



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:18 AM UTC

PDB ID : 4FBK / pdb_00004fbk
Title : Crystal structure of a covalently fused Nbs1-Mre11 complex with one manganese ion per active site
Authors : Schiller, C.B.; Lammens, K.; Hopfner, K.P.
Deposited on : 2012-05-23
Resolution : 2.38 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

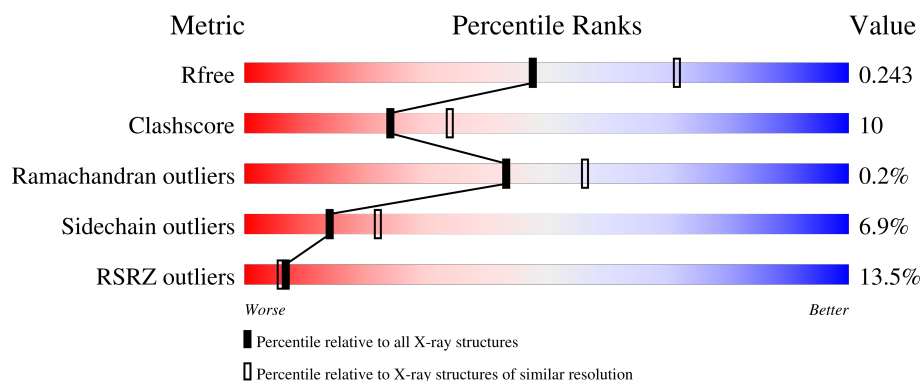
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	472	9% 72% 16% • 10%
1	B	472	15% 66% 16% • 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6934 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 DNA repair and telomere maintenance protein nbs1, DNA repair protein rad32 CHIMERIC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	98	0	0
			3428	2181	597	642	8			
1	B	406	Total	C	N	O	S	123	0	0
			3274	2085	569	612	8			

There are 30 discrepancies between the modelled and reference sequences:

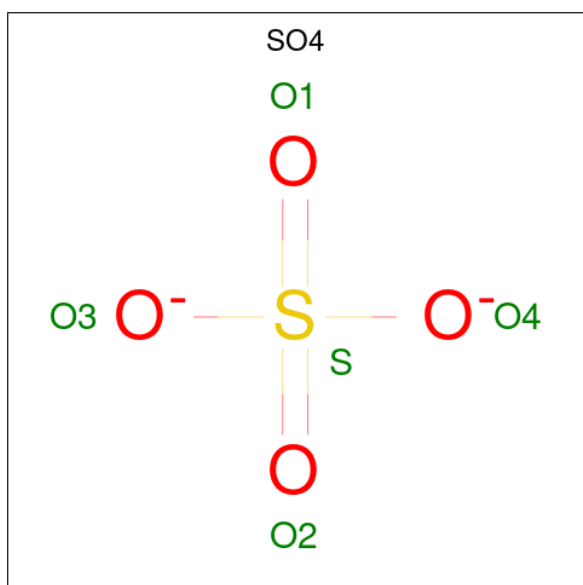
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP O43070
A	-3	PRO	-	expression tag	UNP O43070
A	-2	LEU	-	expression tag	UNP O43070
A	-1	GLY	-	expression tag	UNP O43070
A	0	SER	-	expression tag	UNP O43070
A	532	VAL	-	linker	UNP Q09683
A	533	ASP	-	linker	UNP Q09683
A	534	GLY	-	linker	UNP Q09683
A	535	SER	-	linker	UNP Q09683
A	536	ALA	-	linker	UNP Q09683
A	537	GLY	-	linker	UNP Q09683
A	538	SER	-	linker	UNP Q09683
A	539	ALA	-	linker	UNP Q09683
A	540	GLY	-	linker	UNP Q09683
A	541	SER	-	linker	UNP Q09683
B	-4	GLY	-	expression tag	UNP O43070
B	-3	PRO	-	expression tag	UNP O43070
B	-2	LEU	-	expression tag	UNP O43070
B	-1	GLY	-	expression tag	UNP O43070
B	0	SER	-	expression tag	UNP O43070
B	532	VAL	-	linker	UNP Q09683
B	533	ASP	-	linker	UNP Q09683
B	534	GLY	-	linker	UNP Q09683
B	535	SER	-	linker	UNP Q09683

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	536	ALA	-	linker	UNP Q09683
B	537	GLY	-	linker	UNP Q09683
B	538	SER	-	linker	UNP Q09683
B	539	ALA	-	linker	UNP Q09683
B	540	GLY	-	linker	UNP Q09683
B	541	SER	-	linker	UNP Q09683

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0

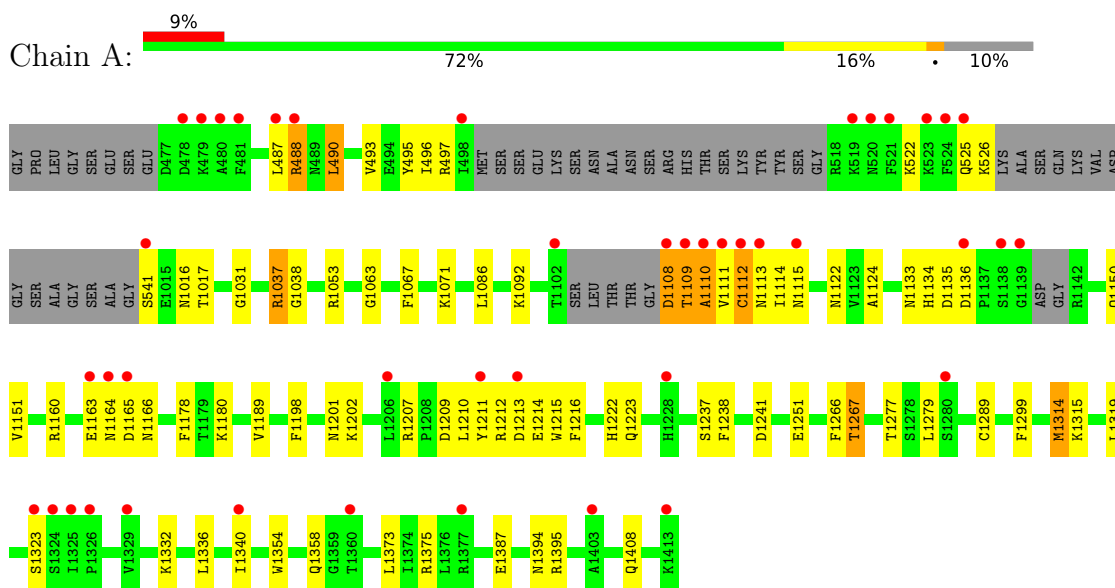
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total 121	O 121	0	0
4	B	89	Total 89	O 89	0	0

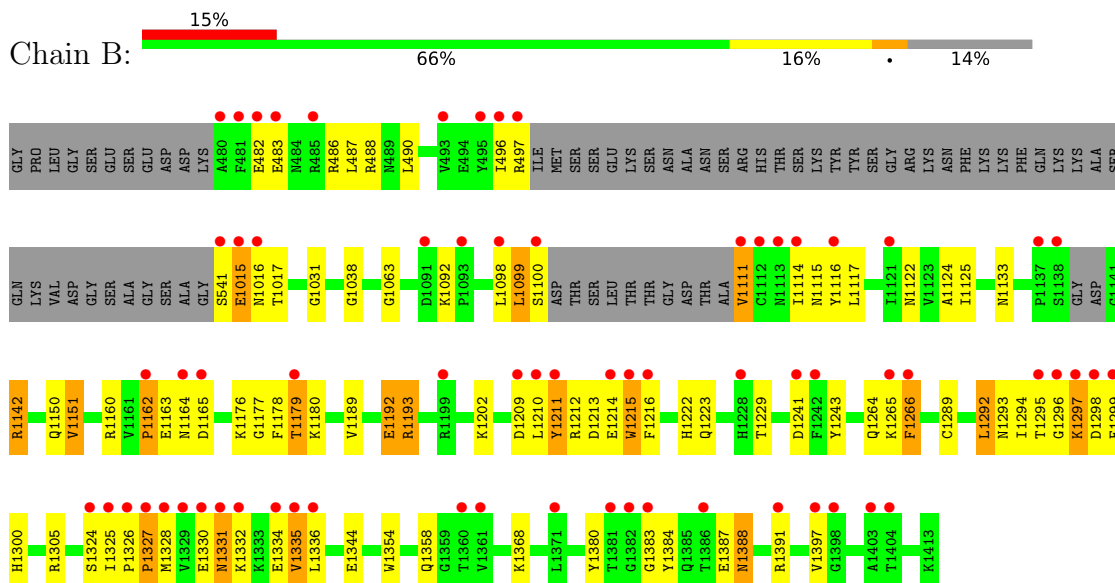
3 Residue-property plots

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: DNA repair and telomere maintenance protein nbs1,DNA repair protein rad32 CHIMERIC PROTEIN



- Molecule 1: DNA repair and telomere maintenance protein nbs1,DNA repair protein rad32 CHIMERIC PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.26Å 78.87Å 222.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.88 – 2.38 47.88 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.88-2.38) 99.5 (47.88-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.222 , 0.242 0.221 , 0.243	Depositor DCC
R_{free} test set	2000 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6934	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: SO4, MN

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	0.77	1/3503 (0.0%)	1.26	20/4746 (0.4%)
1	B	0.71	0/3348	1.24	18/4543 (0.4%)
All	All	0.74	1/6851 (0.0%)	1.25	38/9289 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1314	MET	SD-CE	-5.36	1.66	1.79

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1299	PHE	N-CA-CB	-10.41	95.11	111.56
1	A	1114	ILE	CB-CA-C	9.78	124.77	110.98
1	B	1162	PRO	CA-N-CD	-9.65	98.49	112.00
1	A	1216	PHE	N-CA-C	-9.64	92.80	108.52
1	B	1388	ASN	N-CA-C	-8.63	98.93	109.72
1	A	1109	THR	N-CA-CB	-8.21	97.53	111.50
1	B	1215	TRP	N-CA-C	7.74	121.27	108.96
1	A	1110	ALA	N-CA-C	-7.43	104.36	113.50
1	A	1108	ASP	CB-CA-C	-7.36	96.11	110.10
1	A	1031	GLY	CA-C-N	6.99	129.95	120.38
1	A	1031	GLY	C-N-CA	6.99	129.95	120.38
1	A	1266	PHE	CA-CB-CG	6.82	120.62	113.80
1	B	496	ILE	CB-CA-C	6.81	120.87	111.34
1	A	1135	ASP	CA-C-N	6.59	130.70	120.68
1	A	1135	ASP	C-N-CA	6.59	130.70	120.68
1	B	1031	GLY	CA-C-N	6.56	129.37	120.38
1	B	1031	GLY	C-N-CA	6.56	129.37	120.38
1	B	1298	ASP	CB-CA-C	-6.54	98.38	109.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1136	ASP	CA-CB-CG	6.28	118.88	112.60
1	B	1214	GLU	N-CA-CB	-6.20	100.77	110.44
1	B	1214	GLU	CB-CA-C	6.16	122.05	109.55
1	A	1114	ILE	CA-C-N	5.99	132.97	121.54
1	A	1114	ILE	C-N-CA	5.99	132.97	121.54
1	A	1114	ILE	N-CA-C	-5.93	99.87	108.71
1	B	1038	GLY	N-CA-C	5.60	119.66	112.83
1	A	1241	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	1241	ASP	CA-CB-CG	5.53	118.13	112.60
1	B	482	GLU	CA-C-N	5.38	127.49	120.28
1	B	482	GLU	C-N-CA	5.38	127.49	120.28
1	B	1289	CYS	N-CA-C	-5.35	101.99	109.69
1	A	1038	GLY	N-CA-C	5.25	119.24	112.83
1	B	1387	GLU	CB-CA-C	5.25	122.09	111.60
1	B	1380	TYR	N-CA-C	5.24	119.26	111.87
1	A	1109	THR	N-CA-C	5.23	125.64	111.00
1	B	1216	PHE	N-CA-C	-5.14	102.03	109.59
1	A	1289	CYS	N-CA-C	-5.08	102.37	109.69
1	A	1037	ARG	CA-C-N	5.01	125.64	120.03
1	A	1037	ARG	C-N-CA	5.01	125.64	120.03

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	3428	0	3393	43	0
1	B	3274	0	3238	88	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	121	0	0	0	0
4	B	89	0	0	0	0
All	All	6934	0	6631	129	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 (129) 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:1108:ASP:CB	1:A:1109:THR:HA	1.54	1.31
1:A:1108:ASP:HB3	1:A:1109:THR:CA	1.46	1.29
1:B:1162:PRO:HD2	1:B:1163:GLU:H	1.09	1.08
1:B:1326:PRO:HD2	1:B:1334:GLU:HG2	1.44	0.96
1:B:1211:TYR:O	1:B:1215:TRP:HD1	1.50	0.94
1:B:1211:TYR:HB2	1:B:1215:TRP:HE1	1.31	0.93
1:B:541:SER:HB2	1:B:1017:THR:HB	1.51	0.89
1:B:1266:PHE:O	1:B:1266:PHE:HD2	1.53	0.89
1:B:1162:PRO:HD2	1:B:1163:GLU:N	1.88	0.89
1:A:1108:ASP:HB3	1:A:1109:THR:HA	0.88	0.87
1:B:1383:GLY:O	1:B:1384:TYR:CD2	2.28	0.87
1:B:1016:ASN:ND2	1:B:1177:GLY:HA3	1.88	0.85
1:B:1292:LEU:CD2	1:B:1294:ILE:HG13	2.06	0.85
1:B:1114:ILE:HG21	1:B:1116:TYR:CE1	2.11	0.84
1:B:1331:ASN:O	1:B:1335:VAL:HG23	1.77	0.83
1:B:1292:LEU:HD21	1:B:1294:ILE:HG13	1.60	0.83
1:B:1211:TYR:O	1:B:1215:TRP:CD1	2.30	0.83
1:B:1162:PRO:CD	1:B:1163:GLU:H	1.93	0.80
1:B:1266:PHE:O	1:B:1266:PHE:CD2	2.34	0.80
1:B:1211:TYR:HB2	1:B:1215:TRP:NE1	1.98	0.78
1:A:1108:ASP:CB	1:A:1109:THR:CA	2.30	0.78
1:A:1067:PHE:O	1:A:1134:HIS:HE1	1.67	0.76
1:B:1383:GLY:C	1:B:1384:TYR:CD2	2.63	0.76
1:B:1016:ASN:HD22	1:B:1177:GLY:HA3	1.48	0.75
1:A:1108:ASP:CG	1:A:1109:THR:HA	2.12	0.75
1:B:1292:LEU:C	1:B:1292:LEU:HD23	2.11	0.75
1:A:525:GLN:O	1:B:1122:ASN:ND2	2.20	0.75
1:A:1165:ASP:O	1:A:1202:LYS:HB3	1.86	0.74
1:B:1016:ASN:O	1:B:1179:THR:CG2	2.37	0.73
1:B:1332:LYS:O	1:B:1336:LEU:HD13	1.89	0.72
1:B:1016:ASN:HD22	1:B:1178:PHE:H	1.39	0.69
1:B:1098:LEU:C	1:B:1099:LEU:HD12	2.18	0.69
1:A:488:ARG:HA	1:A:1237:SER:O	1.94	0.68
1:B:1266:PHE:HD2	1:B:1266:PHE:C	2.02	0.67
1:B:1266:PHE:CD2	1:B:1266:PHE:C	2.73	0.66
1:B:1016:ASN:O	1:B:1179:THR:HG21	1.96	0.66
1:B:1162:PRO:CD	1:B:1163:GLU:N	2.57	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1114:ILE:CG2	1:B:1116:TYR:CD1	2.80	0.64
1:B:1115:ASN:OD1	1:B:1116:TYR:N	2.30	0.64
1:A:522:LYS:HE3	1:A:1122:ASN:ND2	2.14	0.63
1:B:1016:ASN:HD22	1:B:1177:GLY:CA	2.12	0.63
1:B:1179:THR:HB	1:B:1296:GLY:H	1.63	0.63
1:A:1108:ASP:CG	1:A:1110:ALA:H	2.05	0.63
1:B:1016:ASN:HD22	1:B:1178:PHE:N	1.96	0.63
1:A:541:SER:HB2	1:A:1017:THR:HB	1.81	0.63
1:A:1209:ASP:OD1	1:A:1210:LEU:N	2.32	0.62
1:B:1264:GLN:O	1:B:1265:LYS:HB2	1.99	0.62
1:B:1332:LYS:O	1:B:1336:LEU:CD1	2.49	0.61
1:B:1209:ASP:O	1:B:1212:ARG:NH1	2.34	0.61
1:A:1189:VAL:H	1:A:1223:GLN:HE22	1.48	0.61
1:B:1383:GLY:O	1:B:1384:TYR:CG	2.53	0.60
1:A:1063:GLY:O	1:A:1222:HIS:HD2	1.84	0.60
1:B:1133:ASN:H	1:B:1222:HIS:CE1	2.20	0.60
1:B:1292:LEU:CD2	1:B:1292:LEU:C	2.74	0.59
1:B:1016:ASN:ND2	1:B:1177:GLY:CA	2.63	0.59
1:A:1111:VAL:HG12	1:A:1112:CYS:N	2.18	0.59
1:B:1189:VAL:H	1:B:1223:GLN:HE22	1.47	0.59
1:A:490:LEU:HD23	1:A:1198:PHE:HB3	1.84	0.59
1:B:487:LEU:HB3	1:B:490:LEU:HD11	1.84	0.59
1:A:1180:LYS:HB3	1:A:1215:TRP:CE3	2.39	0.58
1:B:1114:ILE:HG21	1:B:1116:TYR:CD1	2.40	0.57
1:A:1111:VAL:CG1	1:A:1112:CYS:N	2.68	0.57
1:A:1016:ASN:HD22	1:A:1178:PHE:H	1.53	0.57
1:A:1108:ASP:OD1	1:A:1110:ALA:N	2.33	0.56
1:B:1325:ILE:HG23	1:B:1334:GLU:HB3	1.87	0.56
1:B:1292:LEU:HD21	1:B:1294:ILE:CG1	2.35	0.56
1:B:1331:ASN:H	1:B:1331:ASN:ND2	2.04	0.55
1:A:1211:TYR:O	1:A:1214:GLU:HB2	2.06	0.55
1:B:1115:ASN:C	1:B:1117:LEU:H	2.15	0.55
1:B:1114:ILE:CG2	1:B:1116:TYR:CE1	2.88	0.55
1:A:1133:ASN:H	1:A:1222:HIS:CE1	2.25	0.55
1:B:1264:GLN:HB3	1:B:1266:PHE:CE1	2.43	0.54
1:B:1099:LEU:HD12	1:B:1099:LEU:N	2.23	0.54
1:B:1015:GLU:O	1:B:1176:LYS:HG2	2.09	0.53
1:B:1099:LEU:N	1:B:1099:LEU:CD1	2.71	0.52
1:A:1340:ILE:HD11	1:A:1395:ARG:HE	1.74	0.52
1:B:1328:MET:O	1:B:1328:MET:HG3	2.10	0.52
1:B:1116:TYR:O	1:B:1116:TYR:CD2	2.62	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1092:LYS:HB3	1:B:1124:ALA:HB1	1.92	0.51
1:A:1211:TYR:HB3	1:A:1214:GLU:CB	2.42	0.50
1:A:1037:ARG:HD3	1:A:1373:LEU:HD21	1.94	0.50
1:B:1292:LEU:HD23	1:B:1293:ASN:N	2.27	0.50
1:A:487:LEU:C	1:A:488:ARG:HG2	2.36	0.50
1:B:1326:PRO:CD	1:B:1334:GLU:HG2	2.31	0.50
1:B:1180:LYS:HB3	1:B:1215:TRP:CE3	2.48	0.48
1:A:1211:TYR:HB3	1:A:1214:GLU:HB3	1.96	0.48
1:A:1150:GLN:OE1	1:A:1160:ARG:NH2	2.46	0.48
1:B:488:ARG:HD2	1:B:1264:GLN:OE1	2.14	0.47
1:B:1150:GLN:OE1	1:B:1160:ARG:NH2	2.47	0.47
1:B:1209:ASP:O	1:B:1212:ARG:HG3	2.15	0.46
1:B:1016:ASN:O	1:B:1179:THR:HG23	2.14	0.46
1:B:1124:ALA:C	1:B:1125:ILE:HG13	2.40	0.46
1:B:1116:TYR:CD2	1:B:1116:TYR:C	2.93	0.46
1:B:1063:GLY:O	1:B:1222:HIS:HD2	1.97	0.46
1:A:1211:TYR:O	1:A:1214:GLU:N	2.48	0.46
1:B:1243:TYR:O	1:B:1266:PHE:HB3	2.16	0.45
1:A:490:LEU:HD22	1:A:1238:PHE:CG	2.51	0.45
1:A:522:LYS:HE3	1:A:1122:ASN:HD22	1.82	0.45
1:B:1354:TRP:O	1:B:1358:GLN:HG2	2.17	0.45
1:B:1264:GLN:CB	1:B:1266:PHE:CE1	3.01	0.44
1:A:1354:TRP:O	1:A:1358:GLN:HG2	2.17	0.44
1:B:1117:LEU:HD23	1:B:1117:LEU:HA	1.84	0.44
1:B:1327:PRO:HA	1:B:1328:MET:HA	1.65	0.44
1:A:522:LYS:CE	1:A:1122:ASN:ND2	2.79	0.44
1:B:1295:THR:HG22	1:B:1295:THR:O	2.17	0.44
1:B:1331:ASN:ND2	1:B:1331:ASN:N	2.66	0.43
1:B:1115:ASN:C	1:B:1117:LEU:N	2.76	0.43
1:A:1267:THR:HG21	1:A:1299:PHE:HZ	1.83	0.43
1:A:495:TYR:HA	1:A:1207:ARG:O	2.19	0.43
1:A:1336:LEU:HD11	1:A:1387:GLU:HB2	2.00	0.43
1:B:1165:ASP:O	1:B:1202:LYS:HB3	2.18	0.43
1:A:490:LEU:HD22	1:A:1238:PHE:CD1	2.53	0.43
1:B:1142:ARG:HH11	1:B:1142:ARG:H	1.66	0.42
1:B:1192:GLU:H	1:B:1192:GLU:HG3	1.55	0.42
1:B:1331:ASN:O	1:B:1332:LYS:C	2.63	0.42
1:B:1388:ASN:HD22	1:B:1391:ARG:H	1.66	0.42
1:B:1297:LYS:HA	1:B:1297:LYS:HD3	1.62	0.42
1:A:1086:LEU:HD21	1:B:1111:VAL:HG22	2.01	0.41
1:A:1279:LEU:O	1:A:1314:MET:HE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1179:THR:HB	1:B:1296:GLY:N	2.34	0.41
1:B:1099:LEU:HD22	1:B:1215:TRP:HH2	1.84	0.41
1:B:1331:ASN:O	1:B:1334:GLU:N	2.54	0.41
1:B:1383:GLY:C	1:B:1384:TYR:CG	2.96	0.41
1:A:1375:ARG:HH21	1:A:1408:GLN:HB2	1.85	0.41
1:B:1111:VAL:CG1	1:B:1151:VAL:HG23	2.51	0.41
1:B:1164:ASN:HB3	1:B:1193:ARG:HG2	2.03	0.41
1:B:1334:GLU:N	1:B:1334:GLU:OE1	2.54	0.41
1:A:1053:ARG:HE	1:A:1053:ARG:HB3	1.75	0.41
1:A:1092:LYS:HB3	1:A:1124:ALA:HB1	2.02	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	414/472 (88%)	402 (97%)	12 (3%)	0	100	100
1	B	398/472 (84%)	384 (96%)	12 (3%)	2 (0%)	24	34
All	All	812/944 (86%)	786 (97%)	24 (3%)	2 (0%)	43	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1327	PRO
1	B	1397	VAL

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	384/420 (91%)	359 (94%)	25 (6%)	15	24
1	B	367/420 (87%)	340 (93%)	27 (7%)	13	19
All	All	751/840 (89%)	699 (93%)	52 (7%)	14	22

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	488	ARG
1	A	490	LEU
1	A	493	VAL
1	A	496	ILE
1	A	497	ARG
1	A	526	LYS
1	A	1071	LYS
1	A	1112	CYS
1	A	1113	ASN
1	A	1115	ASN
1	A	1151	VAL
1	A	1163	GLU
1	A	1164	ASN
1	A	1166	ASN
1	A	1201	ASN
1	A	1212	ARG
1	A	1213	ASP
1	A	1251	GLU
1	A	1267	THR
1	A	1277	THR
1	A	1315	LYS
1	A	1319	LEU
1	A	1323	SER
1	A	1332	LYS
1	A	1394	ASN
1	B	483	GLU
1	B	486	ARG
1	B	497	ARG
1	B	1015	GLU
1	B	1099	LEU
1	B	1100	SER
1	B	1111	VAL
1	B	1142	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1151	VAL
1	B	1179	THR
1	B	1192	GLU
1	B	1193	ARG
1	B	1210	LEU
1	B	1211	TYR
1	B	1213	ASP
1	B	1229	THR
1	B	1266	PHE
1	B	1292	LEU
1	B	1297	LYS
1	B	1300	HIS
1	B	1305	ARG
1	B	1324	SER
1	B	1330	GLU
1	B	1331	ASN
1	B	1335	VAL
1	B	1344	GLU
1	B	1368	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1016	ASN
1	A	1122	ASN
1	A	1131	HIS
1	A	1133	ASN
1	A	1188	ASN
1	A	1217	ASN
1	A	1222	HIS
1	A	1223	GLN
1	A	1353	GLN
1	B	1016	ASN
1	B	1120	ASN
1	B	1133	ASN
1	B	1188	ASN
1	B	1217	ASN
1	B	1222	HIS
1	B	1223	GLN
1	B	1331	ASN
1	B	1353	GLN
1	B	1388	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	SO4	A	1503	-	4,4,4	0.49	0	6,6,6	0.39	0
2	SO4	A	1501	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	B	1501	-	4,4,4	0.24	0	6,6,6	0.23	0
2	SO4	A	1502	-	4,4,4	0.31	0	6,6,6	0.25	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 [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	424/472 (89%)	0.50	43 (10%)	12 11	20, 41, 74, 104	36 (8%)
1	B	406/472 (86%)	0.96	69 (16%)	4 4	24, 52, 87, 114	38 (9%)
All	All	830/944 (87%)	0.73	112 (13%)	7 6	20, 46, 82, 114	74 (8%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1139	GLY	8.4
1	A	1165	ASP	7.0
1	B	497	ARG	6.9
1	A	1325	ILE	6.5
1	B	1329	VAL	5.9
1	A	1164	ASN	5.9
1	B	1211	TYR	5.5
1	B	1383	GLY	5.4
1	B	1111	VAL	5.4
1	B	482	GLU	5.3
1	A	1323	SER	5.3
1	B	480	ALA	5.3
1	B	1327	PRO	5.2
1	A	1112	CYS	5.0
1	B	1299	PHE	4.6
1	A	1113	ASN	4.6
1	B	1114	ILE	4.6
1	A	1110	ALA	4.6
1	B	1397	VAL	4.5
1	A	1108	ASP	4.5
1	A	1109	THR	4.4
1	B	541	SER	4.4
1	A	498	ILE	4.3
1	B	1382	GLY	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1016	ASN	4.1
1	B	1330	GLU	4.1
1	B	496	ILE	4.1
1	B	1328	MET	4.0
1	B	1215	TRP	4.0
1	A	478	ASP	3.9
1	B	1015	GLU	3.7
1	A	1213	ASP	3.7
1	A	541	SER	3.6
1	A	1115	ASN	3.6
1	B	1113	ASN	3.6
1	B	1165	ASP	3.5
1	A	1324	SER	3.4
1	B	1138	SER	3.4
1	A	523	LYS	3.4
1	A	1211	TYR	3.3
1	B	1403	ALA	3.3
1	A	525	GLN	3.3
1	A	1163	GLU	3.3
1	B	1214	GLU	3.2
1	B	1265	LYS	3.2
1	B	1228	HIS	3.2
1	B	1295	THR	3.2
1	B	1381	THR	3.1
1	B	495	TYR	3.0
1	B	1209	ASP	3.0
1	A	1326	PRO	3.0
1	B	1335	VAL	3.0
1	B	1326	PRO	2.9
1	A	481	PHE	2.9
1	B	1386	THR	2.9
1	B	1241	ASP	2.9
1	A	480	ALA	2.8
1	A	1403	ALA	2.8
1	B	1324	SER	2.8
1	A	1377	ARG	2.8
1	A	1138	SER	2.8
1	B	1336	LEU	2.8
1	B	1391	ARG	2.8
1	B	1112	CYS	2.7
1	A	1280	SER	2.7
1	B	1093	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1331	ASN	2.6
1	B	481	PHE	2.6
1	B	1164	ASN	2.6
1	B	1162	PRO	2.6
1	A	487	LEU	2.6
1	B	1121	ILE	2.6
1	B	1098	LEU	2.6
1	B	485	ARG	2.6
1	B	1296	GLY	2.6
1	A	1111	VAL	2.6
1	B	1266	PHE	2.5
1	B	1298	ASP	2.5
1	A	1102	THR	2.5
1	B	1361	VAL	2.5
1	B	1210	LEU	2.4
1	A	1228	HIS	2.4
1	B	1116	TYR	2.4
1	B	1091	ASP	2.4
1	B	1332	LYS	2.3
1	A	1360	THR	2.3
1	A	1206	LEU	2.3
1	B	1334	GLU	2.3
1	B	1325	ILE	2.3
1	A	521	PHE	2.3
1	B	1179	THR	2.3
1	A	479	LYS	2.3
1	B	1404	THR	2.3
1	B	493	VAL	2.3
1	A	520	ASN	2.2
1	A	1136	ASP	2.2
1	B	1398	GLY	2.2
1	A	524	PHE	2.2
1	B	1100	SER	2.2
1	B	1371	LEU	2.1
1	A	1340	ILE	2.1
1	A	1329	VAL	2.1
1	B	1199	ARG	2.1
1	A	519	LYS	2.0
1	B	483	GLU	2.0
1	B	1137	PRO	2.0
1	B	1216	PHE	2.0
1	B	1242	PHE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1360	THR	2.0
1	A	488	ARG	2.0
1	A	1413	LYS	2.0
1	B	1297	LYS	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, 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($\text{\AA}^2$)	Q<0.9
3	MN	B	1502	1/1	0.85	0.36	120,120,120,120	0
3	MN	A	1504	1/1	0.93	0.22	97,97,97,97	0
2	SO4	A	1502	5/5	0.96	0.12	49,51,51,52	0
2	SO4	A	1503	5/5	0.97	0.08	44,45,48,48	0
2	SO4	B	1501	5/5	0.98	0.06	35,37,39,39	0
2	SO4	A	1501	5/5	0.99	0.04	35,37,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.