



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:57 PM UTC

PDB ID : 5L6H / pdb_00005l6h
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 : 4-5-2 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

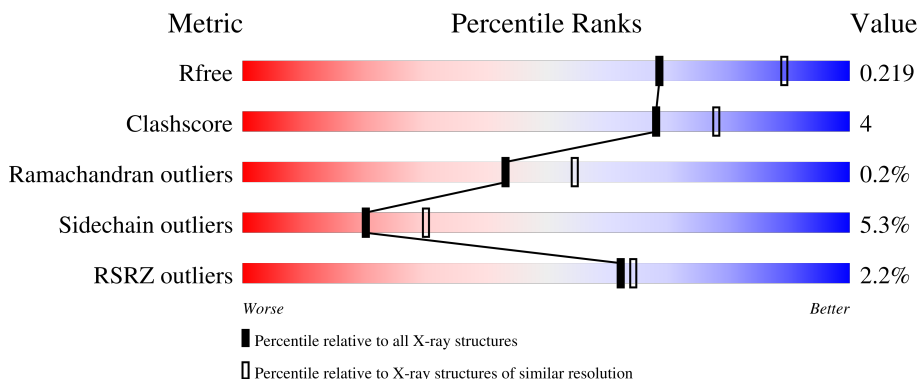
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	 84% 12% . .
1	C	1024	 83% 12% . .
2	B	76	 93% 7%
2	D	76	 89% 9% .
2	E	76	 54% 68% 18% 7% . 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	-

2 Entry composition [i](#)

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.

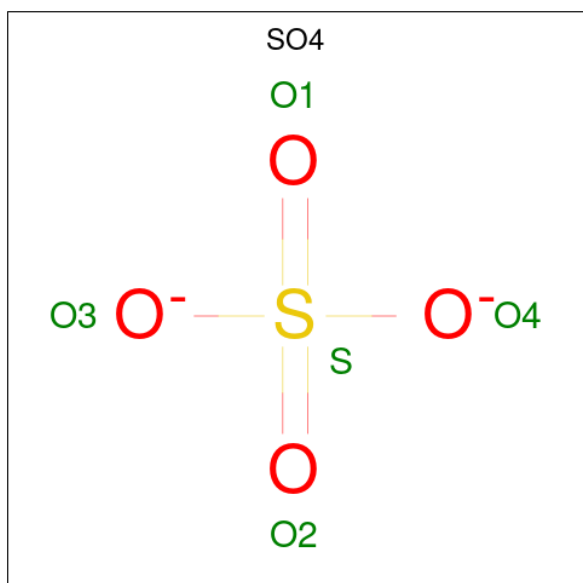
- Molecule 1 is a protein called Ubiquitin-activating enzyme E1 1.

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 (CCD ID: SO4) (formula: O₄S).

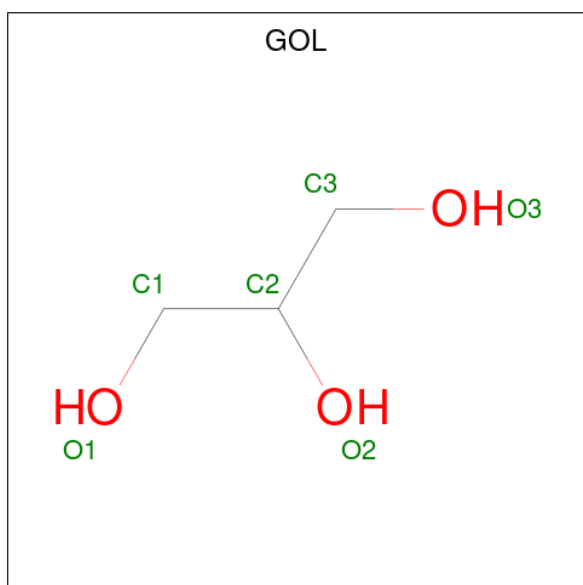


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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

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

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



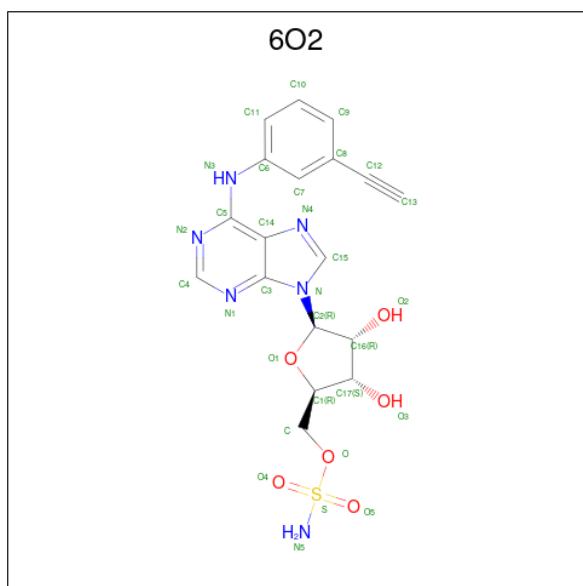
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

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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 (CCD ID: 6O2) (formula: C₁₈H₁₈N₆O₆S).



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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2^-$).



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

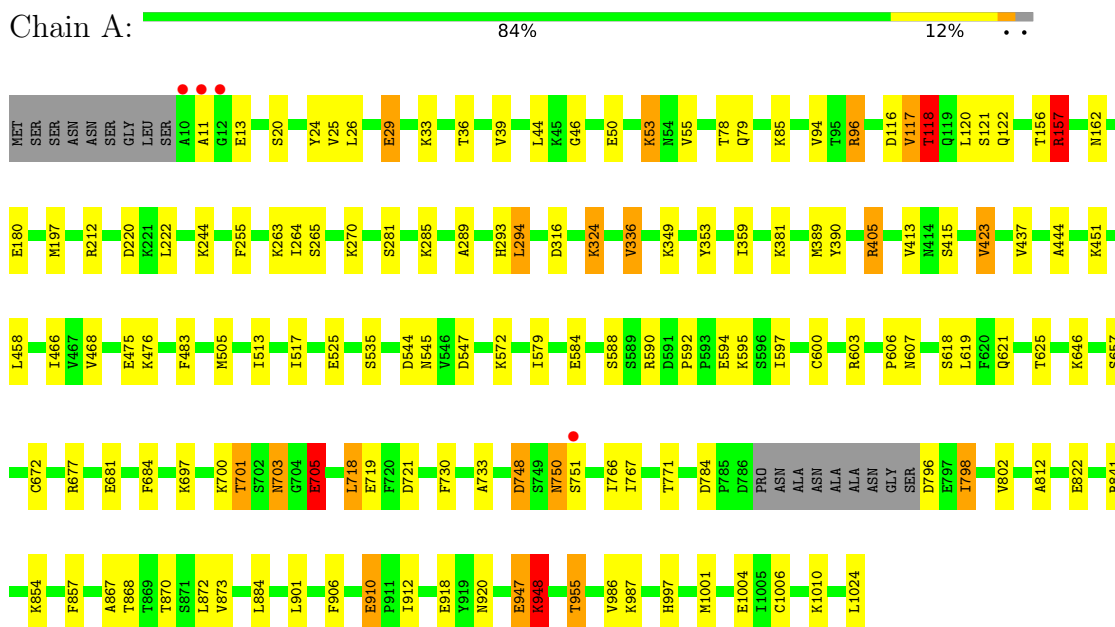
- Molecule 9 is water.

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

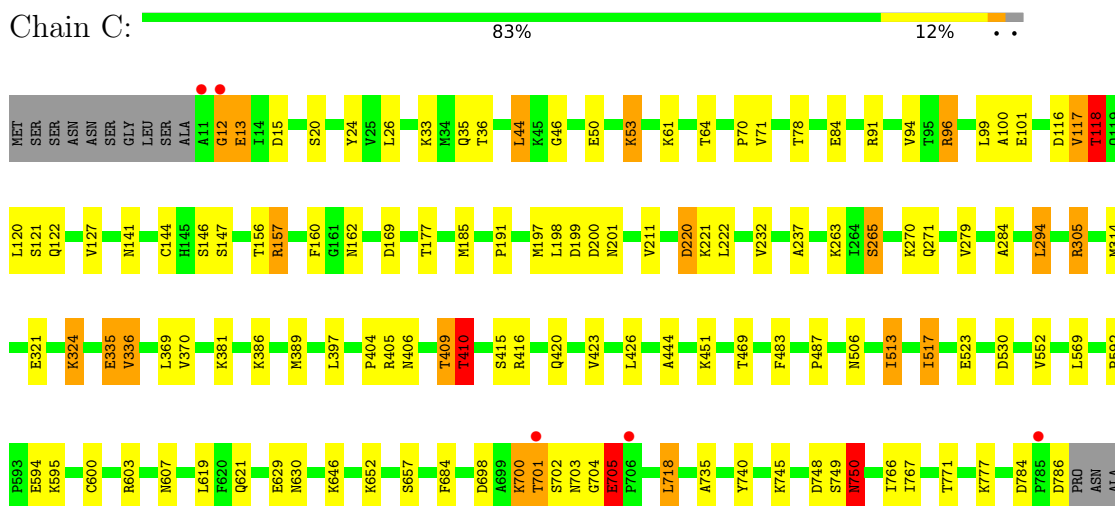
3 Residue-property plots

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

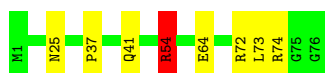
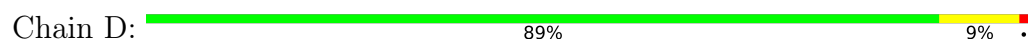




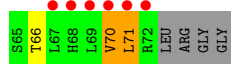
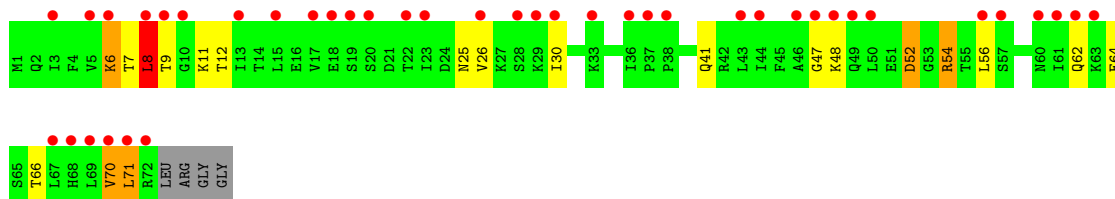
- Molecule 2: Ubiquitin-40S ribosomal protein S31



- Molecule 2: Ubiquitin-40S ribosomal protein S31



- Molecule 2: Ubiquitin-40S ribosomal protein S31



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	72.05Å 194.10Å 230.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.30) 99.2 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.87%)	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 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SO4, ACT, GOL, MG, CSO, 6O2

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	1.54	47/8264 (0.6%)	1.29	38/11181 (0.3%)
1	C	1.53	52/8161 (0.6%)	1.29	32/11039 (0.3%)
2	B	1.28	2/645 (0.3%)	1.12	0/864
2	D	1.32	2/625 (0.3%)	1.23	1/838 (0.1%)
2	E	1.34	2/578 (0.3%)	1.37	6/777 (0.8%)
All	All	1.52	105/18273 (0.6%)	1.28	77/24699 (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
1	C	0	1
All	All	0	2

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	ALA	CA-C	10.52	1.65	1.52
1	C	748	ASP	CA-C	8.74	1.65	1.52
1	A	579	ILE	N-CA	-7.46	1.39	1.46
1	A	547	ASP	C-O	-7.36	1.15	1.24
1	C	12	GLY	N-CA	7.25	1.55	1.45
1	C	101	GLU	C-O	-7.17	1.14	1.24
1	C	873	VAL	C-O	-7.00	1.16	1.24
1	A	607	ASN	C-O	-6.94	1.15	1.24
1	A	606	PRO	N-CA	-6.94	1.38	1.47
2	E	71	LEU	N-CA	6.94	1.54	1.46
1	A	1004	GLU	CG-CD	6.88	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	177	THR	N-CA	6.86	1.55	1.46
1	C	84	GLU	CD-OE1	6.85	1.38	1.25
1	C	36	THR	C-O	-6.73	1.14	1.23
1	C	942	LEU	C-O	6.64	1.31	1.24
1	A	572	LYS	C-O	-6.51	1.15	1.23
1	A	588	SER	C-O	-6.51	1.15	1.24
1	C	64	THR	CA-C	-6.50	1.44	1.52
1	A	289	ALA	CA-C	6.47	1.61	1.52
1	C	99	LEU	C-O	-6.42	1.16	1.24
1	A	359	ILE	N-CA	-6.39	1.40	1.46
1	A	920	ASN	C-O	6.37	1.30	1.24
1	A	36	THR	C-O	-6.27	1.15	1.24
1	A	212	ARG	CZ-NH2	-6.25	1.25	1.33
1	A	13	GLU	N-CA	6.24	1.53	1.45
1	C	735	ALA	N-CA	-6.23	1.39	1.46
1	C	61	LYS	N-CA	-6.19	1.38	1.46
1	C	121	SER	CA-C	-6.18	1.44	1.52
1	A	733	ALA	C-O	-6.04	1.17	1.24
1	C	740	TYR	CA-C	6.01	1.60	1.52
1	A	180	GLU	C-O	-6.01	1.17	1.24
1	C	160	PHE	C-O	-5.99	1.16	1.23
1	A	884	LEU	N-CA	5.98	1.53	1.46
1	A	672	CYS	CA-C	5.96	1.60	1.52
1	C	162	ASN	CG-OD1	-5.95	1.12	1.23
1	C	284	ALA	C-O	-5.94	1.16	1.24
1	A	784	ASP	N-CA	5.94	1.52	1.45
1	C	141	ASN	C-O	-5.89	1.17	1.24
1	A	719	GLU	C-O	-5.88	1.17	1.24
1	C	144	CYS	N-CA	-5.85	1.39	1.46
1	C	397	LEU	CA-C	-5.84	1.47	1.53
2	D	41	GLN	N-CA	-5.82	1.39	1.46
1	A	285	LYS	CA-C	5.80	1.60	1.53
1	A	750	ASN	CA-C	5.80	1.60	1.52
1	C	191	PRO	CA-C	5.79	1.61	1.52
2	E	70	VAL	CA-C	5.79	1.60	1.52
2	B	23	ILE	N-CA	-5.78	1.39	1.46
1	C	96	ARG	C-O	-5.78	1.17	1.24
1	C	369	LEU	CA-C	5.72	1.60	1.52
1	C	386	LYS	N-CA	-5.71	1.39	1.47
1	C	629	GLU	CA-C	5.65	1.60	1.52
1	C	630	ASN	N-CA	-5.65	1.39	1.46
1	C	976	GLU	CD-OE1	5.64	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	748	ASP	CA-C	5.61	1.60	1.52
1	C	963	LEU	C-O	-5.60	1.17	1.24
2	D	37	PRO	C-O	-5.60	1.18	1.24
1	A	625	THR	N-CA	-5.59	1.41	1.46
1	A	868	THR	N-CA	-5.54	1.39	1.46
1	A	13	GLU	CA-C	5.49	1.59	1.52
1	C	127	VAL	N-CA	-5.44	1.40	1.46
1	C	15	ASP	CA-C	5.43	1.60	1.52
1	A	359	ILE	CA-C	5.42	1.57	1.52
1	C	1019	PHE	CG-CD1	5.42	1.50	1.38
1	A	39	VAL	CA-C	-5.38	1.46	1.52
1	C	506	ASN	C-O	-5.37	1.19	1.24
1	C	70	PRO	C-O	-5.36	1.17	1.23
1	C	147	SER	CB-OG	-5.36	1.31	1.42
1	C	265	SER	N-CA	-5.35	1.39	1.46
1	A	997	HIS	CA-C	5.35	1.60	1.52
1	C	232	VAL	C-O	-5.35	1.18	1.24
1	A	812	ALA	CA-CB	5.34	1.60	1.53
1	C	13	GLU	CA-C	5.33	1.59	1.52
1	C	211	VAL	CA-C	-5.31	1.46	1.52
1	A	918	GLU	C-O	-5.31	1.17	1.23
1	C	370	VAL	C-O	-5.29	1.17	1.24
1	A	162	ASN	CG-ND2	-5.26	1.22	1.33
1	A	597	ILE	C-O	-5.25	1.17	1.24
1	A	822	GLU	CA-C	5.25	1.59	1.53
1	C	35	GLN	CD-OE1	5.24	1.33	1.23
1	C	169	ASP	C-O	-5.20	1.18	1.24
1	A	29	GLU	N-CA	5.20	1.52	1.46
1	C	784	ASP	N-CA	5.20	1.53	1.46
1	C	948	LYS	C-O	-5.19	1.18	1.24
1	C	469	THR	CA-C	-5.19	1.46	1.52
1	A	721	ASP	CA-C	-5.18	1.47	1.52
1	A	96	ARG	C-O	-5.15	1.18	1.24
1	C	100	ALA	C-O	-5.14	1.18	1.24
1	A	476	LYS	N-CA	-5.12	1.40	1.46
1	A	423	VAL	C-O	-5.12	1.18	1.23
1	A	910	GLU	CA-C	5.11	1.58	1.53
1	C	523[B]	GLU	CG-CD	5.10	1.64	1.52
1	A	854	LYS	N-CA	-5.09	1.40	1.46
1	A	157	ARG	N-CA	-5.09	1.40	1.46
1	A	468	VAL	C-O	-5.08	1.18	1.24
1	C	607	ASN	C-O	-5.08	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	426	LEU	CA-C	5.07	1.59	1.52
1	C	967	SER	C-O	-5.07	1.17	1.24
1	C	232	VAL	CA-C	-5.07	1.47	1.52
1	C	552	VAL	CA-CB	5.07	1.60	1.54
1	A	868	THR	C-O	-5.06	1.18	1.24
1	A	505	MET	C-N	-5.05	1.29	1.33
1	A	122	GLN	C-O	-5.04	1.17	1.24
1	A	121	SER	C-O	-5.03	1.17	1.24
1	C	122	GLN	C-O	-5.03	1.17	1.24
2	B	73	LEU	N-CA	-5.02	1.40	1.45

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	336	VAL	N-CA-C	9.40	119.37	110.53
1	A	29	GLU	N-CA-CB	8.72	122.65	110.01
1	C	410	THR	N-CA-CB	-8.60	97.76	110.49
1	C	117	VAL	CB-CA-C	-8.38	99.82	112.05
2	E	70	VAL	CB-CA-C	8.15	124.66	111.29
2	E	8	LEU	N-CA-C	7.93	121.91	111.75
1	A	336	VAL	N-CA-C	7.72	117.78	110.53
1	A	212	ARG	NE-CZ-NH2	-7.42	112.52	119.20
1	A	117	VAL	CB-CA-C	-6.98	101.34	112.16
2	E	52	ASP	N-CA-C	6.79	125.27	110.80
1	A	592	PRO	CA-C-N	-6.77	113.81	120.52
1	A	592	PRO	C-N-CA	-6.77	113.81	120.52
1	C	592	PRO	CA-C-N	-6.66	113.93	120.52
1	C	592	PRO	C-N-CA	-6.66	113.93	120.52
2	D	54	ARG	CB-CG-CD	6.37	125.94	111.30
1	A	1010	LYS	N-CA-C	6.25	120.00	112.38
1	C	955	THR	N-CA-CB	-6.14	101.72	110.81
1	C	517	ILE	N-CA-CB	-6.14	104.18	112.16
1	C	920	ASN	CB-CA-C	-5.98	102.99	111.95
1	A	324	LYS	N-CA-CB	5.97	118.89	110.12
1	A	867	ALA	N-CA-C	5.82	118.40	111.71
1	C	20	SER	N-CA-C	5.81	118.08	111.11
1	A	29	GLU	CB-CA-C	-5.79	101.79	110.88
1	C	513	ILE	CB-CA-C	-5.77	102.09	110.63
1	C	305	ARG	NE-CZ-NH2	5.74	124.36	119.20
1	C	705	GLU	CA-C-N	-5.71	114.05	119.76
1	C	705	GLU	C-N-CA	-5.71	114.05	119.76
1	A	584[A]	GLU	CB-CA-C	5.67	122.56	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	584[B]	GLU	CB-CA-C	5.67	122.56	110.19
1	A	96	ARG	CG-CD-NE	-5.67	99.53	112.00
1	A	212	ARG	NE-CZ-NH1	5.65	127.15	121.50
1	C	994	ILE	CA-C-N	-5.63	113.98	119.78
1	C	994	ILE	C-N-CA	-5.63	113.98	119.78
1	C	420	GLN	N-CA-C	-5.61	104.65	112.45
1	A	316	ASP	N-CA-C	5.59	117.38	111.28
1	C	701	THR	N-CA-C	5.57	118.54	109.24
1	A	1004	GLU	OE1-CD-OE2	-5.56	109.55	122.90
1	C	767	ILE	CB-CG1-CD1	5.55	125.46	113.80
1	A	29	GLU	CA-CB-CG	5.52	125.14	114.10
1	C	220	ASP	CB-CA-C	5.47	119.83	110.74
1	A	767	ILE	CA-C-N	-5.47	114.33	119.85
1	A	767	ILE	C-N-CA	-5.47	114.33	119.85
1	C	201	ASN	N-CA-C	-5.45	100.41	109.46
1	A	324	LYS	CB-CG-CD	5.44	123.81	111.30
1	A	802	VAL	N-CA-C	5.43	116.06	110.36
1	C	96	ARG	CG-CD-NE	-5.43	100.06	112.00
1	C	117	VAL	N-CA-C	5.42	118.65	111.17
1	C	517	ILE	CA-CB-CG2	5.42	119.72	110.50
1	C	1011	GLU	CA-CB-CG	5.42	124.93	114.10
1	A	705	GLU	CA-C-N	-5.39	114.37	119.76
1	A	705	GLU	C-N-CA	-5.39	114.37	119.76
1	C	146	SER	N-CA-C	-5.36	106.00	112.54
1	A	20	SER	N-CA-C	5.35	117.53	111.11
1	A	948	LYS	CA-CB-CG	5.34	124.78	114.10
1	C	324	LYS	CB-CG-CD	5.33	123.55	111.30
1	A	475	GLU	CB-CG-CD	5.31	121.63	112.60
1	A	748	ASP	CB-CA-C	-5.30	102.48	111.02
1	C	185	MET	CG-SD-CE	-5.28	89.29	100.90
1	A	525	GLU	N-CA-C	5.25	118.79	112.38
1	C	263	LYS	CG-CD-CE	5.25	123.36	111.30
1	A	841	ARG	N-CA-C	-5.23	105.66	111.36
2	E	54	ARG	CB-CG-CD	5.22	123.31	111.30
1	A	730	PHE	N-CA-C	-5.18	105.53	111.07
1	A	55	VAL	N-CA-C	-5.15	105.52	110.72
1	A	263	LYS	CG-CD-CE	5.13	123.11	111.30
2	E	8	LEU	CA-CB-CG	5.12	134.23	116.30
1	A	25	VAL	CB-CA-C	-5.12	105.49	111.94
1	C	324	LYS	N-CA-CB	5.10	117.62	110.12
1	C	1010	LYS	N-CA-C	5.09	118.98	112.87
1	C	118	THR	N-CA-CB	-5.09	102.10	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	THR	N-CA-CB	-5.08	102.11	110.14
1	A	281	SER	N-CA-C	-5.07	107.15	113.38
1	C	921	ASN	N-CA-C	5.06	119.03	112.86
1	A	594	GLU	CB-CG-CD	-5.05	104.02	112.60
1	A	912	ILE	CB-CA-C	-5.04	103.81	111.33
1	A	405	ARG	NE-CZ-NH2	-5.03	114.67	119.20
2	E	8	LEU	CB-CA-C	-5.01	100.73	110.46

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

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	39	0
1	C	7981	0	7894	73	0
2	B	631	0	664	4	0
2	D	614	0	644	4	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	29	0	0	0	0
9	E	3	0	0	0	0
All	All	18998	0	17882	128	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 4.

All (128) 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
1:C:199:ASP:C	2:E:70:VAL:HB	1.80	1.06
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: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
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:C:279:VAL:HG12	1:C:389[B]:MET:HE2	1.71	0.72
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:703:ASN:CG	2:E:11:LYS:HD2	2.18	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:199:ASP:C	2:E:70:VAL:CB	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:199:ASP:CG	2:E:8:LEU:HB3	2.26	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: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: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:A:156:THR:C	1:A:157:ARG:HG2	2.36	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:156:THR:C	1:C:157:ARG:HG2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:279:VAL:HG12	1:C:389[B]:MET:CE	2.40	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:389[B]:MET:HE1	1:A:906:PHE:CE2	2.52	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:293:HIS:ND1	1:A:390:TYR:OH	2.44	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
1:C:279:VAL:CG1	1:C:389[B]:MET:HE2	2.45	0.43
1:C:703:ASN:ND2	2:E:11:LYS:CD	2.71	0.43
1:A:986:VAL:HG21	1:A:1001:MET:HE1	1.99	0.43
1:C:405:ARG:HA	1:C:409:THR:CG2	2.49	0.43
1:C:271:GLN:HB3	5:C:1108:GOL:H31	2.01	0.43
1:A:796:ASP:C	1:A:798:ILE:H	2.26	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:C:335:GLU:H	1:C:335:GLU:CD	2.27	0.42
1:C:530:ASP:OD2	1:C:999:SER:OG	2.37	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:198:LEU:O	1:C:199:ASP:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:255:PHE:CD1	1:A:255:PHE:C	2.98	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
2:D:72:ARG:C	2:D:73:LEU:HG	2.45	0.41
1:A:349:LYS:HD3	1:A:353:TYR:CZ	2.56	0.41
1:C:197:MET:HE3	1:C:197:MET:HB3	1.86	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:A:197:MET:HB3	1:A:197:MET:HE3	1.91	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1021/1024 (100%)	987 (97%)	32 (3%)	2 (0%)	43	55
1	C	1008/1024 (98%)	970 (96%)	36 (4%)	2 (0%)	43	55
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%)	9	9
All	All	2253/2276 (99%)	2178 (97%)	70 (3%)	5 (0%)	43	55

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 ⓘ

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%)	857 (95%)	49 (5%)	20	29
1	C	894/899 (99%)	850 (95%)	44 (5%)	22	34
2	B	73/69 (106%)	71 (97%)	2 (3%)	39	58
2	D	71/69 (103%)	68 (96%)	3 (4%)	26	40
2	E	67/69 (97%)	59 (88%)	8 (12%)	5	6
All	All	2011/2005 (100%)	1905 (95%)	106 (5%)	20	30

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	33	LYS
1	A	44	LEU
1	A	53	LYS
1	A	79	GLN
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	220	ASP
1	A	222	LEU
1	A	244	LYS

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Mol	Chain	Res	Type
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	513	ILE
1	A	517[A]	ILE
1	A	517[B]	ILE
1	A	535	SER
1	A	590	ARG
1	A	595	LYS
1	A	618	SER
1	A	619	LEU
1	A	621[A]	GLN
1	A	621[B]	GLN
1	A	646	LYS
1	A	657	SER
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	766	ILE
1	A	771	THR
1	A	798	ILE
1	A	873	VAL
1	A	910	GLU
1	A	947	GLU
1	A	948	LYS
1	A	955	THR
1	A	987	LYS
2	B	62	GLN
2	B	64	GLU
1	C	33	LYS
1	C	44	LEU
1	C	53	LYS
1	C	94	VAL
1	C	96	ARG
1	C	117	VAL

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Mol	Chain	Res	Type
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	324	LYS
1	C	335	GLU
1	C	409	THR
1	C	410	THR
1	C	415	SER
1	C	487	PRO
1	C	513	ILE
1	C	517	ILE
1	C	594	GLU
1	C	595	LYS
1	C	619	LEU
1	C	621	GLN
1	C	646	LYS
1	C	652	LYS
1	C	657	SER
1	C	700	LYS
1	C	705	GLU
1	C	718	LEU
1	C	745	LYS
1	C	750	ASN
1	C	766	ILE
1	C	771	THR
1	C	777	LYS
1	C	786	ASP
1	C	873	VAL
1	C	910	GLU
1	C	955	THR
1	C	973	LYS
1	C	987	LYS
2	D	25	ASN
2	D	54	ARG
2	D	64	GLU
2	E	6	LYS

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Mol	Chain	Res	Type
2	E	8	LEU
2	E	12	THR
2	E	25	ASN
2	E	48	LYS
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 (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	429	GLN
1	A	647	GLN
1	A	764	HIS
1	A	781	ASN
1	A	844	ASN
1	A	997	HIS
2	B	60	ASN
1	C	122	GLN
1	C	320	ASN
1	C	411	GLN
1	C	429	GLN
1	C	637	GLN
1	C	639	ASN
1	C	647	GLN
1	C	703	ASN
1	C	844	ASN
1	C	893	GLN
2	D	25	ASN
2	D	40	GLN
2	D	60	ASN
2	E	2	GLN
2	E	25	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	1.22	0	1,6,8	0.27	0
1	CSO	C	1006	1	3,6,7	1.35	0	1,6,8	0.53	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
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
5	GOL	A	1111	-	5,5,5	0.46	0	5,5,5	1.06	0
3	SO4	A	1101	-	4,4,4	0.31	0	6,6,6	0.94	0
5	GOL	C	1109	-	5,5,5	0.92	0	5,5,5	1.55	1 (20%)
5	GOL	A	1109	-	5,5,5	0.72	0	5,5,5	0.66	0
5	GOL	A	1106	-	5,5,5	0.82	0	5,5,5	0.92	0
6	6O2	D	101	2	34,34,34	1.70	5 (14%)	50,50,50	2.45	19 (38%)
5	GOL	A	1110	-	5,5,5	1.01	0	5,5,5	1.75	2 (40%)
8	ACT	C	1111	-	3,3,3	0.88	0	3,3,3	0.76	0
3	SO4	C	1101	-	4,4,4	0.26	0	6,6,6	1.67	1 (16%)
5	GOL	A	1108	-	5,5,5	1.20	0	5,5,5	1.39	0
5	GOL	A	1107	-	5,5,5	0.68	0	5,5,5	1.00	0
6	6O2	B	101	2	34,34,34	1.75	6 (17%)	50,50,50	2.46	21 (42%)
5	GOL	C	1110	-	5,5,5	1.03	0	5,5,5	1.11	0
5	GOL	C	1108	-	5,5,5	0.65	0	5,5,5	0.84	0
5	GOL	C	1107	-	5,5,5	0.33	0	5,5,5	0.88	0
5	GOL	A	1112	-	5,5,5	1.14	0	5,5,5	1.25	1 (20%)

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	1111	-	-	0/4/4/4	-
5	GOL	C	1109	-	-	2/4/4/4	-
5	GOL	A	1109	-	-	2/4/4/4	-
5	GOL	A	1106	-	-	2/4/4/4	-
6	6O2	D	101	2	-	5/16/32/32	0/4/4/4
5	GOL	A	1110	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	1108	-	-	1/4/4/4	-
5	GOL	A	1107	-	-	1/4/4/4	-
6	6O2	B	101	2	-	4/16/32/32	0/4/4/4
5	GOL	C	1110	-	-	4/4/4/4	-
5	GOL	C	1108	-	-	1/4/4/4	-
5	GOL	C	1107	-	-	1/4/4/4	-
5	GOL	A	1112	-	-	2/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	101	6O2	C8-C12	-7.12	1.29	1.44
6	D	101	6O2	C8-C12	-6.15	1.31	1.44
6	D	101	6O2	O-S	-3.57	1.52	1.57
6	D	101	6O2	C12-C13	3.22	1.29	1.18
6	B	101	6O2	C12-C13	2.78	1.27	1.18
6	B	101	6O2	C3-N	-2.74	1.32	1.37
6	D	101	6O2	C15-N	-2.73	1.32	1.37
6	D	101	6O2	C3-N	-2.72	1.32	1.37
6	B	101	6O2	C15-N	-2.64	1.33	1.37
6	B	101	6O2	O-S	-2.46	1.54	1.57
6	B	101	6O2	C14-N4	-2.27	1.34	1.39

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	101	6O2	O5-S-O4	-9.21	110.57	119.94
6	B	101	6O2	C6-C7-C8	6.98	124.96	119.89
6	B	101	6O2	O5-S-O4	-6.61	113.21	119.94
6	D	101	6O2	N2-C4-N1	-5.00	121.01	128.58
6	D	101	6O2	C-O-S	4.48	123.02	117.29
6	B	101	6O2	C14-C3-N1	-4.28	120.83	126.72
6	D	101	6O2	C6-C7-C8	4.27	122.99	119.89
6	D	101	6O2	C14-C3-N1	-3.92	121.32	126.72
6	D	101	6O2	O-S-O5	3.70	117.25	106.28
6	B	101	6O2	C3-C14-N4	-3.66	106.39	110.58
6	D	101	6O2	C3-N-C15	3.61	109.53	105.74
6	B	101	6O2	O5-S-N5	-3.60	103.92	109.13
6	B	101	6O2	N2-C4-N1	-3.58	123.16	128.58
6	B	101	6O2	C11-C6-C7	-3.58	115.33	119.66
6	B	101	6O2	C7-C8-C12	-3.57	115.54	120.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	101	6O2	O-S-O5	3.53	116.75	106.28
6	D	101	6O2	N-C15-N4	-3.51	108.96	113.94
6	B	101	6O2	C9-C8-C12	3.30	125.48	120.66
6	D	101	6O2	C4-N1-C3	3.25	119.76	111.83
6	B	101	6O2	C3-C14-C5	3.15	119.39	116.78
6	D	101	6O2	C3-C14-N4	-3.11	107.03	110.58
6	B	101	6O2	N-C15-N4	-3.09	109.55	113.94
3	C	1101	SO4	O4-S-O3	2.71	123.45	108.54
6	B	101	6O2	C11-C10-C9	2.66	123.67	120.24
6	B	101	6O2	C11-C6-N3	2.62	129.49	120.61
5	C	1109	GOL	O1-C1-C2	2.62	122.16	110.38
6	B	101	6O2	C4-N1-C3	2.55	118.06	111.83
6	D	101	6O2	O4-S-N5	-2.54	105.47	109.13
6	B	101	6O2	C14-N4-C15	2.54	107.44	103.45
6	B	101	6O2	C14-C5-N3	2.50	127.45	120.22
6	D	101	6O2	N1-C3-N	2.47	131.37	127.17
5	A	1112	GOL	O3-C3-C2	2.41	121.25	110.38
6	D	101	6O2	C11-C6-C7	-2.38	116.78	119.66
6	B	101	6O2	C14-C3-N	2.38	108.40	105.81
6	D	101	6O2	C14-N4-C15	2.36	107.17	103.45
6	D	101	6O2	C16-C17-C1	2.32	107.09	102.61
6	B	101	6O2	C3-N-C15	2.29	108.14	105.74
6	B	101	6O2	N3-C5-N2	-2.26	115.66	118.38
6	D	101	6O2	C3-C14-C5	2.11	118.53	116.78
5	A	1110	GOL	O3-C3-C2	2.09	119.78	110.38
6	B	101	6O2	N1-C3-N	2.03	130.62	127.17
5	A	1110	GOL	O2-C2-C3	2.02	117.56	109.18
6	D	101	6O2	C9-C8-C12	2.02	123.61	120.66
6	D	101	6O2	C14-C5-N3	2.02	126.06	120.22
6	D	101	6O2	C11-C6-N3	2.02	127.44	120.61

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

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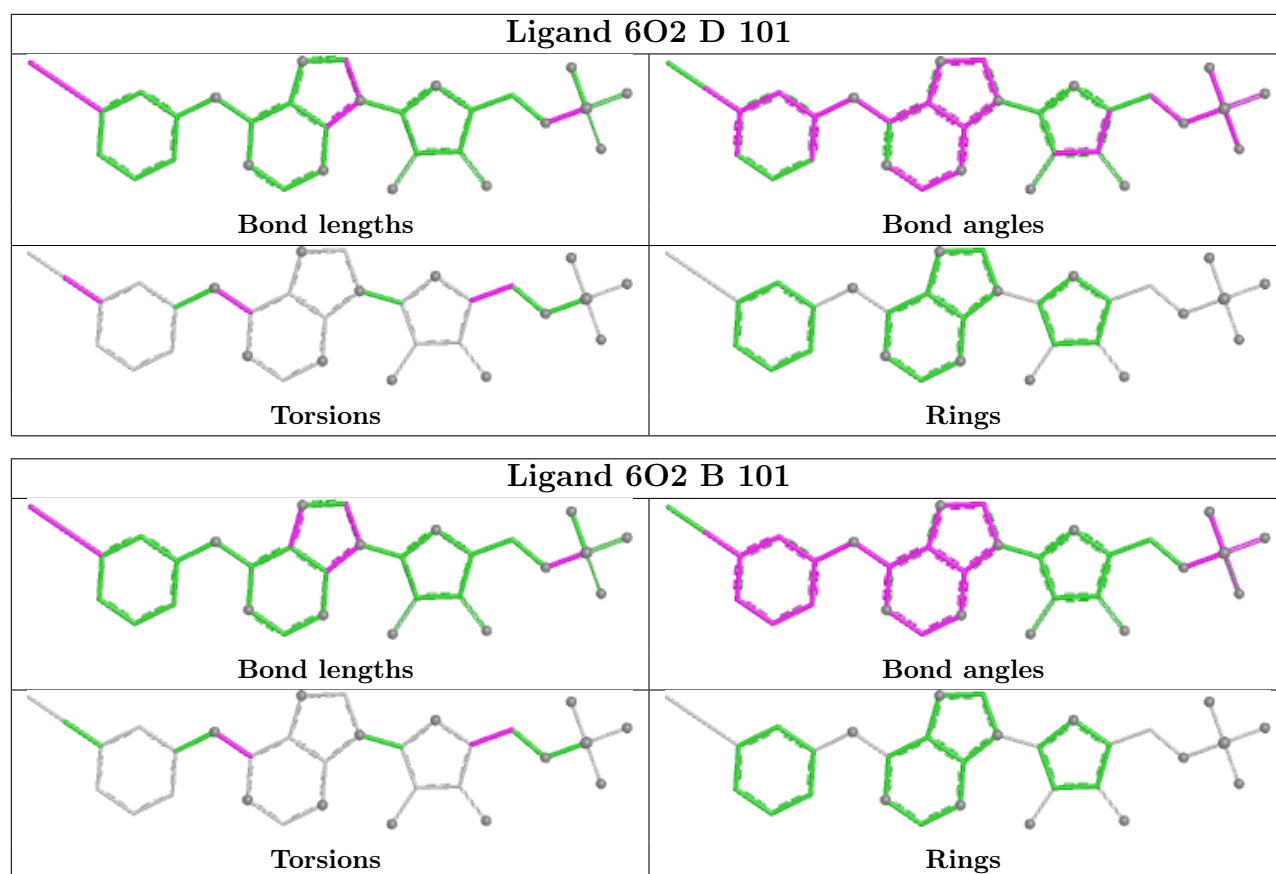
Mol	Chain	Res	Type	Atoms
6	B	101	6O2	C14-C5-N3-C6
6	B	101	6O2	O-C-C1-O1
6	D	101	6O2	C13-C12-C8-C7
6	D	101	6O2	C14-C5-N3-C6
6	B	101	6O2	N2-C5-N3-C6
6	D	101	6O2	N2-C5-N3-C6
5	A	1110	GOL	O1-C1-C2-C3
5	C	1108	GOL	C1-C2-C3-O3
5	A	1106	GOL	O1-C1-C2-O2
5	A	1109	GOL	O2-C2-C3-O3
5	A	1112	GOL	O2-C2-C3-O3
5	C	1109	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
6	D	101	6O2	C13-C12-C8-C9
5	C	1107	GOL	O1-C1-C2-O2
6	D	101	6O2	O-C-C1-O1

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1005/1024 (98%)	-0.56	4 (0%) 88 89	24, 49, 95, 145	20 (1%)
1	C	1004/1024 (98%)	-0.52	5 (0%) 87 87	23, 49, 99, 162	8 (0%)
2	B	76/76 (100%)	-0.53	0 100 100	21, 53, 78, 85	4 (5%)
2	D	76/76 (100%)	-0.44	0 100 100	26, 59, 88, 101	2 (2%)
2	E	72/76 (94%)	2.39	41 (56%) 0 0	135, 153, 183, 193	0
All	All	2233/2276 (98%)	-0.44	50 (2%) 62 64	21, 50, 116, 193	34 (1%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	71	LEU	5.7
1	A	11	ALA	5.0
2	E	56	LEU	4.6
2	E	26	VAL	4.5
2	E	47	GLY	4.4
2	E	8	LEU	4.1
2	E	61	ILE	4.0
2	E	38	PRO	3.8
2	E	43	LEU	3.7
2	E	19	SER	3.7
2	E	20	SER	3.6
2	E	36	ILE	3.6
2	E	70	VAL	3.6
2	E	23	ILE	3.6
2	E	67	LEU	3.6
2	E	46	ALA	3.6
2	E	3	ILE	3.5
2	E	63	LYS	3.4
2	E	17	VAL	3.4
2	E	22	THR	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	50	LEU	3.3
1	C	785	PRO	3.3
1	C	12	GLY	3.2
2	E	48	LYS	3.2
2	E	69	LEU	3.2
2	E	44	ILE	3.2
2	E	9	THR	3.2
2	E	6	LYS	3.1
2	E	30	ILE	3.1
2	E	62	GLN	3.1
2	E	28	SER	2.9
1	A	10	ALA	2.8
2	E	13	ILE	2.8
2	E	57	SER	2.7
2	E	37	PRO	2.7
1	A	12	GLY	2.7
2	E	60	ASN	2.5
1	C	706	PRO	2.5
2	E	15	LEU	2.4
1	C	11	ALA	2.4
2	E	68	HIS	2.4
1	C	701	THR	2.3
1	A	751[A]	SER	2.3
2	E	18	GLU	2.3
2	E	49	GLN	2.3
2	E	5	VAL	2.3
2	E	72	ARG	2.2
2	E	10	GLY	2.2
2	E	29	LYS	2.1
2	E	33	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	CSO	A	1006	7/8	0.97	0.05	45,50,58,63	0
1	CSO	C	1006	7/8	0.98	0.05	39,43,49,55	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

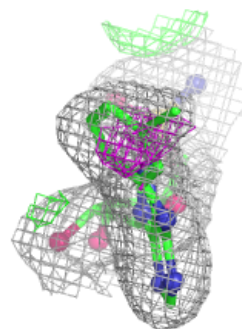
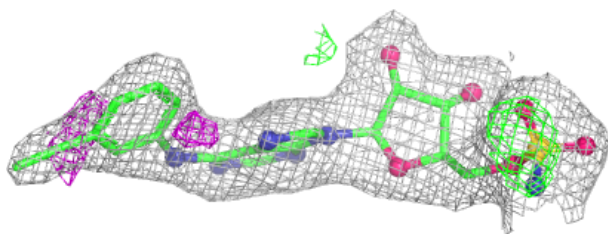
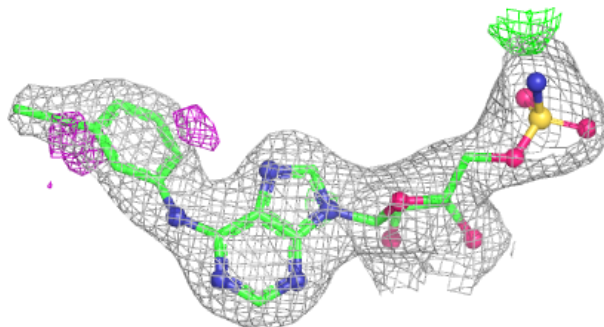
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C	1107	6/6	0.59	0.18	90,92,95,98	0
5	GOL	C	1108	6/6	0.80	0.12	66,82,95,96	0
5	GOL	A	1111	6/6	0.81	0.11	74,79,86,86	0
5	GOL	C	1110	6/6	0.82	0.14	67,84,85,89	0
8	ACT	C	1111	4/4	0.82	0.14	64,74,78,79	0
5	GOL	A	1109	6/6	0.83	0.11	78,89,90,93	0
5	GOL	A	1110	6/6	0.84	0.16	53,59,63,63	0
5	GOL	A	1112	6/6	0.88	0.12	64,79,84,88	0
4	CL	A	1103	1/1	0.90	0.08	77,77,77,77	0
4	CL	C	1104	1/1	0.90	0.07	75,75,75,75	0
5	GOL	A	1108	6/6	0.91	0.12	56,62,68,68	0
5	GOL	A	1107	6/6	0.92	0.08	69,73,76,79	0
4	CL	C	1105	1/1	0.94	0.06	88,88,88,88	0
5	GOL	A	1106	6/6	0.94	0.11	47,56,60,60	0
4	CL	C	1103	1/1	0.94	0.07	85,85,85,85	0
4	CL	A	1105	1/1	0.94	0.09	91,91,91,91	0
5	GOL	C	1109	6/6	0.95	0.11	45,54,55,63	0
4	CL	A	1102	1/1	0.96	0.05	60,60,60,60	0
4	CL	C	1102	1/1	0.97	0.05	65,65,65,65	0
4	CL	A	1104	1/1	0.97	0.09	68,68,68,68	0
6	6O2	D	101	31/31	0.98	0.06	27,44,53,57	0
7	MG	C	1106	1/1	0.98	0.03	45,45,45,45	0
6	6O2	B	101	31/31	0.98	0.05	32,40,45,50	0
3	SO4	C	1101	5/5	0.99	0.06	42,42,43,49	0
3	SO4	A	1101	5/5	0.99	0.03	39,44,45,46	0

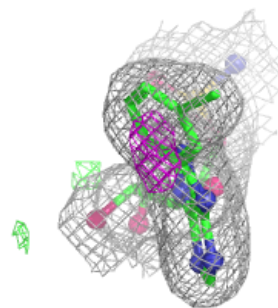
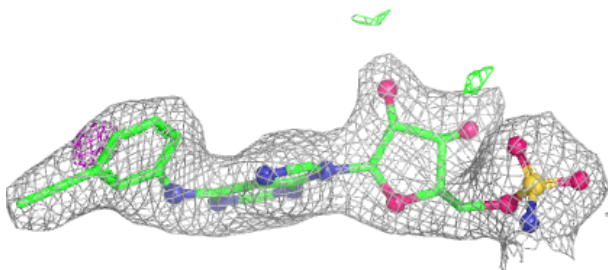
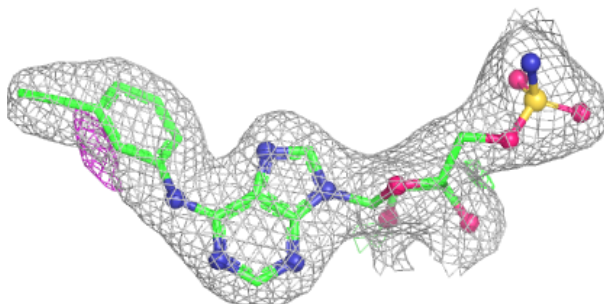
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6O2 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 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.