7.92	124.26	120.30
2	B	54	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	C	416	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	826	ASP	CB-CG-OD1	7.23	124.81	118.30
1	A	182	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	405	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	C	130	ASP	CB-CG-OD1	7.11	124.70	118.30
1	C	262	ARG	NE-CZ-NH2	-7.10	116.75	120.30
2	D	72	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	220	ASP	CB-CG-OD1	-6.95	112.04	118.30
1	C	157	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	A	555	ARG	CG-CD-NE	6.58	125.61	111.80
1	C	157	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	A	929	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	288	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	C	530	ASP	CB-CG-OD1	6.36	124.03	118.30
1	A	405	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	713	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	389	MET	CG-SD-CE	-6.21	90.27	100.20
1	C	851	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	C	175	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	A	603	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	C	418	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	175	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	416	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	918	GLU	OE1-CD-OE2	5.97	130.47	123.30
1	C	175	ASP	CB-CG-OD1	5.96	123.66	118.30
1	C	481	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	157	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	581	ARG	NE-CZ-NH2	-5.86	117.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	530	ASP	CB-CG-OD1	5.76	123.49	118.30
1	C	677	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	825	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	C	603	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	A	783	ASP	CB-CG-OD1	5.70	123.43	118.30
1	C	150	ARG	NE-CZ-NH1	-5.67	117.46	120.30
1	A	220	ASP	CB-CG-OD2	5.63	123.36	118.30
1	C	726	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	726	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	C	44	LEU	CB-CG-CD2	5.57	120.48	111.00
1	A	212	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	410	THR	N-CA-CB	-5.51	99.83	110.30
1	C	481	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	977	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	B	72	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	C	389	MET	CG-SD-CE	-5.31	91.71	100.20
1	A	202	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	810	THR	CA-CB-CG2	5.22	119.71	112.40
1	C	328	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	782	ASP	CB-CG-OD1	5.18	122.96	118.30
1	C	977	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	B	74[A]	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	B	74[B]	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	618	SER	CB-CA-C	-5.07	100.46	110.10
2	B	72	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	797	GLU	N-CA-CB	5.04	119.68	110.60
1	C	784	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	175	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	A	44	LEU	CB-CG-CD2	-5.01	102.49	111.00

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 (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	7945	0	7846	42	0
1	C	7927	0	7838	35	0
2	B	608	0	638	3	0
2	D	608	0	638	2	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	81	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 2.

All (81) 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: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:C:798:ILE:O	1:C:799:ASP:C	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:746:SER:CB	1:A:749:SER:HB3	2.44	0.48
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
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
2:D:72:ARG:C	2:D:73:LEU:HG	2.37	0.43
1:A:852:ARG:HD3	7:A:1494:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:684:PHE:HB3	1:C:718:LEU:HD22	2.00	0.43
1:A:255:PHE:CD1	1:A:255:PHE:C	2.91	0.43
1:A:293:HIS:HA	1:A:390:TYR:CZ	2.54	0.43
2:B:72:ARG:C	2:B:73:LEU:HG	2.39	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:C:255:PHE:C	1:C:255:PHE:CD1	2.92	0.43
1:C:785:PRO:O	1:C:786:ASP:C	2.57	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
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: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: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: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: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%)	51 76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	998/1024 (98%)	966 (97%)	31 (3%)	1 (0%)	51	76
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%)	51	76

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%)	841 (95%)	48 (5%)	22	44
1	C	886/900 (98%)	833 (94%)	53 (6%)	19	39
2	B	70/69 (101%)	66 (94%)	4 (6%)	20	41
2	D	70/69 (101%)	66 (94%)	4 (6%)	20	41
All	All	1915/1938 (99%)	1806 (94%)	109 (6%)	21	41

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	29	GLU
1	A	79	GLN
1	A	96	ARG
1	A	120	LEU
1	A	157	ARG
1	A	212	ARG
1	A	214	SER
1	A	220	ASP

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Mol	Chain	Res	Type
1	A	222	LEU
1	A	244	LYS
1	A	263	LYS
1	A	270	LYS
1	A	294	LEU
1	A	316	ASP
1	A	324	LYS
1	A	336	VAL
1	A	349	LYS
1	A	416	ARG
1	A	451	LYS
1	A	475	GLU
1	A	488	LYS
1	A	555	ARG
1	A	590	ARG
1	A	595	LYS
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	745	LYS
1	A	748	ASP
1	A	750	ASN
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
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

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Mol	Chain	Res	Type
2	B	74[B]	ARG
1	C	16	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	222	LEU
1	C	248	GLU
1	C	262	ARG
1	C	270	LYS
1	C	294	LEU
1	C	335	GLU
1	C	336	VAL
1	C	349	LYS
1	C	360	PRO
1	C	392	ASP
1	C	408	LYS
1	C	409	THR
1	C	410	THR
1	C	413	VAL
1	C	416	ARG
1	C	451	LYS
1	C	475	GLU
1	C	488	LYS
1	C	517	ILE
1	C	523	GLU
1	C	555	ARG
1	C	590	ARG
1	C	619	LEU
1	C	621[A]	GLN
1	C	621[B]	GLN
1	C	657	SER
1	C	663	SER
1	C	665	LYS
1	C	682	LYS
1	C	709	SER
1	C	718	LEU

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Mol	Chain	Res	Type
1	C	749	SER
1	C	750	ASN
1	C	760	SER
1	C	771	THR
1	C	776	LEU
1	C	784	ASP
1	C	800	GLN
1	C	923	LYS
1	C	934	LYS
1	C	948	LYS
1	C	962	SER
1	C	993	ASP
2	D	25	ASN
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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	647	GLN
1	A	984	GLN
1	A	997	HIS
1	C	35	GLN
1	C	201	ASN
1	C	750	ASN
2	D	2	GLN

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 monosaccharides 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	C	1106	-	5,5,5	0.72	0	5,5,5	0.40	0
5	GOL	C	1108	-	5,5,5	1.09	0	5,5,5	1.16	0
5	GOL	A	1110	-	5,5,5	0.63	0	5,5,5	0.79	0
5	GOL	A	1111	-	5,5,5	0.78	0	5,5,5	0.77	0
3	SO4	A	1101	-	4,4,4	0.49	0	6,6,6	0.71	0
6	61T	B	101	2	33,37,37	2.47	9 (27%)	42,56,56	2.66	11 (26%)
3	SO4	A	1102	-	4,4,4	0.37	0	6,6,6	0.19	0
5	GOL	A	1106	-	5,5,5	0.84	0	5,5,5	0.74	0
5	GOL	A	1108	-	5,5,5	0.79	0	5,5,5	0.56	0
5	GOL	A	1109	-	5,5,5	0.83	0	5,5,5	0.66	0
5	GOL	C	1105	-	5,5,5	0.91	0	5,5,5	0.73	0
5	GOL	A	1107	-	5,5,5	0.75	0	5,5,5	0.76	0
5	GOL	C	1111	-	5,5,5	0.53	0	5,5,5	0.81	0
5	GOL	C	1109	-	5,5,5	0.77	0	5,5,5	0.73	0
5	GOL	C	1110	-	5,5,5	0.61	0	5,5,5	0.53	0
5	GOL	A	1105	-	5,5,5	0.75	0	5,5,5	1.28	1 (20%)
6	61T	D	101	2	33,37,37	2.16	8 (24%)	42,56,56	2.68	15 (35%)
5	GOL	C	1112	-	5,5,5	0.44	0	5,5,5	0.48	0
3	SO4	C	1101	-	4,4,4	0.62	0	6,6,6	1.34	1 (16%)
5	GOL	C	1107	-	5,5,5	0.63	0	5,5,5	0.73	0
5	GOL	C	1104	-	5,5,5	0.55	0	5,5,5	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
5	GOL	C	1112	-	-	0/4/4/4	-
5	GOL	A	1107	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	1106	-	-	2/4/4/4	-
5	GOL	C	1108	-	-	1/4/4/4	-
5	GOL	C	1109	-	-	2/4/4/4	-
5	GOL	C	1110	-	-	0/4/4/4	-
5	GOL	A	1105	-	-	1/4/4/4	-
5	GOL	A	1106	-	-	3/4/4/4	-
5	GOL	C	1111	-	-	2/4/4/4	-
5	GOL	A	1108	-	-	2/4/4/4	-
5	GOL	A	1109	-	-	2/4/4/4	-
5	GOL	A	1110	-	-	2/4/4/4	-
5	GOL	C	1107	-	-	0/4/4/4	-
5	GOL	C	1105	-	-	3/4/4/4	-
6	61T	D	101	2	-	5/19/35/35	0/4/4/4
5	GOL	C	1104	-	-	1/4/4/4	-
5	GOL	A	1111	-	-	0/4/4/4	-
6	61T	B	101	2	-	0/19/35/35	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	101	61T	C14-S1	-8.27	1.68	1.78
6	D	101	61T	C14-S1	-6.11	1.71	1.78
6	B	101	61T	C5-C6	6.11	1.51	1.38
6	D	101	61T	C5-C6	5.83	1.50	1.38
6	B	101	61T	C17-C3	-4.56	1.48	1.53
6	D	101	61T	C17-C3	-4.43	1.49	1.53
6	B	101	61T	C8-C9	4.16	1.47	1.39
6	B	101	61T	C4-N1	3.91	1.46	1.37
6	D	101	61T	C8-C9	3.57	1.46	1.39
6	B	101	61T	C2-C3	-3.47	1.48	1.54
6	D	101	61T	C5-C4	-3.21	1.34	1.39
6	D	101	61T	C2-C3	-3.02	1.48	1.54
6	D	101	61T	C4-N1	2.69	1.43	1.37
6	B	101	61T	C5-C4	-2.51	1.35	1.39
6	B	101	61T	S-N	2.40	1.61	1.58
6	D	101	61T	O-S	2.31	1.44	1.42
6	B	101	61T	O1-S	2.26	1.44	1.42

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	101	61T	O-S-O1	-11.17	109.41	119.97
6	D	101	61T	O-S-O1	-10.41	110.12	119.97
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	C2-C1-C	-5.50	102.02	112.68
6	B	101	61T	C16-S1-C14	4.78	111.69	99.21
6	B	101	61T	C17-C3-N1	3.89	120.07	112.32
6	D	101	61T	C2-C1-C18	3.65	111.61	102.66
6	B	101	61T	C-O2-S	3.54	121.65	117.21
6	D	101	61T	C16-S1-C14	3.25	107.69	99.21
6	B	101	61T	C15-C14-S1	-3.16	116.12	120.04
6	D	101	61T	O2-C-C1	3.10	116.05	108.30
6	B	101	61T	C2-C1-C18	3.02	110.08	102.66
6	D	101	61T	C17-C3-N1	2.97	118.24	112.32
6	D	101	61T	C5-C6-N2	-2.97	119.98	124.58
6	D	101	61T	C10-C9-N3	2.86	125.45	120.92
6	B	101	61T	O1-S-N	-2.68	105.08	109.14
6	D	101	61T	O1-S-N	-2.52	105.33	109.14
6	D	101	61T	O4-C18-C17	2.49	119.87	111.82
6	B	101	61T	O4-C18-C1	-2.44	106.43	112.75
6	D	101	61T	C1-C2-C3	-2.39	100.47	103.32
6	D	101	61T	C-O2-S	2.39	120.20	117.21
3	C	1101	SO4	O3-S-O1	2.37	121.69	109.31
6	D	101	61T	C8-C9-N3	-2.17	105.88	109.88
6	D	101	61T	C2-C3-N1	2.11	117.36	112.67
6	B	101	61T	O4-C18-C17	2.10	118.61	111.82
5	A	1105	GOL	O1-C1-C2	2.02	119.88	110.20
6	B	101	61T	F1-C16-F	2.01	111.85	106.55

There are no chirality outliers.

All (28) 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
5	C	1108	GOL	C1-C2-C3-O3
6	D	101	61T	C-O2-S-O1
6	D	101	61T	C-O2-S-O

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

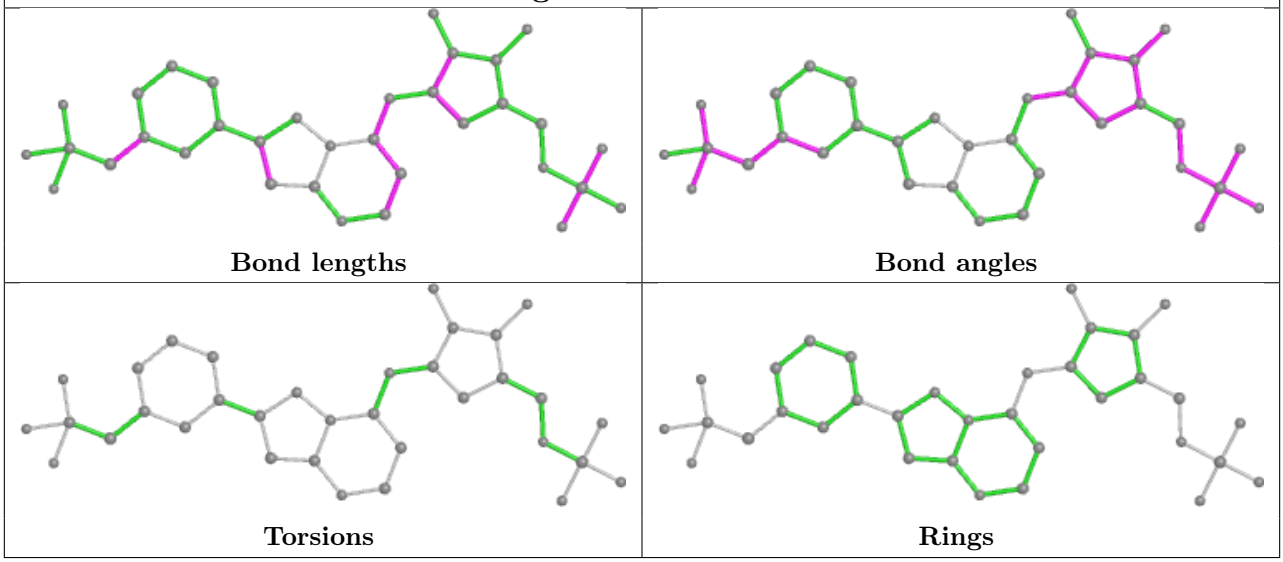
There are no ring outliers.

3 monomers are involved in 3 short contacts:

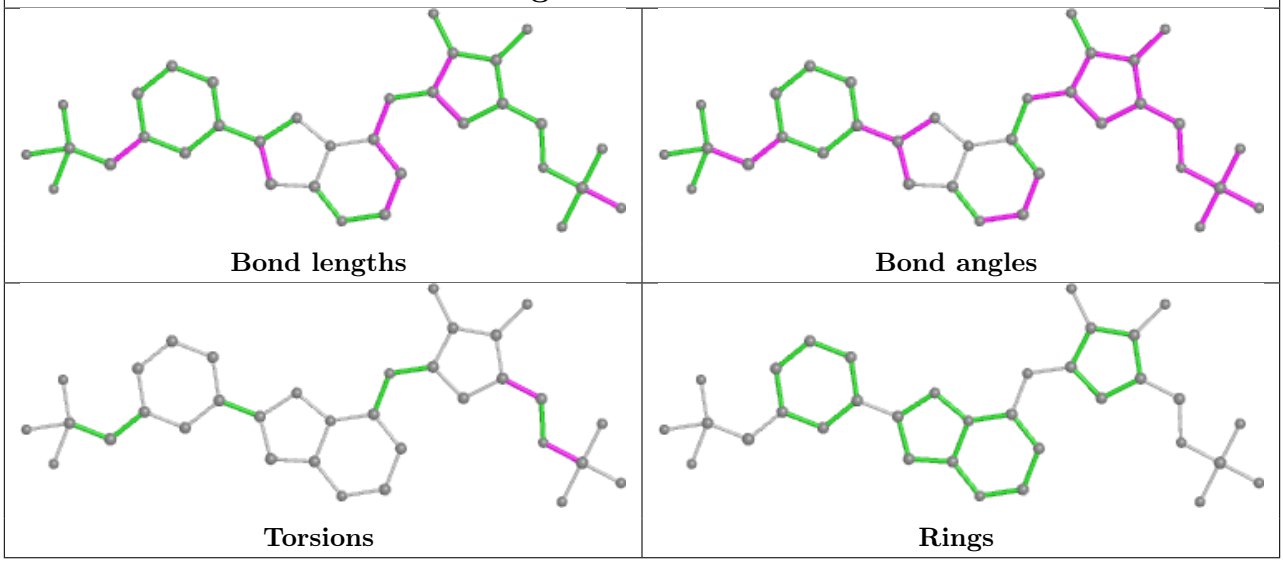
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1110	GOL	1	0
6	D	101	61T	1	0
5	C	1107	GOL	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 61T B 101



Ligand 61T D 101



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%)	-0.36	22 (2%) 62 61	26, 44, 90, 150	0
1	C	1003/1024 (97%)	-0.35	14 (1%) 75 76	26, 45, 91, 141	0
2	B	76/76 (100%)	-0.10	0 100 100	28, 50, 75, 88	0
2	D	76/76 (100%)	-0.23	1 (1%) 77 78	39, 57, 84, 89	0
All	All	2161/2200 (98%)	-0.34	37 (1%) 70 71	26, 45, 89, 150	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	747	ASP	4.3
1	A	647	GLN	4.3
1	A	750	ASN	4.2
1	A	646	LYS	3.7
1	A	748	ASP	3.5
1	A	746	SER	3.4
1	C	11	ALA	3.3
1	C	751	SER	3.2
1	C	994	ILE	3.2
1	A	749	SER	3.2
1	A	996	ALA	3.1
1	A	775	ASN	3.0
1	C	704	GLY	3.0
1	C	996	ALA	2.7
1	C	703	ASN	2.7
1	A	785	PRO	2.6
1	A	648	SER	2.6
1	A	702	SER	2.6
1	C	775	ASN	2.5
1	A	783	ASP	2.5
1	C	776	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	595	LYS	2.4
1	C	785	PRO	2.4
1	A	990	THR	2.3
1	C	647	GLN	2.3
1	A	994	ILE	2.3
1	A	787	PRO	2.3
1	A	997	HIS	2.3
1	C	705	GLU	2.2
1	A	751	SER	2.2
1	C	749	SER	2.1
2	D	62	GLN	2.1
1	A	961	VAL	2.1
1	A	995	PRO	2.1
1	A	993	ASP	2.0
1	C	245	GLU	2.0
1	A	989	VAL	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 monosaccharides 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(Å^2)	Q<0.9
5	GOL	C	1105	6/6	0.57	0.27	56,72,77,77	0
5	GOL	A	1106	6/6	0.66	0.36	71,86,89,90	0
5	GOL	C	1110	6/6	0.82	0.17	76,83,85,87	0
5	GOL	C	1111	6/6	0.82	0.31	51,60,69,75	0
5	GOL	A	1108	6/6	0.83	0.17	60,63,66,67	0
5	GOL	C	1108	6/6	0.84	0.24	57,63,67,69	0
5	GOL	A	1110	6/6	0.86	0.14	50,56,59,66	0

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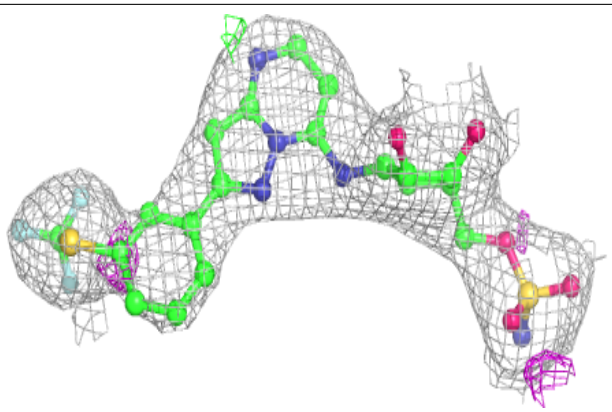
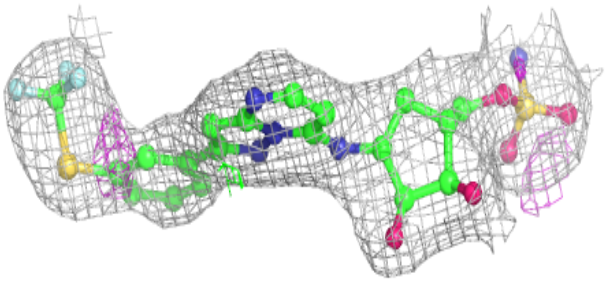
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	C	1104	6/6	0.86	0.16	64,68,71,72	0
5	GOL	A	1109	6/6	0.87	0.33	62,70,75,80	0
5	GOL	C	1107	6/6	0.88	0.34	60,66,67,67	0
4	CL	A	1104	1/1	0.88	0.11	59,59,59,59	0
4	CL	C	1103	1/1	0.89	0.11	64,64,64,64	0
4	CL	C	1102	1/1	0.90	0.08	62,62,62,62	0
3	SO4	A	1102	5/5	0.90	0.17	99,101,110,110	0
5	GOL	A	1111	6/6	0.91	0.24	57,63,66,67	0
5	GOL	A	1105	6/6	0.92	0.23	47,52,56,58	0
4	CL	A	1103	1/1	0.94	0.25	56,56,56,56	0
5	GOL	C	1109	6/6	0.94	0.24	52,63,64,66	0
6	61T	D	101	34/34	0.95	0.16	26,49,79,82	0
5	GOL	A	1107	6/6	0.96	0.21	37,51,54,55	0
6	61T	B	101	34/34	0.96	0.15	26,35,54,57	0
5	GOL	C	1106	6/6	0.96	0.17	38,42,44,47	0
5	GOL	C	1112	6/6	0.97	0.15	42,46,46,49	0
3	SO4	A	1101	5/5	0.99	0.09	28,29,32,33	0
3	SO4	C	1101	5/5	0.99	0.11	26,27,31,33	0

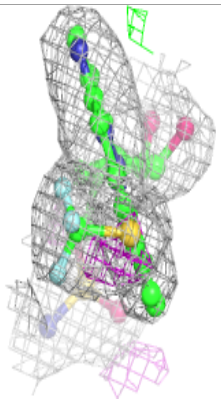
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 61T 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)

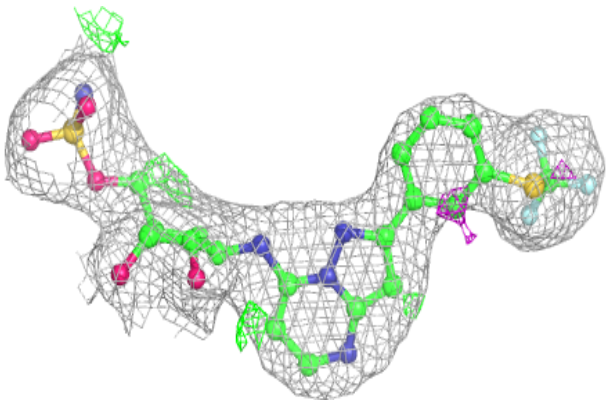


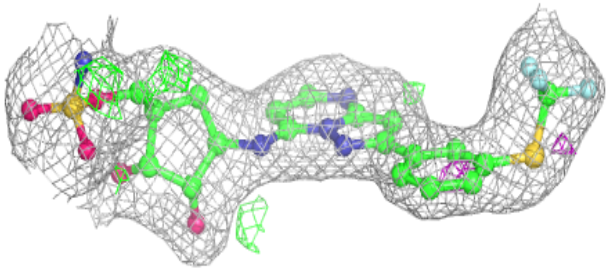


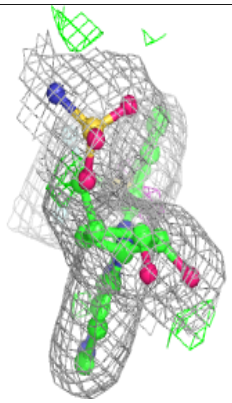


Electron density around 61T B 101:

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







6.5 Other polymers (i)

There are no such residues in this entry.