



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:17 PM GMT

PDB ID : 3THO
Title : Crystal structure of Mre11:Rad50 in its ATP/ADP bound state
Authors : Moeckel, C.; Lammens, K.
Deposited on : 2011-08-19
Resolution : 2.61 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

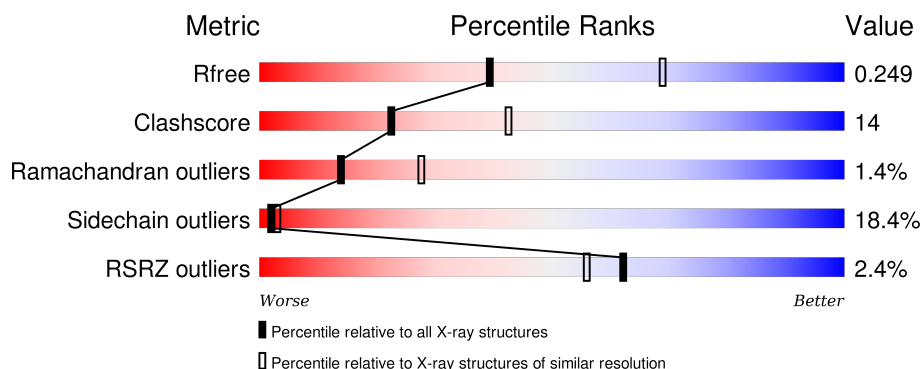
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

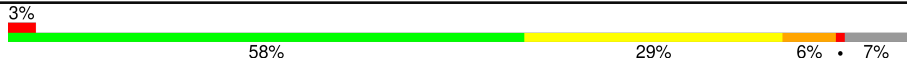

The reported resolution of this entry is 2.61 Å.

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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	382	
2	B	379	

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	SO4	A	854	-	-	X	X
5	SO4	A	855	-	-	X	-
5	SO4	A	857	-	-	X	X
5	SO4	B	387	-	-	X	X
5	SO4	B	5	-	-	X	-
6	PO4	A	859	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5973 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 Probable DNA double-strand break repair Rad50 ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	221	0	0
			2850	1814	494	536	6			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	EXPRESSION TAG	UNP Q9X1X1
A	-15	HIS	-	EXPRESSION TAG	UNP Q9X1X1
A	-14	HIS	-	EXPRESSION TAG	UNP Q9X1X1
A	-13	HIS	-	EXPRESSION TAG	UNP Q9X1X1
A	-12	HIS	-	EXPRESSION TAG	UNP Q9X1X1
A	-11	HIS	-	EXPRESSION TAG	UNP Q9X1X1
A	-10	SER	-	EXPRESSION TAG	UNP Q9X1X1
A	-9	SER	-	EXPRESSION TAG	UNP Q9X1X1
A	-8	GLY	-	EXPRESSION TAG	UNP Q9X1X1
A	-7	GLU	-	EXPRESSION TAG	UNP Q9X1X1
A	-6	ASN	-	EXPRESSION TAG	UNP Q9X1X1
A	-5	LEU	-	EXPRESSION TAG	UNP Q9X1X1
A	-4	TYR	-	EXPRESSION TAG	UNP Q9X1X1
A	-3	PHE	-	EXPRESSION TAG	UNP Q9X1X1
A	-2	GLN	-	EXPRESSION TAG	UNP Q9X1X1
A	-1	GLY	-	EXPRESSION TAG	UNP Q9X1X1
A	0	HIS	-	EXPRESSION TAG	UNP Q9X1X1
A	678	GLY	-	LINKER	UNP Q9X1X1
A	679	GLY	-	LINKER	UNP Q9X1X1
A	680	ALA	-	LINKER	UNP Q9X1X1
A	681	GLY	-	LINKER	UNP Q9X1X1
A	682	GLY	-	LINKER	UNP Q9X1X1
A	683	ALA	-	LINKER	UNP Q9X1X1
A	684	GLY	-	LINKER	UNP Q9X1X1
A	685	GLY	-	LINKER	UNP Q9X1X1
A	804	CYS	ASP	ENGINEERED MUTATION	UNP Q9X1X1
A	830	CYS	HIS	ENGINEERED MUTATION	UNP Q9X1X1

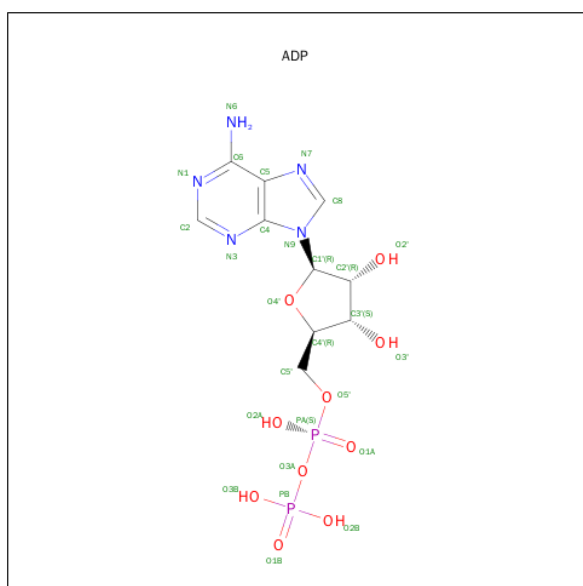
- Molecule 2 is a protein called Exonuclease, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	366	Total	C	N	O	S	270	0	0
			3000	1922	509	562	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	MET	LEU	CONFLICT	UNP Q9X1X0
B	94	GLN	HIS	ENGINEERED MUTATION	UNP Q9X1X0
B	291	SER	PHE	ENGINEERED MUTATION	UNP Q9X1X0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

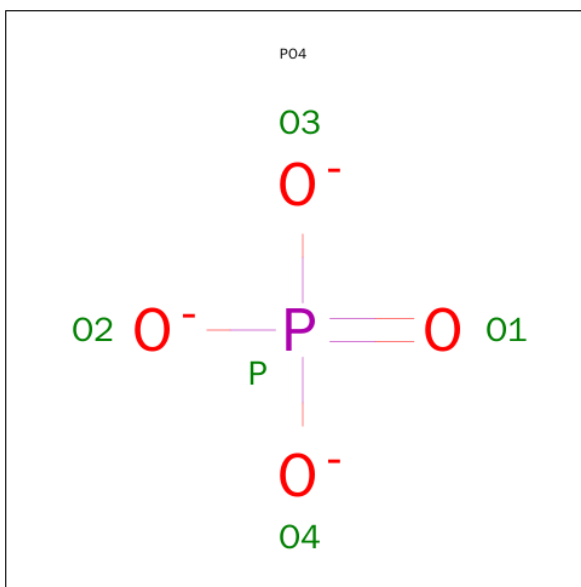
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO₄) (formula: O₄P).



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

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Mn	0	0
			2	2		

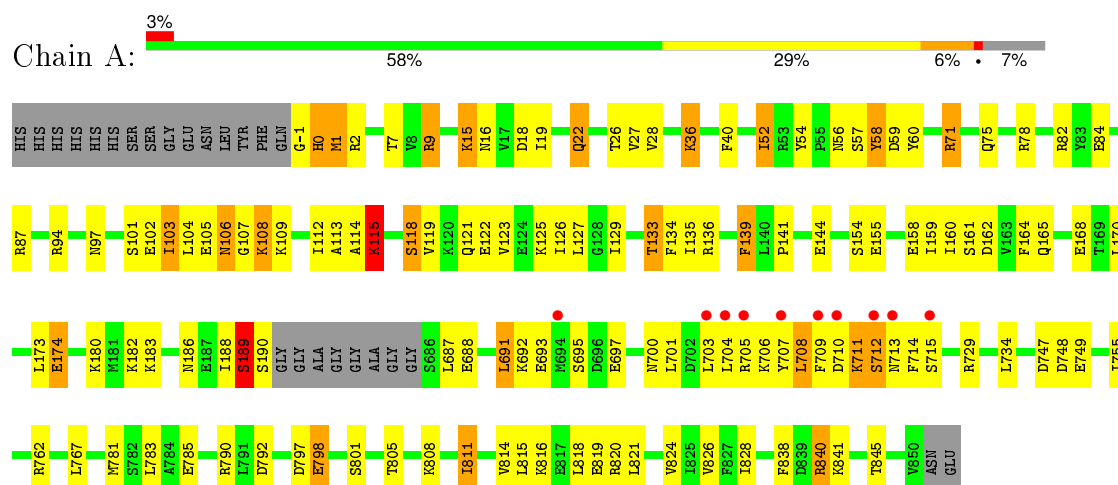
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	18	Total	O	0	0
			18	18		
8	B	25	Total	O	0	0
			25	25		

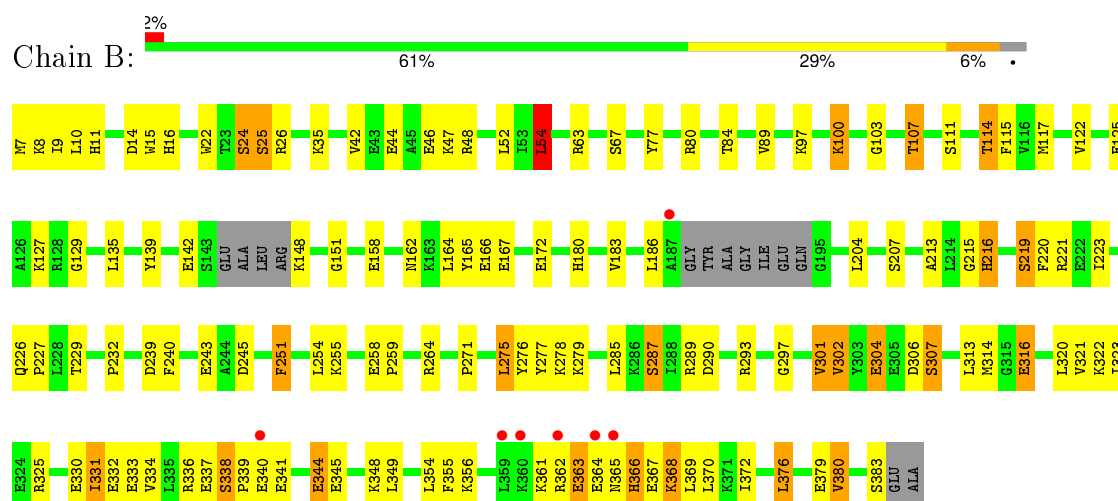
3 Residue-property plots [i](#)

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: Probable DNA double-strand break repair Rad50 ATPase



- Molecule 2: Exonuclease, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.77Å 121.77Å 135.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.12 – 2.61 49.12 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.12-2.61) 99.7 (49.12-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.204 , 0.242 0.210 , 0.249	Depositor DCC
R_{free} test set	1992 reflections (5.92%)	DCC
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.5	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 35647 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5973	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MN, PO4, ADP, 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	0.45	0/2891	0.57	0/3874
2	B	0.46	0/3059	0.59	1/4118 (0.0%)
All	All	0.45	0/5950	0.58	1/7992 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	54	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	ILE	Peptide

5.2 Too-close contacts [i](#)

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	2850	0	2922	78	0
2	B	3000	0	3032	72	0
3	A	27	0	10	0	0
4	A	1	0	0	0	0
5	A	25	0	0	8	0
5	B	20	0	0	4	0
6	A	5	0	0	0	0
7	B	2	0	0	0	0
8	A	18	0	0	1	0
8	B	25	0	0	1	0
All	All	5973	0	5964	147	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 14.

All (147) 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)
2:B:100:LYS:HB3	2:B:117:MET:HG2	1.49	0.95
2:B:135:LEU:HB3	2:B:164:LEU:HD22	1.54	0.89
1:A:106:ASN:O	1:A:108:LYS:N	2.09	0.85
1:A:22:GLN:HB2	1:A:840:ARG:HH22	1.46	0.79
1:A:71:ARG:NH2	5:A:855:SO4:O4	2.16	0.79
1:A:94:ARG:HH11	1:A:94:ARG:HG2	1.54	0.73
1:A:122:GLU:O	1:A:126:ILE:HG12	1.90	0.72
1:A:101:SER:HA	1:A:112:ILE:HD12	1.73	0.69
2:B:166:GLU:HA	5:B:387:SO4:O4	1.91	0.69
2:B:103:GLY:O	2:B:107:THR:HG23	1.94	0.68
2:B:107:THR:HG21	2:B:115:PHE:H	1.59	0.68
2:B:368:LYS:O	2:B:372:ILE:N	2.19	0.67
1:A:26:THR:OG1	5:A:857:SO4:O2	2.09	0.67
1:A:755:ILE:HD13	1:A:767:LEU:HD11	1.77	0.67
2:B:22:TRP:NE1	2:B:239:ASP:OD1	2.27	0.66
1:A:174:GLU:HB2	1:A:709:PHE:CZ	2.31	0.66
2:B:25:SER:OG	2:B:321:VAL:O	2.12	0.66
2:B:275:LEU:HB3	2:B:277:TYR:CE2	2.32	0.65
2:B:301:VAL:HG12	2:B:320:LEU:HD11	1.79	0.65
1:A:57:SER:OG	5:A:854:SO4:O2	2.14	0.64
2:B:26:ARG:NH2	2:B:314:MET:O	2.31	0.63
2:B:240:PHE:O	2:B:243:GLU:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:MET:N	2:B:254:LEU:O	2.32	0.63
1:A:710:ASP:O	1:A:712:SER:N	2.32	0.62
2:B:366:HIS:HB2	2:B:369:LEU:HD22	1.82	0.62
1:A:1:MET:O	1:A:792:ASP:HB2	2.00	0.61
1:A:838:PHE:O	1:A:841:LYS:NZ	2.33	0.61
1:A:7:THR:OG1	1:A:18:ASP:OD1	2.19	0.61
2:B:24:SER:OG	5:B:5:SO4:O4	2.19	0.61
1:A:58:TYR:CE2	1:A:94:ARG:HD3	2.35	0.61
2:B:306:ASP:OD2	2:B:307:SER:N	2.33	0.61
1:A:115:LYS:O	1:A:119:VAL:HG23	2.01	0.61
1:A:729:ARG:NE	8:A:872:HOH:O	2.31	0.60
1:A:54:TYR:HB2	1:A:60:TYR:CE2	2.37	0.60
1:A:71:ARG:NH2	5:A:855:SO4:S	2.75	0.60
2:B:275:LEU:HB3	2:B:277:TYR:HE2	1.66	0.60
1:A:141:PRO:HG2	1:A:144:GLU:HB2	1.85	0.59
2:B:322:LYS:NZ	5:B:5:SO4:O2	2.35	0.59
1:A:711:LYS:C	1:A:713:ASN:H	2.07	0.58
2:B:25:SER:OG	2:B:26:ARG:N	2.34	0.58
1:A:84:GLU:HB2	1:A:103:ILE:HD11	1.85	0.58
1:A:56:ASN:HB3	1:A:58:TYR:CE1	2.40	0.57
1:A:113:ALA:HB1	1:A:118:SER:HB2	1.86	0.57
2:B:368:LYS:O	2:B:372:ILE:HG12	2.05	0.56
2:B:289:ARG:NH2	2:B:316:GLU:OE1	2.38	0.56
1:A:790:ARG:NH2	5:A:858:SO4:O4	2.37	0.56
2:B:363:GLU:O	2:B:365:ASN:N	2.39	0.56
1:A:129:ILE:CD1	1:A:134:PHE:HB2	2.36	0.56
1:A:797:ASP:OD2	1:A:798:GLU:HG3	2.06	0.55
1:A:826:VAL:HG22	5:A:857:SO4:O4	2.06	0.55
2:B:115:PHE:HB3	2:B:117:MET:SD	2.46	0.55
2:B:9:ILE:HG21	2:B:54:LEU:HD22	1.89	0.55
2:B:11:HIS:CE1	2:B:232:PRO:HD3	2.42	0.54
1:A:133:THR:HG21	1:A:162:ASP:OD1	2.07	0.54
2:B:334:VAL:HA	2:B:337:GLU:HG3	1.89	0.54
2:B:251:PHE:C	2:B:251:PHE:CD2	2.80	0.54
2:B:258:GLU:HB3	2:B:259:PRO:HD2	1.89	0.54
1:A:155:GLU:O	1:A:159:ILE:HG23	2.08	0.54
2:B:215:GLY:O	2:B:216:HIS:CB	2.56	0.53
2:B:344:GLU:O	2:B:348:LYS:HG3	2.07	0.53
1:A:188:ILE:C	1:A:190:SER:H	2.12	0.53
1:A:711:LYS:O	1:A:713:ASN:N	2.42	0.52
1:A:28:VAL:HG12	1:A:36:LYS:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:THR:HB	2:B:114:THR:HA	1.92	0.51
2:B:301:VAL:HG13	2:B:323:ILE:HG22	1.91	0.51
1:A:9:ARG:HA	1:A:15:LYS:O	2.11	0.51
1:A:161:SER:O	1:A:165:GLN:HB2	2.11	0.51
1:A:139:PHE:O	1:A:141:PRO:HD3	2.11	0.51
2:B:11:HIS:CE1	2:B:213:ALA:HB1	2.46	0.50
2:B:183:VAL:HG21	2:B:223:ILE:HD12	1.92	0.50
1:A:188:ILE:O	1:A:190:SER:N	2.38	0.50
2:B:264:ARG:NH1	8:B:6:HOH:O	2.44	0.50
1:A:707:TYR:OH	2:B:363:GLU:HG3	2.11	0.50
1:A:815:LEU:O	1:A:818:LEU:HB2	2.11	0.50
1:A:704:LEU:O	1:A:708:LEU:HB2	2.12	0.49
1:A:104:LEU:O	1:A:106:ASN:N	2.45	0.49
2:B:276:TYR:CD1	2:B:302:VAL:HG22	2.46	0.49
2:B:207:SER:HB3	2:B:226:GLN:OE1	2.13	0.49
1:A:57:SER:OG	5:A:854:SO4:S	2.71	0.49
1:A:189:SER:O	1:A:190:SER:OG	2.30	0.49
2:B:42:VAL:O	2:B:46:GLU:HG3	2.12	0.49
2:B:107:THR:CG2	2:B:115:PHE:H	2.23	0.49
2:B:35:LYS:HE3	2:B:77:TYR:CE2	2.49	0.48
2:B:8:LYS:HE3	2:B:48:ARG:O	2.14	0.48
2:B:148:LYS:N	2:B:151:GLY:H	2.12	0.47
1:A:26:THR:OG1	5:A:857:SO4:S	2.66	0.47
2:B:258:GLU:OE2	2:B:258:GLU:N	2.48	0.47
2:B:215:GLY:O	2:B:216:HIS:HB3	2.15	0.47
2:B:314:MET:HA	2:B:320:LEU:HD23	1.97	0.47
1:A:102:GLU:HG3	1:A:103:ILE:N	2.30	0.46
2:B:220:PHE:C	2:B:220:PHE:CD2	2.87	0.46
2:B:14:ASP:O	2:B:16:HIS:HD2	1.98	0.46
2:B:35:LYS:HE3	2:B:77:TYR:OH	2.14	0.46
2:B:278:LYS:HG3	2:B:304:GLU:OE2	2.16	0.46
2:B:290:ASP:OD1	2:B:293:ARG:NH2	2.44	0.46
1:A:119:VAL:O	1:A:123:VAL:HG23	2.17	0.45
2:B:103:GLY:O	2:B:107:THR:CG2	2.62	0.45
1:A:94:ARG:NH1	1:A:94:ARG:HG2	2.28	0.45
1:A:58:TYR:CG	1:A:94:ARG:NH1	2.85	0.45
1:A:747:ASP:OD2	1:A:749:GLU:HG2	2.16	0.45
1:A:707:TYR:CE2	2:B:363:GLU:HG3	2.51	0.45
1:A:134:PHE:CE2	1:A:139:PHE:CG	3.05	0.45
2:B:376:LEU:O	2:B:380:VAL:HG12	2.17	0.44
1:A:697:GLU:O	1:A:701:LEU:HG	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:GLN:HA	2:B:227:PRO:HA	1.81	0.44
1:A:808:LYS:O	1:A:811:ILE:HG22	2.17	0.44
2:B:125:GLU:OE1	2:B:129:GLY:HA2	2.17	0.44
1:A:729:ARG:HD3	1:A:785:GLU:OE1	2.18	0.44
1:A:135:ILE:HA	1:A:139:PHE:O	2.17	0.44
1:A:711:LYS:O	1:A:715:SER:HB2	2.17	0.44
1:A:816:LYS:O	1:A:819:GLU:HB2	2.19	0.43
1:A:19:ILE:HD12	1:A:19:ILE:O	2.19	0.43
2:B:338:SER:CB	2:B:339:PRO:HD2	2.49	0.43
1:A:40:PHE:CZ	1:A:139:PHE:CD1	3.07	0.42
1:A:36:LYS:HB3	1:A:828:ILE:CG2	2.49	0.42
1:A:-1:GLY:HA3	1:A:0:HIS:HA	1.62	0.42
2:B:9:ILE:CG2	2:B:54:LEU:HD22	2.48	0.42
1:A:189:SER:OG	1:A:189:SER:O	2.33	0.42
1:A:797:ASP:OD2	1:A:798:GLU:CG	2.67	0.42
1:A:188:ILE:C	1:A:190:SER:N	2.73	0.42
2:B:338:SER:O	2:B:341:GLU:N	2.53	0.42
2:B:331:ILE:HD12	2:B:331:ILE:HA	1.78	0.42
1:A:101:SER:CA	1:A:112:ILE:HD12	2.47	0.41
1:A:734:LEU:HD23	1:A:734:LEU:HA	1.72	0.41
2:B:277:TYR:HE1	2:B:287:SER:HG	1.68	0.41
1:A:2:ARG:HD3	1:A:792:ASP:HB3	2.02	0.41
2:B:15:TRP:O	2:B:16:HIS:HB2	2.19	0.41
2:B:180:HIS:CD2	2:B:216:HIS:HB2	2.56	0.41
1:A:160:ILE:O	1:A:164:PHE:HD2	2.03	0.41
1:A:56:ASN:HB2	1:A:59:ASP:OD2	2.20	0.41
2:B:52:LEU:HG	2:B:54:LEU:HD13	2.03	0.41
2:B:219:SER:HB3	2:B:245:ASP:HB2	2.02	0.41
2:B:223:ILE:HB	2:B:229:THR:HB	2.02	0.41
1:A:714:PHE:CE1	2:B:355:PHE:HD1	2.39	0.41
1:A:711:LYS:C	1:A:713:ASN:N	2.72	0.41
1:A:700:ASN:O	1:A:703:LEU:N	2.54	0.41
1:A:102:GLU:HG2	1:A:104:LEU:HD21	2.03	0.41
1:A:781:MET:SD	1:A:814:VAL:HG12	2.61	0.41
1:A:114:ALA:O	1:A:115:LYS:HB2	2.21	0.41
1:A:87:ARG:HA	1:A:97:ASN:O	2.21	0.40
2:B:271:PRO:O	2:B:297:GLY:HA3	2.21	0.40
1:A:36:LYS:HE2	1:A:36:LYS:HB2	1.83	0.40
2:B:35:LYS:HE3	2:B:77:TYR:CZ	2.56	0.40
2:B:162:ASN:O	2:B:165:TYR:HB3	2.21	0.40
1:A:691:LEU:HA	1:A:691:LEU:HD12	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:GLU:CA	5:B:387:SO4:O4	2.65	0.40
2:B:139:TYR:HA	2:B:180:HIS:O	2.22	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	353/382 (92%)	323 (92%)	23 (6%)	7 (2%)	9	18
2	B	360/379 (95%)	328 (91%)	29 (8%)	3 (1%)	24	46
All	All	713/761 (94%)	651 (91%)	52 (7%)	10 (1%)	14	28

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	GLU
1	A	712	SER
2	B	364	GLU
1	A	107	GLY
1	A	189	SER
1	A	711	LYS
2	B	216	HIS
2	B	356	LYS
1	A	106	ASN
1	A	115	LYS

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	310/326 (95%)	253 (82%)	57 (18%)	2	3
2	B	333/341 (98%)	272 (82%)	61 (18%)	2	3
All	All	643/667 (96%)	525 (82%)	118 (18%)	2	3

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	1	MET
1	A	9	ARG
1	A	15	LYS
1	A	16	ASN
1	A	22	GLN
1	A	27	VAL
1	A	36	LYS
1	A	52	ILE
1	A	58	TYR
1	A	71	ARG
1	A	75	GLN
1	A	78	ARG
1	A	82	ARG
1	A	103	ILE
1	A	108	LYS
1	A	109	LYS
1	A	115	LYS
1	A	118	SER
1	A	121	GLN
1	A	125	LYS
1	A	127	LEU
1	A	133	THR
1	A	136	ARG
1	A	139	PHE
1	A	154	SER
1	A	158	GLU
1	A	168	GLU
1	A	170	LEU
1	A	173	LEU
1	A	174	GLU
1	A	180	LYS
1	A	182	LYS

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Mol	Chain	Res	Type
1	A	183	LYS
1	A	186	ASN
1	A	189	SER
1	A	687	LEU
1	A	688	GLU
1	A	691	LEU
1	A	692	LYS
1	A	693	GLU
1	A	695	SER
1	A	705	ARG
1	A	706	LYS
1	A	708	LEU
1	A	748	ASP
1	A	762	ARG
1	A	783	LEU
1	A	798	GLU
1	A	801	SER
1	A	805	THR
1	A	811	ILE
1	A	820	ARG
1	A	821	LEU
1	A	824	VAL
1	A	840	ARG
1	A	845	THR
2	B	10	LEU
2	B	24	SER
2	B	25	SER
2	B	44	GLU
2	B	47	LYS
2	B	54	LEU
2	B	63	ARG
2	B	67	SER
2	B	80	ARG
2	B	84	THR
2	B	89	VAL
2	B	97	LYS
2	B	100	LYS
2	B	107	THR
2	B	111	SER
2	B	114	THR
2	B	122	VAL
2	B	127	LYS

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Mol	Chain	Res	Type
2	B	142	GLU
2	B	158	GLU
2	B	167	GLU
2	B	172	GLU
2	B	186	LEU
2	B	204	LEU
2	B	219	SER
2	B	221	ARG
2	B	251	PHE
2	B	255	LYS
2	B	275	LEU
2	B	279	LYS
2	B	285	LEU
2	B	287	SER
2	B	301	VAL
2	B	302	VAL
2	B	304	GLU
2	B	307	SER
2	B	313	LEU
2	B	316	GLU
2	B	325	ARG
2	B	330	GLU
2	B	331	ILE
2	B	332	GLU
2	B	333	GLU
2	B	336	ARG
2	B	338	SER
2	B	340	GLU
2	B	344	GLU
2	B	345	GLU
2	B	349	LEU
2	B	354	LEU
2	B	361	LYS
2	B	362	ARG
2	B	363	GLU
2	B	366	HIS
2	B	367	GLU
2	B	368	LYS
2	B	370	LEU
2	B	376	LEU
2	B	379	GLU
2	B	380	VAL

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Mol	Chain	Res	Type
2	B	383	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	$\# Z > 2$
3	ADP	A	1452	4	22,29,29	1.32	4 (18%)	27,45,45	2.41	4 (14%)
5	SO4	A	854	-	4,4,4	0.11	0	6,6,6	0.17	0
5	SO4	A	855	-	4,4,4	0.04	0	6,6,6	0.23	0
5	SO4	A	856	-	4,4,4	0.11	0	6,6,6	0.19	0
5	SO4	A	857	-	4,4,4	0.22	0	6,6,6	0.10	0
5	SO4	A	858	-	4,4,4	0.12	0	6,6,6	0.09	0
6	PO4	A	859	-	4,4,4	0.30	0	6,6,6	0.28	0
5	SO4	B	386	-	4,4,4	0.13	0	6,6,6	0.11	0
5	SO4	B	387	-	4,4,4	0.22	0	6,6,6	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	B	4	-	4,4,4	0.06	0	6,6,6	0.27	0
5	SO4	B	5	-	4,4,4	0.13	0	6,6,6	0.11	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
3	ADP	A	1452	4	-	0/12/32/32	0/3/3/3
5	SO4	A	854	-	-	0/0/0/0	0/0/0/0
5	SO4	A	855	-	-	0/0/0/0	0/0/0/0
5	SO4	A	856	-	-	0/0/0/0	0/0/0/0
5	SO4	A	857	-	-	0/0/0/0	0/0/0/0
5	SO4	A	858	-	-	0/0/0/0	0/0/0/0
6	PO4	A	859	-	-	0/0/0/0	0/0/0/0
5	SO4	B	386	-	-	0/0/0/0	0/0/0/0
5	SO4	B	387	-	-	0/0/0/0	0/0/0/0
5	SO4	B	4	-	-	0/0/0/0	0/0/0/0
5	SO4	B	5	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1452	ADP	O2'-C2'	-2.88	1.36	1.43
3	A	1452	ADP	O3'-C3'	-2.69	1.36	1.43
3	A	1452	ADP	C5'-C4'	-2.01	1.45	1.51
3	A	1452	ADP	C6-N6	2.25	1.41	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1452	ADP	N3-C2-N1	-10.59	120.79	128.89
3	A	1452	ADP	C1'-N9-C4	-3.29	121.98	126.94
3	A	1452	ADP	O5'-C5'-C4'	2.19	117.20	109.12
3	A	1452	ADP	C2'-C1'-N9	2.20	117.66	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	854	SO4	2	0
5	A	855	SO4	2	0
5	A	857	SO4	3	0
5	A	858	SO4	1	0
5	B	387	SO4	2	0
5	B	5	SO4	2	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	356/382 (93%)	0.00	10 (2%) 56 49	42, 63, 97, 118	72 (20%)
2	B	366/379 (96%)	-0.12	7 (1%) 70 64	42, 60, 104, 119	75 (20%)
All	All	722/761 (94%)	-0.06	17 (2%) 62 56	42, 62, 102, 119	147 (20%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	707	TYR	6.3
2	B	359	LEU	5.6
1	A	703	LEU	4.2
1	A	712	SER	3.7
1	A	705	ARG	3.4
2	B	340	GLU	2.9
1	A	713	ASN	2.9
1	A	704	LEU	2.8
2	B	187	ALA	2.8
1	A	709	PHE	2.8
2	B	360	LYS	2.7
2	B	364	GLU	2.6
1	A	715	SER	2.6
2	B	365	ASN	2.6
1	A	710	ASP	2.2
1	A	694	MET	2.1
2	B	362	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
5	SO4	B	387	5/5	0.86	0.37	9.04	50,50,52,56	5
5	SO4	A	857	5/5	0.90	0.39	6.70	61,62,65,65	5
5	SO4	A	854	5/5	0.95	0.26	2.49	67,68,71,75	5
6	PO4	A	859	5/5	0.96	0.30	2.35	66,69,76,78	5
5	SO4	A	858	5/5	0.83	0.15	1.98	81,82,89,92	5
7	MN	B	2	1/1	0.99	0.20	1.71	38,38,38,38	0
5	SO4	B	5	5/5	0.89	0.16	0.98	77,79,83,95	5
7	MN	B	1	1/1	0.95	0.17	0.60	49,49,49,49	1
3	ADP	A	1452	27/27	0.99	0.20	0.46	38,44,48,49	0
4	MG	A	853	1/1	0.92	0.19	-1.62	56,56,56,56	0
5	SO4	B	386	5/5	0.96	0.10	-3.46	75,76,90,91	0
5	SO4	A	855	5/5	0.92	0.12	-	64,66,74,77	5
5	SO4	B	4	5/5	0.91	0.13	-	97,97,114,118	0
5	SO4	A	856	5/5	0.90	0.14	-	62,75,81,83	5

6.5 Other polymers [i](#)

There are no such residues in this entry.