



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:29 AM GMT

PDB ID : 3AZV
Title : Crystal structure of the receptor binding domain
Authors : Nuemket, N.; Tanaka, Y.; Tsukamoto, K.; Tsuji, T.; Nakamura, K.; Kozaki, S.; Yao, M.; Tanaka, I.
Deposited on : 2011-06-02
Resolution : 3.10 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

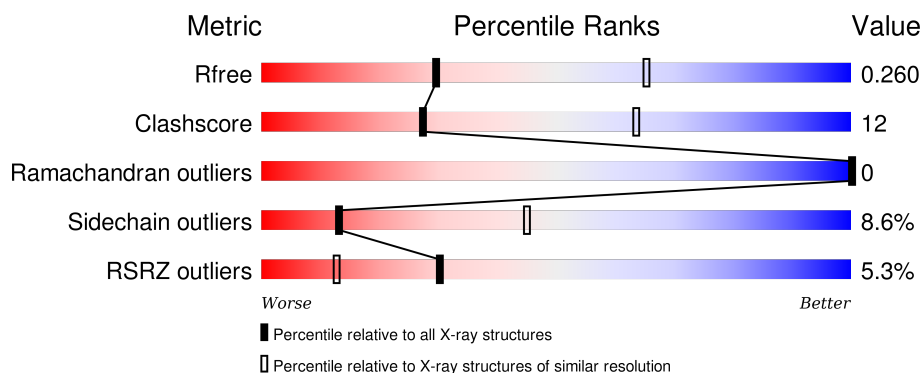
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	443	<div> <div>3%</div> <div>72%</div> <div>21%</div> <div>6%</div> </div>
1	B	443	<div> <div>7%</div> <div>68%</div> <div>22%</div> <div>6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6889 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	Se	0	0	0
			3426	2199	566	647	1	13			
1	B	418	Total	C	N	O	S	Se	0	0	0
			3426	2199	566	647	1	13			

There are 28 discrepancies between the modelled and reference sequences:

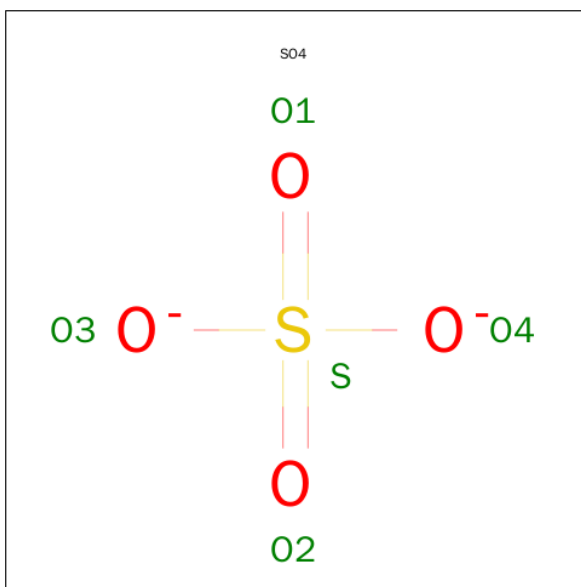
Chain	Residue	Modelled	Actual	Comment	Reference
A	851	MSE	-	EXPRESSION TAG	UNP A5JGM8
A	852	GLU	-	EXPRESSION TAG	UNP A5JGM8
A	853	TYR	-	EXPRESSION TAG	UNP A5JGM8
A	854	PHE	-	EXPRESSION TAG	UNP A5JGM8
A	855	ASN	-	EXPRESSION TAG	UNP A5JGM8
A	856	ASN	-	EXPRESSION TAG	UNP A5JGM8
A	1286	LEU	-	EXPRESSION TAG	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	851	MSE	-	EXPRESSION TAG	UNP A5JGM8
B	852	GLU	-	EXPRESSION TAG	UNP A5JGM8
B	853	TYR	-	EXPRESSION TAG	UNP A5JGM8
B	854	PHE	-	EXPRESSION TAG	UNP A5JGM8
B	855	ASN	-	EXPRESSION TAG	UNP A5JGM8
B	856	ASN	-	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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		

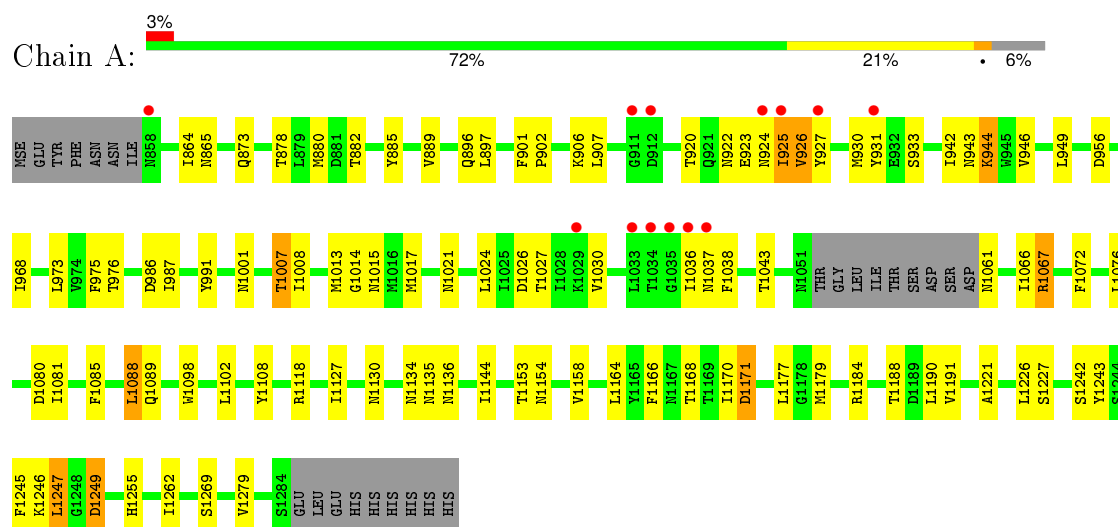
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	9	Total	O	0	0
			9	9		

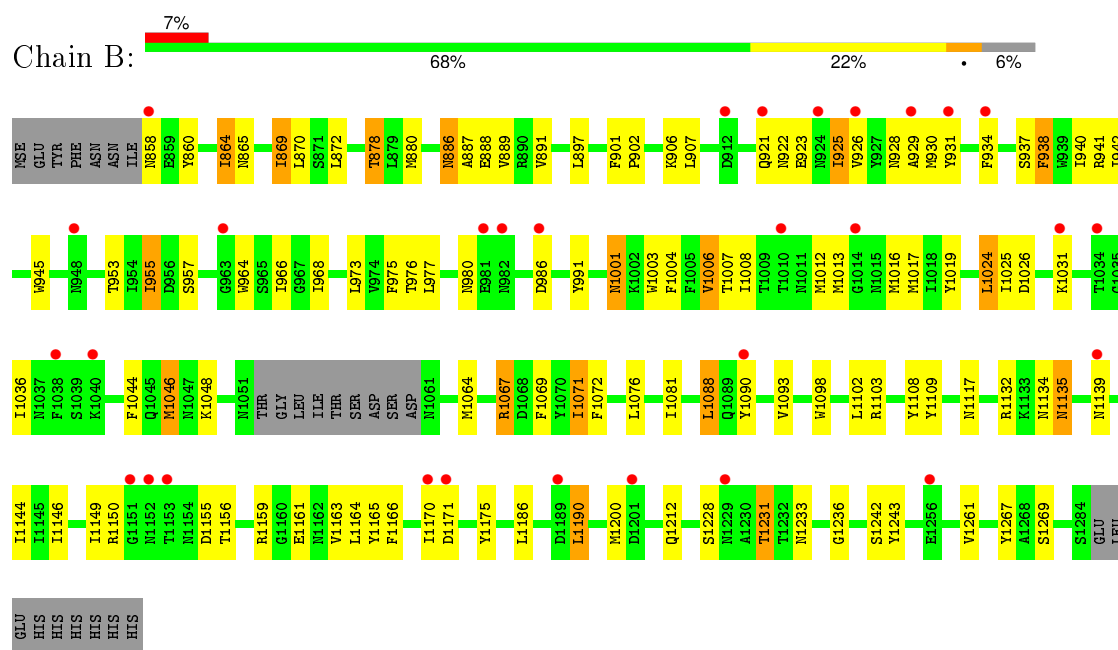
3 Residue-property plots

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 ($RSRZ > 2$). 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: D/C mosaic neurotoxin



• Molecule 1: D/C mosaic neurotoxin



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 138.57Å 162.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.46 – 3.10 44.46 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.46-3.10) 99.3 (44.46-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.6.0091	Depositor
R, R_{free}	0.250 , 0.286 0.233 , 0.260	Depositor DCC
R_{free} test set	1252 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	70.2	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 24383 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6889	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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	0/3492	0.57	0/4704
1	B	0.39	0/3492	0.55	0/4704
All	All	0.41	0/6984	0.56	0/9408

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	78	0
1	B	3426	0	3342	83	0
2	A	10	0	0	1	0
3	A	18	0	0	0	0
3	B	9	0	0	0	0
All	All	6889	0	6684	161	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 12.

All (161) 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:1179:MSE:HE1	1:A:1226:LEU:CD2	1.68	1.22
1:A:1179:MSE:HE1	1:A:1226:LEU:HD21	1.18	1.12
1:A:1179:MSE:CE	1:A:1226:LEU:CD2	2.47	0.92
1:B:922:ASN:O	1:B:926:VAL:HG13	1.69	0.92
1:B:1046:MSE:HE1	1:B:1064:MSE:HB3	1.55	0.87
1:A:1179:MSE:CE	1:A:1226:LEU:CD1	2.53	0.87
1:B:1046:MSE:HE2	1:B:1064:MSE:HE2	1.54	0.86
1:A:1017:MSE:HE2	1:A:1024:LEU:HD11	1.58	0.85
1:A:942:ILE:HD13	1:A:968:ILE:HD13	1.60	0.83
1:B:864:ILE:HD11	1:B:1072:PHE:CE1	2.13	0.82
1:B:955:ILE:HG23	1:B:966:ILE:HB	1.64	0.80
1:A:1017:MSE:CE	1:A:1024:LEU:HD11	2.13	0.79
1:B:1012:MSE:HE1	1:B:1036:ILE:HG21	1.65	0.77
1:A:1179:MSE:HE3	1:A:1226:LEU:HD11	1.66	0.76
1:A:1007:THR:HG21	1:A:1081:ILE:CD1	2.15	0.76
1:B:1007:THR:HG23	1:B:1019:TYR:HB2	1.66	0.76
1:A:1179:MSE:CE	1:A:1226:LEU:HD11	2.17	0.74
1:A:922:ASN:HB2	1:A:925:ILE:HD11	1.68	0.74
1:A:1017:MSE:HE2	1:A:1024:LEU:CD1	2.18	0.73
1:A:1179:MSE:CE	1:A:1226:LEU:HD22	2.19	0.71
1:B:1012:MSE:CE	1:B:1036:ILE:HG21	2.21	0.71
1:A:1127:ILE:CD1	1:A:1177:LEU:HD22	2.20	0.70
1:A:1067:ARG:NH1	1:A:1088:LEU:O	2.25	0.68
1:B:1149:ILE:HG22	1:B:1150:ARG:HG2	1.76	0.68
1:A:1179:MSE:HE3	1:A:1226:LEU:CD1	2.21	0.68
1:B:1190:LEU:HD23	1:B:1261:VAL:HG21	1.75	0.67
1:B:940:ILE:HG23	1:B:1004:PHE:CE2	2.29	0.67
1:A:885:TYR:CD1	1:A:925:ILE:HG21	2.30	0.66
1:B:1067:ARG:NH1	1:B:1088:LEU:O	2.28	0.66
1:B:968:ILE:HG23	1:B:973:LEU:HD12	1.78	0.65
1:A:1127:ILE:HD13	1:A:1177:LEU:HD22	1.79	0.64
1:B:1190:LEU:HD23	1:B:1261:VAL:CG2	2.28	0.64
1:A:1179:MSE:CE	1:A:1226:LEU:HD13	2.29	0.63
1:B:1007:THR:CG2	1:B:1019:TYR:HB2	2.28	0.63
1:A:942:ILE:CD1	1:A:968:ILE:HD13	2.29	0.63
1:B:955:ILE:HD12	1:B:1044:PHE:CE1	2.35	0.62
1:A:1127:ILE:CD1	1:A:1177:LEU:CD2	2.77	0.61
1:A:1007:THR:HG21	1:A:1081:ILE:HD12	1.83	0.61
1:B:891:VAL:O	1:B:891:VAL:HG13	2.01	0.61
1:B:864:ILE:HD11	1:B:1072:PHE:CZ	2.35	0.60
1:B:886:ASN:HD22	1:B:887:ALA:N	1.99	0.60
1:B:921:GLN:HG3	1:B:926:VAL:HG11	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1103:ARG:HG3	1:B:1156:THR:HG22	1.84	0.59
1:B:864:ILE:CD1	1:B:1072:PHE:CE1	2.86	0.58
1:A:1102:LEU:HD12	1:A:1108:TYR:CZ	2.38	0.58
1:B:1046:MSE:CE	1:B:1064:MSE:HB3	2.28	0.58
1:A:1007:THR:HG21	1:A:1081:ILE:HD13	1.86	0.58
1:B:901:PHE:CG	1:B:902:PRO:HA	2.39	0.58
1:B:1228:SER:O	1:B:1231:THR:HG22	2.04	0.57
1:B:1231:THR:HG23	1:B:1233:ASN:H	1.70	0.57
1:B:1135:ASN:HD22	1:B:1135:ASN:N	2.03	0.56
1:A:1170:ILE:HG22	1:A:1171:ASP:N	2.21	0.56
1:B:938:PHE:CE2	1:B:1006:VAL:HG13	2.41	0.56
1:A:901:PHE:CG	1:A:902:PRO:HA	2.41	0.55
1:B:880:MSE:HA	1:B:889:VAL:HG11	1.87	0.55
1:B:869:ILE:HD13	1:B:929:ALA:HB1	1.89	0.55
1:B:942:ILE:HD11	1:B:945:TRP:CD2	2.41	0.54
1:A:976:THR:HG22	1:A:986:ASP:HB3	1.88	0.54
1:A:1072:PHE:CD2	1:A:1076:LEU:HD11	2.43	0.53
1:A:1179:MSE:HE1	1:A:1226:LEU:CG	2.38	0.52
1:B:1072:PHE:CD2	1:B:1076:LEU:HD11	2.44	0.52
1:A:906:LYS:O	1:A:907:LEU:HD12	2.10	0.52
1:A:922:ASN:O	1:A:926:VAL:HG12	2.09	0.52
1:B:1161:GLU:CD	1:B:1212:GLN:HE22	2.12	0.52
1:B:1117:ASN:O	1:B:1132:ARG:HG2	2.10	0.52
1:A:1179:MSE:HE2	1:A:1226:LEU:HD22	1.92	0.51
1:A:987:ILE:HD11	1:A:1026:ASP:O	2.10	0.51
1:B:977:LEU:HD11	1:B:1016:MSE:SE	2.61	0.51
1:B:977:LEU:HD12	1:B:977:LEU:N	2.26	0.51
1:B:1102:LEU:HD12	1:B:1108:TYR:CZ	2.46	0.51
1:B:977:LEU:CD1	1:B:1016:MSE:SE	3.09	0.51
1:B:886:ASN:C	1:B:886:ASN:HD22	2.14	0.50
1:A:1245:PHE:CE1	1:A:1247:LEU:HD13	2.47	0.50
1:B:925:ILE:C	1:B:925:ILE:HD12	2.31	0.50
1:B:860:TYR:O	1:B:864:ILE:HG22	2.12	0.50
1:B:1024:LEU:HD23	1:B:1024:LEU:H	1.77	0.49
1:A:1017:MSE:CE	1:A:1024:LEU:CD1	2.84	0.49
1:A:901:PHE:CD1	1:A:902:PRO:HA	2.47	0.49
1:A:1164:LEU:C	1:A:1164:LEU:HD12	2.32	0.49
1:A:1001:ASN:HB2	1:A:1098:TRP:CZ3	2.47	0.49
1:B:1001:ASN:HD22	1:B:1001:ASN:N	2.10	0.49
1:B:878:THR:HG23	1:B:880:MSE:CE	2.42	0.49
1:A:1127:ILE:HD11	1:A:1177:LEU:CD2	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1144:ILE:HD13	1:B:1166:PHE:HD2	1.77	0.49
1:B:977:LEU:HD22	1:B:1016:MSE:HE2	1.95	0.49
1:A:968:ILE:HG23	1:A:973:LEU:HD12	1.95	0.48
1:A:923:GLU:O	1:A:926:VAL:HG13	2.13	0.48
1:B:976:THR:HG22	1:B:986:ASP:OD1	2.14	0.48
1:B:1046:MSE:HE1	1:B:1064:MSE:CB	2.36	0.47
1:A:1118:ARG:HA	1:A:1130:ASN:O	2.15	0.47
1:A:975:PHE:CG	1:A:1008:ILE:HD13	2.48	0.47
1:A:1153:THR:HG22	1:A:1154:ASN:N	2.30	0.47
1:B:1146:ILE:HG23	1:B:1164:LEU:HD13	1.95	0.47
1:A:930:MSE:HE1	1:A:1037:ASN:OD1	2.14	0.47
1:B:1165:TYR:OH	1:B:1200:MSE:HE1	2.14	0.47
1:A:1144:ILE:HG22	1:A:1168:THR:HB	1.97	0.47
1:B:1046:MSE:CE	1:B:1064:MSE:HE2	2.36	0.47
1:A:1179:MSE:HE1	1:A:1226:LEU:CD1	2.35	0.46
1:A:1245:PHE:CE1	1:A:1247:LEU:CD1	2.98	0.46
1:A:1190:LEU:HD21	1:A:1243:TYR:OH	2.15	0.46
1:B:1007:THR:HG21	1:B:1081:ILE:HG23	1.98	0.46
1:B:1149:ILE:HB	1:B:1163:VAL:HG12	1.97	0.46
1:B:1001:ASN:HB2	1:B:1098:TRP:CZ3	2.50	0.46
1:B:869:ILE:HD13	1:B:929:ALA:CB	2.46	0.46
1:A:1249:ASP:N	1:A:1249:ASP:OD1	2.48	0.45
1:B:1186:LEU:HD22	1:B:1243:TYR:HB3	1.98	0.45
1:A:1134:ASN:ND2	1:A:1136:ASN:HB2	2.31	0.45
1:A:1221:ALA:HB2	1:A:1279:VAL:HG12	1.99	0.45
1:A:975:PHE:CE1	1:A:1008:ILE:HG21	2.51	0.45
1:A:880:MSE:HA	1:A:889:VAL:HG11	1.99	0.45
1:B:872:LEU:HB3	1:B:1069:PHE:HB3	1.99	0.44
1:B:942:ILE:HG13	1:B:945:TRP:HB2	2.00	0.44
1:A:987:ILE:HD11	1:A:1026:ASP:C	2.37	0.44
1:A:930:MSE:HG2	1:A:1038:PHE:HB2	1.98	0.44
1:B:906:LYS:O	1:B:907:LEU:HD12	2.18	0.44
1:B:1090:TYR:CD2	1:B:1093:VAL:HG23	2.53	0.44
1:B:938:PHE:CZ	1:B:1006:VAL:HG11	2.53	0.44
1:B:1090:TYR:HD2	1:B:1093:VAL:HG23	1.83	0.43
1:A:873:GLN:OE1	1:A:882:THR:HG21	2.18	0.43
1:B:1155:ASP:OD1	1:B:1159:ARG:NH1	2.44	0.43
1:B:1170:ILE:HG22	1:B:1171:ASP:N	2.34	0.43
1:A:1017:MSE:HE3	1:A:1024:LEU:HD11	1.93	0.43
1:A:942:ILE:HD13	1:A:968:ILE:CD1	2.38	0.43
1:A:926:VAL:HG22	1:A:927:TYR:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:968:ILE:CG2	1:B:973:LEU:HD12	2.46	0.43
1:B:1025:ILE:HG22	1:B:1026:ASP:N	2.32	0.43
1:B:1170:ILE:HD13	1:B:1175:TYR:CD2	2.53	0.43
1:A:885:TYR:CE1	1:A:925:ILE:HG21	2.54	0.43
1:A:1007:THR:CG2	1:A:1081:ILE:HD12	2.48	0.43
1:A:1127:ILE:HD13	1:A:1177:LEU:CD2	2.45	0.43
1:B:938:PHE:CZ	1:B:1006:VAL:CG1	3.02	0.43
1:A:1144:ILE:HD13	1:A:1166:PHE:HD2	1.84	0.43
1:B:1236:GLY:HA2	1:B:1267:TYR:CE2	2.54	0.43
1:B:1007:THR:HG21	1:B:1081:ILE:HD12	2.01	0.42
1:A:1061:ASN:HD22	1:A:1061:ASN:N	2.17	0.42
1:B:941:ARG:HD3	1:B:1003:TRP:CD1	2.54	0.42
1:B:1134:ASN:OD1	1:B:1134:ASN:N	2.53	0.42
1:B:907:LEU:HD22	1:B:1064:MSE:HE3	2.02	0.42
1:A:1179:MSE:HE2	1:A:1262:ILE:HD12	2.02	0.42
1:A:946:VAL:HG23	1:A:949:LEU:N	2.35	0.42
1:B:870:LEU:HB3	1:B:1071:ILE:HG22	2.02	0.42
1:A:864:ILE:HD11	1:A:1080:ASP:CG	2.40	0.42
1:A:1021:ASN:HA	1:A:1085:PHE:CE1	2.55	0.42
1:A:1144:ILE:C	1:A:1144:ILE:HD12	2.40	0.42
1:B:860:TYR:O	1:B:864:ILE:CG2	2.68	0.41
1:A:926:VAL:HG23	1:A:930:MSE:HG3	2.02	0.41
1:B:938:PHE:N	1:B:938:PHE:CD2	2.89	0.41
1:A:943:ASN:OD1	1:A:944:LYS:N	2.53	0.41
1:B:977:LEU:HD13	1:B:1016:MSE:SE	2.71	0.41
1:A:1015:ASN:ND2	1:A:1027:THR:OG1	2.53	0.41
1:A:1014:GLY:O	1:A:1030:VAL:HG12	2.21	0.41
1:A:1007:THR:CG2	1:A:1081:ILE:CD1	2.93	0.41
1:B:977:LEU:HD22	1:B:1016:MSE:CE	2.50	0.41
1:B:975:PHE:CG	1:B:1008:ILE:HD13	2.55	0.41
1:B:923:GLU:O	1:B:926:VAL:HG22	2.20	0.41
1:B:957:SER:HB3	1:B:964:TRP:CE2	2.56	0.41
1:A:1255:HIS:HE1	2:A:1:SO4:O3	2.03	0.40
1:A:1036:ILE:HG23	1:A:1036:ILE:O	2.21	0.40
1:B:901:PHE:CD1	1:B:902:PRO:HA	2.57	0.40
1:A:1066:ILE:HG22	1:A:1067:ARG:N	2.36	0.40
1:B:1109:TYR:CZ	1:B:1139:ASN:HA	2.57	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	414/443 (94%)	387 (94%)	27 (6%)	0	100	100
1	B	414/443 (94%)	386 (93%)	28 (7%)	0	100	100
All	All	828/886 (94%)	773 (93%)	55 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	383/393 (98%)	352 (92%)	31 (8%)	15	47
1	B	383/393 (98%)	348 (91%)	35 (9%)	12	40
All	All	766/786 (98%)	700 (91%)	66 (9%)	13	45

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	865	ASN
1	A	878	THR
1	A	896	GLN
1	A	897	LEU
1	A	920	THR
1	A	924	ASN
1	A	925	ILE
1	A	926	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	931	TYR
1	A	933	SER
1	A	944	LYS
1	A	956	ASP
1	A	991	TYR
1	A	1007	THR
1	A	1013	MSE
1	A	1043	THR
1	A	1067	ARG
1	A	1088	LEU
1	A	1089	GLN
1	A	1135	ASN
1	A	1158	VAL
1	A	1171	ASP
1	A	1184	ARG
1	A	1188	THR
1	A	1191	VAL
1	A	1227	SER
1	A	1242	SER
1	A	1246	LYS
1	A	1247	LEU
1	A	1249	ASP
1	A	1269	SER
1	B	858	ASN
1	B	864	ILE
1	B	865	ASN
1	B	869	ILE
1	B	878	THR
1	B	886	ASN
1	B	888	GLU
1	B	897	LEU
1	B	925	ILE
1	B	928	ASN
1	B	930	MSE
1	B	931	TYR
1	B	934	PHE
1	B	937	SER
1	B	938	PHE
1	B	953	THR
1	B	955	ILE
1	B	980	ASN
1	B	991	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1001	ASN
1	B	1006	VAL
1	B	1013	MSE
1	B	1017	MSE
1	B	1024	LEU
1	B	1031	LYS
1	B	1046	MSE
1	B	1048	LYS
1	B	1067	ARG
1	B	1071	ILE
1	B	1088	LEU
1	B	1135	ASN
1	B	1190	LEU
1	B	1231	THR
1	B	1242	SER
1	B	1269	SER

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

Mol	Chain	Res	Type
1	A	858	ASN
1	A	865	ASN
1	A	928	ASN
1	A	1015	ASN
1	A	1089	GLN
1	A	1112	ASN
1	A	1134	ASN
1	A	1136	ASN
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	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	0.42	0	6,6,6	0.73	0
2	SO4	A	2	-	4,4,4	0.50	0	6,6,6	0.26	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	SO4	1	0

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, 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	405/443 (91%)	0.13	13 (3%) 51 27	19, 56, 157, 214	0
1	B	405/443 (91%)	0.47	30 (7%) 17 6	41, 97, 171, 220	0
All	All	810/886 (91%)	0.30	43 (5%) 30 13	19, 80, 168, 220	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1035	GLY	11.9
1	A	1034	THR	8.2
1	A	858	ASN	5.7
1	A	1036	ILE	5.1
1	B	1152	ASN	4.9
1	B	1170	ILE	4.5
1	B	931	TYR	4.2
1	A	931	TYR	4.1
1	B	858	ASN	3.8
1	B	1151	GLY	3.5
1	A	1037	ASN	3.3
1	B	1010	THR	3.3
1	B	1040	LYS	3.2
1	B	921	GLN	3.2
1	B	981	GLU	3.0
1	A	1029	LYS	2.8
1	B	1171	ASP	2.8
1	B	1139	ASN	2.8
1	A	927	TYR	2.8
1	B	982	ASN	2.8
1	B	1014	GLY	2.7
1	B	924	ASN	2.6
1	A	912	ASP	2.6
1	B	1256	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1031	LYS	2.6
1	B	934	PHE	2.5
1	B	926	VAL	2.5
1	B	929	ALA	2.4
1	A	1033	LEU	2.4
1	B	1153	THR	2.4
1	B	1034	THR	2.4
1	B	1201	ASP	2.4
1	B	948	ASN	2.3
1	B	1038	PHE	2.3
1	B	1090	TYR	2.2
1	B	912	ASP	2.2
1	B	986	ASP	2.2
1	B	1189	ASP	2.2
1	A	925	ILE	2.1
1	B	1229	ASN	2.1
1	B	963	GLY	2.0
1	A	911	GLY	2.0
1	A	924	ASN	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	2	5/5	0.92	0.19	-0.57	62,65,67,67	0
2	SO4	A	1	5/5	0.95	0.15	-1.23	37,38,39,39	0

6.5 Other polymers

There are no such residues in this entry.