



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:41 AM UTC

PDB ID : 6Z8A / pdb_00006z8a
Title : Outer membrane FoxA in complex with nocardamine
Authors : Josts, I.; Tidow, H.
Deposited on : 2020-06-02
Resolution : 2.95 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

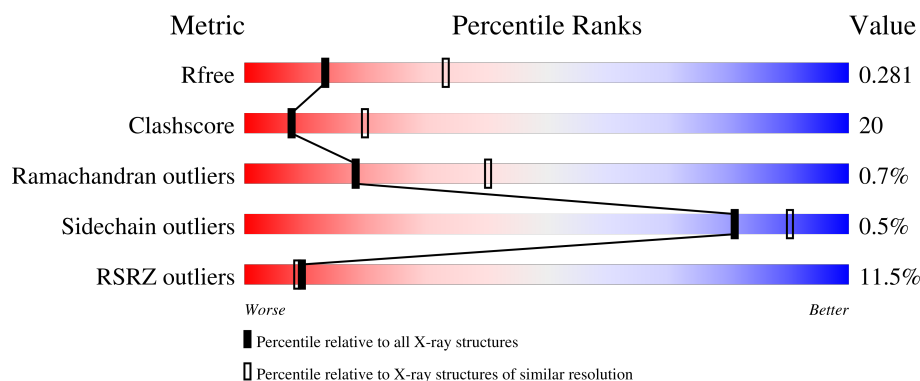
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	776	10% 55% 30% • 13%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5395 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 Ferrioxamine receptor FoxA.

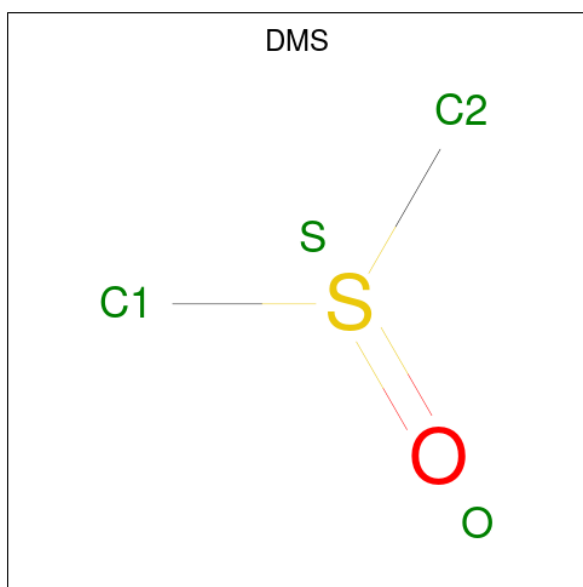
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	677	Total	C	N	O	S	0	0	0
			5325	3345	910	1059	11			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



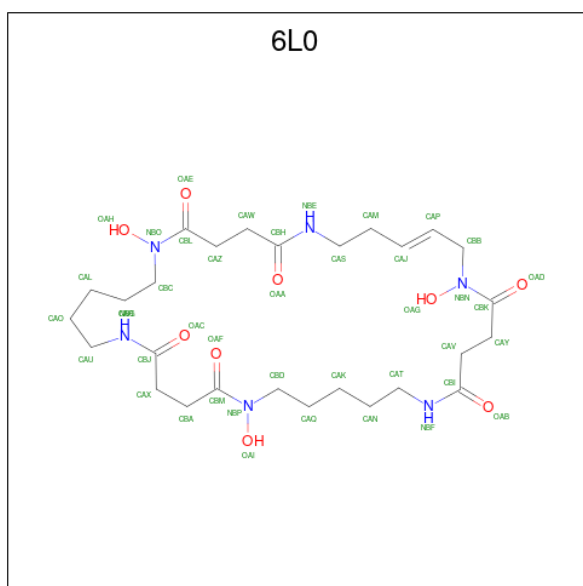
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is (8E)-6,17,28-trihydroxy-1,6,12,17,23,28-hexaazacyclotritriacont-8-ene-2,5,13,16,24,27-hexone (CCD ID: 6L0) (formula: $C_{27}H_{46}N_6O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			42	27	6	9		

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Fe	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.22Å 95.22Å 178.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	82.46 – 2.95 82.46 – 2.95	Depositor EDS
% Data completeness (in resolution range)	73.5 (82.46-2.95) 73.5 (82.46-2.95)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.235 , 0.270 0.245 , 0.281	Depositor DCC
R_{free} test set	709 reflections (3.48%)	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 18.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	5395	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: DMS, 6L0, SO4, FE

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	1.12	6/5451 (0.1%)	1.54	58/7397 (0.8%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	608	PRO	N-CA	15.55	1.67	1.47
1	A	377	VAL	C-N	13.48	1.50	1.33
1	A	620	ALA	C-N	12.45	1.50	1.33
1	A	394	GLU	CA-C	7.43	1.63	1.52
1	A	528	ASP	C-O	5.68	1.31	1.23
1	A	393	ARG	CA-C	5.24	1.59	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	667	VAL	N-CA-C	-14.85	78.44	109.34
1	A	620	ALA	CA-C-N	14.30	134.51	119.78
1	A	620	ALA	C-N-CA	14.30	134.51	119.78
1	A	607	ASN	CA-C-N	12.44	135.39	119.84
1	A	607	ASN	C-N-CA	12.44	135.39	119.84
1	A	377	VAL	CA-C-N	12.08	132.84	119.92
1	A	377	VAL	C-N-CA	12.08	132.84	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	GLU	N-CA-C	10.45	126.34	113.17
1	A	668	GLY	N-CA-C	-10.44	94.93	110.38
1	A	513	ALA	CB-CA-C	-8.77	95.77	110.68
1	A	694	THR	N-CA-C	8.73	123.56	108.02
1	A	762	THR	CB-CA-C	8.51	121.83	110.94
1	A	316	GLU	N-CA-C	-8.45	101.10	111.40
1	A	577	ASP	CA-C-N	7.84	134.70	122.94
1	A	577	ASP	C-N-CA	7.84	134.70	122.94
1	A	314	LEU	N-CA-C	-7.79	103.91	113.50
1	A	608	PRO	N-CA-C	-7.76	96.48	112.47
1	A	772	LEU	CA-C-N	7.72	136.54	121.41
1	A	772	LEU	C-N-CA	7.72	136.54	121.41
1	A	667	VAL	CB-CA-C	7.40	123.43	111.29
1	A	227	ASN	N-CA-C	7.23	126.19	110.80
1	A	272	ARG	CB-CA-C	6.98	118.39	109.80
1	A	393	ARG	N-CA-C	-6.94	104.62	113.23
1	A	392	SER	N-CA-C	6.85	119.57	110.53
1	A	608	PRO	CA-N-CD	-6.79	102.49	112.00
1	A	615	SER	N-CA-C	-6.69	103.32	113.89
1	A	659	PRO	N-CA-C	6.47	125.79	112.47
1	A	390	HIS	CA-C-N	6.40	133.48	121.97
1	A	390	HIS	C-N-CA	6.40	133.48	121.97
1	A	334	GLN	N-CA-C	-6.23	104.48	111.28
1	A	571	THR	CB-CA-C	-6.18	97.24	109.67
1	A	317	GLU	N-CA-C	-6.11	105.79	113.18
1	A	513	ALA	N-CA-C	6.09	118.70	111.33
1	A	694	THR	N-CA-CB	-6.09	101.58	110.84
1	A	436	ASP	CA-CB-CG	-5.93	106.67	112.60
1	A	226	ASP	CB-CA-C	5.90	118.66	110.16
1	A	394	GLU	CA-C-O	5.83	126.17	119.35
1	A	422	ASP	N-CA-C	-5.75	106.11	113.01
1	A	378	PRO	N-CA-C	5.73	120.22	111.34
1	A	813	THR	N-CA-C	5.60	118.60	109.59
1	A	611	TYR	CA-C-N	5.56	130.32	122.09
1	A	611	TYR	C-N-CA	5.56	130.32	122.09
1	A	711	THR	CA-C-O	-5.47	114.89	119.76
1	A	355	ASP	N-CA-C	-5.47	105.42	111.71
1	A	659	PRO	CB-CA-C	-5.41	102.64	111.56
1	A	319	ARG	N-CA-C	-5.40	106.73	113.38
1	A	405	PHE	CA-CB-CG	-5.37	108.43	113.80
1	A	709	GLY	N-CA-C	-5.31	108.76	115.08
1	A	374	HIS	CB-CA-C	5.27	118.48	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	ALA	CA-C-N	5.27	127.59	120.38
1	A	379	ALA	C-N-CA	5.27	127.59	120.38
1	A	490	THR	CA-CB-OG1	-5.26	101.71	109.60
1	A	661	ASP	CB-CA-C	5.25	117.36	110.06
1	A	728	PHE	CB-CA-C	5.24	119.38	109.37
1	A	397	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	227	ASN	CA-C-N	5.12	131.32	121.18
1	A	227	ASN	C-N-CA	5.12	131.32	121.18
1	A	390	HIS	N-CA-C	5.06	118.36	108.18

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	376	GLY	Mainchain

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	5325	0	5038	206	0
2	A	15	0	0	1	0
3	A	4	0	6	0	0
4	A	42	0	0	4	0
5	A	1	0	0	0	0
6	A	8	0	0	1	0
All	All	5395	0	5044	208	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 20.

All (208) 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:240:MET:HE2	1:A:240:MET:HA	1.22	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLN:O	1:A:190:THR:HG22	1.63	0.99
1:A:609:ASN:ND2	1:A:620:ALA:O	1.96	0.97
1:A:818:TYR:CE2	1:A:820:PHE:CD1	2.64	0.85
1:A:772:LEU:H	1:A:772:LEU:HD23	1.41	0.84
1:A:240:MET:HA	1:A:240:MET:CE	2.05	0.84
1:A:512:ASP:O	1:A:516:PRO:HB3	1.79	0.82
1:A:640:SER:HB3	1:A:681:THR:HA	1.65	0.78
1:A:250:GLN:H	1:A:409:GLN:HE22	1.29	0.77
1:A:818:TYR:HE2	1:A:820:PHE:CD1	2.03	0.77
1:A:415:GLN:OE1	1:A:427:ARG:NH2	2.19	0.76
1:A:323:ARG:HD3	1:A:325:ILE:HD11	1.68	0.74
1:A:457:ARG:NH1	1:A:511:LEU:HD22	2.03	0.73
1:A:485:ARG:HB3	1:A:547:ASP:HB2	1.71	0.72
1:A:249:MET:HA	1:A:409:GLN:NE2	2.04	0.72
1:A:245:THR:HG21	1:A:499:THR:HG21	1.73	0.71
1:A:369:PRO:C	1:A:370:ASN:HD22	1.99	0.70
1:A:199:MET:HE1	1:A:219:VAL:HG21	1.74	0.69
1:A:749:TRP:CZ3	1:A:754:ASN:O	2.45	0.69
1:A:609:ASN:ND2	1:A:620:ALA:C	2.50	0.68
1:A:772:LEU:HB2	1:A:775:LEU:HD12	1.74	0.68
1:A:772:LEU:HD23	1:A:772:LEU:N	2.09	0.68
1:A:772:LEU:O	1:A:772:LEU:HG	1.94	0.68
1:A:163:GLN:OE1	1:A:167:LYS:HA	1.94	0.67
1:A:200:ARG:HB3	1:A:743:ARG:HD3	1.76	0.67
1:A:186:GLN:O	1:A:190:THR:CG2	2.41	0.66
1:A:760:ASP:OD1	1:A:760:ASP:O	2.14	0.65
1:A:818:TYR:CE2	1:A:820:PHE:HD1	2.12	0.65
1:A:772:LEU:H	1:A:772:LEU:CD2	2.10	0.65
1:A:645:SER:O	1:A:675:LEU:HA	1.96	0.65
1:A:772:LEU:HD21	1:A:780:LEU:HD23	1.79	0.65
1:A:511:LEU:HD11	1:A:516:PRO:HB2	1.77	0.64
1:A:331:SER:OG	1:A:332:ASP:O	2.13	0.64
1:A:393:ARG:HD3	1:A:793:ASP:OD1	1.98	0.64
1:A:285:LYS:HE3	1:A:415:GLN:HE22	1.62	0.63
1:A:745:VAL:HG21	1:A:761:TYR:CE2	2.33	0.63
1:A:415:GLN:CD	1:A:427:ARG:HH21	2.05	0.62
1:A:167:LYS:HE3	1:A:269:LEU:HB3	1.82	0.62
1:A:295:THR:HG22	1:A:296:GLY:N	2.15	0.61
1:A:164:ILE:HD12	1:A:280:ALA:HB3	1.83	0.61
1:A:214:ASN:O	1:A:250:GLN:NE2	2.34	0.60
1:A:203:PRO:HB3	1:A:692:SER:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ASP:C	1:A:615:SER:H	2.10	0.59
1:A:166:THR:HG22	1:A:168:THR:HG22	1.85	0.59
1:A:393:ARG:CD	1:A:793:ASP:OD1	2.51	0.59
1:A:165:ALA:HB2	1:A:262:LEU:HD13	1.84	0.59
1:A:293:GLN:HG2	1:A:294:ILE:N	2.17	0.58
1:A:686:ASN:HB3	1:A:727:ALA:HB3	1.85	0.58
1:A:451:GLU:HG3	1:A:454:LYS:HE3	1.86	0.58
1:A:250:GLN:N	1:A:409:GLN:HE22	2.00	0.58
1:A:333:THR:OG1	1:A:338:VAL:HG21	2.04	0.58
1:A:166:THR:HG22	1:A:168:THR:CG2	2.33	0.58
1:A:240:MET:HE1	1:A:272:ARG:HH21	1.69	0.57
1:A:315:ASP:HB3	1:A:318:LYS:H	1.69	0.57
1:A:255:PHE:CE1	1:A:325:ILE:HG22	2.39	0.57
1:A:415:GLN:CD	1:A:427:ARG:NH2	2.61	0.57
1:A:233:TYR:CE2	1:A:238:LYS:HG2	2.39	0.57
1:A:389:ARG:NH2	6:A:1002:HOH:O	2.37	0.57
1:A:238:LYS:HB3	1:A:240:MET:HE3	1.86	0.57
1:A:167:LYS:NZ	1:A:472:ASP:OD2	2.38	0.56
1:A:557:LEU:HD22	1:A:582:PHE:CZ	2.41	0.56
1:A:589:LEU:HD12	1:A:599:TYR:HB3	1.87	0.56
1:A:783:SER:HB3	1:A:815:THR:HG23	1.86	0.56
1:A:327:LEU:HD12	1:A:327:LEU:O	2.05	0.56
1:A:268:VAL:HG11	1:A:556:GLY:HA3	1.87	0.56
1:A:454:LYS:HG2	1:A:512:ASP:HA	1.87	0.56
1:A:146:ALA:HB2	1:A:151:LEU:HD12	1.88	0.55
1:A:686:ASN:HB3	1:A:727:ALA:H	1.71	0.55
1:A:548:ILE:HD12	1:A:548:ILE:O	2.06	0.55
1:A:700:TYR:CD2	1:A:710:HIS:O	2.60	0.55
4:A:904:6L0:CAP	4:A:904:6L0:CAY	2.84	0.55
1:A:173:LEU:HD21	1:A:591:LEU:HD11	1.88	0.55
1:A:674:GLY:HA3	1:A:695:TYR:O	2.06	0.55
1:A:150:ASN:N	2:A:901:SO4:O3	2.33	0.54
1:A:444:ALA:HB1	1:A:455:LEU:HD13	1.89	0.54
1:A:700:TYR:HD2	1:A:710:HIS:O	1.91	0.54
1:A:311:SER:HB2	1:A:323:ARG:HG3	1.88	0.54
1:A:541:TYR:HB3	1:A:558:ARG:HG3	1.89	0.54
1:A:559:GLN:HG2	1:A:561:TRP:CZ2	2.44	0.53
1:A:761:TYR:HD2	1:A:763:LEU:HD11	1.73	0.53
1:A:356:ASP:HB2	1:A:419:ARG:HB3	1.88	0.53
1:A:286:PRO:HD3	1:A:348:THR:HG21	1.91	0.53
1:A:315:ASP:HB3	1:A:318:LYS:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:TYR:HB2	1:A:619:LEU:HD12	1.91	0.53
1:A:779:GLY:O	1:A:818:TYR:HA	2.10	0.52
1:A:166:THR:HG22	1:A:168:THR:H	1.74	0.52
1:A:194:THR:HG22	1:A:196:GLN:H	1.74	0.52
1:A:686:ASN:HD22	1:A:727:ALA:HB3	1.75	0.52
1:A:215:ARG:C	1:A:250:GLN:HE21	2.18	0.52
1:A:249:MET:HA	1:A:409:GLN:HE21	1.75	0.52
1:A:249:MET:CA	1:A:409:GLN:NE2	2.72	0.51
1:A:534:ARG:HB2	1:A:565:THR:HB	1.91	0.51
1:A:445:TYR:CD1	1:A:445:TYR:C	2.88	0.51
1:A:671:ARG:NH1	1:A:673:GLN:OE1	2.43	0.51
1:A:421:ASP:HB2	1:A:424:TRP:H	1.75	0.51
1:A:613:ASP:C	1:A:615:SER:N	2.69	0.51
1:A:658:GLU:O	1:A:661:ASP:O	2.29	0.50
1:A:199:MET:CE	1:A:219:VAL:HG21	2.39	0.50
1:A:173:LEU:HD21	1:A:591:LEU:CD1	2.42	0.50
1:A:199:MET:HE1	1:A:219:VAL:CG2	2.41	0.50
1:A:206:PHE:HB3	1:A:220:VAL:HB	1.94	0.50
1:A:393:ARG:HD3	1:A:793:ASP:CG	2.36	0.50
1:A:393:ARG:HG3	1:A:394:GLU:CD	2.36	0.49
1:A:464:GLU:HA	1:A:500:VAL:O	2.12	0.49
1:A:511:LEU:CD1	1:A:516:PRO:HB2	2.41	0.49
1:A:256:LEU:HA	1:A:283:SER:HA	1.93	0.49
1:A:419:ARG:NH2	1:A:422:ASP:HA	2.27	0.49
1:A:808:GLU:OE2	1:A:811:ASN:HB2	2.12	0.49
1:A:389:ARG:HB3	1:A:514:PHE:CE1	2.47	0.49
1:A:745:VAL:HG21	1:A:761:TYR:CZ	2.47	0.49
1:A:818:TYR:CD2	1:A:820:PHE:CD1	3.01	0.49
1:A:713:ASN:ND2	1:A:799:TYR:O	2.46	0.49
1:A:245:THR:HB	1:A:464:GLU:OE1	2.12	0.48
1:A:166:THR:CG2	1:A:168:THR:HG23	2.44	0.48
1:A:237:LEU:HD22	1:A:470:ILE:HG12	1.96	0.48
1:A:670:VAL:CG1	1:A:698:ILE:HD11	2.42	0.48
1:A:333:THR:OG1	1:A:338:VAL:CG2	2.62	0.48
1:A:640:SER:CB	1:A:681:THR:HA	2.39	0.48
1:A:448:SER:OG	1:A:451:GLU:HB2	2.13	0.48
1:A:293:GLN:HB2	1:A:819:GLN:HG2	1.95	0.48
1:A:735:GLY:O	1:A:771:ASP:N	2.35	0.48
1:A:818:TYR:CD2	1:A:820:PHE:HD1	2.31	0.47
1:A:484:ALA:HA	1:A:548:ILE:HG22	1.95	0.47
1:A:153:SER:O	1:A:160:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LEU:HD23	1:A:361:LEU:HD12	1.95	0.47
1:A:725:ASP:OD1	1:A:767:ARG:NH1	2.48	0.47
1:A:211:GLY:HA2	1:A:796:ALA:CB	2.43	0.47
1:A:278:LEU:HD12	1:A:278:LEU:C	2.39	0.47
1:A:683:LEU:HD23	1:A:684:SER:HB3	1.97	0.47
1:A:197:GLN:O	1:A:200:ARG:NE	2.45	0.47
1:A:779:GLY:O	1:A:819:GLN:N	2.47	0.47
1:A:212:ALA:HB2	1:A:808:GLU:N	2.29	0.46
1:A:374:HIS:O	4:A:904:6L0:CAT	2.63	0.46
1:A:295:THR:CG2	1:A:296:GLY:N	2.78	0.46
1:A:613:ASP:HB3	1:A:617:THR:OG1	2.15	0.46
1:A:327:LEU:HD12	1:A:327:LEU:C	2.40	0.46
1:A:369:PRO:C	1:A:370:ASN:ND2	2.70	0.46
1:A:389:ARG:CB	1:A:514:PHE:CE1	2.98	0.46
1:A:445:TYR:C	1:A:445:TYR:HD1	2.24	0.46
1:A:199:MET:CE	1:A:219:VAL:CG2	2.93	0.46
1:A:194:THR:HB	1:A:197:GLN:HB2	1.98	0.46
1:A:686:ASN:OD1	1:A:729:ASP:CG	2.59	0.46
1:A:255:PHE:CE1	1:A:325:ILE:CG2	2.99	0.45
1:A:499:THR:HG22	1:A:501:VAL:HG13	1.97	0.45
1:A:585:ARG:HG3	1:A:603:SER:HB3	1.98	0.45
1:A:780:LEU:HA	1:A:817:ASN:O	2.17	0.45
1:A:242:ASP:C	1:A:244:GLY:H	2.25	0.45
1:A:271:GLY:O	1:A:272:ARG:C	2.59	0.45
1:A:469:TYR:OH	1:A:496:ARG:HD2	2.16	0.45
1:A:609:ASN:HD22	1:A:620:ALA:C	2.23	0.45
1:A:163:GLN:O	1:A:167:LYS:N	2.47	0.45
1:A:206:PHE:HB2	1:A:719:MET:HE1	1.99	0.45
1:A:216:TYR:HB2	1:A:218:TYR:CE1	2.52	0.45
1:A:686:ASN:OD1	1:A:729:ASP:OD2	2.35	0.45
1:A:716:PRO:HG2	1:A:719:MET:HE3	1.99	0.45
1:A:423:VAL:HG13	1:A:424:TRP:CD1	2.53	0.44
1:A:571:THR:O	1:A:571:THR:HG22	2.14	0.44
1:A:756:LEU:HD23	1:A:756:LEU:N	2.33	0.44
1:A:374:HIS:O	4:A:904:6L0:NBF	2.51	0.44
1:A:256:LEU:HD22	1:A:281:LEU:HB3	2.00	0.44
1:A:424:TRP:CZ3	1:A:477:ALA:HB2	2.52	0.44
1:A:700:TYR:HB3	1:A:703:SER:OG	2.18	0.44
1:A:761:TYR:CD2	1:A:763:LEU:HD11	2.51	0.44
1:A:767:ARG:HB3	1:A:785:ASN:ND2	2.33	0.43
1:A:221:MET:HE1	1:A:262:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LEU:HB3	1:A:470:ILE:HD13	1.99	0.43
1:A:212:ALA:HB2	1:A:808:GLU:CA	2.49	0.43
1:A:237:LEU:HB2	1:A:431:ARG:NH2	2.33	0.43
1:A:359:LEU:HD13	1:A:416:LEU:HD13	1.99	0.43
1:A:596:LEU:HD12	1:A:633:PHE:HB2	2.00	0.43
1:A:472:ASP:OD1	1:A:541:TYR:OH	2.32	0.43
1:A:272:ARG:H	1:A:537:GLN:HE22	1.66	0.43
1:A:194:THR:HG22	1:A:196:GLN:N	2.34	0.43
1:A:671:ARG:NH1	1:A:673:GLN:CD	2.76	0.43
1:A:789:LEU:HD12	1:A:810:ARG:HD2	2.00	0.43
1:A:418:HIS:NE2	1:A:420:ILE:HG12	2.34	0.43
1:A:716:PRO:CG	1:A:719:MET:HE3	2.49	0.43
1:A:432:TYR:HD1	1:A:469:TYR:HB3	1.84	0.43
1:A:675:LEU:HD12	1:A:676:GLU:N	2.34	0.42
1:A:728:PHE:HB2	1:A:733:LEU:O	2.19	0.42
1:A:393:ARG:HD2	1:A:793:ASP:OD1	2.19	0.42
1:A:487:THR:O	1:A:545:LEU:HD12	2.19	0.42
1:A:166:THR:CG2	1:A:168:THR:CG2	2.97	0.42
1:A:249:MET:HB3	1:A:409:GLN:NE2	2.35	0.42
1:A:495:GLN:NE2	1:A:537:GLN:OE1	2.52	0.42
1:A:497:ARG:HH11	1:A:497:ARG:HD2	1.70	0.41
1:A:167:LYS:HD2	1:A:269:LEU:HD22	2.01	0.41
1:A:181:VAL:C	1:A:182:ILE:HD13	2.45	0.41
1:A:238:LYS:CB	1:A:240:MET:HE3	2.49	0.41
1:A:390:HIS:O	1:A:390:HIS:ND1	2.53	0.41
1:A:602:TYR:HA	1:A:626:GLN:O	2.19	0.41
1:A:716:PRO:HD2	1:A:719:MET:HE3	2.02	0.41
1:A:210:VAL:HG13	1:A:213:SER:OG	2.20	0.41
1:A:548:ILE:HD12	1:A:548:ILE:C	2.45	0.41
1:A:164:ILE:HD12	1:A:280:ALA:CB	2.49	0.41
1:A:398:GLY:HA2	1:A:442:VAL:O	2.21	0.41
1:A:512:ASP:O	1:A:516:PRO:CB	2.61	0.41
1:A:317:GLU:HB2	1:A:319:ARG:HG3	2.01	0.41
1:A:370:ASN:ND2	1:A:370:ASN:N	2.67	0.41
4:A:904:6L0:CAQ	4:A:904:6L0:CBA	2.97	0.41
1:A:173:LEU:CD2	1:A:591:LEU:HD11	2.50	0.40
1:A:398:GLY:O	1:A:457:ARG:NH1	2.54	0.40
1:A:406:ASP:O	1:A:437:VAL:HA	2.21	0.40
1:A:748:THR:O	1:A:758:VAL:N	2.54	0.40
1:A:499:THR:HG22	1:A:501:VAL:CG1	2.52	0.40
1:A:365:LEU:HD23	1:A:365:LEU:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:LEU:HD12	1:A:564:VAL:HG22	2.03	0.40
1:A:167:LYS:CE	1:A:269:LEU:HB3	2.49	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	675/776 (87%)	614 (91%)	56 (8%)	5 (1%)	18 40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	391	ILE
1	A	145	PHE
1	A	791	ASP
1	A	227	ASN
1	A	240	MET

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	566/635 (89%)	563 (100%)	3 (0%)	81 90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	497	ARG
1	A	515	ASN
1	A	799	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	250	GLN
1	A	293	GLN
1	A	370	ASN
1	A	374	HIS
1	A	390	HIS
1	A	409	GLN
1	A	456	ASN
1	A	495	GLN
1	A	639	ASN
1	A	648	HIS
1	A	707	ASN
1	A	710	HIS
1	A	714	GLN
1	A	785	ASN
1	A	811	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
2	SO4	A	902	-	4,4,4	0.45	0	6,6,6	0.10	0
3	DMS	A	903	-	3,3,3	0.16	0	3,3,3	0.07	0
2	SO4	A	901	-	4,4,4	0.46	0	6,6,6	0.16	0
2	SO4	A	906	-	4,4,4	0.31	0	6,6,6	0.16	0
4	6L0	A	904	5	41,42,42	1.97	3 (7%)	37,51,51	0.60	1 (2%)

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
4	6L0	A	904	5	-	28/53/54/54	0/0/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	904	6L0	OAG-NBN	-7.27	1.34	1.40
4	A	904	6L0	OAI-NBP	-6.94	1.35	1.40
4	A	904	6L0	OAH-NBO	-6.59	1.35	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904	6L0	CAS-CAM-CAJ	2.14	114.23	111.95

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	904	6L0	CAL-CAR-CBC-NBO
4	A	904	6L0	CAW-CAZ-CBL-NBO
4	A	904	6L0	CAJ-CAM-CAS-NBE
4	A	904	6L0	CAP-CBB-NBN-CBK
4	A	904	6L0	OAD-CBK-NBN-CBB
4	A	904	6L0	CAY-CBK-NBN-CBB
4	A	904	6L0	OAD-CBK-NBN-OAG
4	A	904	6L0	CAY-CBK-NBN-OAG
4	A	904	6L0	CAK-CAQ-CBD-NBP
4	A	904	6L0	CBA-CBM-NBP-OAI
4	A	904	6L0	OAF-CBM-NBP-OAI
4	A	904	6L0	CAN-CAT-NBF-CBI
4	A	904	6L0	CAO-CAU-NBG-CBJ
4	A	904	6L0	CAK-CAN-CAT-NBF
4	A	904	6L0	CAL-CAO-CAU-NBG
4	A	904	6L0	CBH-CAW-CAZ-CBL
4	A	904	6L0	CBA-CAX-CBJ-NBG
4	A	904	6L0	CAW-CAZ-CBL-OAE
4	A	904	6L0	CBA-CAX-CBJ-OAC
4	A	904	6L0	CAN-CAK-CAQ-CBD
4	A	904	6L0	CAQ-CAK-CAN-CAT
4	A	904	6L0	CAO-CAL-CAR-CBC
4	A	904	6L0	CAR-CAL-CAO-CAU
4	A	904	6L0	CAM-CAJ-CAP-CBB
4	A	904	6L0	CBI-CAV-CAY-CBK
4	A	904	6L0	CAX-CBA-CBM-NBP
4	A	904	6L0	CAQ-CBD-NBP-OAI
4	A	904	6L0	OAE-CBL-NBO-OAH

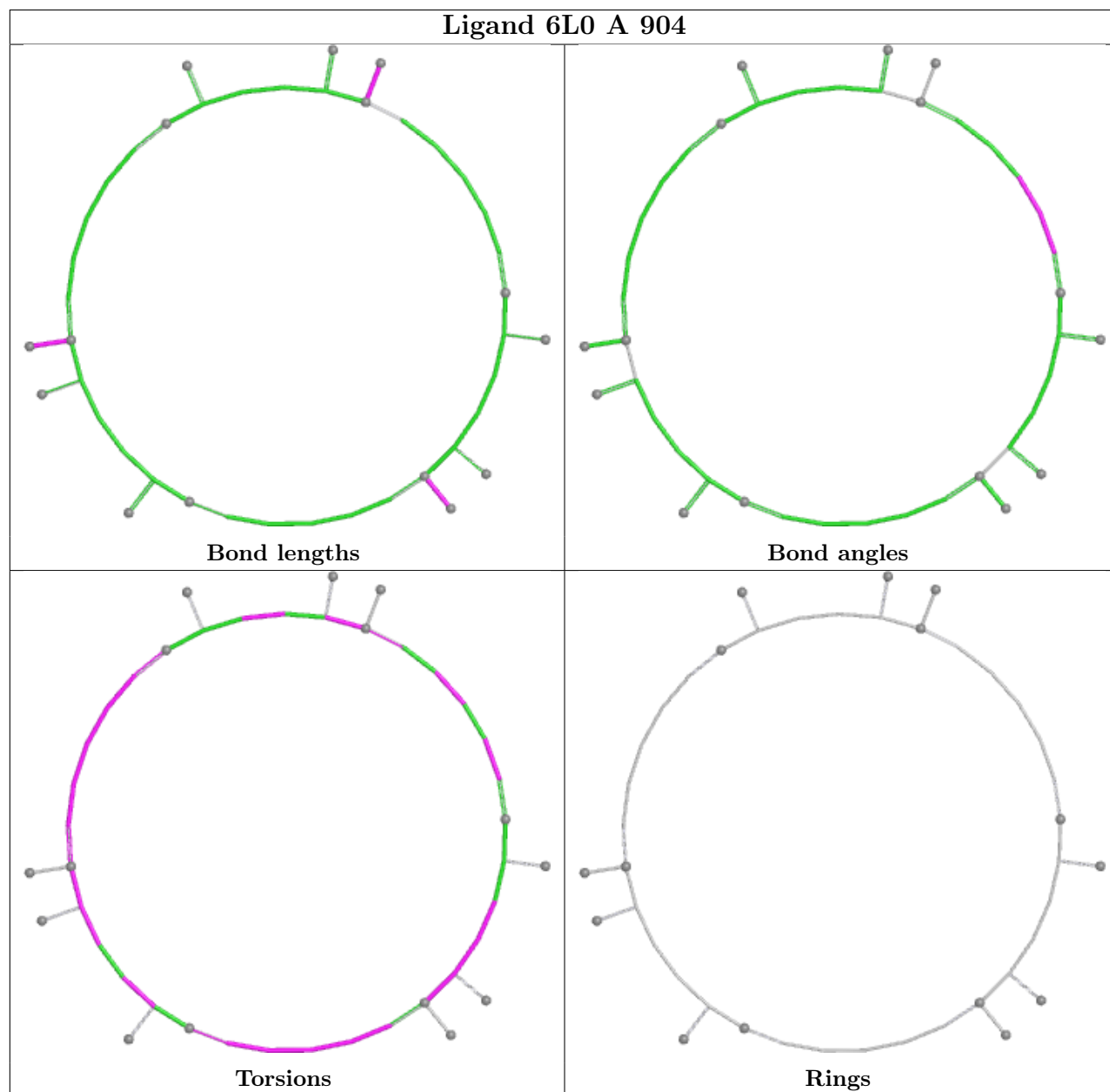
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	SO4	1	0
4	A	904	6L0	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	677/776 (87%)	0.73	78 (11%) 9 9	42, 67, 105, 131	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	756	LEU	9.9
1	A	750	ALA	7.9
1	A	390	HIS	7.6
1	A	463	ARG	7.2
1	A	754	ASN	7.0
1	A	620	ALA	6.5
1	A	755	THR	6.3
1	A	382	THR	5.9
1	A	803	PHE	5.8
1	A	445	TYR	5.7
1	A	802	ASP	5.5
1	A	391	ILE	5.5
1	A	275	PRO	5.3
1	A	749	TRP	5.2
1	A	393	ARG	5.0
1	A	753	GLU	4.9
1	A	145	PHE	4.8
1	A	223	GLY	4.8
1	A	383	LEU	4.7
1	A	806	PHE	4.5
1	A	801	LEU	4.4
1	A	426	ALA	4.3
1	A	713	ASN	4.0
1	A	462	ALA	3.9
1	A	440	SER	3.9
1	A	446	GLY	3.8
1	A	404	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	378	PRO	3.7
1	A	475	LEU	3.7
1	A	304	LYS	3.7
1	A	800	SER	3.6
1	A	666	SER	3.5
1	A	664	TYR	3.5
1	A	425	SER	3.5
1	A	751	ASP	3.5
1	A	392	SER	3.4
1	A	461	GLY	3.3
1	A	757	ARG	3.3
1	A	460	SER	3.3
1	A	752	LYS	3.2
1	A	643	THR	3.2
1	A	381	GLY	3.1
1	A	489	LEU	3.0
1	A	799	TYR	3.0
1	A	379	ALA	3.0
1	A	804	CYS	2.9
1	A	424	TRP	2.9
1	A	244	GLY	2.9
1	A	469	TYR	2.9
1	A	793	ASP	2.8
1	A	609	ASN	2.7
1	A	184	ARG	2.6
1	A	619	LEU	2.5
1	A	667	VAL	2.5
1	A	798	CYS	2.4
1	A	544	ASP	2.4
1	A	306	MET	2.4
1	A	298	ILE	2.4
1	A	365	LEU	2.4
1	A	503	TRP	2.3
1	A	683	LEU	2.3
1	A	513	ALA	2.2
1	A	403	ASP	2.2
1	A	455	LEU	2.2
1	A	618	PRO	2.2
1	A	183	THR	2.2
1	A	280	ALA	2.1
1	A	401	SER	2.1
1	A	377	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	504	ARG	2.1
1	A	818	TYR	2.1
1	A	624	GLY	2.1
1	A	564	VAL	2.0
1	A	227	ASN	2.0
1	A	224	PHE	2.0
1	A	412	PHE	2.0
1	A	438	ASP	2.0
1	A	732	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

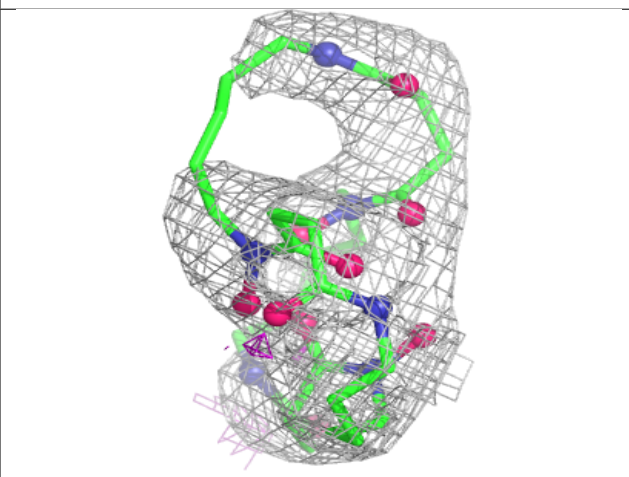
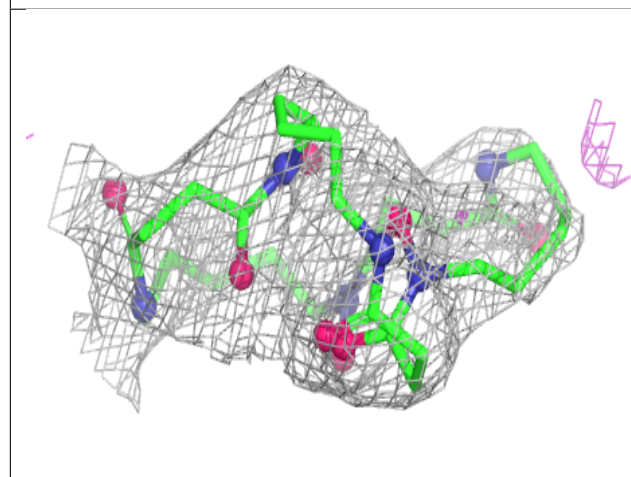
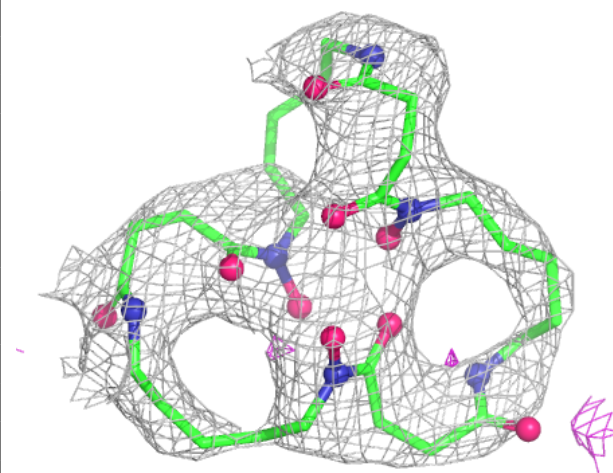
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DMS	A	903	4/4	0.23	0.36	106,113,115,119	0
2	SO4	A	901	5/5	0.71	0.22	62,64,66,66	5
2	SO4	A	906	5/5	0.85	0.19	102,113,117,124	0
2	SO4	A	902	5/5	0.88	0.20	93,96,100,104	5
4	6L0	A	904	42/42	0.90	0.11	51,62,69,73	0
5	FE	A	905	1/1	1.00	0.08	70,70,70,70	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 6L0 A 904:

$2mF_o-DF_c$ (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.