



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 06:49 AM EDT

PDB ID : 4K6M
Title : Crystal Structure of the full-length Japanese encephalitis virus NS5
Authors : Lu, G.; Gong, P.
Deposited on : 2013-04-16
Resolution : 2.60 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

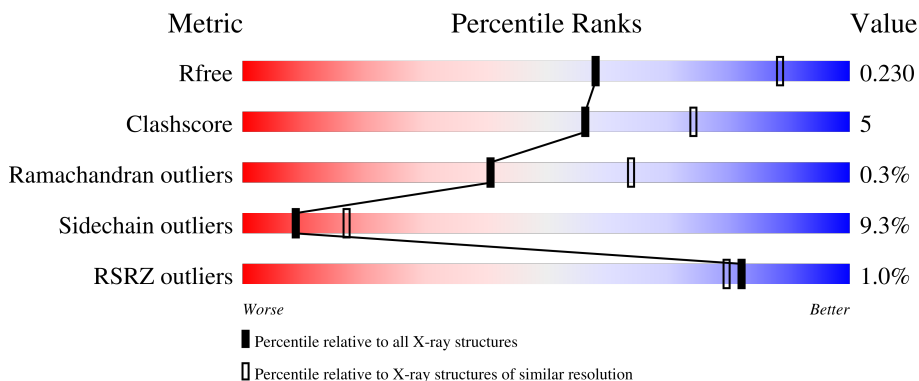
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	915	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>• •</div> </div> </div>
1	B	915	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14758 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 Polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	888	Total	C	N	O	S	0	0	0
			7135	4497	1291	1303	44			
1	B	888	Total	C	N	O	S	0	0	0
			7135	4497	1291	1303	44			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	906	GLY	-	expression tag	UNP Q5NT71
A	907	SER	-	expression tag	UNP Q5NT71
A	908	SER	-	expression tag	UNP Q5NT71
A	909	SER	-	expression tag	UNP Q5NT71
A	910	HIS	-	expression tag	UNP Q5NT71
A	911	HIS	-	expression tag	UNP Q5NT71
A	912	HIS	-	expression tag	UNP Q5NT71
A	913	HIS	-	expression tag	UNP Q5NT71
A	914	HIS	-	expression tag	UNP Q5NT71
A	915	HIS	-	expression tag	UNP Q5NT71
B	906	GLY	-	expression tag	UNP Q5NT71
B	907	SER	-	expression tag	UNP Q5NT71
B	908	SER	-	expression tag	UNP Q5NT71
B	909	SER	-	expression tag	UNP Q5NT71
B	910	HIS	-	expression tag	UNP Q5NT71
B	911	HIS	-	expression tag	UNP Q5NT71
B	912	HIS	-	expression tag	UNP Q5NT71
B	913	HIS	-	expression tag	UNP Q5NT71
B	914	HIS	-	expression tag	UNP Q5NT71
B	915	HIS	-	expression tag	UNP Q5NT71

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		

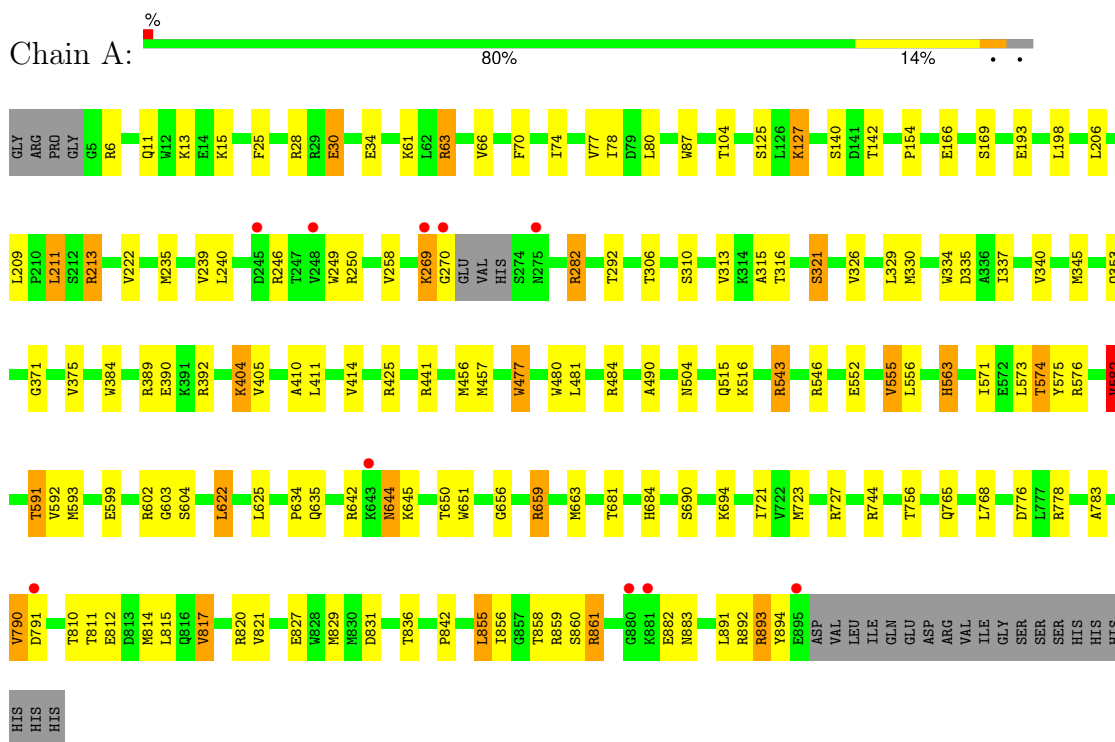
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	183	Total 183	O 183	0	0
5	B	159	Total 159	O 159	0	0

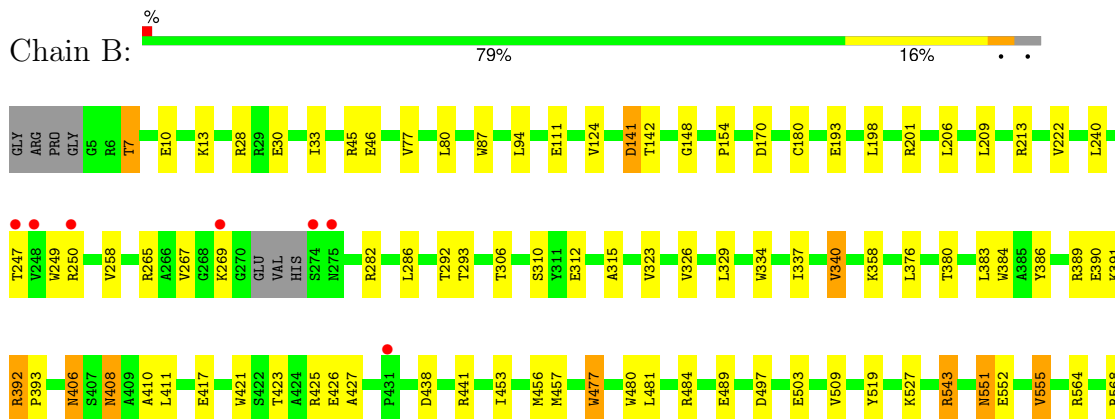
3 Residue-property plots [i](#)

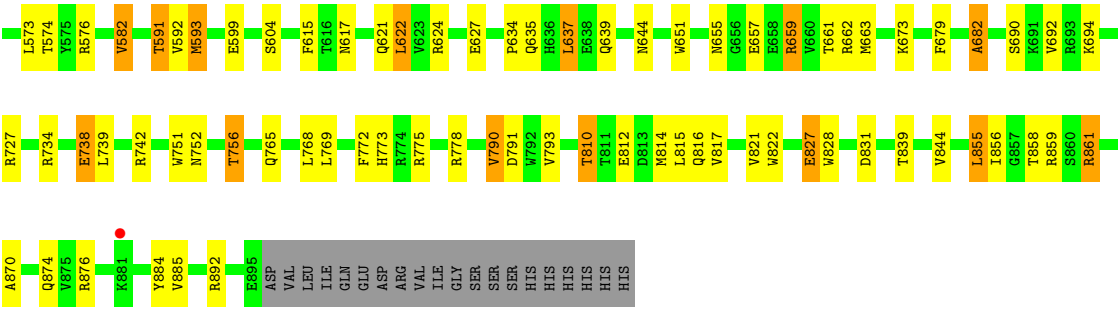
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Polyprotein



• Molecule 1: Polyprotein





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	272.29Å 272.29Å 177.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.22 – 2.60 46.18 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.22-2.60) 98.5 (46.18-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.196 , 0.228 0.200 , 0.230	Depositor DCC
R_{free} test set	7461 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.599	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.006 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14758	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN, SAH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/7303	0.58	1/9867 (0.0%)
1	B	0.44	1/7303 (0.0%)	0.59	0/9867
All	All	0.43	1/14606 (0.0%)	0.58	1/19734 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	GLU	CG-CD	5.17	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	582	VAL	CB-CA-C	-5.93	100.13	111.40

There are no chirality outliers.

There are no planarity outliers.

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	7135	0	7038	63	0
1	B	7135	0	7038	81	0
2	A	26	0	19	1	0
2	B	26	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	50	0	0	2	0
3	B	40	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	183	0	0	4	0
5	B	159	0	0	1	0
All	All	14758	0	14114	143	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 5.

All (143) 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:315:ALA:HB2	1:A:591:THR:HG21	1.51	0.90
1:A:30:GLU:HG3	1:A:249:TRP:HE3	1.36	0.89
1:B:30:GLU:HG3	1:B:249:TRP:HE3	1.41	0.85
1:B:810:THR:HB	1:B:812:GLU:H	1.47	0.79
1:B:13:LYS:HG2	1:B:154:PRO:HG3	1.63	0.77
1:A:727:ARG:HD3	1:A:831:ASP:HB3	1.68	0.76
1:A:30:GLU:HG3	1:A:249:TRP:CE3	2.21	0.75
1:B:391:LYS:NZ	1:B:497:ASP:O	2.22	0.72
1:B:315:ALA:HB2	1:B:591:THR:HG21	1.71	0.71
1:A:34:GLU:OE1	1:A:213:ARG:NH2	2.25	0.69
1:B:282:ARG:NH2	1:B:573:LEU:O	2.26	0.68
1:A:410:ALA:O	1:A:484:ARG:NH2	2.26	0.67
1:B:855:LEU:O	1:B:858:THR:HB	1.94	0.67
1:A:30:GLU:OE2	1:A:250:ARG:N	2.23	0.67
1:B:477:TRP:H	1:B:604:SER:HB3	1.59	0.67
1:A:776:ASP:OD1	1:A:861:ARG:NH1	2.27	0.66
1:A:765:GLN:HB3	1:A:814:MET:HE3	1.78	0.65
1:B:441:ARG:NH1	1:B:489:GLU:OE1	2.30	0.64
1:B:738:GLU:HG2	1:B:742:ARG:NH1	2.12	0.64
1:B:564:ARG:HE	1:B:568:ARG:HH21	1.48	0.62
1:A:330:MET:HE2	1:A:783:ALA:HB1	1.82	0.62
1:A:856:ILE:HA	1:A:861:ARG:HD3	1.82	0.61
1:B:752:ASN:O	1:B:756:THR:HG23	2.00	0.61
1:B:30:GLU:OE2	1:B:250:ARG:N	2.34	0.61
1:B:423:THR:HG22	1:B:425:ARG:H	1.65	0.61
1:A:384:TRP:CH2	1:A:555:VAL:HG13	2.35	0.61
1:A:456:MET:HB3	1:A:582:VAL:HG13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:GLU:HG3	1:B:249:TRP:CE3	2.29	0.60
1:B:389:ARG:HG2	1:B:390:GLU:HG3	1.84	0.60
1:B:392:ARG:HD3	1:B:393:PRO:HD2	1.84	0.59
1:A:30:GLU:HG2	5:A:1217:HOH:O	2.03	0.59
1:B:617:ASN:O	1:B:621:GLN:HG2	2.02	0.59
1:B:775:ARG:NH2	1:B:844:VAL:O	2.36	0.58
1:B:87:TRP:HZ3	1:B:180:CYS:HG	1.49	0.58
1:A:282:ARG:NH2	1:A:573:LEU:O	2.30	0.58
1:A:335:ASP:OD1	1:A:744:ARG:NH2	2.28	0.58
1:A:337:ILE:HB	1:A:340:VAL:HG13	1.86	0.57
1:A:127:LYS:HE2	5:A:1190:HOH:O	2.04	0.57
1:B:337:ILE:HB	1:B:340:VAL:HG13	1.87	0.57
1:A:812:GLU:OE1	1:A:820:ARG:NH2	2.37	0.57
1:B:423:THR:HG22	1:B:425:ARG:N	2.20	0.57
1:B:408:ASN:OD1	1:B:408:ASN:N	2.38	0.56
1:A:70:PHE:HB3	1:A:222:VAL:HG21	1.88	0.56
1:A:855:LEU:O	1:A:858:THR:HB	2.06	0.56
1:B:141:ASP:N	1:B:141:ASP:OD1	2.40	0.55
1:B:727:ARG:HD3	1:B:831:ASP:HB3	1.89	0.55
1:B:456:MET:HB3	1:B:582:VAL:HG13	1.89	0.54
1:B:624:ARG:HG2	1:B:679:PHE:CE1	2.42	0.54
1:B:651:TRP:CZ2	1:B:659:ARG:HD3	2.42	0.54
1:B:406:ASN:ND2	1:B:408:ASN:OD1	2.41	0.54
1:A:389:ARG:NH2	1:A:504:ASN:O	2.41	0.54
1:B:410:ALA:O	1:B:484:ARG:NH2	2.36	0.53
1:A:77:VAL:HG22	1:A:142:THR:HB	1.90	0.53
1:B:751:TRP:HB3	1:B:756:THR:HG22	1.91	0.53
1:B:384:TRP:CH2	1:B:555:VAL:HG13	2.44	0.52
3:A:1003:SO4:O4	1:B:45:ARG:NH1	2.42	0.52
1:B:334:TRP:CE2	1:B:855:LEU:HD22	2.45	0.52
1:B:790:VAL:HG21	1:B:885:VAL:HG23	1.92	0.52
1:A:546:ARG:HG2	5:A:1250:HOH:O	2.09	0.51
1:A:721:ILE:HG21	1:A:842:PRO:HB2	1.91	0.51
1:A:817:VAL:O	1:A:821:VAL:HG13	2.10	0.51
1:B:124:VAL:O	1:B:358:LYS:NZ	2.43	0.50
1:A:321:SER:HB3	1:A:345:MET:H	1.77	0.50
1:B:386:TYR:CE1	1:B:657:GLU:HG2	2.46	0.50
1:B:856:ILE:HA	1:B:861:ARG:HD3	1.94	0.50
1:B:634:PRO:HA	1:B:637:LEU:HD22	1.94	0.50
1:B:527:LYS:HE3	1:B:661:THR:OG1	2.12	0.49
1:A:552:GLU:O	1:A:555:VAL:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:738:GLU:HG2	1:B:742:ARG:HH12	1.76	0.49
1:B:858:THR:HG22	1:B:861:ARG:H	1.77	0.49
1:A:543:ARG:HD3	1:A:690:SER:O	2.13	0.49
1:A:812:GLU:CD	1:A:820:ARG:HH22	2.14	0.49
1:A:371:GLY:O	1:A:375:VAL:HG23	2.12	0.49
1:A:477:TRP:CD1	1:A:477:TRP:N	2.81	0.49
1:A:723:MET:HG2	1:A:842:PRO:HG3	1.93	0.49
1:A:574:THR:HG22	1:A:575:TYR:CD1	2.48	0.48
1:A:28:ARG:NH1	3:A:1006:SO4:O4	2.45	0.48
1:A:790:VAL:HG23	1:A:883:ASN:O	2.13	0.48
1:A:644:ASN:OD1	1:A:644:ASN:N	2.43	0.48
1:B:639:GLN:NE2	5:B:1115:HOH:O	2.46	0.48
1:A:330:MET:CE	1:A:783:ALA:HB1	2.43	0.48
1:B:7:THR:HG23	1:B:10:GLU:HG3	1.95	0.48
1:B:552:GLU:O	1:B:555:VAL:HG22	2.13	0.48
1:B:543:ARG:HD3	1:B:690:SER:O	2.13	0.48
1:A:634:PRO:HG3	1:A:684:HIS:CG	2.49	0.47
1:A:13:LYS:HG2	1:A:154:PRO:HG3	1.95	0.47
1:B:384:TRP:CZ2	1:B:555:VAL:HG13	2.49	0.47
1:A:556:LEU:HD21	1:A:571:ILE:HD12	1.96	0.47
1:A:651:TRP:CZ2	1:A:659:ARG:HD2	2.49	0.47
1:A:810:THR:OG1	1:A:811:THR:N	2.48	0.47
1:A:78:ILE:HD12	1:A:140:SER:HB3	1.97	0.46
1:A:404:LYS:HE2	1:A:404:LYS:HB2	1.79	0.46
1:B:28:ARG:NH1	3:B:1005:SO4:O3	2.48	0.46
1:A:61:LYS:HA	1:A:211:LEU:HD23	1.97	0.46
1:B:876:ARG:HG2	1:B:884:TYR:CE1	2.50	0.46
1:B:564:ARG:HH11	1:B:568:ARG:HH22	1.64	0.46
1:B:768:LEU:O	1:B:772:PHE:HB3	2.17	0.45
1:B:94:LEU:O	1:B:265:ARG:NH2	2.47	0.45
1:B:87:TRP:CD1	2:B:1001:SAH:N	2.84	0.45
1:B:383:LEU:HD23	1:B:615:PHE:CE1	2.52	0.45
1:B:564:ARG:HH11	1:B:568:ARG:NH2	2.15	0.44
1:B:477:TRP:N	1:B:477:TRP:CD1	2.85	0.44
1:B:286:LEU:HD11	1:B:453:ILE:HD13	1.99	0.44
1:B:421:TRP:CD1	1:B:427:ALA:HA	2.53	0.44
1:B:576:ARG:O	1:B:599:GLU:HA	2.18	0.44
1:A:11:GLN:O	1:A:15:LYS:HG3	2.18	0.44
1:B:7:THR:HG23	1:B:10:GLU:OE1	2.17	0.44
1:B:423:THR:HB	1:B:426:GLU:HG3	1.99	0.44
1:A:576:ARG:O	1:A:599:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ALA:O	1:A:563:HIS:HE1	2.01	0.43
1:A:768:LEU:HD23	1:A:768:LEU:HA	1.74	0.43
1:A:87:TRP:CD1	2:A:1001:SAH:N	2.86	0.43
1:A:625:LEU:HD13	1:A:659:ARG:HG2	2.00	0.43
1:B:821:VAL:HG22	1:B:822:TRP:CD1	2.53	0.43
1:B:870:ALA:O	1:B:874:GLN:HG3	2.18	0.43
1:B:651:TRP:O	1:B:655:ASN:HB2	2.19	0.43
1:B:734:ARG:HD3	1:B:739:LEU:HD21	2.00	0.42
1:B:773:HIS:CD2	1:B:773:HIS:H	2.36	0.42
1:A:516:LYS:NZ	1:A:827:GLU:OE1	2.50	0.42
1:A:166:GLU:O	1:A:169:SER:OG	2.32	0.42
1:A:269:LYS:HB2	1:A:270:GLY:H	1.53	0.42
1:A:477:TRP:CE2	1:A:603:GLY:HA2	2.55	0.42
1:B:694:LYS:HE3	1:B:694:LYS:HB2	1.79	0.42
1:B:77:VAL:HG22	1:B:142:THR:HB	2.02	0.42
1:B:662:ARG:HD3	1:B:673:LYS:O	2.20	0.42
1:A:334:TRP:CE2	1:A:855:LEU:HD22	2.54	0.42
1:B:380:THR:HG21	1:B:551:ASN:HB3	2.01	0.42
1:B:310:SER:HA	1:B:593:MET:O	2.19	0.41
1:A:334:TRP:HA	1:A:337:ILE:HG12	2.01	0.41
1:A:63:ARG:HD2	5:A:1124:HOH:O	2.20	0.41
1:A:622:LEU:HD13	1:A:663:MET:CE	2.51	0.41
1:B:293:THR:HB	1:B:312:GLU:HG3	2.01	0.41
1:B:876:ARG:HG2	1:B:884:TYR:CZ	2.56	0.41
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.94	0.41
1:B:765:GLN:HB3	1:B:814:MET:HE3	2.03	0.41
1:B:827:GLU:H	1:B:827:GLU:HG2	1.31	0.41
1:A:25:PHE:CD1	1:B:46:GLU:HG2	2.56	0.41
1:A:893:ARG:HD2	1:A:894:TYR:CE2	2.56	0.41
1:B:627:GLU:HG2	1:B:682:ALA:HB1	2.02	0.41
1:A:235:MET:O	1:A:239:VAL:HG23	2.21	0.41
1:B:519:TYR:HB3	1:B:828:TRP:CE2	2.56	0.40
1:B:622:LEU:HD13	1:B:663:MET:CE	2.52	0.40
1:B:817:VAL:O	1:B:821:VAL:HG13	2.20	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	884/915 (97%)	861 (97%)	22 (2%)	1 (0%)	51	75
1	B	884/915 (97%)	847 (96%)	33 (4%)	4 (0%)	29	52
All	All	1768/1830 (97%)	1708 (97%)	55 (3%)	5 (0%)	41	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	269	LYS
1	B	682	ALA
1	B	148	GLY
1	B	509	VAL
1	A	656	GLY

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	753/777 (97%)	676 (90%)	77 (10%)	7	14
1	B	753/777 (97%)	690 (92%)	63 (8%)	11	21
All	All	1506/1554 (97%)	1366 (91%)	140 (9%)	9	17

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG

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Mol	Chain	Res	Type
1	A	30	GLU
1	A	63	ARG
1	A	66	VAL
1	A	74	ILE
1	A	80	LEU
1	A	104	THR
1	A	125	SER
1	A	127	LYS
1	A	193	GLU
1	A	198	LEU
1	A	206	LEU
1	A	209	LEU
1	A	211	LEU
1	A	213	ARG
1	A	240	LEU
1	A	246	ARG
1	A	258	VAL
1	A	269	LYS
1	A	282	ARG
1	A	292	THR
1	A	306	THR
1	A	310	SER
1	A	313	VAL
1	A	316	THR
1	A	321	SER
1	A	326	VAL
1	A	329	LEU
1	A	353	GLN
1	A	390	GLU
1	A	392	ARG
1	A	404	LYS
1	A	405	VAL
1	A	411	LEU
1	A	414	VAL
1	A	425	ARG
1	A	441	ARG
1	A	457	MET
1	A	477	TRP
1	A	480	TRP
1	A	481	LEU
1	A	515	GLN
1	A	543	ARG

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Mol	Chain	Res	Type
1	A	555	VAL
1	A	563	HIS
1	A	574	THR
1	A	582	VAL
1	A	591	THR
1	A	592	VAL
1	A	593	MET
1	A	602	ARG
1	A	604	SER
1	A	622	LEU
1	A	635	GLN
1	A	642	ARG
1	A	644	ASN
1	A	645	LYS
1	A	650	THR
1	A	659	ARG
1	A	681	THR
1	A	694	LYS
1	A	756	THR
1	A	778	ARG
1	A	790	VAL
1	A	791	ASP
1	A	815	LEU
1	A	817	VAL
1	A	829	MET
1	A	836	THR
1	A	855	LEU
1	A	859	ARG
1	A	860	SER
1	A	861	ARG
1	A	882	GLU
1	A	891	LEU
1	A	892	ARG
1	A	893	ARG
1	B	7	THR
1	B	33	ILE
1	B	80	LEU
1	B	141	ASP
1	B	170	ASP
1	B	193	GLU
1	B	198	LEU
1	B	201	ARG

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Mol	Chain	Res	Type
1	B	206	LEU
1	B	209	LEU
1	B	213	ARG
1	B	222	VAL
1	B	240	LEU
1	B	247	THR
1	B	258	VAL
1	B	267	VAL
1	B	292	THR
1	B	306	THR
1	B	323	VAL
1	B	326	VAL
1	B	329	LEU
1	B	340	VAL
1	B	392	ARG
1	B	406	ASN
1	B	408	ASN
1	B	411	LEU
1	B	417	GLU
1	B	438	ASP
1	B	457	MET
1	B	477	TRP
1	B	480	TRP
1	B	481	LEU
1	B	503	GLU
1	B	543	ARG
1	B	551	ASN
1	B	555	VAL
1	B	574	THR
1	B	582	VAL
1	B	591	THR
1	B	592	VAL
1	B	593	MET
1	B	622	LEU
1	B	635	GLN
1	B	637	LEU
1	B	644	ASN
1	B	659	ARG
1	B	692	VAL
1	B	738	GLU
1	B	756	THR
1	B	769	LEU

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Mol	Chain	Res	Type
1	B	778	ARG
1	B	790	VAL
1	B	791	ASP
1	B	793	VAL
1	B	810	THR
1	B	815	LEU
1	B	816	GLN
1	B	827	GLU
1	B	839	THR
1	B	855	LEU
1	B	859	ARG
1	B	861	ARG
1	B	892	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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
3	SO4	A	1011	-	4,4,4	0.25	0	6,6,6	0.24	0
2	SAH	A	1001	-	23,28,28	1.35	3 (13%)	22,40,40	2.01	4 (18%)
3	SO4	A	1010	-	4,4,4	0.22	0	6,6,6	0.33	0
3	SO4	B	1006	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	A	1002	-	4,4,4	0.25	0	6,6,6	0.12	0
3	SO4	A	1008	-	4,4,4	0.24	0	6,6,6	0.46	0
3	SO4	A	1005	-	4,4,4	0.24	0	6,6,6	0.18	0
3	SO4	A	1007	-	4,4,4	0.28	0	6,6,6	0.33	0
2	SAH	B	1001	-	23,28,28	1.32	3 (13%)	22,40,40	2.17	4 (18%)
3	SO4	B	1003	-	4,4,4	0.22	0	6,6,6	0.23	0
3	SO4	A	1009	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	B	1002	-	4,4,4	0.32	0	6,6,6	0.25	0
3	SO4	B	1005	-	4,4,4	0.31	0	6,6,6	0.30	0
3	SO4	B	1007	-	4,4,4	0.28	0	6,6,6	0.40	0
3	SO4	A	1004	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	B	1009	-	4,4,4	0.26	0	6,6,6	0.25	0
3	SO4	B	1004	-	4,4,4	0.28	0	6,6,6	0.12	0
3	SO4	A	1003	-	4,4,4	0.33	0	6,6,6	0.26	0
3	SO4	A	1006	-	4,4,4	0.32	0	6,6,6	0.42	0
3	SO4	B	1008	-	4,4,4	0.21	0	6,6,6	0.16	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
2	SAH	B	1001	-	-	1/11/31/31	0/3/3/3
2	SAH	A	1001	-	-	1/11/31/31	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	SAH	C2-N3	4.48	1.39	1.32
2	B	1001	SAH	C2-N3	4.01	1.38	1.32
2	B	1001	SAH	C2-N1	3.18	1.39	1.33
2	A	1001	SAH	C2-N1	2.94	1.39	1.33
2	A	1001	SAH	OXT-C	-2.25	1.23	1.30
2	B	1001	SAH	OXT-C	-2.20	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	SAH	N3-C2-N1	-6.06	120.45	128.67
2	A	1001	SAH	N3-C2-N1	-5.84	120.75	128.67
2	B	1001	SAH	O4'-C1'-N9	4.99	115.36	108.75
2	B	1001	SAH	C5'-SD-CG	-4.61	88.57	102.26
2	A	1001	SAH	C5'-SD-CG	-4.43	89.10	102.26
2	A	1001	SAH	O4'-C1'-N9	3.20	112.98	108.75
2	A	1001	SAH	OXT-C-O	-3.04	117.19	124.08
2	B	1001	SAH	OXT-C-O	-2.68	118.01	124.08

There are no chirality outliers.

All (2) torsion outliers are listed below:

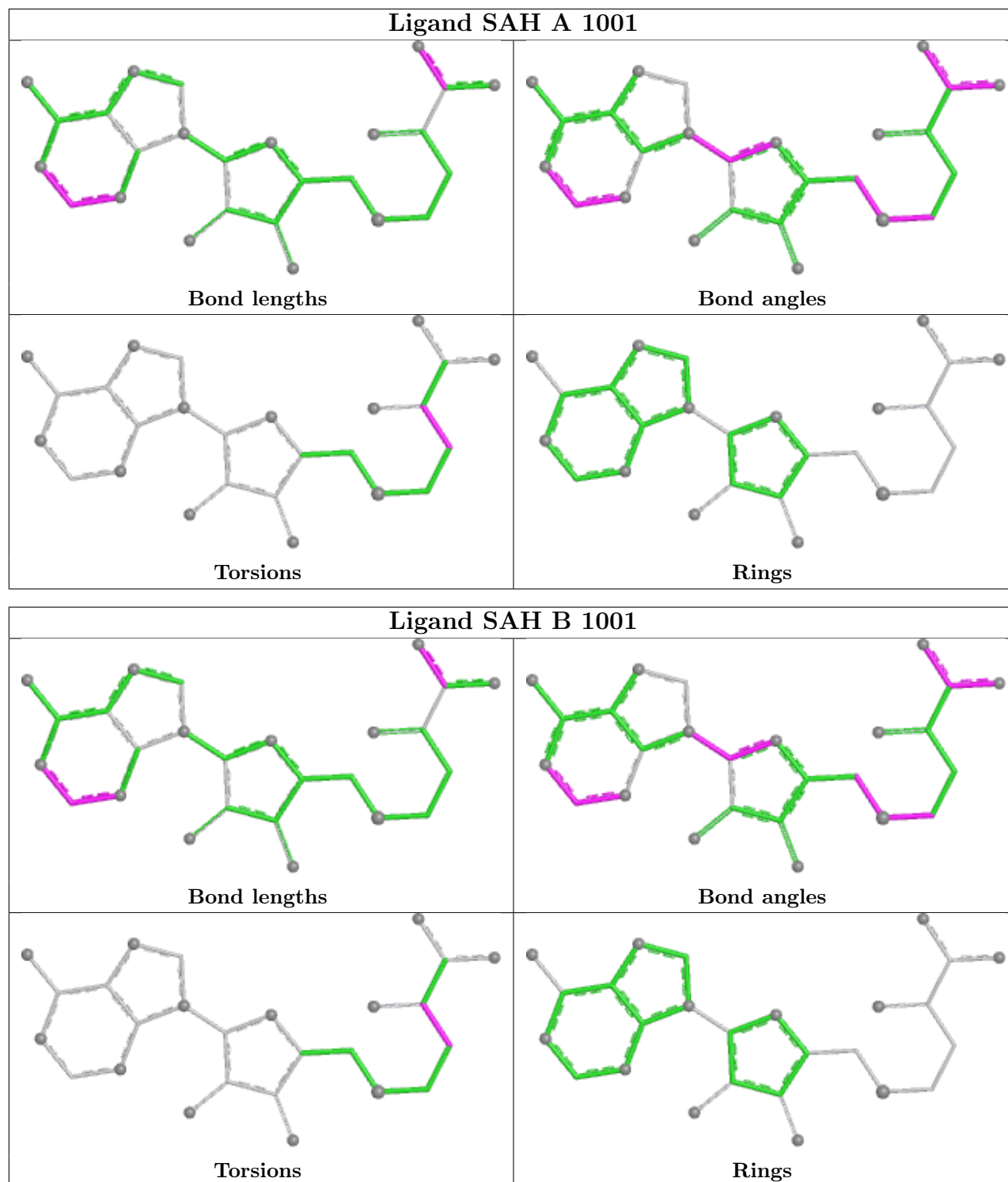
Mol	Chain	Res	Type	Atoms
2	B	1001	SAH	C-CA-CB-CG
2	A	1001	SAH	C-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	SAH	1	0
2	B	1001	SAH	1	0
3	B	1005	SO4	1	0
3	A	1003	SO4	1	0
3	A	1006	SO4	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	888/915 (97%)	-0.14	10 (1%) 80 78	39, 55, 79, 114	0
1	B	888/915 (97%)	-0.18	8 (0%) 84 82	37, 55, 83, 115	0
All	All	1776/1830 (97%)	-0.16	18 (1%) 82 80	37, 55, 81, 115	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	GLY	4.7
1	B	274	SER	4.3
1	B	275	ASN	3.2
1	B	250	ARG	3.1
1	A	248	VAL	2.8
1	A	269	LYS	2.7
1	A	881	LYS	2.5
1	A	245	ASP	2.5
1	A	275	ASN	2.4
1	A	791	ASP	2.4
1	B	431	PRO	2.4
1	B	881	LYS	2.3
1	B	248	VAL	2.2
1	A	895	GLU	2.2
1	B	269	LYS	2.2
1	A	880	GLY	2.1
1	A	643	LYS	2.1
1	B	247	THR	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

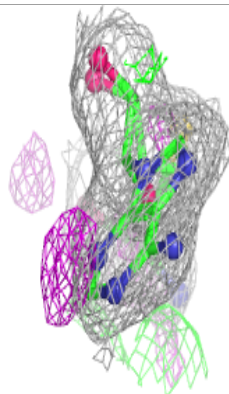
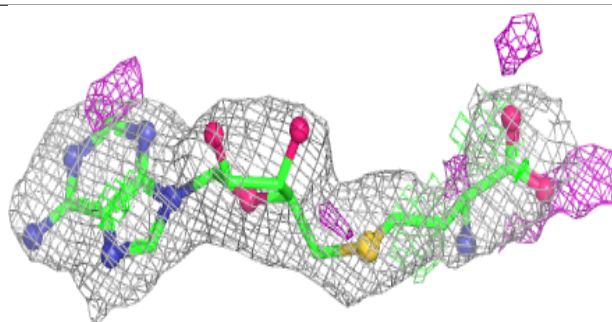
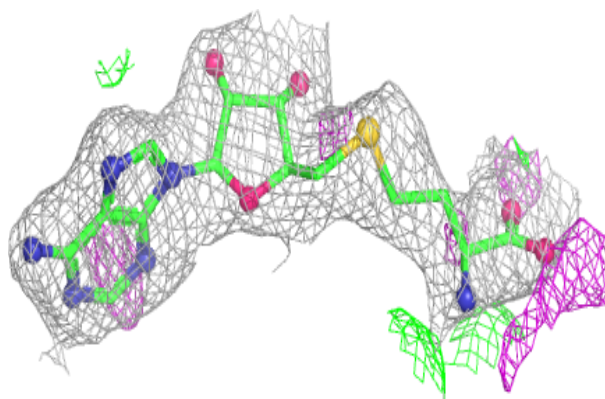
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	1005	5/5	0.77	0.31	64,74,86,87	5
3	SO4	A	1003	5/5	0.83	0.21	59,66,74,74	5
3	SO4	A	1011	5/5	0.85	0.26	64,65,72,74	5
3	SO4	B	1004	5/5	0.89	0.26	69,74,83,88	5
3	SO4	B	1002	5/5	0.90	0.15	56,65,70,72	5
3	SO4	B	1009	5/5	0.90	0.20	55,57,67,68	5
3	SO4	B	1005	5/5	0.92	0.16	50,53,71,73	5
3	SO4	B	1007	5/5	0.93	0.22	51,52,61,64	5
3	SO4	A	1009	5/5	0.94	0.18	62,67,69,77	5
3	SO4	A	1010	5/5	0.94	0.12	62,62,73,83	5
2	SAH	A	1001	26/26	0.94	0.18	47,60,67,89	0
3	SO4	A	1006	5/5	0.94	0.16	50,56,72,79	5
3	SO4	A	1008	5/5	0.95	0.22	59,63,70,71	0
3	SO4	A	1002	5/5	0.96	0.18	61,62,70,70	5
3	SO4	B	1006	5/5	0.96	0.09	66,68,78,78	5
2	SAH	B	1001	26/26	0.96	0.14	44,54,62,77	0
3	SO4	A	1007	5/5	0.96	0.15	42,44,50,55	5
3	SO4	B	1008	5/5	0.97	0.23	62,63,72,73	5
4	ZN	B	1010	1/1	0.98	0.04	74,74,74,74	0
3	SO4	B	1003	5/5	0.99	0.13	60,61,61,62	0
4	ZN	A	1013	1/1	0.99	0.06	89,89,89,89	0
3	SO4	A	1004	5/5	0.99	0.17	49,54,58,59	0
4	ZN	B	1011	1/1	0.99	0.12	70,70,70,70	0
4	ZN	A	1012	1/1	1.00	0.17	45,45,45,45	0

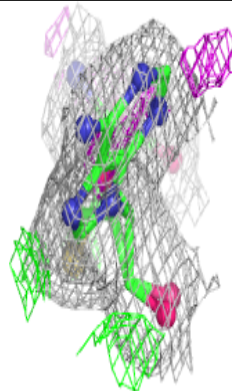
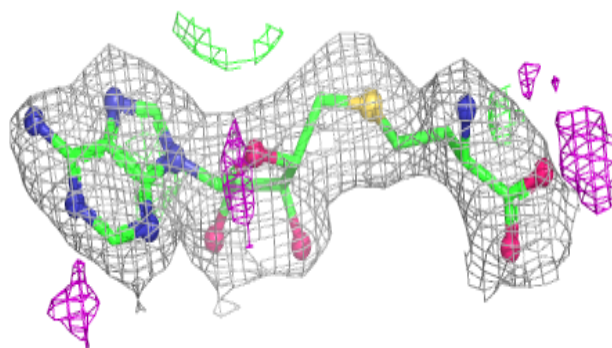
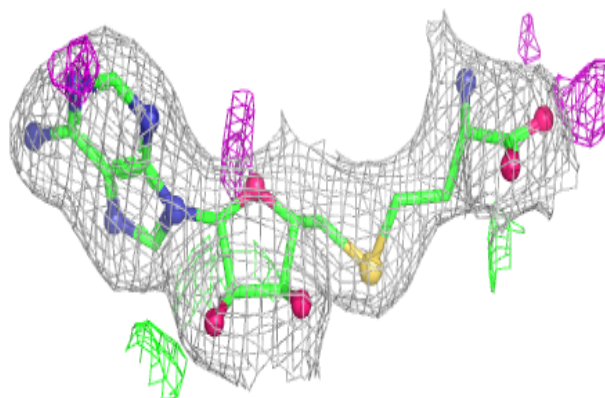
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH A 1001:

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

**Electron density around SAH B 1001:**

$2mF_o-DF_c$ (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.