Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 09:07 PM EDT

PDB ID	:	6N6M
Title	:	Crystal Structure of ATPase delta1-79 Spa47 R189A
Authors	:	Morales, Y.; Johnson, S.J.; Demler, H.J.; Dickenson, N.E.
Deposited on	:	2018-11-26
Resolution	:	2.79 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 (i) 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 (1)) were used in the production of this report:

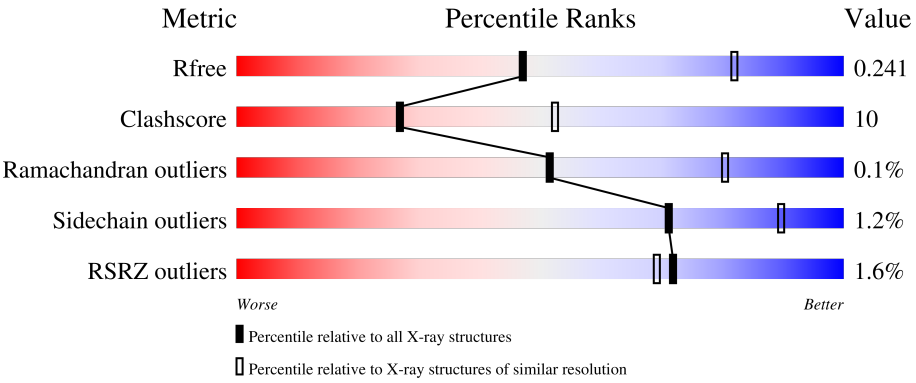
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

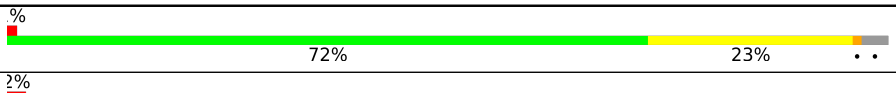
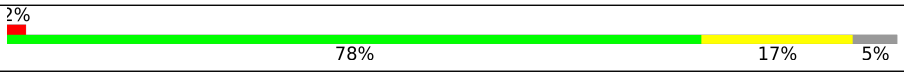
The reported resolution of this entry is 2.79 Å.

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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 <=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	352	
1	B	352	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5334 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.

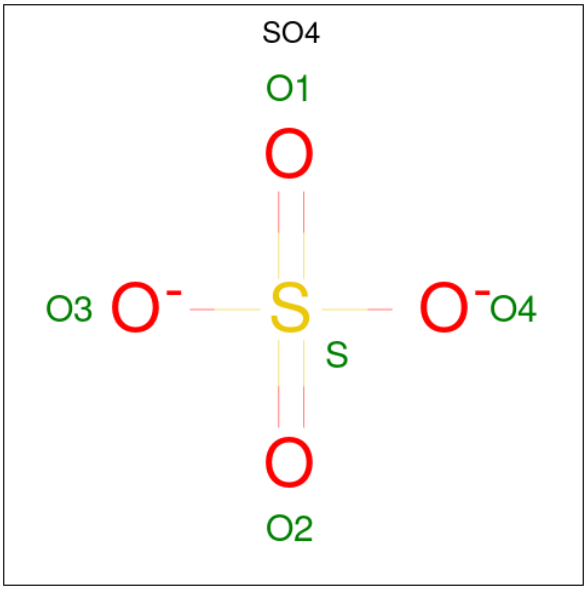
- Molecule 1 is a protein called ATP synthase SpaL/MxiB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2665	1694	455	507	9			
1	B	334	Total	C	N	O	S	0	0	0
			2602	1652	441	500	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ASN	-	expression tag	UNP P0A1C1
A	189	ALA	ARG	engineered mutation	UNP P0A1C1
B	79	ASN	-	expression tag	UNP P0A1C1
B	189	ALA	ARG	engineered mutation	UNP P0A1C1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

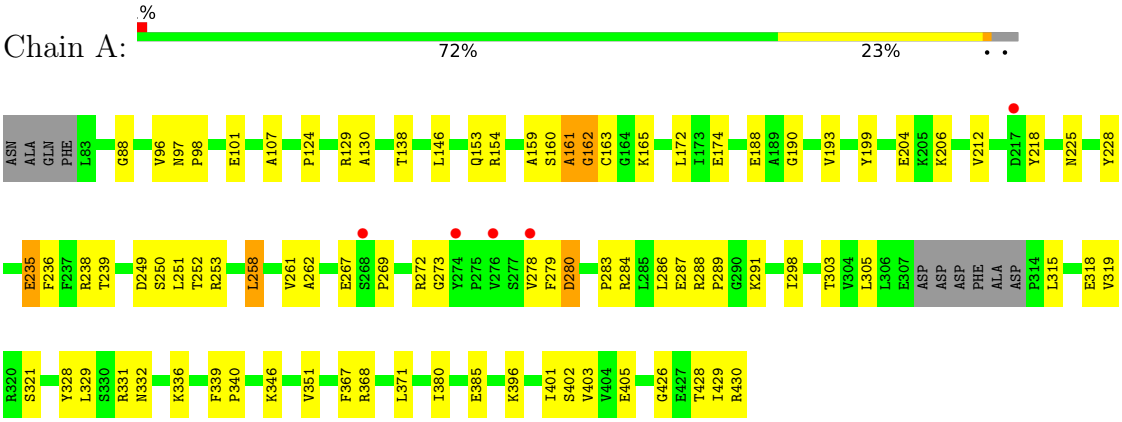
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	31	Total O 31 31	0	0
3	B	26	Total O 26 26	0	0

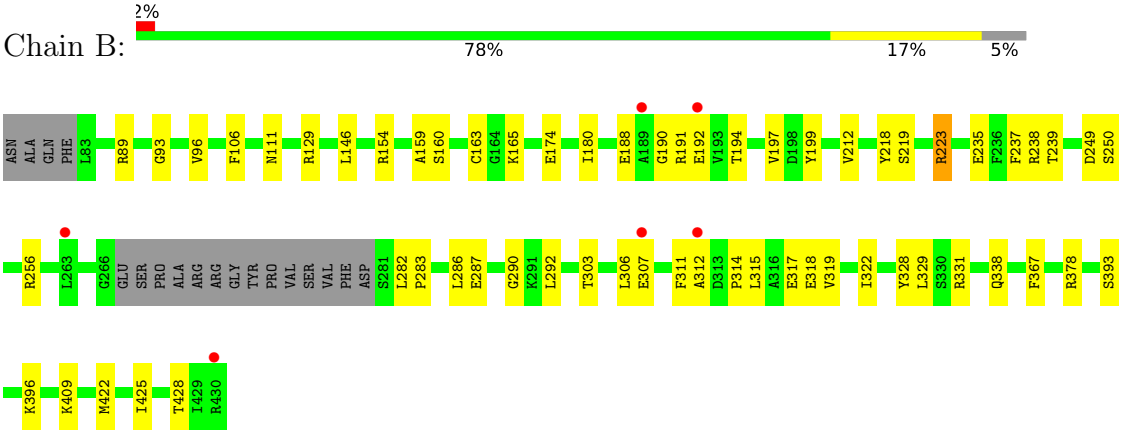
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ATP synthase SpaL/MxiB



• Molecule 1: ATP synthase SpaL/MxiB



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.93Å 154.07Å 54.92Å 90.00° 109.65° 90.00°	Depositor
Resolution (Å)	39.95 – 2.79 41.37 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.2 (39.95-2.79) 87.4 (41.37-2.79)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.182 , 0.241 0.182 , 0.241	Depositor DCC
R_{free} test set	827 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5334	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	1/2710 (0.0%)	0.77	9/3660 (0.2%)
1	B	0.39	0/2644	0.66	1/3571 (0.0%)
All	All	0.42	1/5354 (0.0%)	0.72	10/7231 (0.1%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	GLU	CB-CG	6.70	1.64	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	253	ARG	NE-CZ-NH2	9.63	125.11	120.30
1	A	253	ARG	NE-CZ-NH1	-8.75	115.93	120.30
1	B	378	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	321	SER	CB-CA-C	-5.83	99.03	110.10
1	A	258	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	162	GLY	C-N-CA	5.32	135.00	121.70
1	A	331	ARG	CG-CD-NE	-5.31	100.65	111.80
1	A	318	GLU	CA-CB-CG	5.26	124.97	113.40
1	A	331	ARG	CB-CG-CD	5.17	125.05	111.60
1	A	162	GLY	N-CA-C	-5.09	100.37	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ALA	Peptide
1	A	235	GLU	Sidechain

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	2665	0	2689	73	0
1	B	2602	0	2614	35	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	31	0	0	1	0
3	B	26	0	0	0	0
All	All	5334	0	5303	108	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 (108) 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:269:PRO:O	1:A:272:ARG:NH1	1.94	1.01
1:A:272:ARG:NH1	1:A:272:ARG:HB2	1.78	0.98
1:A:272:ARG:HB2	1:A:272:ARG:HH11	1.26	0.97
1:B:218:TYR:O	1:B:223:ARG:NH2	2.06	0.89
1:A:272:ARG:HH11	1:A:272:ARG:CB	1.88	0.86
1:B:317:GLU:N	1:B:317:GLU:OE1	2.24	0.71
1:A:153:GLN:NE2	1:A:351:VAL:HG22	2.06	0.71
1:A:367:PHE:HA	1:A:429:ILE:HD11	1.74	0.69
1:B:238:ARG:HD3	1:B:292:LEU:HG	1.75	0.67
1:B:283:PRO:O	1:B:287:GLU:HG2	1.94	0.67
1:B:129:ARG:NH2	1:B:287:GLU:O	2.28	0.67
1:A:258:LEU:HD11	1:A:279:PHE:HA	1.77	0.66
1:A:225:ASN:HA	1:A:228:TYR:CD1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ALA:HB2	1:A:329:LEU:HB2	1.78	0.66
1:A:367:PHE:CE2	1:A:371:LEU:HD21	2.32	0.64
1:A:146:LEU:HD11	1:A:367:PHE:CD2	2.33	0.64
1:A:272:ARG:HG3	1:A:279:PHE:HD1	1.63	0.63
1:A:315:LEU:O	1:A:319:VAL:HG23	1.97	0.63
1:A:426:GLY:O	1:A:430:ARG:HG2	1.98	0.63
1:A:154:ARG:HG2	1:A:289:PRO:HB2	1.81	0.62
1:B:194:THR:HA	1:B:197:VAL:HG22	1.82	0.62
1:A:252:THR:HG21	1:A:305:LEU:H	1.66	0.60
1:B:315:LEU:O	1:B:319:VAL:HG12	2.01	0.60
1:B:89:ARG:HH21	1:B:111:ASN:HD22	1.51	0.59
1:A:367:PHE:O	1:A:371:LEU:HD23	2.03	0.59
1:A:174:GLU:HG2	1:A:199:TYR:OH	2.03	0.58
1:A:146:LEU:O	1:A:368:ARG:NH2	2.36	0.58
1:A:162:GLY:HA2	1:A:163:CYS:HB2	1.86	0.56
1:A:225:ASN:HA	1:A:228:TYR:HD1	1.68	0.56
1:A:272:ARG:NE	1:A:279:PHE:CD1	2.74	0.56
1:A:238:ARG:HD3	1:A:298:ILE:HG13	1.87	0.56
1:B:312:ALA:HB1	1:B:317:GLU:OE2	2.05	0.56
1:A:146:LEU:HD11	1:A:367:PHE:HD2	1.71	0.55
1:A:252:THR:HG22	1:A:315:LEU:HD23	1.89	0.54
1:B:174:GLU:HG2	1:B:199:TYR:OH	2.08	0.54
1:A:272:ARG:HG3	1:A:279:PHE:CD1	2.41	0.53
1:B:188:GLU:HB3	1:B:192:GLU:CD	2.29	0.53
1:B:367:PHE:HE1	1:B:428:THR:HG21	1.73	0.53
1:A:97:ASN:OD1	1:A:101:GLU:HG2	2.08	0.53
1:B:89:ARG:HE	1:B:111:ASN:ND2	2.07	0.53
1:A:96:VAL:HG22	1:A:212:VAL:HG22	1.90	0.53
1:A:252:THR:CG2	1:A:305:LEU:H	2.21	0.52
1:A:272:ARG:NE	1:A:279:PHE:HD1	2.06	0.52
1:A:130:ALA:HB3	1:A:291:LYS:HG3	1.92	0.51
1:A:280:ASP:O	1:A:284:ARG:HD2	2.10	0.51
1:A:218:TYR:OH	3:A:601:HOH:O	2.18	0.51
1:A:258:LEU:HD21	1:A:278:VAL:O	2.11	0.51
1:A:262:ALA:HB2	1:A:278:VAL:CG2	2.41	0.50
1:A:88:GLY:HA2	1:A:236:PHE:CE2	2.47	0.50
1:A:269:PRO:HA	1:A:272:ARG:NH2	2.27	0.49
1:A:262:ALA:HB2	1:A:278:VAL:HG22	1.93	0.49
1:A:280:ASP:O	1:A:283:PRO:HD2	2.13	0.49
1:B:238:ARG:NH1	1:B:290:GLY:O	2.46	0.49
1:A:107:ALA:HB2	1:A:206:LYS:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:VAL:CG1	1:B:212:VAL:HG22	2.43	0.49
1:A:153:GLN:HE22	1:A:351:VAL:HG22	1.75	0.48
1:A:261:VAL:HG12	1:A:278:VAL:HG11	1.96	0.48
1:B:163:CYS:SG	1:B:331:ARG:HB2	2.53	0.48
1:B:93:GLY:HA2	1:B:106:PHE:CE1	2.48	0.48
1:A:249:ASP:HA	1:A:250:SER:HA	1.60	0.48
1:A:161:ALA:H	1:A:305:LEU:HD21	1.80	0.47
1:A:252:THR:HA	1:A:315:LEU:CD2	2.44	0.47
1:A:380:ILE:HG23	1:A:385:GLU:HB2	1.97	0.47
1:A:124:PRO:HD2	1:A:129:ARG:NH2	2.30	0.46
1:A:267:GLU:OE2	1:A:273:GLY:N	2.32	0.46
1:B:307:GLU:HG3	1:B:311:PHE:HD2	1.80	0.46
1:B:422:MET:HA	1:B:425:ILE:HG22	1.98	0.46
1:B:235:GLU:O	1:B:239:THR:HG23	2.15	0.46
1:B:338:GLN:HG3	1:B:409:LYS:HG3	1.96	0.46
1:B:146:LEU:HD11	1:B:367:PHE:CD2	2.51	0.46
1:A:98:PRO:HG2	1:A:218:TYR:CD2	2.51	0.46
1:A:332:ASN:O	1:A:336:LYS:HG2	2.15	0.46
1:B:160:SER:OG	1:B:163:CYS:SG	2.69	0.45
1:A:258:LEU:HD13	1:A:278:VAL:HG23	1.97	0.45
1:B:318:GLU:O	1:B:322:ILE:HG13	2.16	0.45
1:A:190:GLY:O	1:A:193:VAL:HG22	2.16	0.45
1:A:235:GLU:O	1:A:239:THR:HG23	2.16	0.45
1:A:272:ARG:HE	1:A:279:PHE:HB2	1.82	0.45
1:A:154:ARG:HD2	1:A:286:LEU:O	2.17	0.44
1:A:165:LYS:HD2	1:A:303:THR:HB	1.99	0.44
1:A:174:GLU:OE2	1:A:204:GLU:HG2	2.17	0.44
1:A:403:VAL:HG13	1:A:428:THR:HG23	1.99	0.44
1:B:190:GLY:O	1:B:194:THR:HG23	2.18	0.44
1:A:272:ARG:NH1	1:A:272:ARG:CB	2.58	0.43
1:A:401:ILE:O	1:A:405:GLU:HG3	2.18	0.43
1:A:96:VAL:CG2	1:A:212:VAL:HG22	2.48	0.43
1:B:154:ARG:HD2	1:B:286:LEU:O	2.18	0.43
1:B:159:ALA:HB2	1:B:329:LEU:HB2	2.01	0.42
1:A:262:ALA:HB1	1:A:267:GLU:HG3	2.01	0.42
1:B:165:LYS:HD2	1:B:303:THR:HG21	2.01	0.42
1:A:288:ARG:NH2	1:A:288:ARG:HG3	2.35	0.42
1:A:339:PHE:CD2	1:A:340:PRO:HA	2.55	0.42
1:B:180:ILE:HG21	1:B:237:PHE:CD2	2.54	0.41
1:A:160:SER:HA	1:A:305:LEU:HD23	2.01	0.41
1:A:98:PRO:HD2	1:A:218:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:TYR:CE1	1:A:346:LYS:HD2	2.55	0.41
1:A:159:ALA:CB	1:A:329:LEU:HB2	2.47	0.41
1:B:282:LEU:N	1:B:283:PRO:HD2	2.35	0.41
1:B:306:LEU:HD22	1:B:311:PHE:O	2.21	0.41
1:A:138:THR:HB	1:A:172:LEU:HD23	2.02	0.41
1:B:249:ASP:HA	1:B:250:SER:HA	1.55	0.41
1:A:251:LEU:HD23	1:A:251:LEU:HA	1.87	0.40
1:A:129:ARG:NH2	1:A:287:GLU:O	2.53	0.40
1:B:393:SER:O	1:B:396:LYS:HG2	2.20	0.40
1:A:165:LYS:HD2	1:A:303:THR:CB	2.51	0.40
1:A:288:ARG:HG3	1:A:288:ARG:HH21	1.86	0.40
1:B:165:LYS:HD2	1:B:303:THR:CG2	2.51	0.40
1:B:219:SER:O	1:B:223:ARG:HG2	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	338/352 (96%)	332 (98%)	6 (2%)	0	100 100
1	B	330/352 (94%)	319 (97%)	10 (3%)	1 (0%)	41 70
All	All	668/704 (95%)	651 (98%)	16 (2%)	1 (0%)	51 80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	314	PRO

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	285/293 (97%)	282 (99%)	3 (1%)	73 90
1	B	278/293 (95%)	274 (99%)	4 (1%)	67 87
All	All	563/586 (96%)	556 (99%)	7 (1%)	71 90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	ASP
1	A	396	LYS
1	A	402	SER
1	B	191	ARG
1	B	223	ARG
1	B	256	ARG
1	B	328	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	111	ASN

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 monosaccharides 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	B	501	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.05	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, 95^{th} 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	342/352 (97%)	-0.17	5 (1%)	73	71	28, 57, 112, 149	0
1	B	334/352 (94%)	-0.17	6 (1%)	68	65	30, 57, 110, 186	0
All	All	676/704 (96%)	-0.17	11 (1%)	72	69	28, 57, 111, 186	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	430	ARG	3.0
1	A	278	VAL	2.6
1	B	307	GLU	2.5
1	A	217	ASP	2.5
1	B	192	GLU	2.5
1	A	276	VAL	2.4
1	A	274	TYR	2.2
1	B	189	ALA	2.2
1	A	268	SER	2.1
1	B	263	LEU	2.1
1	B	312	ALA	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

There are no monosaccharides in this entry.

6.4 Ligands

LIGAND-RSR INFOmissingINFO

6.5 Other polymers

There are no such residues in this entry.