Full wwPDB X-ray Structure Validation Report ⓘ

Jan 29, 2024 – 12:16 am GMT

PDB ID	:	5L6H
Title	:	Uba1 in complex with Ub-ABPA3 covalent adduct
Authors	:	Misra, M.; Schindelin, H.
Deposited on	:	2016-05-30
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

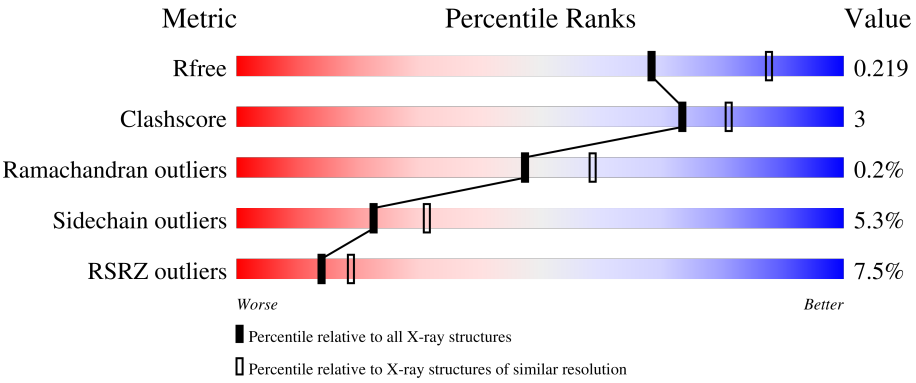
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	4% 86% 11%
1	C	1024	5% 86% 10%
2	B	76	% 93% 5%
2	D	76	% 89% 7%
2	E	76	89% 70% 20% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	C	1104	-	-	X	-
5	GOL	A	1109	-	-	-	X
5	GOL	C	1108	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18998 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.

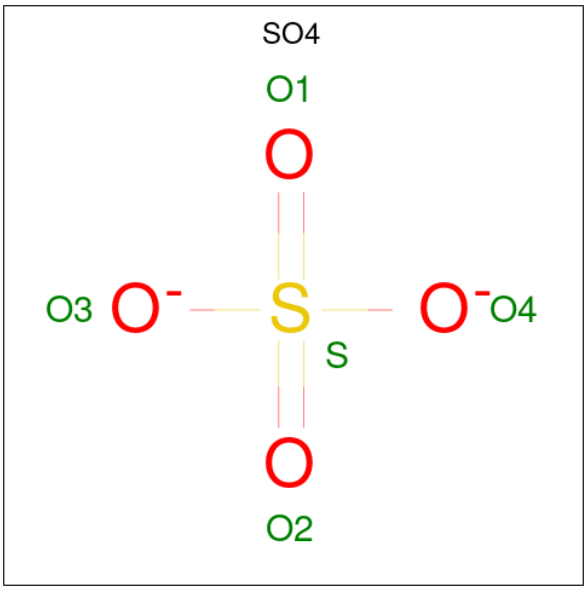
- Molecule 1 is a protein called Ubiquitin-activating enzyme E1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1006	Total	C	N	O	S	0	20	0
			8057	5136	1326	1568	27			
1	C	1005	Total	C	N	O	S	0	9	0
			7981	5086	1314	1556	25			

- 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	4	0
			631	394	113	123	1			
2	D	76	Total	C	N	O	S	0	2	0
			614	384	108	121	1			
2	E	72	Total	C	N	O	S	0	0	0
			573	359	98	115	1			

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

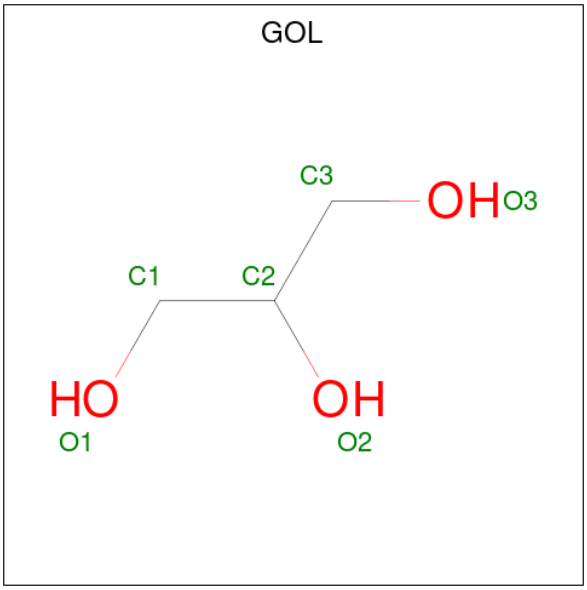


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Cl 4 4	0	0
4	C	4	Total Cl 4 4	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
5	A	1	Total C O 6 3 3	0	0

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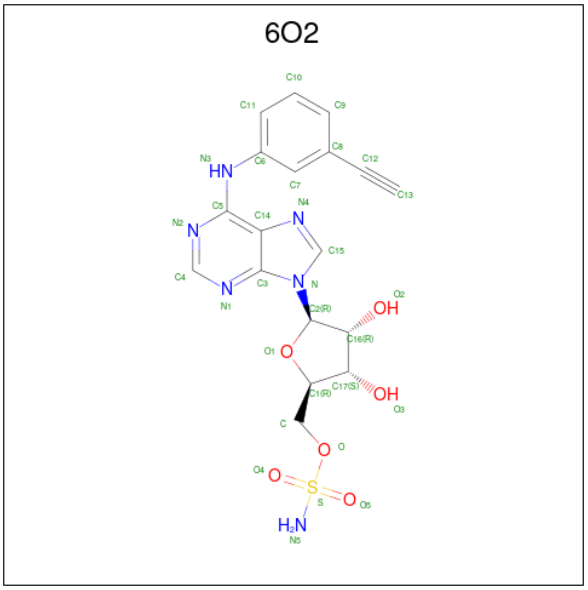
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

- Molecule 6 is [(2 {R},3 {S},4 {R},5 {R})-5-[6-[(3-ethynylphenyl)amino]purin-9-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methyl sulfamate (three-letter code: 6O2) (formula: $C_{18}H_{18}N_6O_6S$).

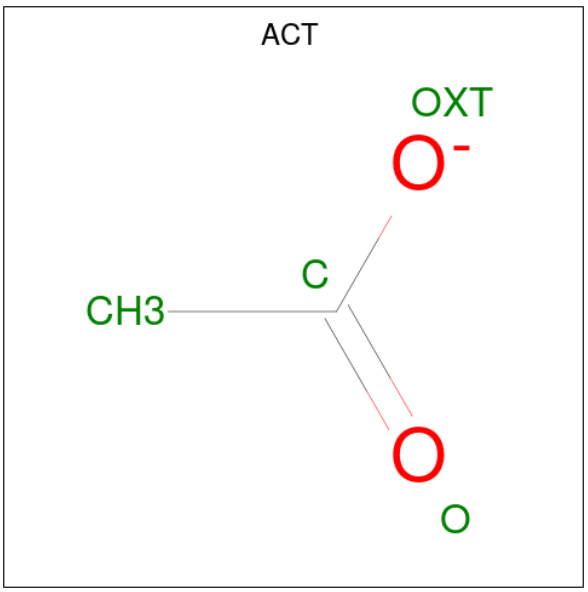


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O S 31 18 6 6 1	0	0
6	D	1	Total C N O S 31 18 6 6 1	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total Mg 1 1	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 4 2 2	0	0

- Molecule 9 is water.

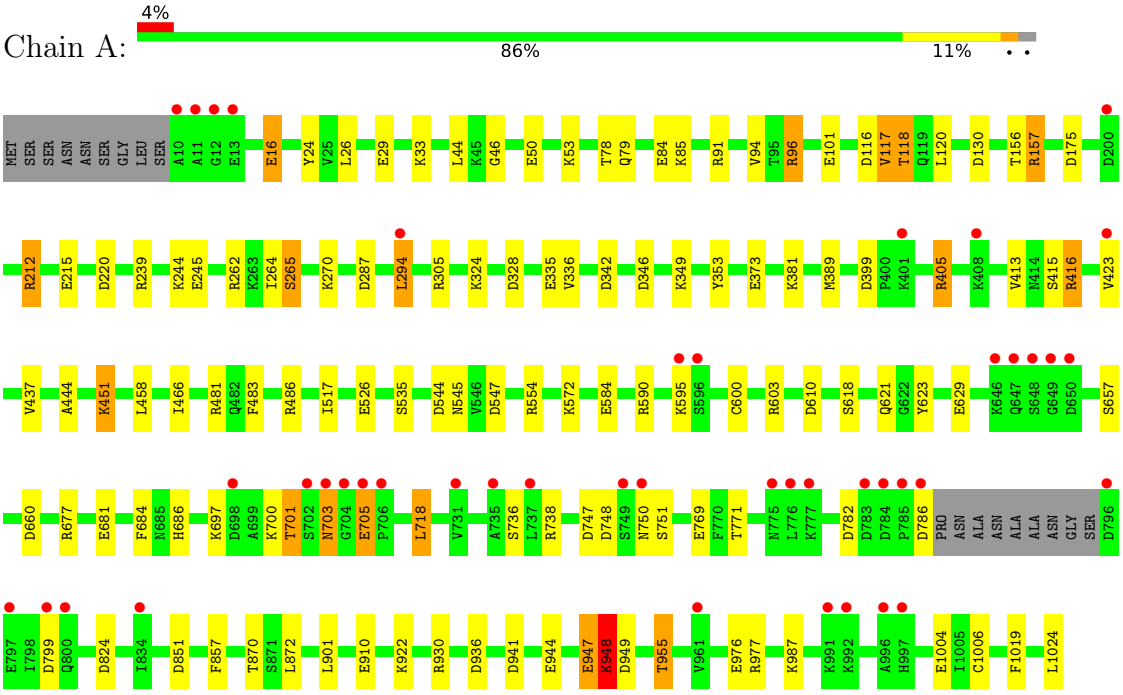
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	485	Total O 485 485	0	0
9	B	33	Total O 33 33	0	0
9	C	441	Total O 441 441	0	0
9	D	29	Total O 29 29	0	0
9	E	3	Total O 3 3	0	0

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.

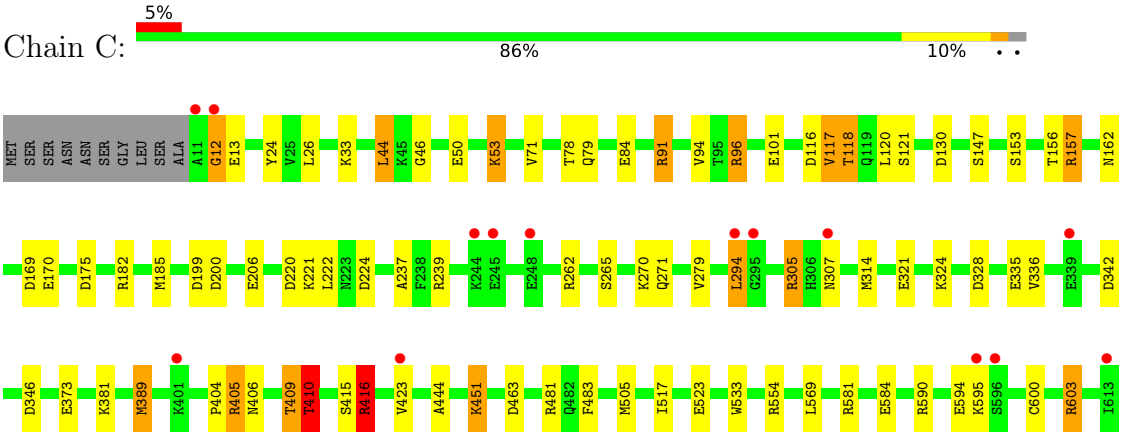
• Molecule 1: Ubiquitin-activating enzyme E1 1

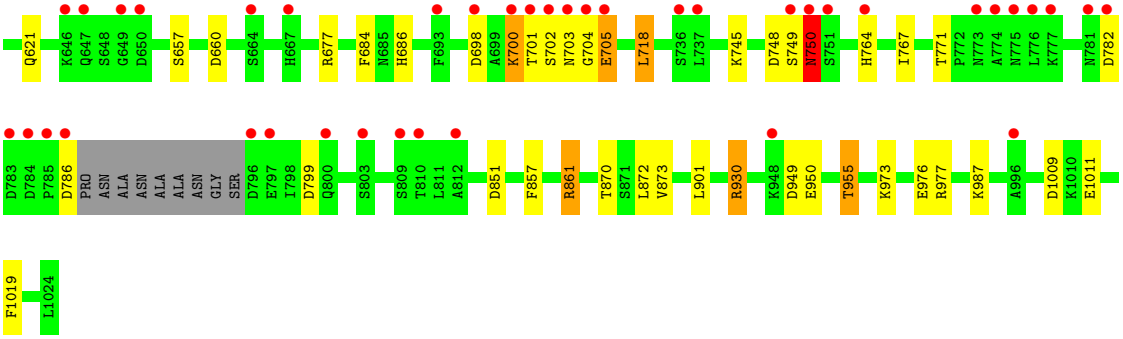
Chain A:



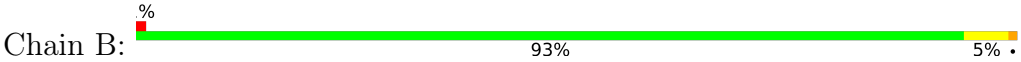
• Molecule 1: Ubiquitin-activating enzyme E1 1

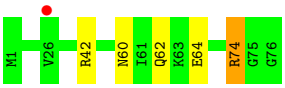
Chain C:



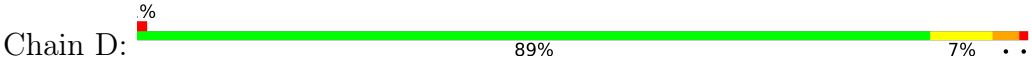


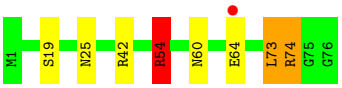
• Molecule 2: Ubiquitin-40S ribosomal protein S31



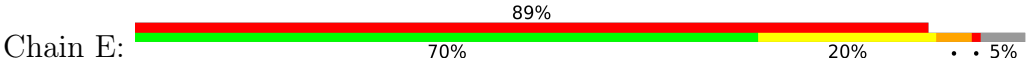


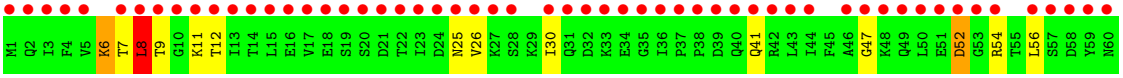
• Molecule 2: Ubiquitin-40S ribosomal protein S31

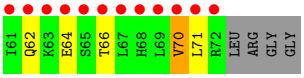




• Molecule 2: Ubiquitin-40S ribosomal protein S31







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.05Å 194.10Å 230.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.30) 99.4 (19.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.172 , 0.218 0.178 , 0.219	Depositor DCC
R_{free} test set	7006 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 31.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18998	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: ACT, GOL, SO4, CSO, 6O2, MG, CL

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	21/8264 (0.3%)	1.17	56/11181 (0.5%)
1	C	1.21	20/8161 (0.2%)	1.14	53/11039 (0.5%)
2	B	0.98	0/645	1.12	3/864 (0.3%)
2	D	1.00	1/625 (0.2%)	1.15	8/838 (1.0%)
2	E	0.88	0/578	1.17	3/777 (0.4%)
All	All	1.19	42/18273 (0.2%)	1.15	123/24699 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	84	GLU	CD-OE1	11.57	1.38	1.25
1	A	1004	GLU	CG-CD	11.53	1.69	1.51
1	C	976	GLU	CD-OE1	9.47	1.36	1.25
1	C	523[B]	GLU	CG-CD	8.57	1.64	1.51
1	C	147	SER	CB-OG	-8.31	1.31	1.42
1	A	944	GLU	CD-OE2	8.15	1.34	1.25
1	C	1019	PHE	CG-CD1	7.65	1.50	1.38
1	C	976	GLU	CD-OE2	7.62	1.34	1.25
1	A	976	GLU	CD-OE2	7.16	1.33	1.25
1	C	101	GLU	CD-OE1	7.05	1.33	1.25
1	A	335	GLU	CG-CD	6.73	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1019	PHE	CG-CD2	6.72	1.48	1.38
1	C	12	GLY	N-CA	6.58	1.55	1.46
1	A	1019	PHE	CG-CD1	6.54	1.48	1.38
1	A	84	GLU	CD-OE1	6.54	1.32	1.25
1	A	910	GLU	CD-OE1	6.51	1.32	1.25
1	A	976	GLU	CD-OE1	6.27	1.32	1.25
1	A	623	TYR	CG-CD2	6.07	1.47	1.39
1	A	629	GLU	CD-OE1	5.96	1.32	1.25
1	A	212	ARG	CZ-NH2	-5.95	1.25	1.33
1	A	265	SER	CB-OG	-5.83	1.34	1.42
1	C	873	VAL	CB-CG1	-5.77	1.40	1.52
1	C	533	TRP	CB-CG	-5.75	1.39	1.50
1	C	170	GLU	CG-CD	5.66	1.60	1.51
1	A	736[A]	SER	CB-OG	5.61	1.49	1.42
1	A	736[B]	SER	CB-OG	5.61	1.49	1.42
1	C	153	SER	CB-OG	-5.59	1.34	1.42
1	A	976	GLU	CG-CD	5.59	1.60	1.51
1	C	169	ASP	CB-CG	-5.58	1.40	1.51
1	C	976	GLU	CG-CD	5.55	1.60	1.51
1	A	623	TYR	CE1-CZ	5.51	1.45	1.38
1	A	526	GLU	CD-OE2	5.50	1.31	1.25
2	D	19	SER	CB-OG	-5.36	1.35	1.42
1	C	950	GLU	CD-OE1	5.35	1.31	1.25
1	C	206	GLU	CD-OE2	5.34	1.31	1.25
1	C	162	ASN	CG-OD1	-5.32	1.12	1.24
1	A	245	GLU	CG-CD	5.29	1.59	1.51
1	C	121	SER	CB-OG	-5.18	1.35	1.42
1	C	523[B]	GLU	CD-OE1	5.18	1.31	1.25
1	A	16	GLU	CD-OE1	5.13	1.31	1.25
1	A	215	GLU	CG-CD	5.06	1.59	1.51
1	A	101	GLU	CD-OE1	5.04	1.31	1.25

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	212	ARG	NE-CZ-NH2	-15.55	112.52	120.30
1	A	212	ARG	NE-CZ-NH1	13.70	127.15	120.30
1	A	1004	GLU	OE1-CD-OE2	-11.46	109.55	123.30
1	A	405	ARG	NE-CZ-NH2	-11.25	114.67	120.30
1	A	405	ARG	NE-CZ-NH1	11.24	125.92	120.30
1	C	416	ARG	NE-CZ-NH1	11.01	125.81	120.30
1	C	405	ARG	NE-CZ-NH1	10.68	125.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	91	ARG	NE-CZ-NH1	9.61	125.11	120.30
1	C	416	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	C	169	ASP	CB-CG-OD1	-9.23	109.99	118.30
1	A	262	ARG	NE-CZ-NH1	9.23	124.91	120.30
1	C	861	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	C	91	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	A	949	ASP	CB-CG-OD1	8.37	125.83	118.30
2	E	8	LEU	CA-CB-CG	8.23	134.23	115.30
1	C	305	ARG	NE-CZ-NH2	8.12	124.36	120.30
1	C	405	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	A	239	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	A	96	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	A	130	ASP	CB-CG-OD1	7.92	125.42	118.30
1	A	91	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	C	91	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	287[A]	ASP	CB-CG-OD1	7.72	125.25	118.30
1	A	287[B]	ASP	CB-CG-OD1	7.72	125.25	118.30
1	A	239	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	A	416[A]	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	A	416[B]	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	A	346	ASP	CB-CG-OD1	7.33	124.90	118.30
1	C	851	ASP	CB-CG-OD1	7.19	124.77	118.30
1	C	130	ASP	CB-CG-OD1	7.19	124.77	118.30
1	C	96	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	287[A]	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	A	287[B]	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	A	416[A]	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	416[B]	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	328	ASP	CB-CG-OD2	-7.13	111.88	118.30
2	B	42	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	C	305	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	C	581	ARG	NE-CZ-NH1	7.02	123.81	120.30
2	E	70	VAL	CB-CA-C	6.98	124.66	111.40
1	C	861	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	C	185	MET	CG-SD-CE	-6.82	89.29	100.20
1	A	305	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	A	29	GLU	N-CA-CB	6.70	122.65	110.60
1	C	328	ASP	CB-CG-OD1	6.68	124.31	118.30
1	C	410	THR	N-CA-CB	-6.60	97.76	110.30
1	A	584[A]	GLU	CB-CA-C	-6.59	97.22	110.40
1	A	584[B]	GLU	CB-CA-C	-6.59	97.22	110.40
1	A	738	ARG	NE-CZ-NH1	6.53	123.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	590	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	C	481	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	C	584[A]	GLU	CB-CA-C	-6.37	97.67	110.40
1	C	584[B]	GLU	CB-CA-C	-6.37	97.67	110.40
1	C	523[B]	GLU	OE1-CD-OE2	-6.34	115.69	123.30
1	C	767	ILE	CG1-CB-CG2	-6.33	97.47	111.40
1	A	486	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	175	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	44	LEU	CB-CG-CD2	-6.25	100.38	111.00
2	D	73	LEU	CA-CB-CG	-6.24	100.96	115.30
1	C	977	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	851	ASP	CB-CG-OD1	6.17	123.86	118.30
1	A	660	ASP	CB-CG-OD1	6.17	123.86	118.30
1	C	239	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	C	117	VAL	CB-CA-C	-6.09	99.82	111.40
1	C	949	ASP	CB-CG-OD1	6.08	123.77	118.30
1	C	748	ASP	CB-CG-OD2	6.06	123.75	118.30
2	D	74[A]	ARG	NE-CZ-NH2	-6.03	117.29	120.30
2	D	74[B]	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	C	603	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	182	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	C	262[A]	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	C	262[B]	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	547	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	389[A]	MET	CG-SD-CE	-5.93	90.72	100.20
1	A	389[B]	MET	CG-SD-CE	-5.93	90.72	100.20
1	A	342	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	C	239	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	769	GLU	OE1-CD-OE2	-5.87	116.26	123.30
1	A	936	ASP	CB-CG-OD1	5.86	123.58	118.30
1	A	977	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	C	660	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	481	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	96	ARG	CG-CD-NE	-5.84	99.53	111.80
1	A	373	GLU	OE1-CD-OE2	-5.81	116.32	123.30
1	A	305	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	44	LEU	CB-CG-CD1	5.77	120.80	111.00
1	C	389[A]	MET	CG-SD-CE	-5.75	90.99	100.20
1	C	389[B]	MET	CG-SD-CE	-5.75	90.99	100.20
1	A	44	LEU	CB-CG-CD1	5.66	120.62	111.00
1	A	481	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	96	ARG	CG-CD-NE	-5.59	100.06	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	505	MET	CG-SD-CE	-5.52	91.37	100.20
2	D	54	ARG	CB-CG-CD	5.52	125.94	111.60
2	D	42	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	C	342	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	C	554	ARG	NE-CZ-NH1	-5.35	117.63	120.30
1	C	463	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	29	GLU	CA-CB-CG	5.34	125.14	113.40
2	D	74[A]	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	D	74[B]	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	481	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	175	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	117	VAL	CB-CA-C	-5.29	101.34	111.40
2	E	52	ASP	N-CA-C	5.29	125.27	111.00
1	C	930	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	C	1011	GLU	CA-CB-CG	5.24	124.93	113.40
1	A	554	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	C	44	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	A	399	ASP	CB-CG-OD1	5.22	122.99	118.30
1	C	346	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	C	224	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	C	373	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	A	824	ASP	CB-CG-OD1	5.17	122.96	118.30
1	A	948	LYS	CA-CB-CG	5.17	124.78	113.40
1	A	941	ASP	CB-CG-OD1	5.15	122.93	118.30
2	D	73	LEU	CB-CG-CD2	5.10	119.67	111.00
1	A	747	ASP	CB-CG-OD1	5.05	122.85	118.30
1	C	677	ARG	NE-CZ-NH2	-5.02	117.79	120.30
2	B	74[A]	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	B	74[B]	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	A	262	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	572	LYS	CD-CE-NZ	-5.01	100.19	111.70
1	C	1009	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	750	ASN	Peptide
1	C	44	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	8057	0	7994	33	0
1	C	7981	0	7894	69	0
2	B	631	0	664	4	0
2	D	614	0	644	3	0
2	E	573	0	595	39	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
4	A	4	0	0	1	0
4	C	4	0	0	3	0
5	A	42	0	56	0	0
5	C	24	0	32	1	0
6	B	31	0	0	0	0
6	D	31	0	0	0	0
7	C	1	0	0	0	0
8	C	4	0	3	0	0
9	A	485	0	0	2	0
9	B	33	0	0	1	0
9	C	441	0	0	6	0
9	D	29	0	0	0	0
9	E	3	0	0	0	0
All	All	18998	0	17882	117	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 (117) 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)
2:B:74[B]:ARG:NH2	9:B:201:HOH:O	1.83	1.07
4:C:1102:CL:CL	9:C:1442:HOH:O	2.08	1.05
1:C:199:ASP:OD1	2:E:8:LEU:HB3	1.56	1.05
1:C:199:ASP:C	2:E:70:VAL:HB	1.80	1.02
1:C:705:GLU:HG3	2:E:9:THR:OG1	1.62	0.99
1:C:703:ASN:ND2	2:E:11:LYS:HD2	1.85	0.91
1:C:705:GLU:HB3	2:E:11:LYS:HB3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:703:ASN:HD22	2:E:11:LYS:HD2	1.39	0.87
1:C:703:ASN:CB	2:E:11:LYS:HD2	2.08	0.84
2:E:30:ILE:HG21	2:E:41:GLN:OE1	1.78	0.83
2:E:30:ILE:CG2	2:E:41:GLN:OE1	2.28	0.81
1:C:701:THR:O	1:C:703:ASN:N	2.13	0.81
1:C:955:THR:HG21	9:C:1205:HOH:O	1.83	0.77
1:C:116:ASP:OD1	1:C:118:THR:HB	1.85	0.76
1:C:703:ASN:HB3	2:E:11:LYS:HD2	1.68	0.75
1:C:406:ASN:H	1:C:409:THR:HG22	1.53	0.74
1:C:703:ASN:HB2	1:C:705:GLU:OE1	1.88	0.73
1:C:705:GLU:HG3	2:E:9:THR:CB	2.19	0.73
1:A:116:ASP:OD1	1:A:118:THR:HB	1.91	0.71
1:C:404:PRO:O	1:C:409:THR:HG21	1.91	0.70
1:C:861:ARG:NH1	4:C:1104:CL:CL	2.62	0.70
1:A:703:ASN:HB2	1:A:705:GLU:OE2	1.92	0.70
4:C:1104:CL:CL	2:D:74[A]:ARG:NH2	2.62	0.69
1:C:13:GLU:HB2	9:C:1563:HOH:O	1.92	0.68
1:C:749:SER:O	1:C:750:ASN:HB2	1.94	0.68
1:C:705:GLU:CG	2:E:9:THR:OG1	2.41	0.67
1:A:294:LEU:HD11	1:A:336:VAL:HG11	1.77	0.67
1:A:703:ASN:N	1:A:703:ASN:OD1	2.29	0.66
1:A:50:GLU:OE2	1:A:53:LYS:NZ	2.29	0.65
1:A:600[B]:CYS:SG	1:A:603:ARG:NH2	2.69	0.65
1:C:703:ASN:CB	2:E:11:LYS:CD	2.75	0.65
1:C:703:ASN:CG	2:E:11:LYS:HD2	2.18	0.64
1:C:294:LEU:HD11	1:C:336:VAL:HG11	1.79	0.64
1:C:569:LEU:HB3	2:D:73:LEU:HD22	1.82	0.62
1:C:199:ASP:C	2:E:70:VAL:CB	2.64	0.61
1:A:600[A]:CYS:SG	9:A:1579:HOH:O	2.56	0.61
1:C:405:ARG:HD2	1:C:423:VAL:O	2.01	0.60
1:C:600[A]:CYS:SG	1:C:603:ARG:NH2	2.75	0.59
1:A:684:PHE:HB3	1:A:718:LEU:HD22	1.84	0.59
1:C:684:PHE:HB3	1:C:718:LEU:HD22	1.86	0.58
1:A:405:ARG:HD2	1:A:423:VAL:O	2.04	0.58
1:C:705:GLU:CG	2:E:9:THR:CB	2.82	0.57
1:C:199:ASP:CA	2:E:70:VAL:HB	2.34	0.57
1:C:701:THR:HB	1:C:705:GLU:OE2	2.05	0.57
1:C:199:ASP:HA	2:E:70:VAL:HA	1.87	0.57
1:A:701:THR:OG1	1:A:705:GLU:HG3	2.04	0.56
1:C:405:ARG:CD	1:C:423:VAL:O	2.54	0.55
1:C:199:ASP:CG	2:E:8:LEU:HB3	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:703:ASN:HB3	2:E:11:LYS:CD	2.36	0.55
1:C:336:VAL:HG22	9:C:1595:HOH:O	2.07	0.54
1:A:677[B]:ARG:NH2	1:A:681:GLU:OE2	2.40	0.54
1:C:199:ASP:O	2:E:70:VAL:CG1	2.56	0.54
1:C:294:LEU:CD1	1:C:336:VAL:HG11	2.38	0.53
1:C:749:SER:O	1:C:750:ASN:CB	2.56	0.53
1:C:701:THR:O	1:C:704:GLY:N	2.40	0.52
1:A:405:ARG:CD	1:A:423:VAL:O	2.58	0.52
1:C:279:VAL:HG12	1:C:389[B]:MET:CE	2.40	0.52
1:A:294:LEU:CD1	1:A:336:VAL:HG11	2.39	0.52
1:A:46:GLY:HA3	1:A:78:THR:OG1	2.11	0.51
1:A:336:VAL:HG22	9:A:1634:HOH:O	2.10	0.51
1:C:705:GLU:CG	2:E:9:THR:HB	2.41	0.51
1:C:12:GLY:HA3	9:C:1307:HOH:O	2.11	0.50
1:C:199:ASP:OD1	2:E:8:LEU:CB	2.44	0.50
1:C:50[B]:GLU:OE2	1:C:53:LYS:NZ	2.45	0.49
1:C:444:ALA:HB1	1:C:870:THR:HG21	1.95	0.48
2:E:30:ILE:HG22	2:E:41:GLN:OE1	2.10	0.48
1:C:200:ASP:N	2:E:70:VAL:HB	2.28	0.48
1:C:199:ASP:O	2:E:70:VAL:HG11	2.12	0.48
1:C:46:GLY:HA3	1:C:78:THR:OG1	2.14	0.47
2:E:8:LEU:HD22	2:E:9:THR:HG23	1.96	0.47
1:C:199:ASP:HA	2:E:70:VAL:CB	2.44	0.47
1:C:279:VAL:CG1	1:C:389[B]:MET:CE	2.93	0.47
1:C:705:GLU:HG2	2:E:9:THR:HB	1.96	0.47
1:C:199:ASP:O	2:E:70:VAL:CB	2.63	0.46
2:E:6:LYS:HG3	2:E:66:THR:CG2	2.45	0.46
1:A:545:ASN:HA	2:B:74[A]:ARG:HH11	1.80	0.46
1:C:24:TYR:CE1	1:C:857:PHE:HB2	2.51	0.45
2:E:7:THR:HG21	2:E:11:LYS:HE3	1.98	0.45
1:A:437[B]:VAL:HG11	1:A:458:LEU:HD21	1.98	0.45
1:A:156:THR:C	1:A:157:ARG:HG2	2.36	0.45
1:C:199:ASP:O	2:E:70:VAL:HB	2.12	0.45
1:A:24:TYR:CE1	1:A:857:PHE:HB2	2.51	0.45
2:E:8:LEU:HD11	2:E:71:LEU:HD12	1.99	0.45
1:A:872:LEU:HD13	1:A:901:LEU:HD21	1.98	0.45
1:A:544:ASP:O	2:B:74[A]:ARG:NH1	2.51	0.44
1:A:26:LEU:O	1:A:381:LYS:HE2	2.18	0.44
1:C:451:LYS:HG3	1:C:483:PHE:HZ	1.83	0.43
2:E:6:LYS:HG3	2:E:66:THR:HG21	2.00	0.43
2:E:8:LEU:HD22	2:E:9:THR:CG2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:THR:C	1:C:157:ARG:HG2	2.39	0.43
1:C:703:ASN:ND2	2:E:11:LYS:CD	2.71	0.43
1:C:405:ARG:HA	1:C:409:THR:CG2	2.49	0.43
1:C:279:VAL:CG1	1:C:389[B]:MET:HE2	2.49	0.43
1:C:271:GLN:HB3	5:C:1108:GOL:H31	2.01	0.43
1:C:872:LEU:HD13	1:C:901:LEU:HD21	2.00	0.43
1:A:947:GLU:HG3	1:A:948:LYS:N	2.33	0.42
1:A:955:THR:HG22	1:A:1006:CSO:HB3	2.00	0.42
1:A:444:ALA:HB1	1:A:870:THR:HG21	2.00	0.42
1:C:305:ARG:NH2	1:C:321:GLU:OE2	2.53	0.42
1:A:437[A]:VAL:HG21	1:A:458:LEU:HD21	2.01	0.42
2:D:54:ARG:NH2	2:D:54:ARG:HG2	2.34	0.42
2:E:26:VAL:HG21	2:E:56:LEU:HD21	2.01	0.42
1:A:947:GLU:OE2	1:A:948:LYS:HE2	2.20	0.42
1:C:26:LEU:O	1:C:381:LYS:HE2	2.20	0.41
1:A:264:ILE:HD13	1:A:264:ILE:HG21	1.83	0.41
1:C:279:VAL:HG12	1:C:389[B]:MET:HE2	2.02	0.41
4:A:1103:CL:CL	2:B:74[A]:ARG:NH2	2.90	0.41
1:A:705:GLU:H	1:A:705:GLU:HG2	1.49	0.41
1:C:71:VAL:HG22	1:C:91:ARG:HG2	2.02	0.41
1:C:314:MET:CG	1:C:410:THR:HG21	2.51	0.41
1:A:349:LYS:HD3	1:A:353:TYR:CZ	2.56	0.41
1:C:237:ALA:HB3	2:E:47:GLY:CA	2.51	0.41
1:C:698:ASP:O	1:C:700:LYS:HE2	2.20	0.40
1:A:437[B]:VAL:CG2	1:A:466:ILE:HG12	2.51	0.40
1:A:451:LYS:HG3	1:A:483:PHE:HZ	1.86	0.40
1:A:1024:LEU:HD23	1:A:1024:LEU:HA	1.93	0.40
1:C:416:ARG:HD3	9:C:1323:HOH:O	2.22	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	1021/1024 (100%)	987 (97%)	32 (3%)	2 (0%)	47	58
1	C	1008/1024 (98%)	970 (96%)	36 (4%)	2 (0%)	47	58
2	B	78/76 (103%)	78 (100%)	0	0	100	100
2	D	76/76 (100%)	76 (100%)	0	0	100	100
2	E	70/76 (92%)	67 (96%)	2 (3%)	1 (1%)	11	11
All	All	2253/2276 (99%)	2178 (97%)	70 (3%)	5 (0%)	47	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	702	SER
1	C	750	ASN
1	A	751[A]	SER
1	A	751[B]	SER
2	E	52	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	906/899 (101%)	856 (94%)	50 (6%)	21	30
1	C	894/899 (99%)	851 (95%)	43 (5%)	25	36
2	B	73/69 (106%)	70 (96%)	3 (4%)	30	43
2	D	71/69 (103%)	67 (94%)	4 (6%)	21	29
2	E	67/69 (97%)	60 (90%)	7 (10%)	7	8
All	All	2011/2005 (100%)	1904 (95%)	107 (5%)	22	31

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	33	LYS
1	A	79	GLN

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Mol	Chain	Res	Type
1	A	85	LYS
1	A	94	VAL
1	A	96	ARG
1	A	117	VAL
1	A	118	THR
1	A	120	LEU
1	A	157	ARG
1	A	212	ARG
1	A	220	ASP
1	A	244	LYS
1	A	265	SER
1	A	270	LYS
1	A	294	LEU
1	A	324	LYS
1	A	413	VAL
1	A	415	SER
1	A	416[A]	ARG
1	A	416[B]	ARG
1	A	451	LYS
1	A	517[A]	ILE
1	A	517[B]	ILE
1	A	535	SER
1	A	590	ARG
1	A	595	LYS
1	A	610	ASP
1	A	618	SER
1	A	621[A]	GLN
1	A	621[B]	GLN
1	A	657	SER
1	A	686	HIS
1	A	697	LYS
1	A	700	LYS
1	A	701	THR
1	A	703	ASN
1	A	705	GLU
1	A	718	LEU
1	A	748	ASP
1	A	771	THR
1	A	782	ASP
1	A	786	ASP
1	A	799	ASP
1	A	922	LYS

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Mol	Chain	Res	Type
1	A	930	ARG
1	A	947	GLU
1	A	948	LYS
1	A	955	THR
1	A	987	LYS
2	B	60	ASN
2	B	62	GLN
2	B	64	GLU
1	C	33	LYS
1	C	53	LYS
1	C	79	GLN
1	C	94	VAL
1	C	96	ARG
1	C	117	VAL
1	C	118	THR
1	C	120	LEU
1	C	157	ARG
1	C	220	ASP
1	C	221	LYS
1	C	222	LEU
1	C	265	SER
1	C	270	LYS
1	C	294	LEU
1	C	307	ASN
1	C	324	LYS
1	C	335	GLU
1	C	409	THR
1	C	410	THR
1	C	415	SER
1	C	416	ARG
1	C	451	LYS
1	C	517	ILE
1	C	594	GLU
1	C	595	LYS
1	C	621	GLN
1	C	657	SER
1	C	686	HIS
1	C	700	LYS
1	C	705	GLU
1	C	718	LEU
1	C	745	LYS
1	C	750	ASN

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Mol	Chain	Res	Type
1	C	764	HIS
1	C	771	THR
1	C	782	ASP
1	C	786	ASP
1	C	799	ASP
1	C	930	ARG
1	C	955	THR
1	C	973	LYS
1	C	987	LYS
2	D	25	ASN
2	D	54	ARG
2	D	60	ASN
2	D	64	GLU
2	E	6	LYS
2	E	8	LEU
2	E	12	THR
2	E	25	ASN
2	E	54	ARG
2	E	62	GLN
2	E	64	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	647	GLN
1	C	647	GLN
1	C	703	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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSO	A	1006	1	3,6,7	1.18	0	0,6,8	-	-
1	CSO	C	1006	1	3,6,7	1.33	0	0,6,8	-	-

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
1	CSO	A	1006	1	-	0/1/5/7	-
1	CSO	C	1006	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1006	CSO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 9 are monoatomic - leaving 16 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	$\#\|Z\|>2$
8	ACT	C	1111	-	3,3,3	0.83	0	3,3,3	0.76	0
5	GOL	A	1107	-	5,5,5	0.66	0	5,5,5	0.96	0
5	GOL	A	1109	-	5,5,5	0.69	0	5,5,5	0.64	0
5	GOL	C	1107	-	5,5,5	0.31	0	5,5,5	0.81	0
5	GOL	C	1110	-	5,5,5	0.99	0	5,5,5	1.06	0
6	6O2	D	101	2	30,34,34	1.73	4 (13%)	35,50,50	2.73	11 (31%)
6	6O2	B	101	2	30,34,34	1.73	5 (16%)	35,50,50	2.65	13 (37%)
5	GOL	A	1111	-	5,5,5	0.45	0	5,5,5	0.99	0
3	SO4	C	1101	-	4,4,4	0.18	0	6,6,6	1.83	1 (16%)
5	GOL	A	1110	-	5,5,5	0.96	0	5,5,5	1.67	0
5	GOL	C	1109	-	5,5,5	0.89	0	5,5,5	1.47	1 (20%)
5	GOL	A	1106	-	5,5,5	0.79	0	5,5,5	0.88	0
5	GOL	A	1108	-	5,5,5	1.17	0	5,5,5	1.32	0
5	GOL	C	1108	-	5,5,5	0.64	0	5,5,5	0.80	0
5	GOL	A	1112	-	5,5,5	1.10	0	5,5,5	1.20	1 (20%)
3	SO4	A	1101	-	4,4,4	0.24	0	6,6,6	0.95	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	A	1107	-	-	2/4/4/4	-
5	GOL	A	1109	-	-	2/4/4/4	-
5	GOL	C	1107	-	-	1/4/4/4	-
5	GOL	C	1110	-	-	4/4/4/4	-
6	6O2	D	101	2	-	4/12/32/32	0/4/4/4
6	6O2	B	101	2	-	3/12/32/32	0/4/4/4
5	GOL	A	1111	-	-	0/4/4/4	-
5	GOL	A	1110	-	-	1/4/4/4	-
5	GOL	C	1109	-	-	2/4/4/4	-
5	GOL	A	1106	-	-	2/4/4/4	-
5	GOL	A	1108	-	-	2/4/4/4	-
5	GOL	C	1108	-	-	1/4/4/4	-
5	GOL	A	1112	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	101	6O2	C8-C12	-6.85	1.29	1.44
6	D	101	6O2	C8-C12	-5.92	1.31	1.44
6	D	101	6O2	O-S	-3.61	1.52	1.57
6	D	101	6O2	C12-C13	3.27	1.29	1.17
6	B	101	6O2	C12-C13	2.84	1.27	1.17
6	B	101	6O2	O-S	-2.50	1.54	1.57
6	B	101	6O2	O1-C2	2.42	1.44	1.41
6	B	101	6O2	O4-S	2.17	1.44	1.42
6	D	101	6O2	O1-C2	2.15	1.44	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	101	6O2	O5-S-O4	-9.94	110.57	119.97
6	B	101	6O2	O5-S-O4	-7.14	113.21	119.97
6	B	101	6O2	C6-C7-C8	6.23	124.96	119.89
6	D	101	6O2	C4-N2-C5	5.91	121.66	116.59
6	B	101	6O2	C4-N2-C5	5.76	121.53	116.59
6	D	101	6O2	N1-C4-N2	-4.90	121.01	128.68
6	D	101	6O2	C-O-S	4.64	123.02	117.21
6	D	101	6O2	C6-C7-C8	3.82	122.99	119.89
6	D	101	6O2	O-S-O5	3.66	117.25	106.38
6	B	101	6O2	C11-C6-C7	-3.65	115.33	119.65
6	B	101	6O2	C7-C8-C12	-3.55	115.54	120.09
6	B	101	6O2	N1-C4-N2	-3.53	123.16	128.68
6	B	101	6O2	O-S-O5	3.50	116.75	106.38
6	B	101	6O2	O5-S-N5	-3.45	103.92	109.14
3	C	1101	SO4	O4-S-O3	3.37	123.45	109.06
6	B	101	6O2	C9-C8-C12	3.24	125.48	120.65
6	B	101	6O2	C3-C14-N4	-2.88	106.39	109.40
6	B	101	6O2	C11-C6-N3	2.64	129.49	120.64
5	C	1109	GOL	O1-C1-C2	2.49	122.16	110.20
6	D	101	6O2	O4-S-N5	-2.43	105.47	109.14
6	D	101	6O2	C11-C6-C7	-2.42	116.78	119.65
6	B	101	6O2	C11-C10-C9	2.41	123.67	120.25
5	A	1112	GOL	O3-C3-C2	2.30	121.25	110.20
6	D	101	6O2	C16-C17-C1	2.29	107.09	102.64
6	B	101	6O2	N3-C5-N2	-2.29	115.66	118.72
6	D	101	6O2	C3-C14-N4	-2.27	107.03	109.40
6	D	101	6O2	C11-C6-N3	2.03	127.44	120.64

There are no chirality outliers.

All (26) 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	1112	GOL	C1-C2-C3-O3
5	C	1109	GOL	O1-C1-C2-C3
5	C	1110	GOL	O1-C1-C2-O2
5	C	1110	GOL	O1-C1-C2-C3
5	C	1110	GOL	C1-C2-C3-O3
6	B	101	6O2	N2-C5-N3-C6
6	B	101	6O2	C14-C5-N3-C6
6	D	101	6O2	C13-C12-C8-C7
6	D	101	6O2	N2-C5-N3-C6
6	D	101	6O2	C14-C5-N3-C6
5	A	1110	GOL	O1-C1-C2-C3
5	C	1108	GOL	C1-C2-C3-O3
5	A	1106	GOL	O1-C1-C2-O2
5	A	1109	GOL	O2-C2-C3-O3
5	A	1112	GOL	O2-C2-C3-O3
5	C	1109	GOL	O1-C1-C2-O2
5	C	1110	GOL	O2-C2-C3-O3
5	A	1108	GOL	O1-C1-C2-O2
5	A	1107	GOL	O1-C1-C2-O2
6	B	101	6O2	O-C-C1-C17
5	A	1107	GOL	O1-C1-C2-C3
5	A	1108	GOL	O1-C1-C2-C3
6	D	101	6O2	C13-C12-C8-C9
5	C	1107	GOL	O1-C1-C2-O2

There are no ring outliers.

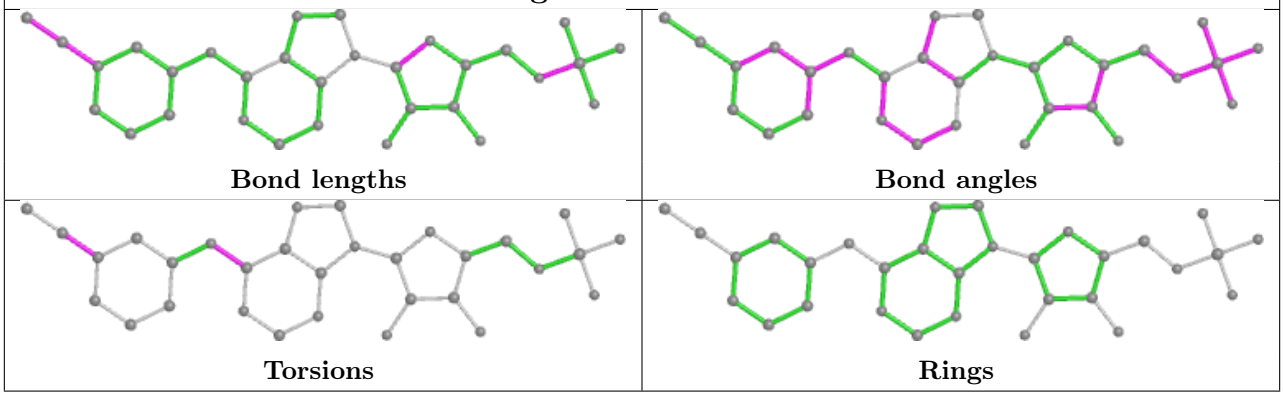
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1108	GOL	1	0

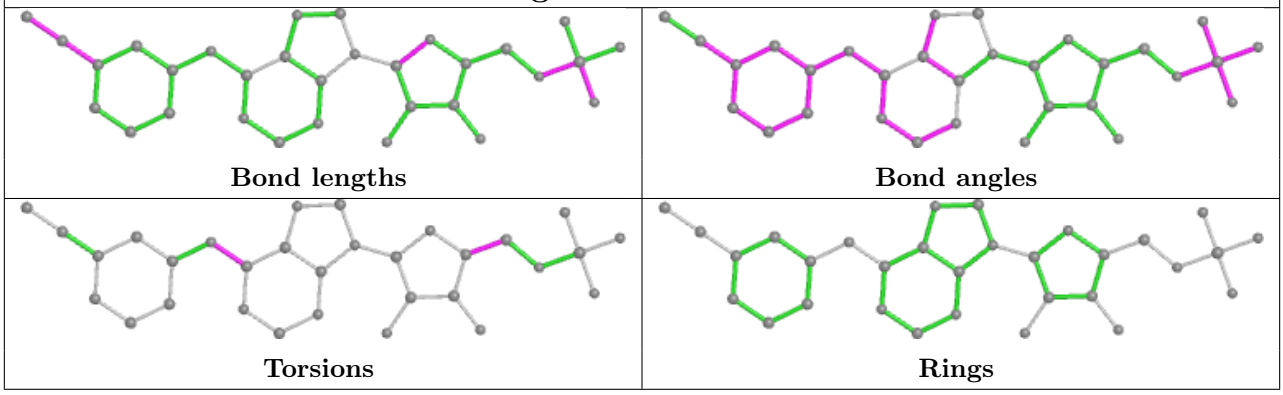
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 6O2 D 101



Ligand 6O2 B 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

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, 95^{th} 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	1005/1024 (98%)	-0.05	44 (4%) 34 41	31, 49, 95, 145	0
1	C	1004/1024 (98%)	-0.05	54 (5%) 25 32	32, 50, 99, 162	0
2	B	76/76 (100%)	-0.12	1 (1%) 77 81	35, 54, 79, 85	0
2	D	76/76 (100%)	-0.16	1 (1%) 77 81	39, 59, 89, 101	0
2	E	72/76 (94%)	5.14	68 (94%) 0 0	135, 153, 183, 193	0
All	All	2233/2276 (98%)	0.11	168 (7%) 14 19	31, 50, 116, 193	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	26	VAL	11.0
2	E	37	PRO	10.7
2	E	39	ASP	9.9
2	E	17	VAL	9.6
2	E	43	LEU	9.1
2	E	63	LYS	8.1
1	C	750	ASN	7.8
2	E	56	LEU	7.8
2	E	31	GLN	7.8
1	A	785	PRO	7.7
2	E	8	LEU	7.4
2	E	67	LEU	7.4
2	E	40	GLN	7.3
2	E	36	ILE	7.0
2	E	70	VAL	6.9
2	E	28	SER	6.9
2	E	50	LEU	6.8
2	E	30	ILE	6.7
2	E	53	GLY	6.7
2	E	18	GLU	6.5

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Mol	Chain	Res	Type	RSRZ
2	E	34	GLU	6.5
1	A	10	ALA	6.5
2	E	59	TYR	6.4
2	E	38	PRO	6.2
1	A	776	LEU	6.0
2	E	4	PHE	6.0
2	E	23	ILE	6.0
2	E	72	ARG	5.9
1	C	776	LEU	5.9
1	C	703	ASN	5.9
1	A	750	ASN	5.8
1	C	785	PRO	5.8
2	E	14	THR	5.7
2	E	71	LEU	5.7
2	E	48	LYS	5.6
1	C	704	GLY	5.6
2	E	1	MET	5.5
2	E	9	THR	5.5
2	E	42	ARG	5.5
1	C	775	ASN	5.4
2	E	12	THR	5.4
1	C	749	SER	5.4
2	E	33	LYS	5.3
2	E	25	ASN	5.3
2	E	54	ARG	5.3
1	A	647	GLN	5.2
2	E	3	ILE	5.2
2	E	27	LYS	5.2
1	A	702	SER	5.2
2	E	58	ASP	5.1
2	E	60	ASN	5.1
2	E	49	GLN	5.1
2	E	35	GLY	5.1
1	C	702	SER	5.0
2	E	69	LEU	4.9
2	E	65	SER	4.9
2	E	64	GLU	4.9
2	E	47	GLY	4.9
2	E	11	LYS	4.8
1	C	783	ASP	4.8
1	C	800	GLN	4.7
1	A	11	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
2	E	51	GLU	4.3
2	E	19	SER	4.3
2	E	24	ASP	4.2
2	E	2	GLN	4.2
2	E	61	ILE	4.2
1	A	783	ASP	4.2
1	A	777	LYS	4.2
2	E	20	SER	4.1
1	A	703	ASN	4.0
2	E	32	ASP	4.0
2	E	52	ASP	4.0
1	C	784	ASP	3.9
1	A	749	SER	3.8
1	A	294	LEU	3.7
2	E	16	GLU	3.7
1	C	774	ALA	3.7
1	A	646	LYS	3.6
1	A	800	GLN	3.6
1	A	775	ASN	3.6
2	E	15	LEU	3.5
1	C	705	GLU	3.5
2	E	41	GLN	3.4
1	A	649	GLY	3.4
1	C	737	LEU	3.4
1	C	646	LYS	3.3
2	E	5	VAL	3.3
1	C	693	PHE	3.3
1	C	797	GLU	3.3
1	A	200	ASP	3.3
1	C	786	ASP	3.3
1	C	12	GLY	3.2
1	A	797	GLU	3.2
1	A	12	GLY	3.2
1	C	996	ALA	3.2
1	A	786	ASP	3.2
1	A	704	GLY	3.2
1	A	961	VAL	3.2
1	C	701	THR	3.2
1	C	649	GLY	3.2
1	C	777	LYS	3.2
1	C	595	LYS	3.2
2	E	46	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	698	ASP	3.1
1	C	248	GLU	3.0
1	C	294	LEU	2.9
1	A	650	ASP	2.9
1	A	648	SER	2.9
1	A	996	ALA	2.9
1	C	698	ASP	2.9
1	C	647	GLN	2.8
1	C	700	LYS	2.8
1	C	736[A]	SER	2.8
1	C	11	ALA	2.8
1	A	784	ASP	2.7
1	A	423	VAL	2.7
1	A	834	ILE	2.7
2	E	44	ILE	2.7
1	C	596	SER	2.7
2	E	21	ASP	2.7
1	A	595	LYS	2.7
1	C	810	THR	2.7
2	E	66	THR	2.6
1	C	423	VAL	2.6
1	A	796	ASP	2.5
1	C	773	ASN	2.5
1	C	613	ILE	2.4
2	E	62	GLN	2.4
1	C	803	SER	2.4
2	E	57	SER	2.4
2	E	13	ILE	2.4
1	C	667	HIS	2.3
1	C	339	GLU	2.3
1	C	948	LYS	2.3
1	C	764	HIS	2.3
1	C	245	GLU	2.3
1	C	295	GLY	2.2
1	A	799	ASP	2.2
1	A	705	GLU	2.2
1	A	401	LYS	2.2
1	A	408	LYS	2.2
1	A	735	ALA	2.2
1	C	664	SER	2.2
1	C	751	SER	2.2
1	A	991	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	992	LYS	2.2
1	A	997	HIS	2.2
2	E	68	HIS	2.2
1	A	13	GLU	2.2
1	C	307	ASN	2.1
1	A	706	PRO	2.1
2	E	7	THR	2.1
1	C	809	SER	2.1
2	E	10	GLY	2.1
2	E	22	THR	2.1
1	C	650	ASP	2.1
1	C	782	ASP	2.1
1	C	796	ASP	2.1
1	C	812	ALA	2.1
1	A	737	LEU	2.1
2	B	26	VAL	2.1
1	C	244	LYS	2.0
1	C	401	LYS	2.0
1	A	731	VAL	2.0
2	D	64	GLU	2.0
1	C	781	ASN	2.0
1	A	596	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	CSO	A	1006	7/8	0.96	0.06	45,50,58,63	0
1	CSO	C	1006	7/8	0.98	0.11	39,43,49,55	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

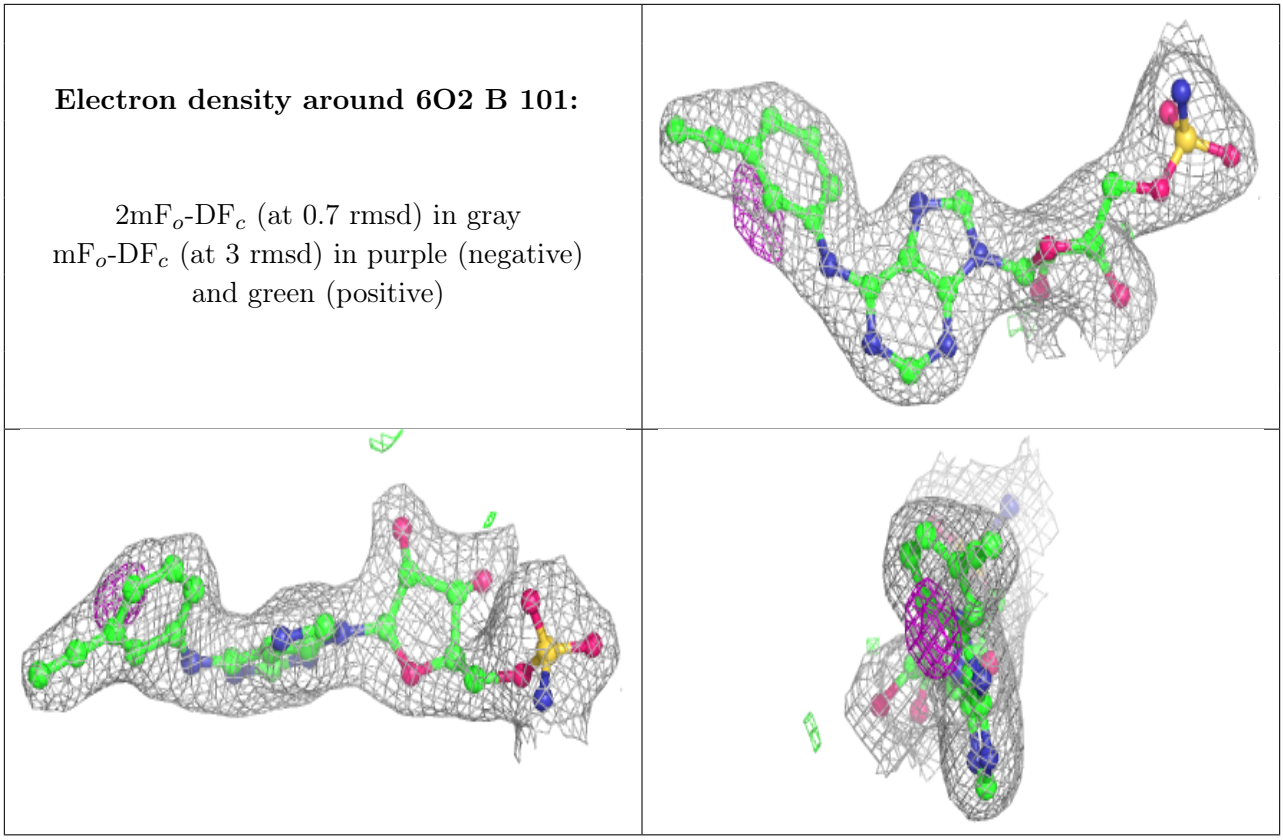
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	1110	6/6	0.64	0.24	67,84,85,89	0
5	GOL	C	1108	6/6	0.69	0.49	66,82,95,96	0
5	GOL	A	1110	6/6	0.71	0.27	53,59,63,63	0
5	GOL	A	1112	6/6	0.72	0.28	64,79,84,88	0
5	GOL	A	1109	6/6	0.79	0.43	78,89,90,93	0
5	GOL	A	1107	6/6	0.80	0.24	69,73,76,79	0
5	GOL	A	1111	6/6	0.83	0.16	74,79,86,86	0
4	CL	C	1104	1/1	0.87	0.13	75,75,75,75	0
4	CL	A	1105	1/1	0.90	0.09	91,91,91,91	0
5	GOL	C	1107	6/6	0.90	0.19	90,92,95,98	0
4	CL	A	1103	1/1	0.91	0.14	77,77,77,77	0
5	GOL	A	1108	6/6	0.91	0.18	56,62,68,68	0
4	CL	C	1105	1/1	0.91	0.21	88,88,88,88	0
8	ACT	C	1111	4/4	0.91	0.15	64,74,78,79	0
5	GOL	A	1106	6/6	0.94	0.16	47,56,60,60	0
7	MG	C	1106	1/1	0.96	0.06	45,45,45,45	0
5	GOL	C	1109	6/6	0.96	0.14	45,54,55,63	0
4	CL	A	1104	1/1	0.97	0.03	68,68,68,68	0
6	6O2	B	101	31/31	0.97	0.10	32,40,45,50	0
6	6O2	D	101	31/31	0.97	0.12	27,44,53,57	0
4	CL	C	1102	1/1	0.97	0.09	65,65,65,65	0
4	CL	C	1103	1/1	0.97	0.24	85,85,85,85	0
4	CL	A	1102	1/1	0.98	0.12	60,60,60,60	0
3	SO4	C	1101	5/5	0.99	0.08	42,42,43,49	0
3	SO4	A	1101	5/5	0.99	0.09	39,44,45,46	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.

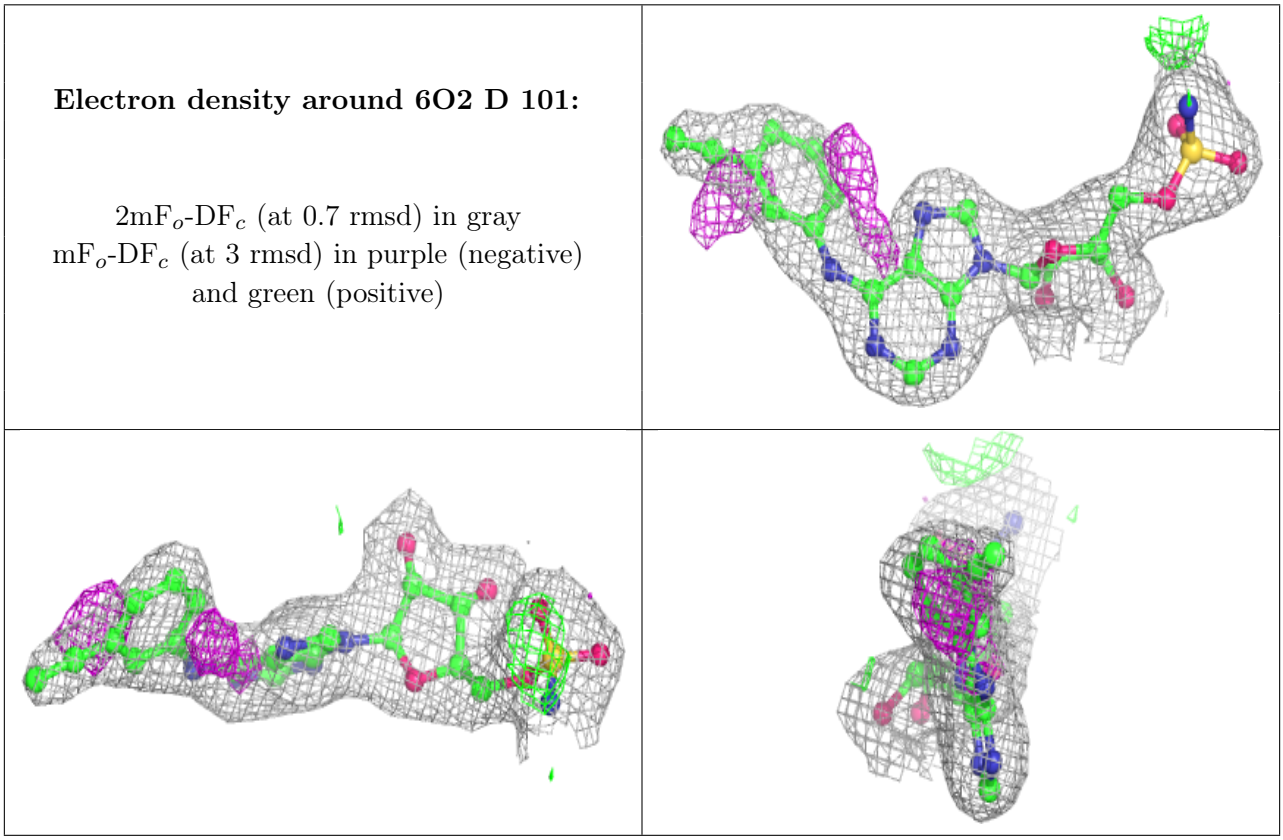
Electron density around 6O2 B 101:

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



Electron density around 6O2 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.