



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:29 AM GMT

PDB ID : 3AZW
Title : Crystal structure of the receptor binding domain
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Deposited on : 2011-06-02
Resolution : 2.99 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

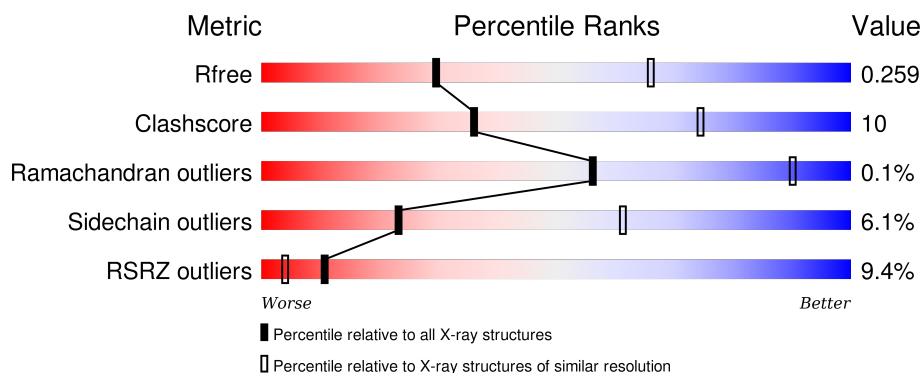
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	438	<div> <div>4%</div> <div>75%</div> <div>19%</div> <div>• 5%</div> </div>
1	B	438	<div> <div>14%</div> <div>72%</div> <div>21%</div> <div>• 5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6874 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 D/C mosaic neurotoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3426	2199	566	647	14			
1	B	418	Total	C	N	O	S	0	0	0
			3426	2199	566	647	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1286	LEU	-	EXPRESSION TAG	UNP A5JGM8
A	1287	GLU	-	EXPRESSION TAG	UNP A5JGM8
A	1288	HIS	-	EXPRESSION TAG	UNP A5JGM8
A	1289	HIS	-	EXPRESSION TAG	UNP A5JGM8
A	1290	HIS	-	EXPRESSION TAG	UNP A5JGM8
A	1291	HIS	-	EXPRESSION TAG	UNP A5JGM8
A	1292	HIS	-	EXPRESSION TAG	UNP A5JGM8
A	1293	HIS	-	EXPRESSION TAG	UNP A5JGM8
B	1286	LEU	-	EXPRESSION TAG	UNP A5JGM8
B	1287	GLU	-	EXPRESSION TAG	UNP A5JGM8
B	1288	HIS	-	EXPRESSION TAG	UNP A5JGM8
B	1289	HIS	-	EXPRESSION TAG	UNP A5JGM8
B	1290	HIS	-	EXPRESSION TAG	UNP A5JGM8
B	1291	HIS	-	EXPRESSION TAG	UNP A5JGM8
B	1292	HIS	-	EXPRESSION TAG	UNP A5JGM8
B	1293	HIS	-	EXPRESSION TAG	UNP A5JGM8

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

- Chain A:
-
- 4% 75% 19% 5%

- [illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.96Å 141.55Å 162.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.22 – 2.99 43.22 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.22-2.99) 99.3 (43.22-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0091	Depositor
R, R_{free}	0.255 , 0.291 0.234 , 0.259	Depositor DCC
R_{free} test set	1424 reflections (5.44%)	DCC
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 27615 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6874	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4

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	0.44	0/3505	0.58	0/4743
1	B	0.38	0/3505	0.56	0/4743
All	All	0.41	0/7010	0.57	0/9486

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	3426	0	3342	66	0
1	B	3426	0	3342	65	0
2	A	10	0	0	0	0
3	A	12	0	0	1	0
All	All	6874	0	6684	130	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 10.

All (130) 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:922:ASN:HB2	1:A:925:ILE:HD11	1.49	0.93
1:B:1007:THR:HG23	1:B:1019:TYR:HB2	1.47	0.93
1:A:1179:MET:CE	1:A:1226:LEU:HD21	2.01	0.91
1:A:1179:MET:CE	1:A:1226:LEU:CD2	2.50	0.90
1:A:1179:MET:HE1	1:A:1226:LEU:CD2	2.02	0.89
1:B:955:ILE:HG23	1:B:966:ILE:HB	1.61	0.82
1:A:885:TYR:CD1	1:A:925:ILE:HG21	2.17	0.80
1:A:1007:THR:HG21	1:A:1081:ILE:CD1	2.11	0.79
1:A:1127:ILE:CD1	1:A:1177:LEU:HD22	2.14	0.78
1:A:1179:MET:HE1	1:A:1226:LEU:HD21	1.64	0.77
1:A:1179:MET:HE1	1:A:1226:LEU:HD22	1.69	0.73
1:A:1179:MET:HE3	1:A:1226:LEU:HD21	1.73	0.71
1:A:976:THR:HG22	1:A:986:ASP:HB3	1.72	0.71
1:B:864:ILE:HD11	1:B:1072:PHE:CE1	2.25	0.70
1:A:1127:ILE:CD1	1:A:1177:LEU:CD2	2.69	0.70
1:B:955:ILE:HD12	1:B:1044:PHE:CE1	2.27	0.70
1:B:1067:ARG:NH1	1:B:1088:LEU:O	2.25	0.69
1:B:1146:ILE:HG23	1:B:1164:LEU:HD13	1.77	0.66
1:A:1127:ILE:HD11	1:A:1177:LEU:CD2	2.26	0.66
1:A:1067:ARG:NH1	1:A:1088:LEU:O	2.29	0.66
1:A:1179:MET:CE	1:A:1226:LEU:HD22	2.25	0.65
1:B:940:ILE:HG23	1:B:1004:PHE:CE2	2.32	0.65
1:B:886:ASN:C	1:B:886:ASN:HD22	2.01	0.64
1:A:1007:THR:HG21	1:A:1081:ILE:HD12	1.80	0.62
1:B:1046:MET:HE1	1:B:1064:MET:HB3	1.81	0.62
1:B:1149:ILE:HG22	1:B:1150:ARG:HG2	1.82	0.62
1:A:1017:MET:CE	1:A:1024:LEU:HD11	2.30	0.61
1:B:922:ASN:O	1:B:926:VAL:HG13	1.99	0.61
1:B:1161:GLU:CD	1:B:1212:GLN:HE22	2.05	0.60
1:A:1170:ILE:HG22	1:A:1171:ASP:N	2.15	0.60
1:A:1144:ILE:C	1:A:1144:ILE:HD12	2.21	0.60
1:B:860:TYR:O	1:B:864:ILE:HG22	1.99	0.60
1:A:873:GLN:OE1	1:A:882:THR:HG21	2.03	0.58
1:B:938:PHE:CE2	1:B:1006:VAL:HG13	2.38	0.58
1:A:889:VAL:HG13	1:A:889:VAL:O	2.04	0.57
1:A:942:ILE:HD13	1:A:968:ILE:HD13	1.87	0.57
1:B:1149:ILE:HB	1:B:1163:VAL:HG12	1.87	0.56
1:B:1103:ARG:HG3	1:B:1156:THR:HG22	1.86	0.56
1:B:1144:ILE:HD13	1:B:1166:PHE:HD2	1.69	0.56
1:B:942:ILE:HD11	1:B:945:TRP:CD2	2.41	0.56
1:B:1231:THR:HG23	1:B:1233:ASN:H	1.69	0.56
1:B:901:PHE:CG	1:B:902:PRO:HA	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:LEU:O	1:A:889:VAL:HG11	2.07	0.55
1:A:1017:MET:HE2	1:A:1024:LEU:HD11	1.87	0.55
1:B:942:ILE:HD11	1:B:945:TRP:CE3	2.41	0.55
1:B:878:THR:HG23	1:B:880:MET:CE	2.37	0.55
1:A:1249:ASP:N	1:A:1249:ASP:OD1	2.39	0.55
1:A:1153:THR:HG22	1:A:1154:ASN:N	2.22	0.55
1:B:1020:ILE:HG22	1:B:1217:PHE:HE1	1.72	0.54
1:B:1090:TYR:CD2	1:B:1093:VAL:HG23	2.42	0.54
1:B:1188:THR:O	1:B:1190:LEU:HD12	2.08	0.54
1:B:976:THR:HG22	1:B:986:ASP:OD1	2.07	0.54
1:A:901:PHE:CG	1:A:902:PRO:HA	2.42	0.53
1:B:1046:MET:CE	1:B:1064:MET:HB3	2.39	0.53
1:B:1001:ASN:N	1:B:1001:ASN:HD22	2.07	0.53
1:B:977:LEU:HD12	1:B:977:LEU:N	2.24	0.53
1:B:921:GLN:HG3	1:B:926:VAL:HG11	1.90	0.52
1:A:939:TRP:HB2	1:A:1067:ARG:HD3	1.90	0.52
1:A:1001:ASN:HB2	1:A:1098:TRP:CZ3	2.44	0.52
1:A:1002:LYS:NZ	1:A:1218:ASP:O	2.43	0.51
1:B:938:PHE:CZ	1:B:1006:VAL:HG11	2.45	0.51
1:A:1135:ASN:ND2	3:A:223:HOH:O	2.43	0.51
1:B:864:ILE:HD11	1:B:1072:PHE:CZ	2.45	0.51
1:B:1144:ILE:HD12	1:B:1144:ILE:C	2.31	0.51
1:B:886:ASN:HD22	1:B:887:ALA:N	2.08	0.51
1:A:1090:TYR:CE1	1:B:859:GLU:HA	2.46	0.51
1:A:975:PHE:CG	1:A:1008:ILE:HD13	2.46	0.50
1:B:938:PHE:CZ	1:B:1006:VAL:CG1	2.95	0.50
1:B:975:PHE:CG	1:B:1008:ILE:HD13	2.47	0.50
1:B:999:GLY:C	1:B:1001:ASN:HD22	2.16	0.50
1:A:885:TYR:CE1	1:A:925:ILE:HG21	2.47	0.49
1:A:1164:LEU:HD12	1:A:1164:LEU:C	2.32	0.49
1:B:1007:THR:CG2	1:B:1019:TYR:HB2	2.31	0.48
1:B:872:LEU:HB3	1:B:1069:PHE:HB3	1.95	0.48
1:B:939:TRP:HB2	1:B:1067:ARG:HD3	1.96	0.48
1:B:1001:ASN:HB2	1:B:1098:TRP:CZ3	2.49	0.48
1:B:939:TRP:HE1	1:B:1088:LEU:HB3	1.78	0.48
1:A:1153:THR:HG22	1:A:1154:ASN:H	1.78	0.48
1:B:1090:TYR:HD2	1:B:1093:VAL:HG23	1.79	0.47
1:A:1192:PRO:HB3	1:A:1259:ILE:HD12	1.95	0.47
1:A:939:TRP:HE1	1:A:1088:LEU:HB3	1.80	0.47
1:B:1117:ASN:O	1:B:1132:ARG:HG2	2.15	0.47
1:A:987:ILE:HD11	1:A:1026:ASP:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1190:LEU:HD23	1:B:1261:VAL:HG21	1.97	0.47
1:A:1245:PHE:CE1	1:A:1247:LEU:HD13	2.50	0.47
1:A:1102:LEU:HD12	1:A:1108:TYR:CZ	2.50	0.47
1:A:914:ARG:NH1	1:A:1047:ASN:OD1	2.47	0.47
1:A:872:LEU:HB3	1:A:1069:PHE:HB3	1.97	0.46
1:B:1170:ILE:HG22	1:B:1171:ASP:N	2.30	0.46
1:B:891:VAL:HG13	1:B:891:VAL:O	2.17	0.45
1:A:942:ILE:CD1	1:A:968:ILE:HD13	2.45	0.45
1:A:1094:VAL:HG22	1:A:1213:PRO:HB3	1.98	0.45
1:A:976:THR:HG22	1:A:986:ASP:CB	2.44	0.45
1:A:1017:MET:HE3	1:A:1024:LEU:HD11	1.98	0.45
1:B:885:TYR:O	1:B:886:ASN:C	2.55	0.45
1:A:860:TYR:HB3	1:A:1083:ILE:HD13	1.99	0.45
1:B:1228:SER:O	1:B:1231:THR:HG22	2.17	0.45
1:A:871:SER:OG	1:A:882:THR:HG23	2.18	0.44
1:B:1262:ILE:HG22	1:B:1263:LYS:O	2.17	0.44
1:B:907:LEU:HB3	1:B:1046:MET:CE	2.46	0.44
1:A:906:LYS:O	1:A:907:LEU:HD12	2.17	0.44
1:A:1118:ARG:HA	1:A:1130:ASN:O	2.18	0.44
1:A:1179:MET:HE3	1:A:1226:LEU:HD11	2.00	0.44
1:B:1072:PHE:CD2	1:B:1076:LEU:HD11	2.52	0.43
1:A:1046:MET:HE1	1:A:1062:ILE:HD11	1.99	0.43
1:A:1179:MET:CE	1:A:1226:LEU:CD1	2.97	0.43
1:A:1014:GLY:O	1:A:1030:VAL:HG12	2.18	0.43
1:B:860:TYR:CB	1:B:1083:ILE:HD13	2.49	0.43
1:A:870:LEU:HD12	1:A:881:ASP:OD2	2.18	0.43
1:B:869:ILE:HD11	1:B:1073:ALA:HB2	2.01	0.43
1:B:873:GLN:O	1:B:879:LEU:HD12	2.18	0.43
1:B:1036:ILE:HG23	1:B:1036:ILE:O	2.20	0.42
1:B:999:GLY:C	1:B:1001:ASN:ND2	2.73	0.42
1:B:1115:TYR:CD2	1:B:1258:LEU:HD21	2.55	0.42
1:B:1102:LEU:HD12	1:B:1108:TYR:CZ	2.55	0.42
1:A:930:MET:HG2	1:A:1038:PHE:HB2	2.01	0.41
1:A:935:SER:OG	1:A:1009:THR:HG22	2.19	0.41
1:A:1128:VAL:O	1:A:1128:VAL:HG23	2.21	0.41
1:A:1102:LEU:HB3	1:A:1158:VAL:HG13	2.03	0.41
1:A:1036:ILE:HG23	1:A:1036:ILE:O	2.21	0.41
1:A:901:PHE:CD1	1:A:902:PRO:HA	2.56	0.41
1:A:900:ILE:HG22	1:A:901:PHE:N	2.35	0.41
1:B:938:PHE:N	1:B:938:PHE:CD2	2.89	0.40
1:A:943:ASN:OD1	1:A:944:LYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:977:LEU:HD11	1:B:1016:MET:SD	2.61	0.40
1:A:987:ILE:HD11	1:A:1026:ASP:C	2.42	0.40
1:B:1094:VAL:HG22	1:B:1213:PRO:HB3	2.03	0.40
1:B:968:ILE:HG23	1:B:973:LEU:HD12	2.03	0.40
1:A:1244:SER:HA	1:A:1255:HIS:O	2.22	0.40
1:B:1214:CYS:HG	1:B:1277:HIS:CD2	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	414/438 (94%)	389 (94%)	24 (6%)	1 (0%)	52	88
1	B	414/438 (94%)	390 (94%)	24 (6%)	0	100	100
All	All	828/876 (94%)	779 (94%)	48 (6%)	1 (0%)	56	90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	886	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	383/402 (95%)	362 (94%)	21 (6%)	27	65
1	B	383/402 (95%)	357 (93%)	26 (7%)	20	56
All	All	766/804 (95%)	719 (94%)	47 (6%)	23	61

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	866	ASP
1	A	896	GLN
1	A	897	LEU
1	A	925	ILE
1	A	926	VAL
1	A	931	TYR
1	A	933	SER
1	A	944	LYS
1	A	1067	ARG
1	A	1088	LEU
1	A	1089	GLN
1	A	1120	MET
1	A	1135	ASN
1	A	1158	VAL
1	A	1168	THR
1	A	1171	ASP
1	A	1184	ARG
1	A	1227	SER
1	A	1246	LYS
1	A	1247	LEU
1	A	1249	ASP
1	B	858	ASN
1	B	864	ILE
1	B	865	ASN
1	B	869	ILE
1	B	875	LYS
1	B	886	ASN
1	B	888	GLU
1	B	930	MET
1	B	934	PHE
1	B	937	SER
1	B	938	PHE
1	B	953	THR
1	B	955	ILE
1	B	956	ASP

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Mol	Chain	Res	Type
1	B	980	ASN
1	B	984	GLU
1	B	1001	ASN
1	B	1006	VAL
1	B	1013	MET
1	B	1024	LEU
1	B	1031	LYS
1	B	1048	LYS
1	B	1067	ARG
1	B	1071	ILE
1	B	1088	LEU
1	B	1231	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	858	ASN
1	A	865	ASN
1	A	928	ASN
1	A	1089	GLN
1	A	1112	ASN
1	A	1198	GLN
1	B	858	ASN
1	B	886	ASN
1	B	928	ASN
1	B	980	ASN
1	B	1089	GLN
1	B	1135	ASN
1	B	1212	GLN
1	B	1223	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	1	-	4,4,4	0.45	0	6,6,6	0.70	0
2	SO4	A	2	-	4,4,4	0.53	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
2	SO4	A	1	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	418/438 (95%)	0.34	16 (3%)	44 18	25, 56, 140, 194	1 (0%)
1	B	418/438 (95%)	0.91	63 (15%)	3 1	49, 93, 149, 204	1 (0%)
All	All	836/876 (95%)	0.63	79 (9%)	11 4	25, 75, 146, 204	2 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	858	ASN	11.1
1	B	931	TYR	6.1
1	B	858	ASN	5.8
1	A	931	TYR	5.7
1	B	860	TYR	5.2
1	B	1139	ASN	4.9
1	A	927	TYR	4.8
1	B	1170	ILE	4.6
1	A	861	PHE	4.0
1	B	912	ASP	3.9
1	B	1090	TYR	3.9
1	A	912	ASP	3.9
1	A	930	MET	3.9
1	B	908	GLY	3.8
1	B	927	TYR	3.7
1	B	1152	ASN	3.6
1	B	928	ASN	3.6
1	B	978	LYS	3.6
1	B	964	TRP	3.6
1	B	1206	TYR	3.6
1	B	1016	MET	3.5
1	B	977	LEU	3.4
1	B	985	GLN	3.4
1	B	1151	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	913	ASP	3.3
1	B	1177	LEU	3.3
1	B	1270	LEU	3.2
1	B	1138	PHE	3.2
1	B	894	ASN	3.2
1	A	929	ALA	3.1
1	B	948	ASN	3.0
1	B	981	GLU	2.9
1	A	862	ASN	2.9
1	A	859	GLU	2.9
1	B	859	GLU	2.9
1	B	1179	MET	2.9
1	A	913	ASP	2.8
1	A	1035	GLY	2.8
1	B	1195	ALA	2.8
1	B	911	GLY	2.7
1	B	1171	ASP	2.7
1	B	1256	GLU	2.6
1	B	1026	ASP	2.5
1	B	961	ASN	2.5
1	B	1028	ILE	2.5
1	B	862	ASN	2.4
1	B	1051	ASN	2.4
1	B	1087	SER	2.4
1	B	1125	ASN	2.4
1	B	1136	ASN	2.4
1	B	930	MET	2.4
1	B	1196	LEU	2.4
1	B	910	SER	2.4
1	A	860	TYR	2.4
1	B	968	ILE	2.4
1	B	1032	GLU	2.4
1	B	1038	PHE	2.3
1	A	926	VAL	2.3
1	B	1137	ASP	2.3
1	B	1193	LEU	2.3
1	B	861	PHE	2.3
1	B	1189	ASP	2.3
1	B	1044	PHE	2.3
1	B	982	ASN	2.3
1	B	1251	TYR	2.3
1	B	917	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1153	THR	2.3
1	B	1013	MET	2.2
1	B	984	GLU	2.2
1	B	932	GLU	2.2
1	A	1026	ASP	2.2
1	B	1264	ILE	2.2
1	B	918	ILE	2.1
1	B	1025	ILE	2.1
1	A	916	LYS	2.1
1	B	1268	ALA	2.1
1	B	1247	LEU	2.1
1	A	891	VAL	2.0
1	B	1014	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	1	5/5	0.97	0.14	-1.08	39,39,40,40	0
2	SO4	A	2	5/5	0.95	0.13	-2.62	72,73,76,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.