



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 01:22 AM UTC

PDB ID : 7HK8 / pdb\_00007hk8  
Title : Crystal Structure of N-methylhydantoinase in complex with 1-methylimidazole-2,4-dione, C2221 form  
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Deposited on : 2024-10-10  
Resolution : 2.80 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](mailto: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>.

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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

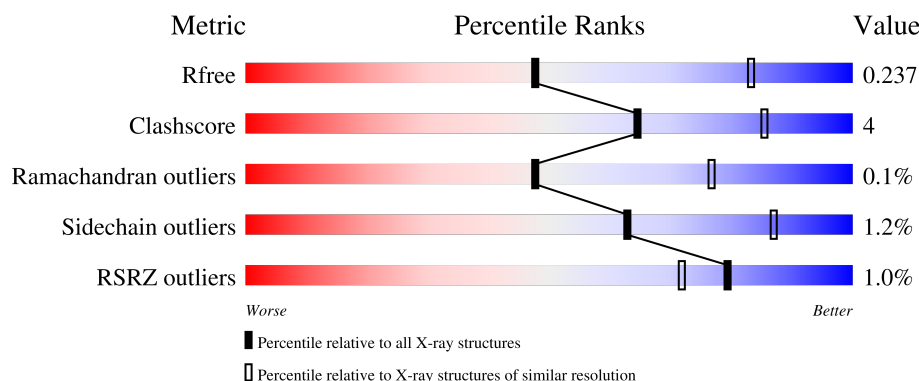
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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  $\geq 3$ , 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	1288	<div> <div></div> <div>91%</div> <div>9%</div> </div>
1	B	1288	<div> <div></div> <div>89%</div> <div>10%</div> </div>

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
5	MES	B	1306	-	-	X	-
6	SO4	A	1308	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 19901 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.

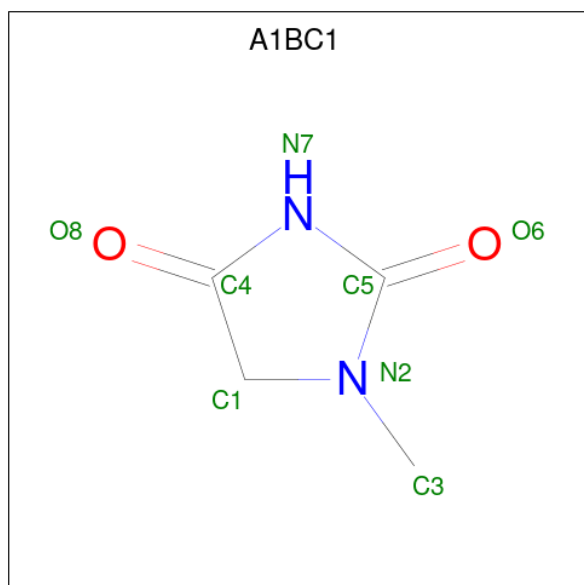
- Molecule 1 is a protein called N-methylhydantoinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1283	Total	C	N	O	S	0	0	0
			9810	6156	1697	1917	40			
1	B	1281	Total	C	N	O	S	0	0	0
			9795	6148	1695	1912	40			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

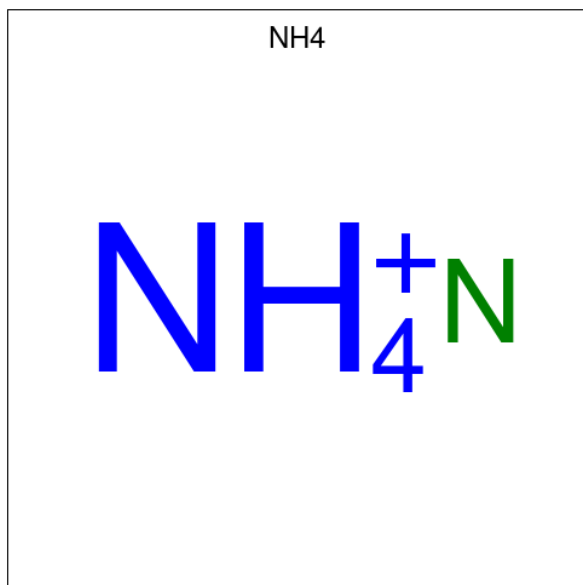
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 1-methylimidazolidine-2,4-dione (CCD ID: A1BC1) (formula: C<sub>4</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	2	2		
3	B	1	Total	C	N	O	0	0
			8	4	2	2		

- Molecule 4 is AMMONIUM ION (CCD ID: NH4) (formula:  $\text{H}_4\text{N}$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	N	0	0
			1	1		
4	B	1	Total	N	0	0
			1	1		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula:  $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

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

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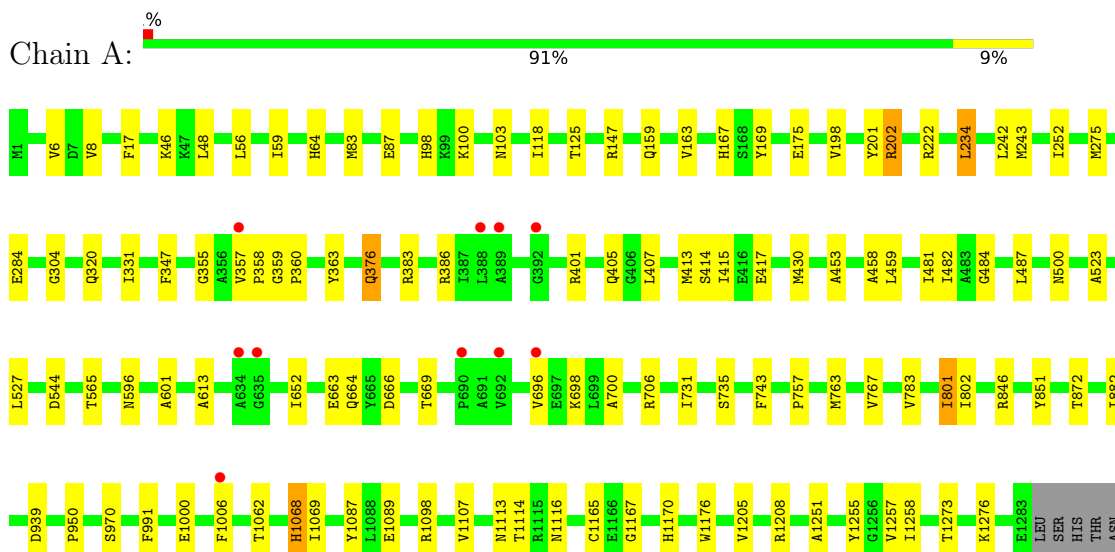
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

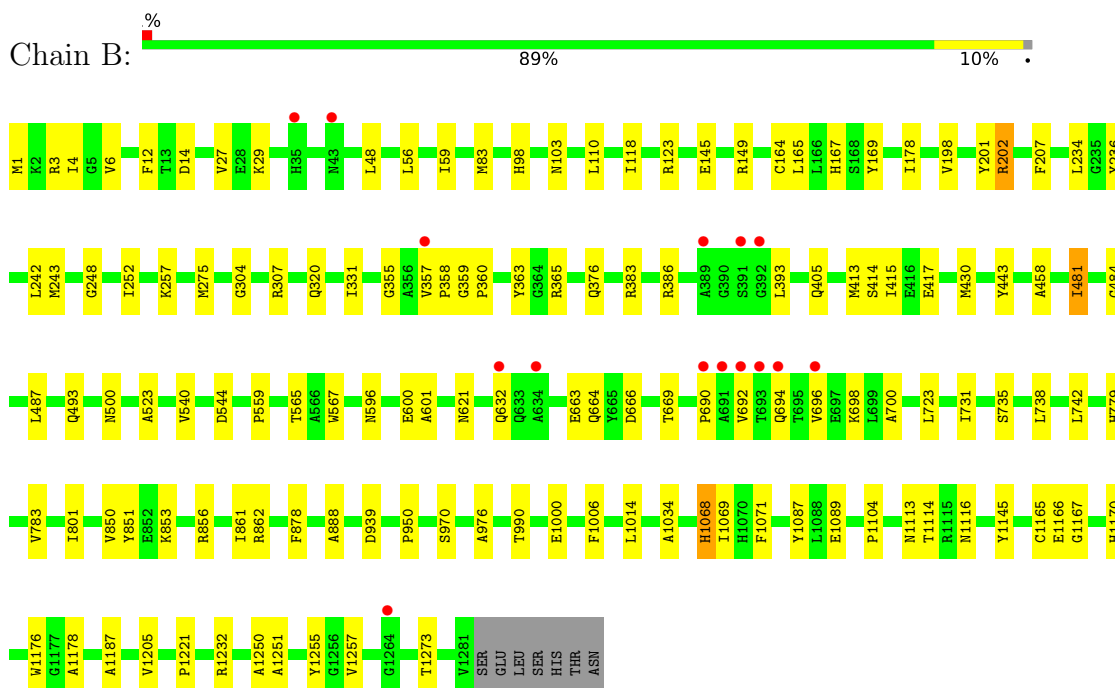
### 3 Residue-property plots [i](#)

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: N-methylhydantoinase



#### • Molecule 1: N-methylhydantoinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	257.41Å 265.92Å 120.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.20 – 2.80 45.20 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.20-2.80) 95.9 (45.20-2.80)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.192 , 0.231 0.198 , 0.237	Depositor DCC
$R_{free}$ test set	5136 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.8	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19901	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NH4, MES, SO4, A1BC1, CA

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	0.10	0/10004	0.32	0/13582
1	B	0.10	0/9989	0.32	0/13562
All	All	0.10	0/19993	0.32	0/27144

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	9810	0	9610	69	0
1	B	9795	0	9599	82	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	48	0	52	2	0
5	B	48	0	52	6	0
6	A	85	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	95	0	0	3	0
All	All	19901	0	19313	151	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 (151) 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:307:ARG:NH2	1:B:443:TYR:OH	2.22	0.72
1:B:692:VAL:HB	1:B:694:GLN:HG2	1.72	0.71
1:B:861:ILE:HG23	5:B:1306:MES:H32	1.71	0.70
1:A:405:GLN:HG2	1:A:415:ILE:HD12	1.74	0.68
1:B:850:VAL:HG21	5:B:1306:MES:H61	1.73	0.68
1:A:357:VAL:HB	1:A:358:PRO:HD3	1.78	0.66
1:B:357:VAL:HB	1:B:358:PRO:HD3	1.77	0.66
1:B:856:ARG:NH1	5:B:1306:MES:O2S	2.28	0.66
1:B:331:ILE:HD11	1:B:430:MET:HG2	1.78	0.65
1:A:386:ARG:NH2	1:A:664:GLN:O	2.28	0.65
1:B:735:SER:HA	1:B:1114:THR:HB	1.78	0.65
1:A:331:ILE:HD11	1:A:430:MET:HG2	1.80	0.63
1:B:386:ARG:NH2	1:B:664:GLN:O	2.31	0.61
1:B:393:LEU:H	1:B:393:LEU:HD12	1.66	0.61
1:A:222:ARG:NH2	6:A:1308:SO4:O1	2.33	0.61
1:A:872:THR:N	5:A:1306:MES:O3S	2.33	0.60
1:A:783:VAL:HB	1:A:851:TYR:HB2	1.83	0.60
1:B:103:ASN:OD1	1:B:1113:ASN:ND2	2.33	0.59
1:B:386:ARG:HD2	1:B:663:GLU:CD	2.28	0.59
1:A:735:SER:HA	1:A:1114:THR:HB	1.86	0.57
1:A:46:LYS:HE2	1:A:234:LEU:HD11	1.86	0.57
1:A:167:HIS:HA	1:A:169:TYR:CE1	2.40	0.56
1:A:98:HIS:CD2	1:A:1116:ASN:HB3	2.40	0.56
1:A:159:GLN:NE2	6:A:1308:SO4:O4	2.38	0.56
1:B:783:VAL:HB	1:B:851:TYR:HB2	1.88	0.56
1:A:383:ARG:NH1	1:A:663:GLU:OE1	2.38	0.55
1:A:1087:TYR:CZ	1:A:1089:GLU:HB2	2.41	0.55
1:B:243:MET:HE2	1:B:487:LEU:HD23	1.88	0.55
1:A:386:ARG:HD2	1:A:663:GLU:CD	2.33	0.54
1:B:540:VAL:HG13	1:B:600:GLU:HB2	1.90	0.53
1:B:14:ASP:HB3	1:B:481:ILE:HG13	1.90	0.53
1:A:1251:ALA:HA	1:A:1255:TYR:HD1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:632:GLN:HE21	1:B:696:VAL:HG21	1.71	0.53
1:A:98:HIS:O	1:A:98:HIS:ND1	2.40	0.53
1:A:1165:CYS:HB3	1:A:1205:VAL:HG22	1.91	0.53
1:A:950:PRO:HD2	1:A:970:SER:HB2	1.91	0.52
1:B:856:ARG:NH1	5:B:1306:MES:O3S	2.42	0.52
1:B:1087:TYR:CZ	1:B:1089:GLU:HB2	2.44	0.52
1:B:696:VAL:HG12	1:B:698:LYS:O	2.10	0.52
1:B:98:HIS:CD2	1:B:1116:ASN:HB3	2.45	0.52
1:B:98:HIS:O	1:B:98:HIS:ND1	2.43	0.52
1:A:56:LEU:HA	1:A:59:ILE:HD13	1.91	0.52
1:B:862:ARG:NH2	6:B:1316:SO4:O3	2.39	0.52
1:B:383:ARG:NH1	1:B:663:GLU:OE1	2.43	0.51
1:B:878:PHE:HB3	5:B:1306:MES:HN4	1.75	0.51
1:B:27:VAL:HG13	1:B:481:ILE:HG12	1.93	0.51
1:A:731:ILE:O	1:A:735:SER:HB2	2.11	0.51
1:B:1250:ALA:HB2	6:B:1323:SO4:O3	2.11	0.50
1:A:413:MET:HB3	1:A:417:GLU:HG3	1.93	0.50
1:A:1258:ILE:HD11	1:A:1276:LYS:HD3	1.92	0.49
1:A:666:ASP:OD1	1:A:666:ASP:N	2.46	0.49
1:A:8:VAL:HG23	1:A:64:HIS:HE1	1.78	0.49
1:A:243:MET:HE2	1:A:487:LEU:HD23	1.94	0.49
1:B:167:HIS:HA	1:B:169:TYR:CE1	2.47	0.49
1:B:856:ARG:NH1	5:B:1306:MES:S	2.77	0.49
1:B:83:MET:HB2	1:B:118:ILE:HG21	1.94	0.48
1:B:544:ASP:HB2	1:B:596:ASN:HB2	1.96	0.48
1:B:731:ILE:O	1:B:735:SER:HB2	2.13	0.48
1:A:275:MET:HE3	1:A:304:GLY:HA2	1.96	0.48
1:A:355:GLY:O	1:A:359:GLY:HA2	2.13	0.48
1:A:706:ARG:NH2	5:A:1304:MES:O2S	2.45	0.48
1:B:1251:ALA:HA	1:B:1255:TYR:HD1	1.78	0.48
1:B:275:MET:HE3	1:B:304:GLY:HA2	1.95	0.47
1:B:1145:TYR:HA	1:B:1232:ARG:NH1	2.29	0.47
1:A:523:ALA:HB1	1:A:601:ALA:HB2	1.95	0.47
1:B:405:GLN:HG2	1:B:415:ILE:HD12	1.96	0.47
1:B:363:TYR:HB3	1:B:365:ARG:HG3	1.97	0.47
1:B:523:ALA:HB1	1:B:601:ALA:HB2	1.95	0.47
1:B:1068:HIS:CG	1:B:1069:ILE:N	2.82	0.47
1:B:1257:VAL:HA	1:B:1273:THR:HG23	1.96	0.47
1:A:801:ILE:HD12	1:A:882:ILE:HG13	1.97	0.47
1:A:1069:ILE:O	1:A:1167:GLY:HA2	2.14	0.47
1:B:666:ASP:OD1	1:B:666:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ALA:HB1	1:A:652:ILE:HD11	1.97	0.47
1:A:743:PHE:CZ	1:A:763:MET:HB3	2.50	0.47
1:A:360:PRO:HD2	1:A:363:TYR:CD2	2.51	0.46
1:A:696:VAL:HG12	1:A:698:LYS:O	2.15	0.46
1:B:56:LEU:HA	1:B:59:ILE:HD13	1.98	0.46
1:A:767:VAL:HG22	1:A:802:ILE:HD12	1.98	0.46
1:B:1187:ALA:HB2	1:B:1221:PRO:HD3	1.96	0.46
1:A:939:ASP:OD2	1:A:1170:HIS:HB2	2.16	0.46
1:A:527:LEU:HD11	1:A:601:ALA:HB1	1.98	0.46
1:B:242:LEU:HD11	1:B:252:ILE:HD13	1.97	0.46
1:B:413:MET:HB3	1:B:417:GLU:HG3	1.97	0.46
1:B:357:VAL:HB	1:B:358:PRO:CD	2.44	0.46
1:B:1176:TRP:CD1	1:B:1176:TRP:H	2.33	0.46
1:A:357:VAL:HB	1:A:358:PRO:CD	2.44	0.45
1:B:383:ARG:HD3	1:B:663:GLU:OE2	2.16	0.45
1:B:355:GLY:O	1:B:359:GLY:HA2	2.15	0.45
1:A:414:SER:OG	1:A:417:GLU:HG2	2.16	0.45
1:A:83:MET:HB2	1:A:118:ILE:HG21	1.97	0.45
1:A:743:PHE:HZ	1:A:763:MET:HB3	1.82	0.45
1:A:1176:TRP:CD1	1:A:1176:TRP:H	2.34	0.45
1:B:1069:ILE:O	1:B:1167:GLY:HA2	2.16	0.45
1:A:17:PHE:HB2	1:A:48:LEU:HD21	1.98	0.45
1:B:360:PRO:HD2	1:B:363:TYR:CE2	2.52	0.45
1:A:98:HIS:HB2	1:A:1107:VAL:HA	1.99	0.45
1:A:1068:HIS:CG	1:A:1069:ILE:N	2.85	0.45
1:B:12:PHE:CG	1:B:29:LYS:HE3	2.51	0.45
1:A:103:ASN:OD1	1:A:1113:ASN:ND2	2.45	0.45
1:A:383:ARG:HD3	1:A:663:GLU:OE2	2.17	0.45
1:B:83:MET:HB3	1:B:123:ARG:HA	1.99	0.44
1:B:559:PRO:O	1:B:567:TRP:NE1	2.43	0.44
1:B:165:LEU:HD11	1:B:178:ILE:HD12	2.00	0.44
1:A:242:LEU:HD11	1:A:252:ILE:HD13	2.00	0.44
1:B:145:GLU:O	1:B:149:ARG:HG2	2.18	0.44
1:A:453:ALA:HB1	1:A:482:ILE:HG21	2.00	0.43
1:A:846:ARG:HE	1:A:846:ARG:HB2	1.52	0.43
1:B:110:LEU:HG	1:B:1104:PRO:HB3	2.00	0.43
1:B:414:SER:OG	1:B:417:GLU:HG2	2.18	0.43
1:A:401:ARG:HG3	1:A:415:ILE:CD1	2.48	0.43
1:A:757:PRO:HB3	1:A:991:PHE:CE1	2.54	0.43
1:A:1062:THR:HG22	1:A:1098:ARG:HG3	2.00	0.43
1:B:59:ILE:HG22	1:B:236:TYR:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ASP:HB2	1:A:596:ASN:HB2	2.00	0.43
1:A:1000:GLU:HG3	1:A:1006:PHE:CD1	2.54	0.43
1:B:851:TYR:CE2	1:B:856:ARG:HB2	2.53	0.43
1:B:1176:TRP:HZ3	1:B:1178:ALA:HB2	1.84	0.43
1:A:87:GLU:HA	1:A:125:THR:HB	2.01	0.42
1:B:248:GLY:HA3	1:B:493:GLN:HG2	2.00	0.42
1:A:458:ALA:HB1	1:A:669:THR:HA	2.00	0.42
1:B:458:ALA:HB1	1:B:669:THR:HA	2.01	0.42
1:B:1068:HIS:CE1	1:B:1221:PRO:HD2	2.54	0.42
1:B:413:MET:HE2	1:B:700:ALA:HB1	2.01	0.42
1:B:950:PRO:HD2	1:B:970:SER:HB2	2.02	0.42
1:A:347:PHE:CE1	1:A:407:LEU:HD21	2.55	0.42
1:A:413:MET:HE2	1:A:700:ALA:HB1	2.01	0.42
1:B:164:CYS:HB3	1:B:207:PHE:CE1	2.54	0.42
1:B:1165:CYS:HB3	1:B:1205:VAL:HG22	2.00	0.42
1:B:621:ASN:ND2	6:B:1322:SO4:O4	2.44	0.42
1:A:163:VAL:HG12	1:A:175:GLU:HG2	2.02	0.42
1:A:201:TYR:O	1:A:202:ARG:HB2	2.20	0.41
1:B:484:GLY:HA2	1:B:487:LEU:HD12	2.01	0.41
1:B:742:LEU:HD21	1:B:888:ALA:HB1	2.01	0.41
1:B:779:HIS:CG	1:B:853:LYS:HE3	2.55	0.41
1:A:484:GLY:HA2	1:A:487:LEU:HD12	2.02	0.41
1:B:939:ASP:OD2	1:B:1170:HIS:HB2	2.20	0.41
1:A:1208:ARG:NH1	6:A:1321:SO4:O1	2.44	0.41
1:A:1257:VAL:HA	1:A:1273:THR:HG23	2.03	0.41
1:A:331:ILE:HD11	1:A:430:MET:CG	2.48	0.41
1:B:257:LYS:HB2	1:B:257:LYS:HE3	1.76	0.41
1:B:976:ALA:HA	1:B:1034:ALA:HB3	2.02	0.41
1:B:990:THR:HG21	1:B:1014:LEU:HD22	2.03	0.41
1:A:100:LYS:HE2	1:A:100:LYS:HB2	1.88	0.41
1:A:376:GLN:HG2	1:A:459:LEU:HD13	2.03	0.41
1:B:723:LEU:HD23	1:B:738:LEU:HD13	2.03	0.41
1:B:201:TYR:O	1:B:202:ARG:HB2	2.21	0.40
1:B:1071:PHE:HB3	1:B:1166:GLU:HB3	2.02	0.40
1:B:690:PRO:O	1:B:692:VAL:HG23	2.21	0.40
1:B:1000:GLU:HG3	1:B:1006:PHE:CD1	2.57	0.40
1:B:4:ILE:HD13	1:B:48:LEU:HD23	2.04	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	1281/1288 (100%)	1243 (97%)	37 (3%)	1 (0%)	48	77
1	B	1279/1288 (99%)	1242 (97%)	36 (3%)	1 (0%)	48	77
All	All	2560/2576 (99%)	2485 (97%)	73 (3%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	ARG
1	B	202	ARG

### 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	1034/1039 (100%)	1022 (99%)	12 (1%)	63	87
1	B	1032/1039 (99%)	1020 (99%)	12 (1%)	63	87
All	All	2066/2078 (99%)	2042 (99%)	24 (1%)	63	87

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	147	ARG
1	A	198	VAL
1	A	234	LEU

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Mol	Chain	Res	Type
1	A	284	GLU
1	A	320	GLN
1	A	376	GLN
1	A	481	ILE
1	A	500	ASN
1	A	565	THR
1	A	801	ILE
1	A	1068	HIS
1	B	1	MET
1	B	3	ARG
1	B	6	VAL
1	B	198	VAL
1	B	234	LEU
1	B	320	GLN
1	B	376	GLN
1	B	481	ILE
1	B	500	ASN
1	B	565	THR
1	B	801	ILE
1	B	1068	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	183	ASN
1	A	230	GLN
1	A	319	HIS
1	A	320	GLN
1	A	472	HIS
1	A	500	ASN
1	A	694	GLN
1	B	174	HIS
1	B	183	ASN
1	B	493	GLN
1	B	526	GLN
1	B	632	GLN
1	B	748	ASN
1	B	857	GLN

### 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 50 ligands modelled in this entry, 2 are monoatomic and 2 are modelled with single atom - leaving 46 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$
6	SO4	B	1323	-	4,4,4	0.66	0	6,6,6	0.09	0
3	A1BC1	B	1302	2	8,8,8	1.21	1 (12%)	10,11,11	1.80	2 (20%)
5	MES	A	1304	-	12,12,12	1.07	1 (8%)	15,16,16	0.95	1 (6%)
6	SO4	B	1321	-	4,4,4	0.67	0	6,6,6	0.12	0
6	SO4	B	1310	-	4,4,4	0.68	0	6,6,6	0.17	0
6	SO4	A	1317	-	4,4,4	0.67	0	6,6,6	0.13	0
5	MES	A	1307	-	12,12,12	1.14	1 (8%)	15,16,16	0.79	0
6	SO4	B	1326	-	4,4,4	0.67	0	6,6,6	0.07	0
5	MES	B	1306	-	12,12,12	1.10	1 (8%)	15,16,16	0.88	1 (6%)
6	SO4	A	1311	-	4,4,4	0.67	0	6,6,6	0.15	0
6	SO4	A	1318	-	4,4,4	0.68	0	6,6,6	0.05	0
6	SO4	A	1322	-	4,4,4	0.68	0	6,6,6	0.14	0
6	SO4	B	1312	-	4,4,4	0.68	0	6,6,6	0.09	0
6	SO4	B	1319	-	4,4,4	0.67	0	6,6,6	0.07	0
6	SO4	A	1308	-	4,4,4	0.68	0	6,6,6	0.06	0
6	SO4	A	1315	-	4,4,4	0.68	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	B	1317	-	4,4,4	0.67	0	6,6,6	0.10	0
6	SO4	A	1323	-	4,4,4	0.67	0	6,6,6	0.08	0
6	SO4	A	1321	-	4,4,4	0.67	0	6,6,6	0.11	0
6	SO4	B	1308	-	4,4,4	0.67	0	6,6,6	0.10	0
6	SO4	B	1318	-	4,4,4	0.67	0	6,6,6	0.06	0
3	A1BC1	A	1302	2	8,8,8	1.20	1 (12%)	10,11,11	1.78	3 (30%)
6	SO4	A	1309	-	4,4,4	0.67	0	6,6,6	0.13	0
6	SO4	A	1316	-	4,4,4	0.67	0	6,6,6	0.13	0
6	SO4	B	1311	-	4,4,4	0.68	0	6,6,6	0.11	0
6	SO4	B	1314	-	4,4,4	0.68	0	6,6,6	0.10	0
5	MES	B	1307	-	12,12,12	1.16	1 (8%)	15,16,16	0.72	0
6	SO4	A	1324	-	4,4,4	0.68	0	6,6,6	0.08	0
6	SO4	A	1310	-	4,4,4	0.66	0	6,6,6	0.12	0
6	SO4	B	1324	-	4,4,4	0.67	0	6,6,6	0.08	0
6	SO4	B	1320	-	4,4,4	0.67	0	6,6,6	0.13	0
6	SO4	B	1315	-	4,4,4	0.68	0	6,6,6	0.07	0
5	MES	B	1305	-	12,12,12	1.13	1 (8%)	15,16,16	0.86	1 (6%)
6	SO4	A	1314	-	4,4,4	0.67	0	6,6,6	0.10	0
6	SO4	B	1322	-	4,4,4	0.67	0	6,6,6	0.08	0
6	SO4	A	1312	-	4,4,4	0.67	0	6,6,6	0.15	0
5	MES	A	1306	-	12,12,12	1.08	1 (8%)	15,16,16	0.74	0
6	SO4	A	1319	-	4,4,4	0.67	0	6,6,6	0.09	0
6	SO4	A	1320	-	4,4,4	0.67	0	6,6,6	0.13	0
6	SO4	B	1309	-	4,4,4	0.67	0	6,6,6	0.10	0
5	MES	A	1305	-	12,12,12	1.12	1 (8%)	15,16,16	0.74	0
5	MES	B	1304	-	12,12,12	1.10	1 (8%)	15,16,16	0.89	0
6	SO4	B	1313	-	4,4,4	0.67	0	6,6,6	0.11	0
6	SO4	B	1325	-	4,4,4	0.67	0	6,6,6	0.08	0
6	SO4	B	1316	-	4,4,4	0.66	0	6,6,6	0.47	0
6	SO4	A	1313	-	4,4,4	0.68	0	6,6,6	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MES	B	1305	-	-	4/6/14/14	0/1/1/1
3	A1BC1	B	1302	2	-	-	0/1/1/1
5	MES	A	1304	-	-	0/6/14/14	0/1/1/1
3	A1BC1	A	1302	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MES	A	1306	-	-	0/6/14/14	0/1/1/1
5	MES	B	1307	-	-	5/6/14/14	0/1/1/1
5	MES	A	1307	-	-	5/6/14/14	0/1/1/1
5	MES	A	1305	-	-	3/6/14/14	0/1/1/1
5	MES	B	1304	-	-	2/6/14/14	0/1/1/1
5	MES	B	1306	-	-	4/6/14/14	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1307	MES	C8-S	3.02	1.81	1.77
5	A	1307	MES	C8-S	2.99	1.81	1.77
5	B	1305	MES	C8-S	2.86	1.81	1.77
5	A	1305	MES	C8-S	2.85	1.81	1.77
5	B	1306	MES	C8-S	2.83	1.81	1.77
5	B	1304	MES	C8-S	2.76	1.81	1.77
5	A	1306	MES	C8-S	2.73	1.81	1.77
5	A	1304	MES	C8-S	2.71	1.81	1.77
3	B	1302	A1BC1	C4-N7	2.41	1.41	1.37
3	A	1302	A1BC1	C4-N7	2.29	1.40	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1302	A1BC1	C4-N7-C5	-3.80	109.14	112.47
3	A	1302	A1BC1	C4-N7-C5	-3.32	109.56	112.47
5	A	1304	MES	O2S-S-C8	-2.56	102.86	106.73
3	B	1302	A1BC1	C1-C4-N7	2.32	109.04	106.81
5	B	1306	MES	O2S-S-C8	-2.28	103.28	106.73
5	B	1305	MES	O2S-S-C8	-2.13	103.51	106.73
3	A	1302	A1BC1	O8-C4-N7	-2.06	122.31	125.06
3	A	1302	A1BC1	C1-C4-N7	2.01	108.74	106.81

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1305	MES	C7-C8-S-O1S
5	A	1305	MES	C7-C8-S-O3S
5	B	1306	MES	C7-C8-S-O1S

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Mol	Chain	Res	Type	Atoms
5	B	1306	MES	C7-C8-S-O3S
5	B	1307	MES	C7-C8-S-O2S
5	B	1307	MES	C7-C8-S-O3S
5	A	1307	MES	C7-C8-S-O3S
5	B	1305	MES	C7-C8-S-O3S
5	B	1306	MES	N4-C7-C8-S
5	A	1307	MES	C8-C7-N4-C3
5	A	1307	MES	C8-C7-N4-C5
5	B	1307	MES	C8-C7-N4-C3
5	B	1307	MES	C8-C7-N4-C5
5	A	1305	MES	C7-C8-S-O2S
5	A	1307	MES	C7-C8-S-O1S
5	A	1307	MES	C7-C8-S-O2S
5	B	1304	MES	C7-C8-S-O2S
5	B	1305	MES	C7-C8-S-O1S
5	B	1305	MES	C7-C8-S-O2S
5	B	1306	MES	C7-C8-S-O2S
5	B	1307	MES	C7-C8-S-O1S
5	B	1304	MES	C7-C8-S-O3S
5	B	1305	MES	C8-C7-N4-C3

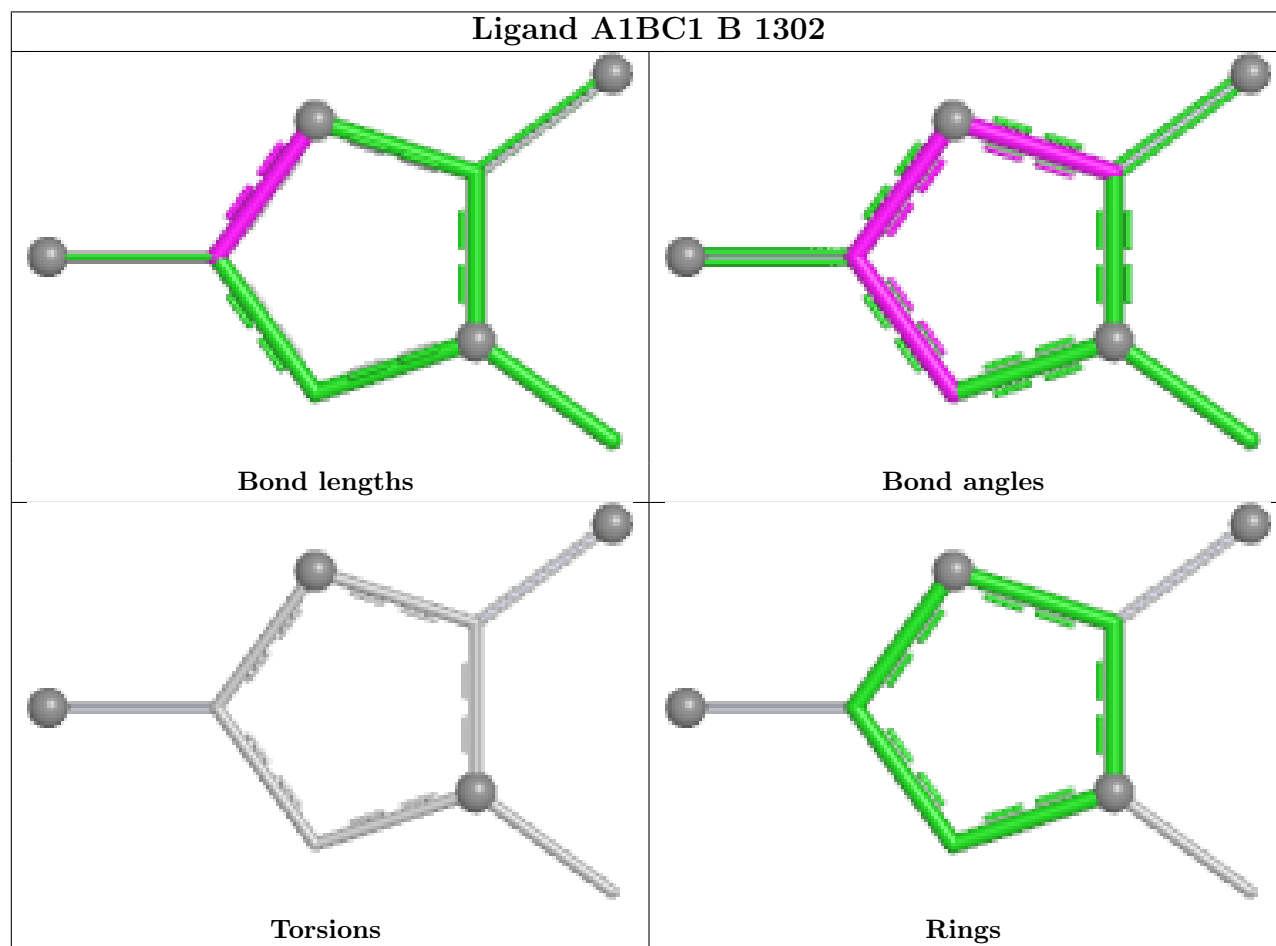
There are no ring outliers.

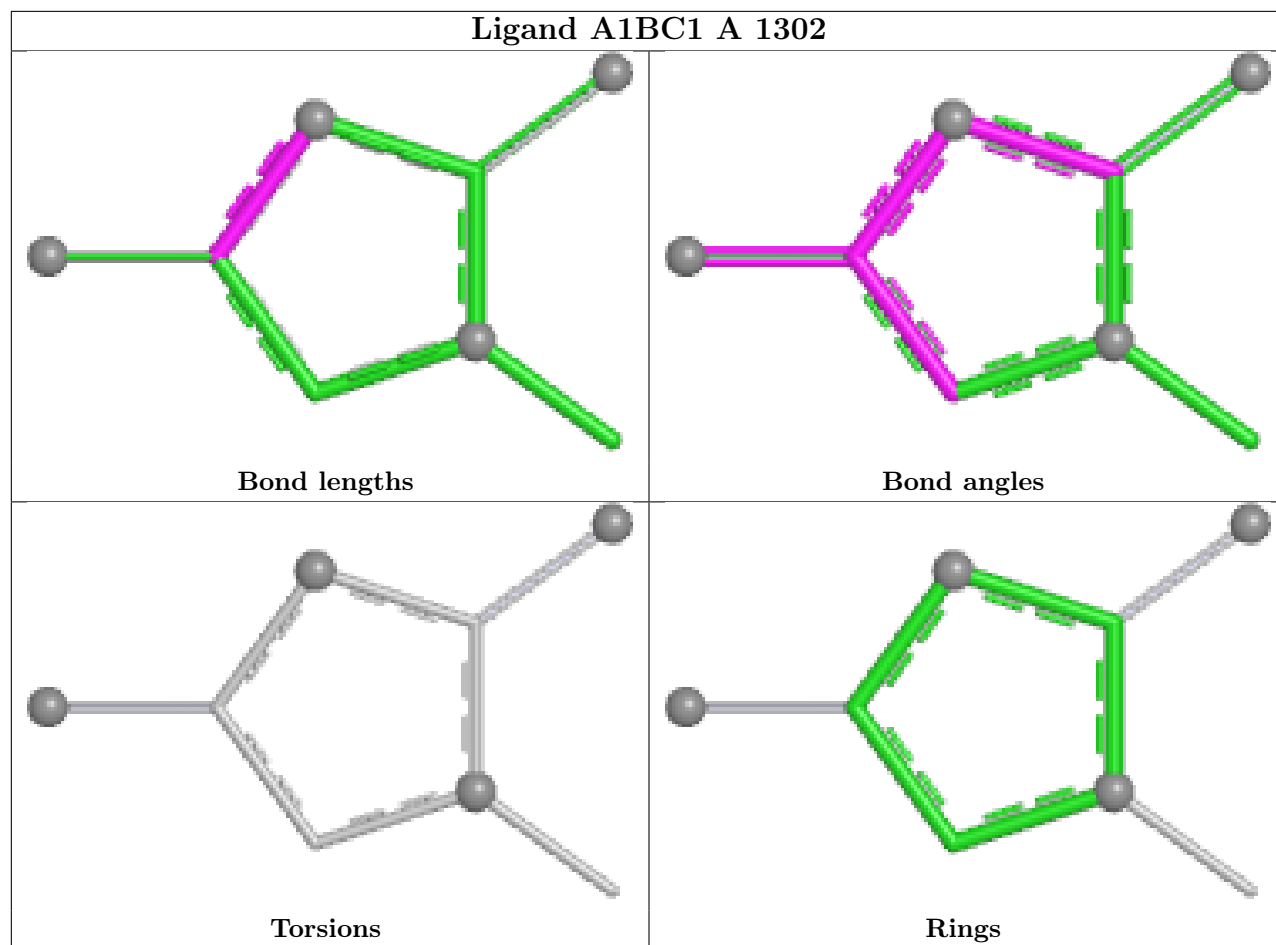
8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1323	SO4	1	0
5	A	1304	MES	1	0
5	B	1306	MES	6	0
6	A	1308	SO4	2	0
6	A	1321	SO4	1	0
6	B	1322	SO4	1	0
5	A	1306	MES	1	0
6	B	1316	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 [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	1283/1288 (99%)	-0.16	10 (0%)	82 75	46, 64, 94, 129	0
1	B	1281/1288 (99%)	-0.23	15 (1%)	76 68	45, 60, 92, 133	0
All	All	2564/2576 (99%)	-0.19	25 (0%)	79 72	45, 62, 93, 133	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	692	VAL	4.7
1	B	696	VAL	4.2
1	A	696	VAL	4.2
1	B	357	VAL	3.8
1	B	694	GLN	3.4
1	B	1264	GLY	3.4
1	A	357	VAL	3.2
1	A	634	ALA	3.0
1	B	690	PRO	3.0
1	A	690	PRO	3.0
1	B	691	ALA	3.0
1	B	392	GLY	2.8
1	A	635	GLY	2.8
1	A	692	VAL	2.7
1	B	634	ALA	2.7
1	B	693	THR	2.7
1	A	388	LEU	2.6
1	B	35	HIS	2.6
1	A	392	GLY	2.5
1	B	389	ALA	2.4
1	B	632	GLN	2.4
1	A	1006	PHE	2.4
1	B	391	SER	2.3
1	B	43	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	389	ALA	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	SO4	B	1326	5/5	0.53	0.12	109,113,127,147	0
6	SO4	A	1317	5/5	0.56	0.11	111,111,144,151	0
6	SO4	B	1324	5/5	0.58	0.09	128,132,151,156	0
6	SO4	A	1323	5/5	0.66	0.09	112,123,130,142	0
6	SO4	A	1322	5/5	0.69	0.15	95,102,124,152	0
4	NH4	A	1303	1/1	0.70	0.14	64,64,64,64	0
6	SO4	A	1324	5/5	0.71	0.08	106,108,132,143	0
6	SO4	B	1323	5/5	0.72	0.13	104,113,126,132	0
6	SO4	A	1319	5/5	0.73	0.10	98,112,129,135	0
6	SO4	B	1322	5/5	0.74	0.08	104,121,142,149	0
6	SO4	A	1314	5/5	0.74	0.14	105,108,116,120	0
6	SO4	B	1313	5/5	0.74	0.09	101,110,123,126	0
6	SO4	B	1321	5/5	0.74	0.23	98,100,125,143	0
6	SO4	B	1320	5/5	0.75	0.28	88,98,123,129	0
6	SO4	B	1325	5/5	0.76	0.07	105,106,134,135	0
6	SO4	A	1309	5/5	0.76	0.11	87,98,102,120	0
4	NH4	B	1303	1/1	0.77	0.21	48,48,48,48	0
5	MES	A	1307	12/12	0.78	0.17	80,92,111,116	0
6	SO4	B	1318	5/5	0.79	0.27	86,97,124,141	0
6	SO4	A	1311	5/5	0.79	0.12	89,99,106,119	0
5	MES	B	1307	12/12	0.79	0.17	88,95,118,127	0
6	SO4	B	1316	5/5	0.79	0.10	111,112,133,138	0

*Continued on next page...*

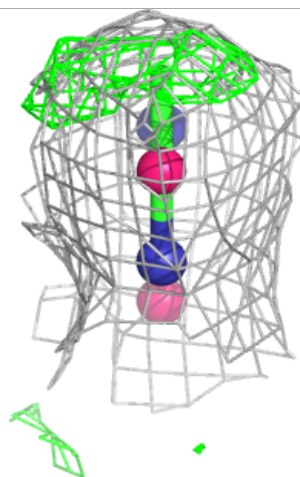
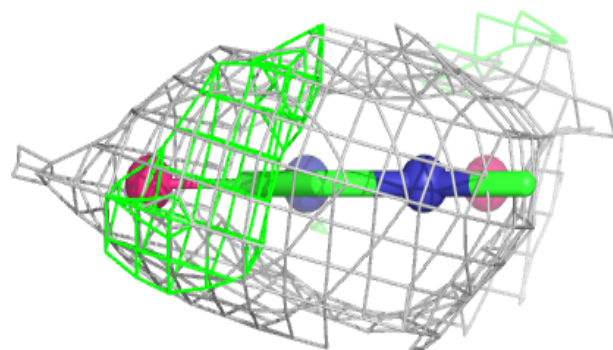
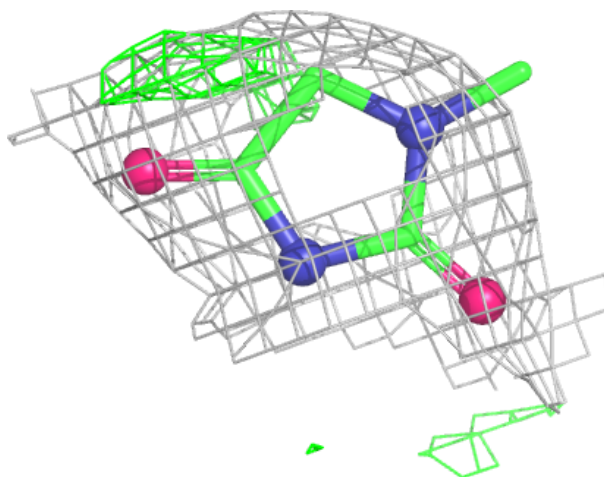
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	A	1316	5/5	0.80	0.12	103,108,143,152	0
6	SO4	A	1320	5/5	0.80	0.28	94,106,108,139	0
6	SO4	A	1315	5/5	0.80	0.09	103,113,139,142	0
6	SO4	A	1318	5/5	0.81	0.15	83,105,119,122	0
6	SO4	B	1311	5/5	0.81	0.15	84,92,111,115	0
6	SO4	A	1321	5/5	0.81	0.22	85,93,111,129	0
6	SO4	B	1314	5/5	0.82	0.08	90,102,119,119	0
6	SO4	B	1319	5/5	0.82	0.09	101,103,128,130	0
6	SO4	A	1313	5/5	0.82	0.24	104,107,120,133	0
6	SO4	B	1317	5/5	0.83	0.23	97,97,120,131	0
6	SO4	B	1309	5/5	0.83	0.08	80,90,92,115	0
6	SO4	B	1308	5/5	0.84	0.22	92,94,98,120	0
6	SO4	A	1312	5/5	0.84	0.14	97,101,121,127	0
6	SO4	A	1310	5/5	0.85	0.16	101,102,113,128	0
6	SO4	B	1310	5/5	0.85	0.12	76,77,116,123	0
6	SO4	A	1308	5/5	0.86	0.17	83,86,100,116	0
6	SO4	B	1315	5/5	0.88	0.21	81,83,114,119	0
6	SO4	B	1312	5/5	0.88	0.10	97,99,120,120	0
5	MES	B	1306	12/12	0.89	0.16	84,94,114,129	0
5	MES	B	1305	12/12	0.90	0.14	67,79,86,89	0
5	MES	A	1305	12/12	0.92	0.13	75,89,95,96	0
5	MES	A	1306	12/12	0.92	0.15	81,90,107,109	0
3	A1BC1	A	1302	8/8	0.93	0.14	49,66,72,73	0
3	A1BC1	B	1302	8/8	0.93	0.13	46,57,62,62	0
5	MES	A	1304	12/12	0.93	0.11	59,69,80,81	0
2	CA	A	1301	1/1	0.95	0.08	57,57,57,57	0
5	MES	B	1304	12/12	0.96	0.09	53,63,77,80	0
2	CA	B	1301	1/1	0.96	0.10	57,57,57,57	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.

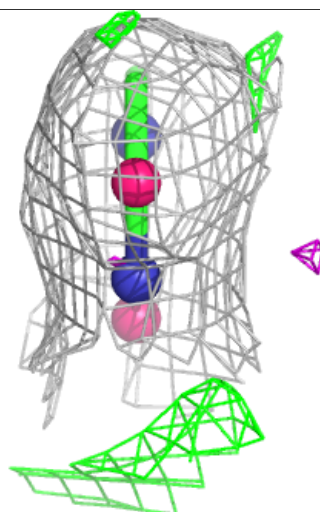
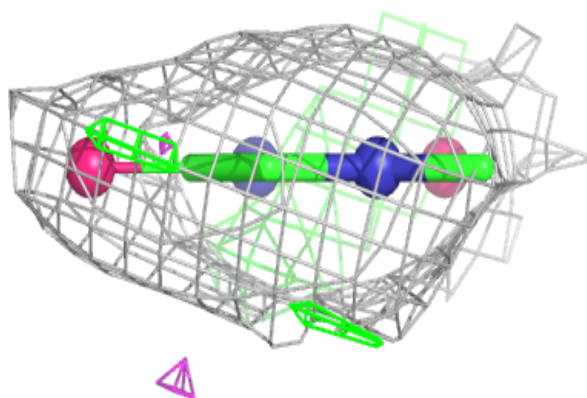
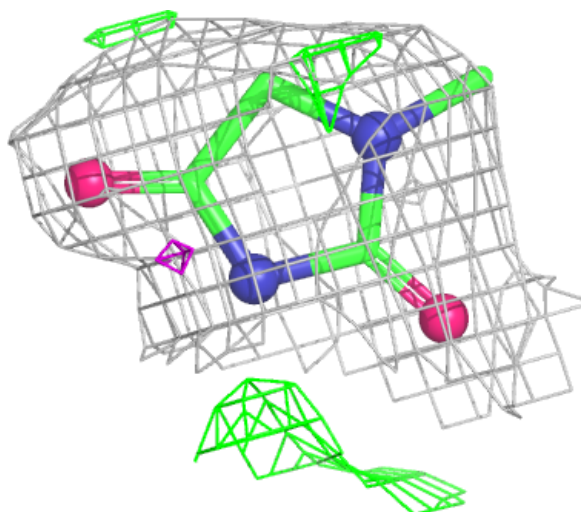
**Electron density around A1BC1 A 1302:**

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



**Electron density around A1BC1 B 1302:**

$2mF_o-DF_c$  (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.