



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2026 – 01:17 pm BST

PDB ID : 9SXD / pdb_00009sxd
Title : Basic membrane protein D in complex with a nucleoside analog
Authors : Airenne, T.T.; Brunell, J.; Huhtala, M.; Salminen, T.A.
Deposited on : 2025-10-09
Resolution : 2.00 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 Phenix2.2
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.2
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

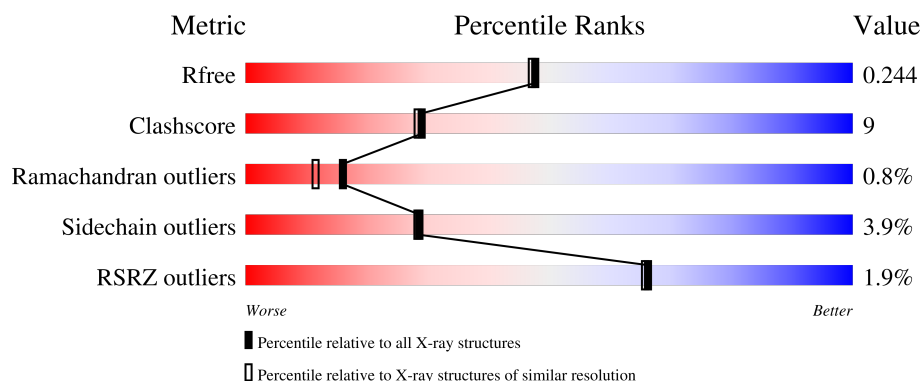
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	321	
1	B	321	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10018 atoms, of which 4896 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.

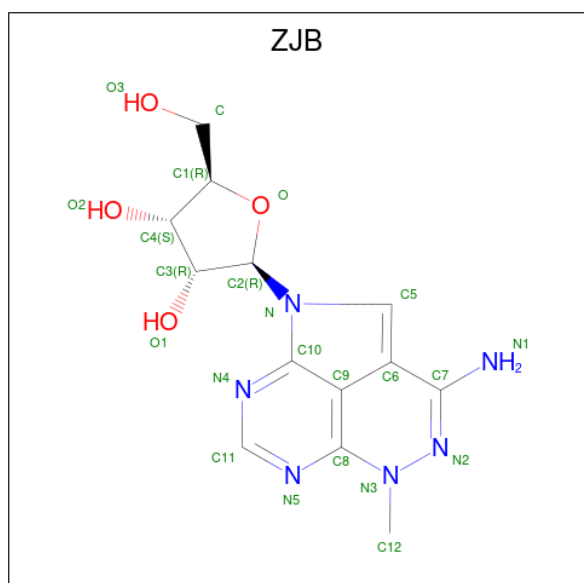
- Molecule 1 is a protein called Basic membrane protein D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	314	Total	C	H	N	O	S	57	1	0
			4820	1536	2416	392	470	6			
1	B	313	Total	C	H	N	O	S	57	3	0
			4828	1537	2424	393	468	6			

There are 4 discrepancies between the modelled and reference sequences:

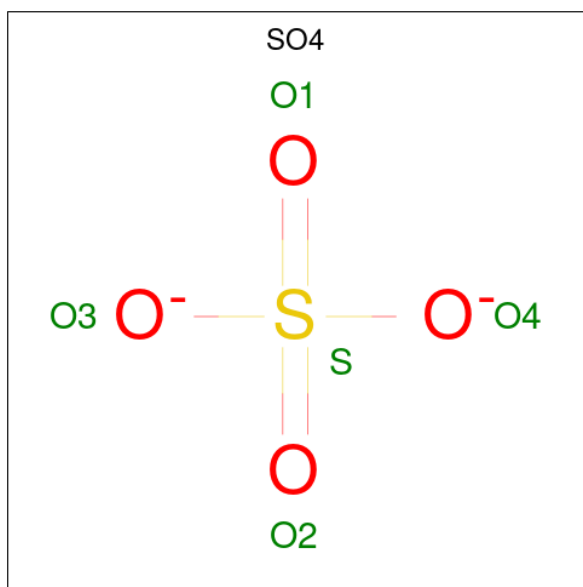
Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	-	expression tag	UNP P0CL55
A	6	PRO	-	expression tag	UNP P0CL55
B	5	GLY	-	expression tag	UNP P0CL55
B	6	PRO	-	expression tag	UNP P0CL55

- Molecule 2 is (2R,3R,4S,5R)-2-(3-AMINO-5-METHYL-1,4,5,6,8-PENTAAZAACENAPH THYLEN-1(5H)-YL)-5-(HYDROXYMETHYL)TETRAHYDROFURAN-3,4-DIOL (CCD ID: ZJB) (formula: C₁₃H₁₆N₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	6	0
			39	13	16	6	4		
2	B	1	Total	C	H	N	O	6	0
			39	13	16	6	4		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

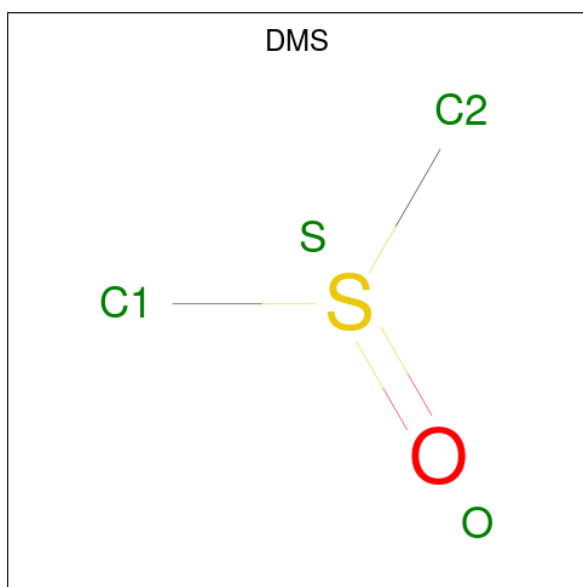


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Cl	0	0
			5	5		
4	B	2	Total	Cl	0	0
			2	2		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

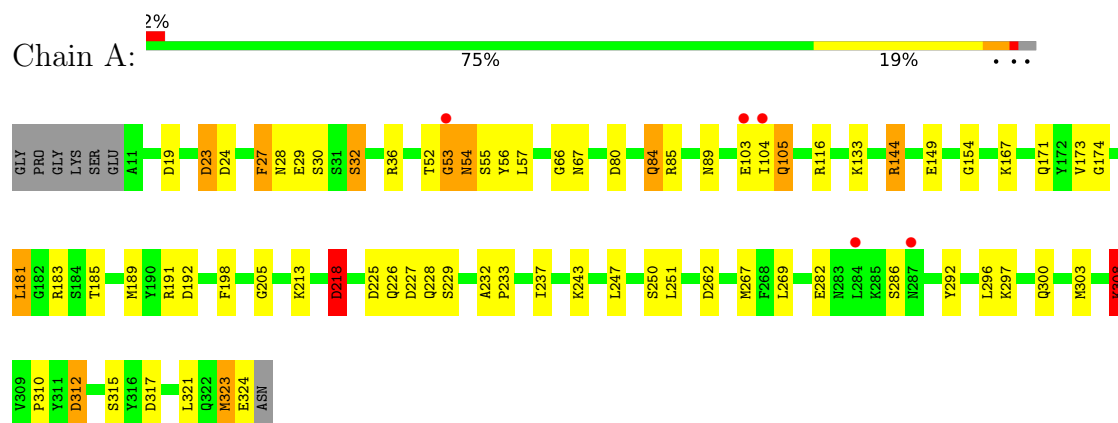
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	125	Total	O	0	0
			125	125		
6	B	105	Total	O	0	0
			105	105		

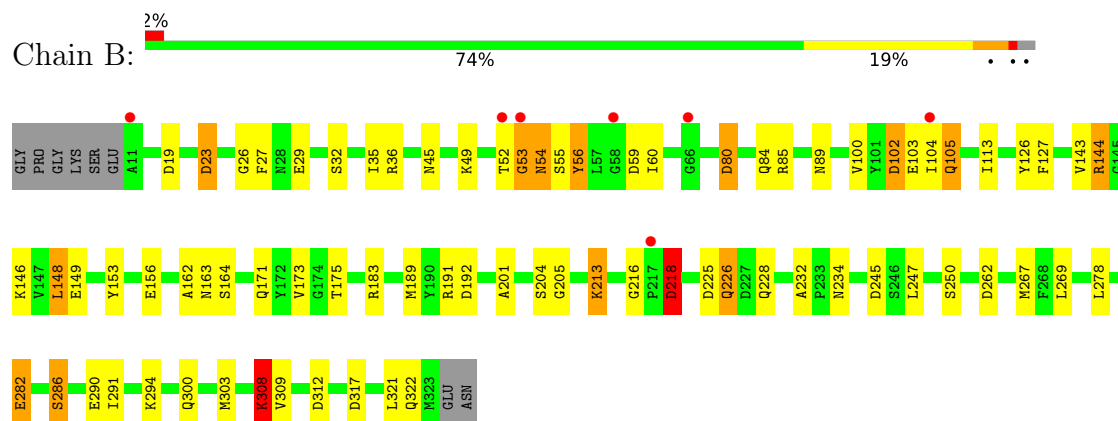
3 Residue-property plots

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: Basic membrane protein D



• Molecule 1: Basic membrane protein D



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.57Å 57.43Å 67.16Å 90.80° 108.44° 102.37°	Depositor
Resolution (Å)	19.86 – 2.00 19.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.86-2.00) 99.5 (19.86-2.00)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.187 , 0.243 0.188 , 0.244	Depositor DCC
R_{free} test set	2031 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.52 , 72.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10018	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.74% 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, ZJB, DMS

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	1.00	2/2444 (0.1%)	1.58	27/3292 (0.8%)
1	B	0.99	0/2452	1.54	27/3302 (0.8%)
All	All	1.00	2/4896 (0.0%)	1.56	54/6594 (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	3
1	B	0	4
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	SER	CA-CB	-5.82	1.44	1.53
1	A	174	GLY	C-O	-5.48	1.17	1.24

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	ASP	CA-CB-CG	-8.46	104.14	112.60
1	A	192	ASP	CA-CB-CG	8.19	120.79	112.60
1	B	312	ASP	CA-CB-CG	8.06	120.66	112.60
1	A	218	ASP	CB-CA-C	-8.02	98.22	111.13
1	B	144	ARG	NE-CZ-NH2	7.67	126.10	119.20
1	B	163	ASN	CB-CA-C	-7.07	100.96	110.79
1	A	218	ASP	CA-CB-CG	-7.04	105.56	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ARG	NE-CZ-NH1	-6.97	114.53	121.50
1	B	262	ASP	CA-CB-CG	6.78	119.38	112.60
1	B	218	ASP	CB-CA-C	-6.72	100.20	111.02
1	B	192	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	267	MET	CB-CA-C	-6.63	98.93	109.80
1	B	156	GLU	CG-CD-OE2	-6.57	103.29	118.40
1	A	144	ARG	NE-CZ-NH1	-6.56	114.94	121.50
1	A	308	LYS	CA-C-N	-6.51	116.27	123.43
1	A	308	LYS	C-N-CA	-6.51	116.27	123.43
1	A	89	ASN	CB-CA-C	-6.42	102.02	112.03
1	A	251	LEU	N-CA-CB	6.31	119.50	110.16
1	B	89	ASN	CB-CA-C	-6.24	102.29	112.03
1	B	282	GLU	CB-CG-CD	6.23	123.19	112.60
1	A	144	ARG	CG-CD-NE	-6.17	98.41	112.00
1	A	23	ASP	CA-CB-CG	-6.14	106.46	112.60
1	B	309	VAL	O-C-N	-6.07	116.72	121.46
1	A	262	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	323	MET	CB-CA-C	-5.99	103.43	111.88
1	B	80	ASP	CA-CB-CG	5.95	118.55	112.60
1	B	23	ASP	CA-CB-CG	-5.93	106.67	112.60
1	A	228	GLN	N-CA-CB	-5.83	102.01	110.70
1	A	144	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	A	312	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	27	PHE	N-CA-CB	-5.76	101.50	109.91
1	B	144	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	B	45	ASN	CB-CA-C	5.53	118.88	109.53
1	A	154	GLY	CA-C-N	5.53	127.63	120.44
1	A	154	GLY	C-N-CA	5.53	127.63	120.44
1	B	56	TYR	N-CA-CB	5.52	118.34	110.06
1	A	233	PRO	CB-CA-C	-5.49	104.05	111.85
1	A	181	LEU	CB-CG-CD2	-5.47	94.28	110.70
1	B	308	LYS	CA-C-N	-5.46	117.34	123.02
1	B	308	LYS	C-N-CA	-5.46	117.34	123.02
1	B	27	PHE	N-CA-CB	-5.41	101.59	109.82
1	B	85	ARG	N-CA-CB	5.37	117.79	110.01
1	B	228	GLN	N-CA-CB	-5.33	103.20	110.56
1	B	317	ASP	CA-C-N	5.21	127.27	120.28
1	B	317	ASP	C-N-CA	5.21	127.27	120.28
1	B	245	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	102	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	234	ASN	CB-CA-C	-5.17	100.66	109.65
1	B	213	LYS	CB-CA-C	-5.05	100.97	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ASP	CA-C-N	5.04	127.03	120.28
1	A	317	ASP	C-N-CA	5.04	127.03	120.28
1	A	243	LYS	N-CA-CB	-5.03	104.11	110.45
1	A	133	LYS	CB-CA-C	5.02	119.59	110.11
1	A	198	PHE	CA-CB-CG	5.01	118.81	113.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	GLN	Peptide
1	A	183	ARG	Sidechain
1	A	191	ARG	Sidechain
1	B	105	GLN	Peptide
1	B	183	ARG	Sidechain
1	B	191	ARG	Sidechain
1	B	216	GLY	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	2404	2416	2414	41	0
1	B	2404	2424	2410	43	0
2	A	23	16	0	1	0
2	B	23	16	0	1	0
3	A	5	0	0	1	0
3	B	10	0	0	0	0
4	A	5	0	0	0	0
4	B	2	0	0	1	0
5	A	4	6	6	0	0
5	B	12	18	18	3	0
6	A	125	0	0	5	1
6	B	105	0	0	9	1
All	All	5122	4896	4848	85	1

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 9.

All (85) 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:B:218:ASP:OD1	1:B:218:ASP:N	1.92	1.02
1:B:143:VAL:O	1:B:148:LEU:HD23	1.60	1.00
1:A:218:ASP:OD1	1:A:218:ASP:N	1.97	0.92
1:A:282:GLU:OE2	6:A:501:HOH:O	1.95	0.83
1:B:143:VAL:O	1:B:148:LEU:CD2	2.31	0.79
1:A:171:GLN:HG3	1:A:189:MET:CE	2.20	0.71
1:B:322:GLN:O	6:B:501:HOH:O	2.09	0.71
1:B:23:ASP:OD1	1:B:29:GLU:OE1	2.08	0.70
1:A:36:ARG:NH2	6:A:502:HOH:O	2.25	0.69
1:A:32:SER:O	1:A:36:ARG:HG3	1.97	0.65
1:A:52:THR:HG22	1:A:53:GLY:O	1.98	0.63
1:B:113:ILE:HG21	1:B:247:LEU:HD21	1.81	0.63
1:A:19:ASP:OD1	1:A:56:TYR:OH	2.12	0.63
4:B:405:CL:CL	6:B:561:HOH:O	2.53	0.62
1:A:171:GLN:CG	1:A:189:MET:CE	2.78	0.61
1:B:19:ASP:OD1	1:B:56:TYR:OH	2.15	0.59
1:B:113:ILE:HG21	1:B:247:LEU:CD2	2.33	0.59
1:B:32:SER:O	1:B:36:ARG:HG3	2.04	0.57
1:B:100:VAL:HG22	5:B:407:DMS:H13	1.86	0.56
1:A:213:LYS:HE2	1:A:232:ALA:HB2	1.87	0.56
1:A:225:ASP:OD1	2:A:401:ZJB:O2	2.24	0.56
1:A:323:MET:O	1:A:324:GLU:CG	2.53	0.56
1:A:323:MET:O	1:A:324:GLU:HG3	2.06	0.55
1:B:267:MET:HE2	1:B:269:LEU:HD21	1.88	0.54
1:B:300:GLN:HG2	1:B:303:MET:CE	2.37	0.54
1:A:171:GLN:CG	1:A:189:MET:HE2	2.38	0.53
1:B:201:ALA:O	1:B:204:SER:HB2	2.07	0.53
1:A:171:GLN:HG3	1:A:189:MET:HE2	1.89	0.52
1:B:104:ILE:HG22	1:B:105:GLN:H	1.74	0.52
1:A:205:GLY:HA3	6:A:528:HOH:O	2.10	0.52
1:A:300:GLN:HG2	1:A:303:MET:CE	2.40	0.52
1:B:171:GLN:HG3	1:B:189:MET:HE3	1.92	0.51
1:B:103:GLU:CA	6:B:505:HOH:O	2.58	0.51
1:B:49:LYS:NZ	6:B:507:HOH:O	2.43	0.51
1:B:286:SER:OG	6:B:502:HOH:O	2.18	0.51
1:A:144:ARG:NH2	6:A:504:HOH:O	2.43	0.50
1:B:205:GLY:HA3	6:B:543:HOH:O	2.10	0.50
1:A:80:ASP:O	1:A:84:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLN:HG3	1:A:189:MET:HE3	1.91	0.50
1:B:300:GLN:HG2	1:B:303:MET:HE3	1.94	0.50
1:B:278:LEU:H	5:B:408:DMS:H21	1.77	0.49
1:A:149:GLU:OE2	1:A:312:ASP:HB2	2.11	0.49
1:A:269:LEU:HD12	1:A:269:LEU:N	2.27	0.49
1:A:292:TYR:CE2	1:A:296:LEU:HD11	2.47	0.49
1:B:52:THR:HG22	1:B:53:GLY:O	2.13	0.48
1:A:23:ASP:OD1	1:A:29:GLU:OE2	2.32	0.48
1:A:104:ILE:HG22	1:A:105:GLN:H	1.78	0.48
1:A:104:ILE:HG22	1:A:105:GLN:N	2.30	0.47
1:B:126:TYR:CD2	1:B:162:ALA:HB2	2.50	0.47
1:B:102:ASP:O	1:B:103:GLU:HB2	2.13	0.47
1:B:308:LYS:HD2	1:B:308:LYS:HA	1.76	0.46
1:B:282:GLU:H	1:B:282:GLU:HG3	1.48	0.46
1:B:144:ARG:NH2	6:B:508:HOH:O	2.44	0.46
1:B:173:VAL:HG12	1:B:175:THR:HG22	1.98	0.46
1:B:225:ASP:OD1	2:B:401:ZJB:O2	2.33	0.46
1:A:24:ASP:OD2	1:A:28:ASN:HB2	2.17	0.45
1:B:300:GLN:HA	1:B:303:MET:HE3	1.99	0.45
1:A:167:LYS:HA	3:A:402:SO4:O2	2.17	0.45
1:A:300:GLN:HG2	1:A:303:MET:HE3	1.99	0.44
1:B:103:GLU:N	6:B:505:HOH:O	2.36	0.44
1:A:173:VAL:HG13	1:A:181:LEU:HG	1.99	0.44
1:A:237:ILE:O	1:A:237:ILE:HG22	2.17	0.44
1:B:213:LYS:HE2	1:B:232:ALA:HB2	1.98	0.44
1:A:185:THR:O	1:A:189:MET:HG3	2.17	0.43
1:A:247:LEU:HD13	1:A:269:LEU:HD21	2.00	0.43
1:B:103:GLU:HA	6:B:505:HOH:O	2.18	0.43
1:B:127:PHE:CD2	1:B:291:ILE:HG22	2.53	0.43
1:A:53:GLY:O	1:A:54:ASN:HB2	2.19	0.43
1:A:297:LYS:HD3	6:A:522:HOH:O	2.19	0.43
1:B:171:GLN:CG	1:B:189:MET:HE3	2.49	0.43
1:A:27:PHE:O	1:A:30[A]:SER:HB2	2.20	0.42
1:B:146:LYS:HZ1	5:B:407:DMS:H23	1.84	0.42
1:A:57:LEU:HD11	1:A:85:ARG:NH1	2.34	0.42
1:B:149:GLU:HG3	1:B:153:TYR:CE2	2.55	0.41
1:A:104:ILE:C	1:A:105:GLN:HG3	2.45	0.41
1:A:308:LYS:HD2	1:A:308:LYS:HA	1.70	0.41
1:B:104:ILE:C	1:B:105:GLN:HG3	2.45	0.41
1:B:26:GLY:HA2	1:B:226:GLN:HG3	2.03	0.41
1:A:66:GLY:O	1:A:67:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:GLY:O	1:B:54:ASN:HB2	2.21	0.41
1:B:290:GLU:OE2	1:B:294:LYS:HE2	2.21	0.41
1:B:104:ILE:HG22	1:B:105:GLN:N	2.36	0.41
1:A:227:ASP:OD1	1:A:229:SER:OG	2.36	0.40
1:B:59:ASP:O	1:B:60:ILE:C	2.62	0.40
1:A:310:PRO:HB3	1:A:315:SER:C	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:581:HOH:O	6:B:575:HOH:O[1_455]	2.15	0.05

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	313/321 (98%)	296 (95%)	14 (4%)	3 (1%)	12	8
1	B	314/321 (98%)	297 (95%)	15 (5%)	2 (1%)	21	17
All	All	627/642 (98%)	593 (95%)	29 (5%)	5 (1%)	16	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	B	54	ASN
1	A	103	GLU
1	B	53	GLY
1	A	53	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	258/262 (98%)	250 (97%)	8 (3%)	35	37
1	B	259/262 (99%)	246 (95%)	13 (5%)	22	20
All	All	517/524 (99%)	496 (96%)	21 (4%)	28	26

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	SER
1	A	84	GLN
1	A	218	ASP
1	A	226	GLN
1	A	250	SER
1	A	286	SER
1	A	308	LYS
1	A	321	LEU
1	B	35	ILE
1	B	55	SER
1	B	80	ASP
1	B	84	GLN
1	B	148	LEU
1	B	164	SER
1	B	218	ASP
1	B	226	GLN
1	B	250[A]	SER
1	B	250[B]	SER
1	B	286	SER
1	B	308	LYS
1	B	321	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN

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Mol	Chain	Res	Type
1	A	62	ASN
1	A	84	GLN
1	A	89	ASN
1	A	105	GLN
1	A	219	HIS
1	B	45	ASN
1	B	62	ASN
1	B	67	ASN
1	B	105	GLN
1	B	219	HIS

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 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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	ZJB	A	401	-	25,26,26	2.17	4 (16%)	32,40,40	3.05	10 (31%)
5	DMS	B	407	-	3,3,3	0.32	0	3,3,3	0.42	0
5	DMS	B	406	-	3,3,3	0.30	0	3,3,3	0.22	0
3	SO4	A	402	-	4,4,4	0.25	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	402	-	4,4,4	0.43	0	6,6,6	0.16	0
3	SO4	B	403	-	4,4,4	0.34	0	6,6,6	0.13	0
5	DMS	A	408	-	3,3,3	0.49	0	3,3,3	0.66	0
5	DMS	B	408	-	3,3,3	0.78	0	3,3,3	0.39	0
2	ZJB	B	401	-	25,26,26	2.23	5 (20%)	32,40,40	2.73	7 (21%)

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	ZJB	A	401	-	-	0/6/22/22	0/4/4/4
2	ZJB	B	401	-	-	0/6/22/22	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ZJB	C7-N2	6.69	1.37	1.30
2	B	401	ZJB	C9-C10	-6.14	1.33	1.40
2	A	401	ZJB	C7-N2	5.75	1.36	1.30
2	A	401	ZJB	C9-C10	-5.74	1.33	1.40
2	A	401	ZJB	C9-C6	-4.75	1.36	1.45
2	A	401	ZJB	C5-N	3.53	1.43	1.38
2	B	401	ZJB	C5-N	3.37	1.43	1.38
2	B	401	ZJB	C9-C6	-3.10	1.39	1.45
2	B	401	ZJB	C9-C8	-2.40	1.37	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ZJB	C10-C9-C8	9.23	123.56	114.93
2	B	401	ZJB	C10-C9-C8	9.02	123.37	114.93
2	A	401	ZJB	C10-C9-C6	8.79	113.88	107.17
2	B	401	ZJB	C10-C9-C6	8.12	113.36	107.17
2	A	401	ZJB	C9-C10-N4	-6.41	120.21	126.94
2	B	401	ZJB	C9-C10-N4	-6.12	120.52	126.94
2	A	401	ZJB	C10-N-C5	-4.04	106.36	108.09
2	A	401	ZJB	C12-N3-C8	3.71	123.67	120.15
2	A	401	ZJB	N5-C8-N3	3.52	123.95	117.29
2	B	401	ZJB	N5-C8-N3	3.14	123.22	117.29
2	B	401	ZJB	C10-N-C5	-2.90	106.85	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ZJB	N4-C10-N	2.84	131.76	127.08
2	A	401	ZJB	C3-C2-N	2.72	120.20	113.30
2	B	401	ZJB	N4-C10-N	2.57	131.32	127.08
2	A	401	ZJB	O2-C4-C1	2.57	118.47	111.05
2	B	401	ZJB	C9-C6-C5	-2.30	102.92	105.81
2	A	401	ZJB	C11-N5-C8	2.15	116.82	111.75

There are no chirality outliers.

There are no torsion outliers.

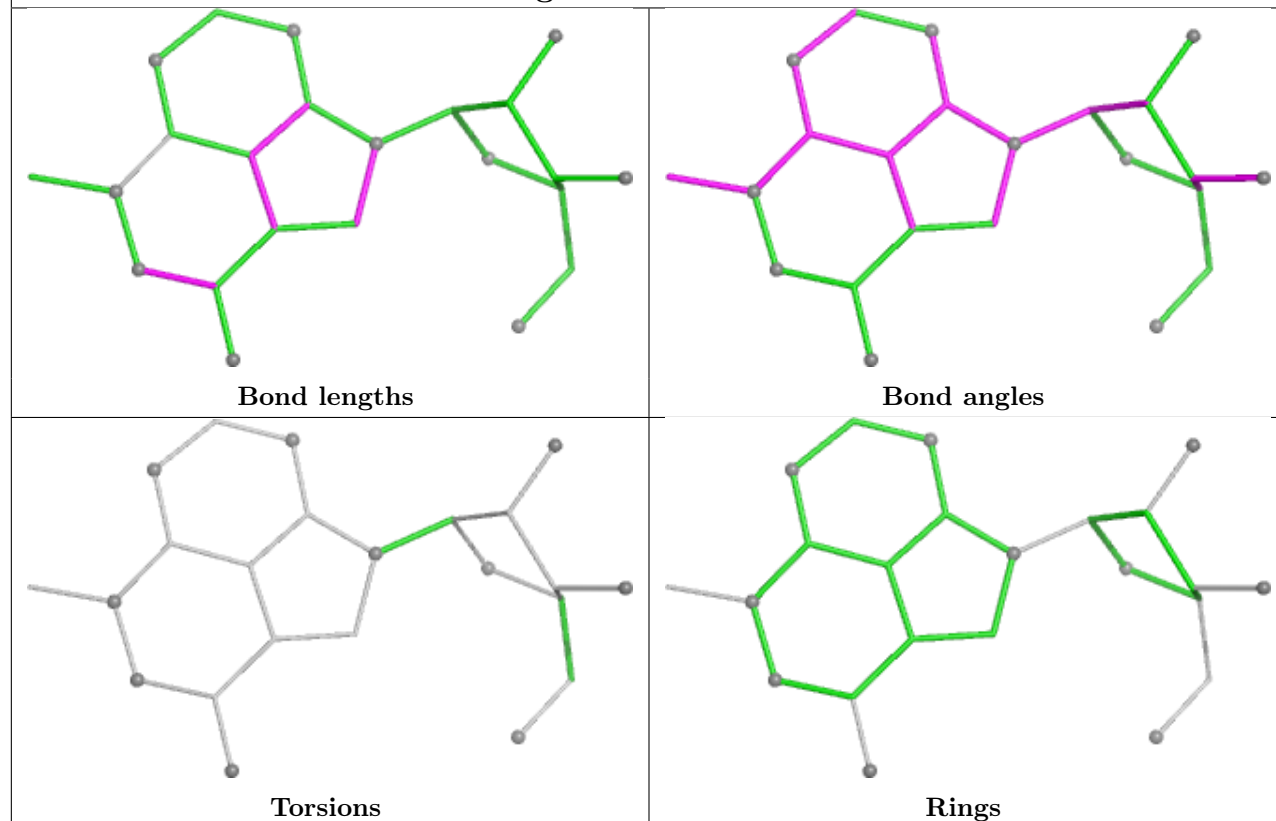
There are no ring outliers.

5 monomers are involved in 6 short contacts:

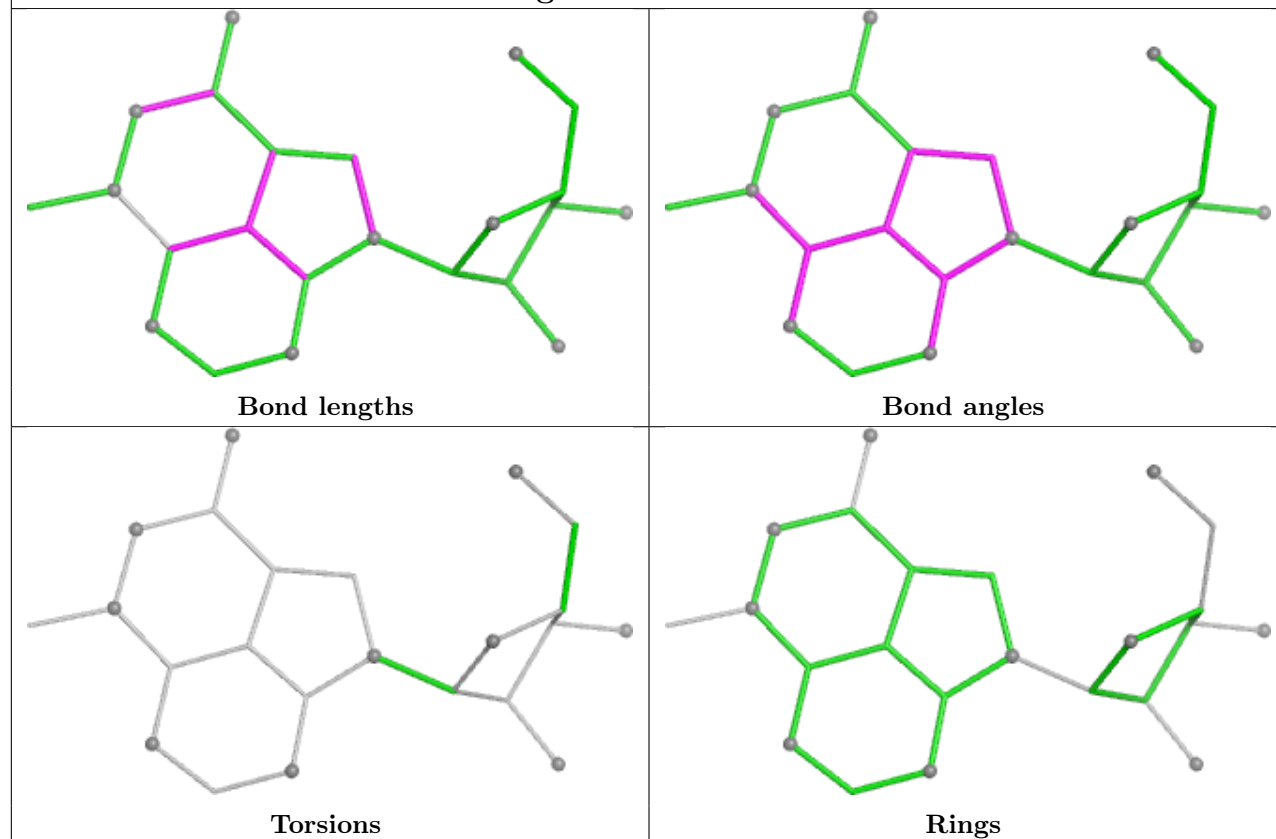
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ZJB	1	0
5	B	407	DMS	2	0
3	A	402	SO4	1	0
5	B	408	DMS	1	0
2	B	401	ZJB	1	0

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.

Ligand ZJB A 401



Ligand ZJB B 401



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	314/321 (97%)	-0.08	5 (1%) 70 70	13, 35, 64, 86	2 (0%)
1	B	313/321 (97%)	-0.04	7 (2%) 62 61	16, 36, 66, 82	3 (0%)
All	All	627/642 (97%)	-0.06	12 (1%) 66 66	13, 35, 65, 86	5 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	PRO	3.0
1	B	11	ALA	2.9
1	B	52	THR	2.9
1	A	53	GLY	2.6
1	B	53	GLY	2.6
1	A	287	ASN	2.5
1	B	104	ILE	2.2
1	A	103	GLU	2.1
1	A	104	ILE	2.1
1	A	284	LEU	2.1
1	B	58	GLY	2.0
1	B	66	GLY	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 ⓘ

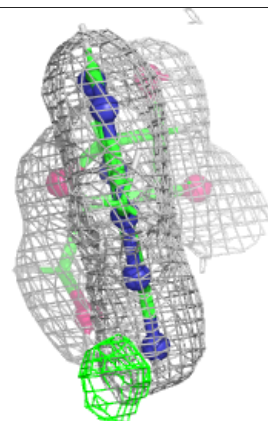
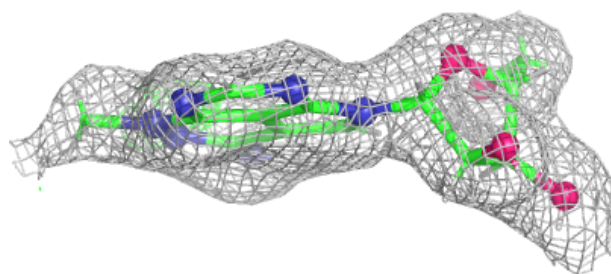
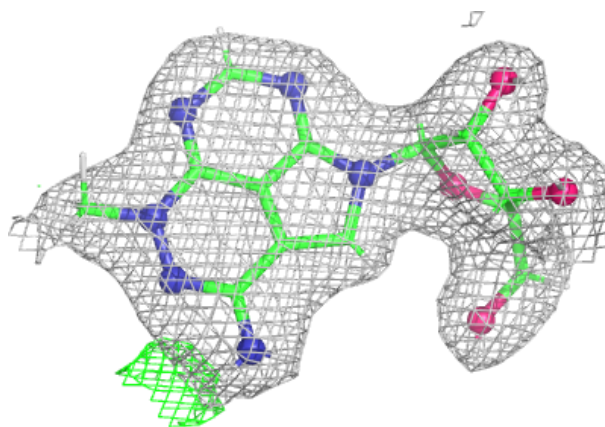
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DMS	B	408	4/4	0.65	0.18	48,54,58,72	0
5	DMS	A	408	4/4	0.79	0.15	52,61,62,74	0
5	DMS	B	406	4/4	0.88	0.13	51,56,80,82	0
3	SO4	B	403	5/5	0.89	0.09	50,69,74,86	0
4	CL	A	406	1/1	0.89	0.20	72,72,72,72	0
4	CL	B	405	1/1	0.89	0.14	67,67,67,67	0
5	DMS	B	407	4/4	0.90	0.10	54,59,61,69	0
3	SO4	A	402	5/5	0.91	0.12	45,51,54,56	0
4	CL	A	405	1/1	0.91	0.10	66,66,66,66	0
3	SO4	B	402	5/5	0.92	0.13	50,52,53,56	0
4	CL	A	407	1/1	0.94	0.16	65,65,65,65	0
4	CL	A	404	1/1	0.94	0.09	60,60,60,60	0
2	ZJB	A	401	23/23	0.95	0.05	21,27,30,30	6
2	ZJB	B	401	23/23	0.96	0.05	22,26,32,34	6
4	CL	A	403	1/1	0.97	0.05	27,27,27,27	0
4	CL	B	404	1/1	0.99	0.04	28,28,28,28	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.

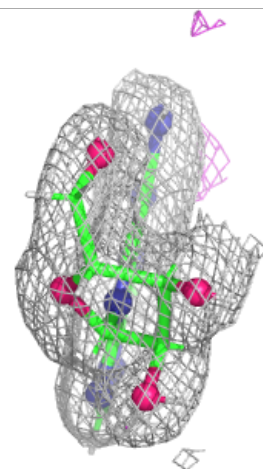
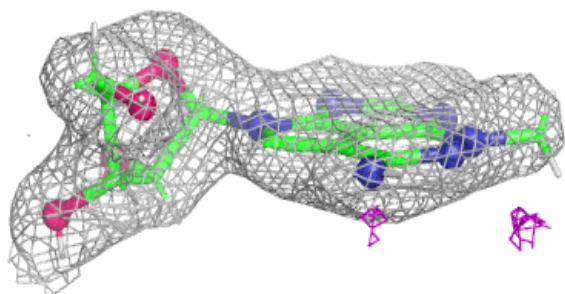
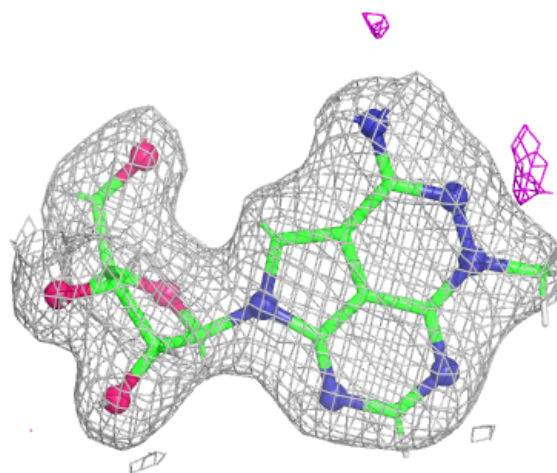
Electron density around ZJB A 401:

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



Electron density around ZJB B 401:

$2mF_o-DF_c$ (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.