Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 11:14 PM GMT

PDB ID	:	5ES5
Title	:	Crystal structure of the initiation module of LgrA in the "open" and "closed " adenylation states
Authors	:	Reimer, J.M.; Aloise, M.N.; Schmeing, T.M.
Deposited on	:	2015-11-16
Resolution	:	2.80 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 ①) were used in the production of this report:

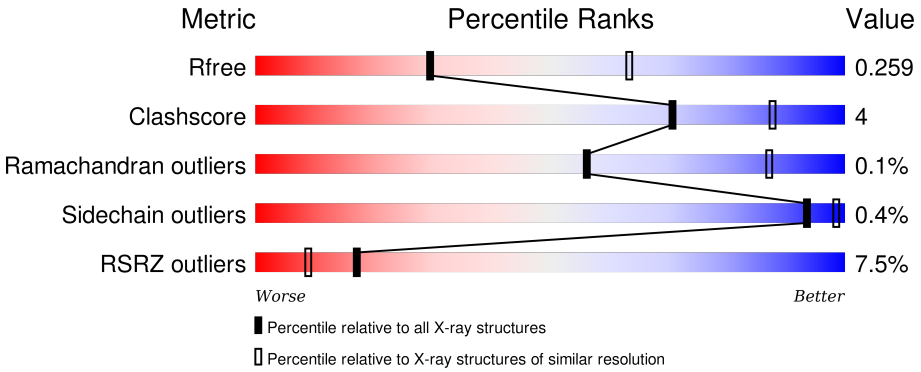
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 <=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	776	5% 81% 7% 12%
1	B	776	9% 78% 10% • 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21585 atoms, of which 10679 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.

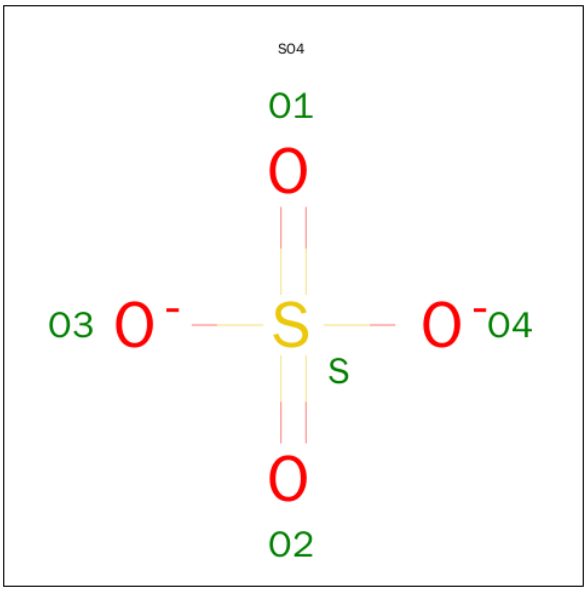
- Molecule 1 is a protein called Linear gramicidin synthetase subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	683	Total	C	H	N	O	S	0	0	0
			10764	3471	5324	930	1014	25			
1	B	685	Total	C	H	N	O	S	0	0	0
			10802	3476	5355	930	1016	25			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q70LM7
B	2	GLY	-	expression tag	UNP Q70LM7
B	768	ALA	-	expression tag	UNP Q70LM7
B	769	ALA	-	expression tag	UNP Q70LM7
B	770	ALA	-	expression tag	UNP Q70LM7
B	771	GLU	-	expression tag	UNP Q70LM7
B	772	ASN	-	expression tag	UNP Q70LM7
B	773	LEU	-	expression tag	UNP Q70LM7
B	774	TYR	-	expression tag	UNP Q70LM7
B	775	PHE	-	expression tag	UNP Q70LM7
B	776	GLN	-	expression tag	UNP Q70LM7
A	1	MET	-	initiating methionine	UNP Q70LM7
A	2	GLY	-	expression tag	UNP Q70LM7
A	768	ALA	-	expression tag	UNP Q70LM7
A	769	ALA	-	expression tag	UNP Q70LM7
A	770	ALA	-	expression tag	UNP Q70LM7
A	771	GLU	-	expression tag	UNP Q70LM7
A	772	ASN	-	expression tag	UNP Q70LM7
A	773	LEU	-	expression tag	UNP Q70LM7
A	774	TYR	-	expression tag	UNP Q70LM7
A	775	PHE	-	expression tag	UNP Q70LM7
A	776	GLN	-	expression tag	UNP Q70LM7

- 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	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

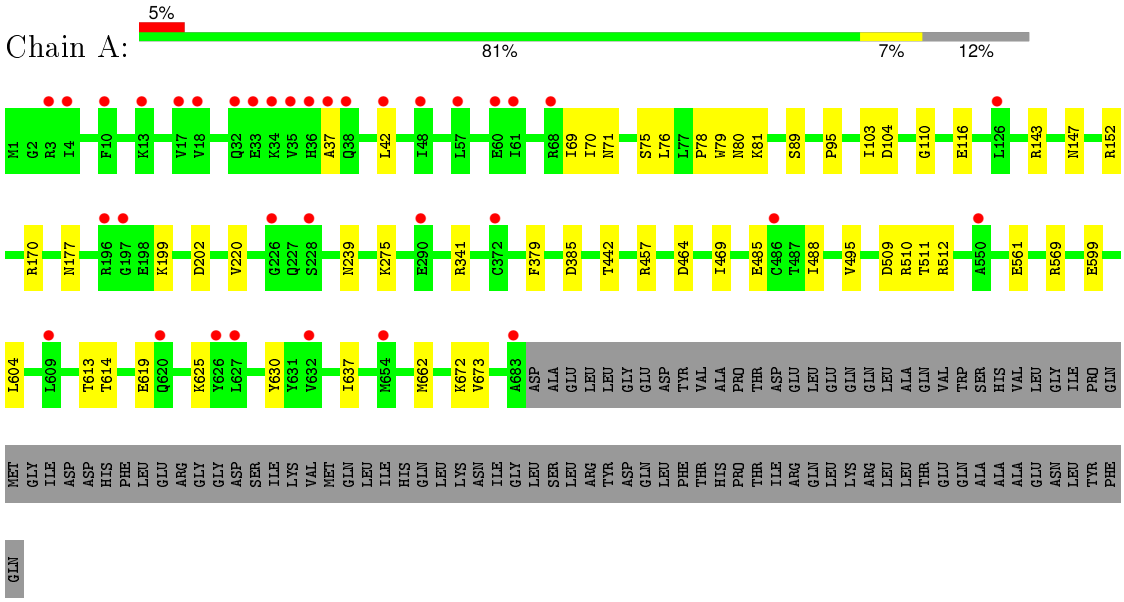
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	4	Total O 4 4	0	0

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.

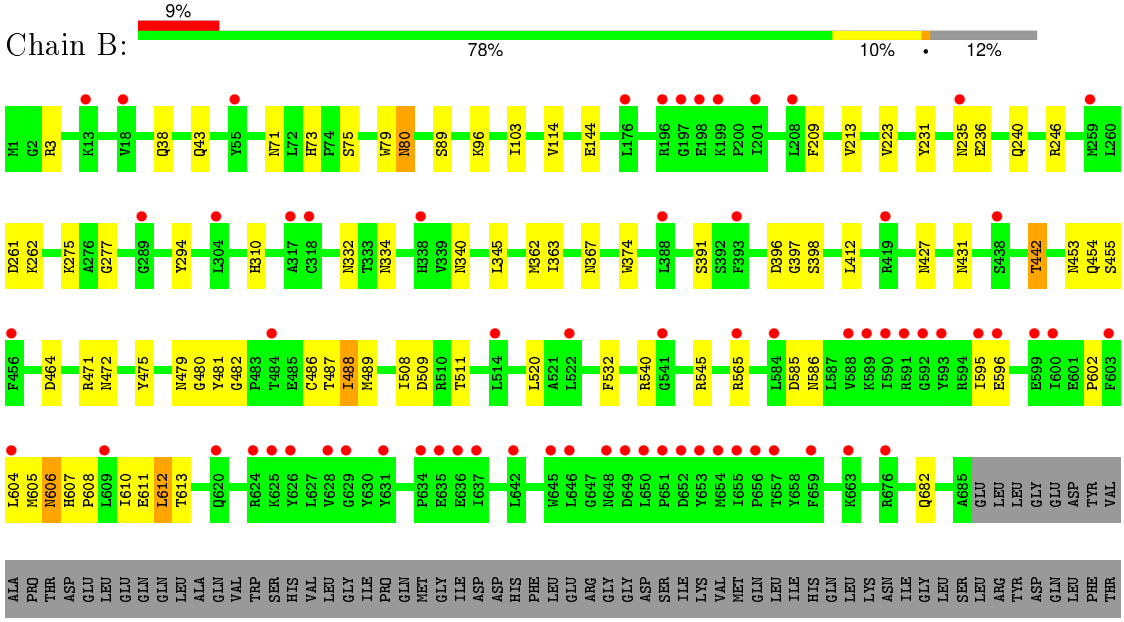
- Molecule 1: Linear gramicidin synthetase subunit A

Chain A:



- Molecule 1: Linear gramicidin synthetase subunit A

Chain B:



HIS
PRO
THR
ILE
ARG
GLN
LEU
LYS
ARG
LEU
LEU
THR
GLU
GLN
ALA
ALA
ALA
GLU
ASN
LEU
TYR
PHE
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	278.84Å 278.84Å 82.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.05 – 2.80 46.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.05-2.80) 92.3 (46.05-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.227 , 0.263 0.222 , 0.259	Depositor DCC
R_{free} test set	2757 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	78.1	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 86.3	EDS
Estimated twinning fraction	0.012 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 59120 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21585	wwPDB-VP
Average B, all atoms (Å^2)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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, 0.375 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	0.25	0/5569	0.43	0/7564
1	B	0.26	0/5576	0.44	0/7574
All	All	0.26	0/11145	0.44	0/15138

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	5440	5324	5357	31	2
1	B	5447	5355	5362	64	1
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	5	0	0	0	0
3	B	4	0	0	0	0
All	All	10906	10679	10719	95	2

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 4.

All (95) 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:B:611:GLU:C	1:B:612:LEU:HD23	1.64	1.17
1:A:199:LYS:O	1:A:510:ARG:NH1	2.03	0.91
1:A:512:ARG:NH2	1:A:561:GLU:OE2	2.14	0.80
1:B:611:GLU:O	1:B:612:LEU:HD23	1.85	0.75
1:B:231:TYR:O	1:B:235:ASN:ND2	2.23	0.72
1:B:612:LEU:N	1:B:612:LEU:HD23	2.03	0.71
1:B:367:ASN:HB3	1:B:487:THR:HG21	1.73	0.71
1:B:605:MET:HA	1:B:610:ILE:HD12	1.76	0.67
1:B:488:ILE:HG22	1:B:489:MET:H	1.61	0.66
1:B:80:ASN:OD1	1:B:89:SER:N	2.34	0.60
1:B:454:GLN:N	1:B:454:GLN:OE1	2.34	0.60
1:B:486:CYS:O	1:B:487:THR:OG1	2.20	0.59
1:A:75:SER:OG	1:A:79:TRP:O	2.18	0.59
1:B:585:ASP:OD1	1:B:586:ASN:N	2.36	0.59
1:B:605:MET:HE1	1:B:611:GLU:O	2.04	0.58
1:B:427:ASN:OD1	1:B:431:ASN:ND2	2.37	0.58
1:B:209:PHE:O	1:B:213:VAL:HG23	2.04	0.57
1:B:391:SER:OG	1:B:398:SER:HA	2.05	0.56
1:A:78:PRO:O	1:A:81:LYS:HE3	2.05	0.56
1:A:71:ASN:HB2	1:A:103:ILE:HD11	1.86	0.56
1:B:374:TRP:CG	1:B:508:ILE:HG23	2.40	0.56
1:B:89:SER:O	1:B:96:LYS:NZ	2.37	0.56
1:A:442:THR:OG1	1:A:464:ASP:HB2	2.06	0.55
1:B:363:ILE:HD12	1:B:487:THR:HG22	1.89	0.55
1:A:464:ASP:OD1	1:A:672:LYS:NZ	2.28	0.54
1:B:277:GLY:O	1:B:340:ASN:ND2	2.37	0.54
1:B:75:SER:OG	1:B:79:TRP:O	2.27	0.52
1:B:606:ASN:OD1	1:B:606:ASN:N	2.41	0.52
1:B:332:ASN:OD1	1:B:334:ASN:N	2.39	0.52
1:B:345:LEU:HD11	1:B:540:ARG:NH1	2.25	0.52
1:A:80:ASN:OD1	1:A:89:SER:N	2.43	0.51
1:B:602:PRO:O	1:B:606:ASN:OD1	2.29	0.51
1:B:209:PHE:CE2	1:B:235:ASN:OD1	2.64	0.51
1:B:374:TRP:CD1	1:B:508:ILE:HG23	2.47	0.50
1:B:605:MET:CE	1:B:611:GLU:O	2.60	0.49
1:A:619:GLU:OE2	1:A:625:LYS:NZ	2.39	0.49
1:B:479:ASN:OD1	1:B:480:GLY:N	2.47	0.48
1:A:104:ASP:OD2	1:A:110:GLY:N	2.45	0.48
1:B:508:ILE:O	1:B:511:THR:OG1	2.25	0.48
1:B:453:ASN:OD1	1:B:455:SER:N	2.46	0.48
1:B:362:MET:HE2	1:B:540:ARG:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:HIS:HB3	1:B:610:ILE:HG12	1.95	0.48
1:A:379:PHE:O	1:A:457:ARG:NH1	2.45	0.48
1:B:213:VAL:CG1	1:B:235:ASN:HD22	2.26	0.47
1:B:213:VAL:CG2	1:B:235:ASN:ND2	2.77	0.47
1:B:520:LEU:N	1:B:520:LEU:HD23	2.29	0.47
1:B:604:LEU:O	1:B:610:ILE:HD13	2.14	0.47
1:B:345:LEU:H	1:B:345:LEU:HD12	1.79	0.47
1:B:246:ARG:NH2	1:B:275:LYS:O	2.48	0.46
1:A:170:ARG:NH2	1:A:177:ASN:OD1	2.48	0.46
1:B:482:GLY:HA3	1:B:489:MET:HA	1.98	0.46
1:A:80:ASN:OD1	1:A:89:SER:CA	2.63	0.46
1:A:385:ASP:OD2	1:A:457:ARG:NH2	2.49	0.46
1:A:512:ARG:HH22	1:A:561:GLU:CD	2.14	0.46
1:B:605:MET:HA	1:B:610:ILE:CD1	2.45	0.46
1:A:147:ASN:OD1	1:A:152:ARG:NH2	2.41	0.46
1:B:442:THR:HB	1:B:464:ASP:HB3	1.98	0.45
1:A:614:THR:HG21	1:A:673:VAL:HG21	1.97	0.45
1:B:236:GLU:O	1:B:240:GLN:HG3	2.17	0.45
1:B:532:PHE:CE2	1:B:565:ARG:HG2	2.51	0.45
1:A:469:ILE:HD12	1:A:495:VAL:HG11	1.99	0.45
1:A:630:TYR:HD1	1:A:662:MET:HE1	1.81	0.45
1:B:3:ARG:NH1	1:B:43:GLN:O	2.50	0.45
1:A:509:ASP:O	1:A:511:THR:HG23	2.18	0.44
1:A:37:ALA:HA	1:A:42:LEU:HD11	1.98	0.44
1:B:480:GLY:HA3	1:B:489:MET:SD	2.57	0.44
1:B:262:LYS:HE2	1:B:391:SER:O	2.17	0.44
1:B:508:ILE:HG22	1:B:509:ASP:N	2.33	0.44
1:B:595:ILE:HG22	1:B:596:GLU:N	2.33	0.44
1:A:76:LEU:HD23	1:A:95:PRO:HB2	2.00	0.44
1:B:396:ASP:OD1	1:B:397:GLY:N	2.51	0.44
1:A:103:ILE:HG22	1:A:104:ASP:N	2.34	0.43
1:B:612:LEU:C	1:B:613:THR:HG23	2.39	0.43
1:B:73:HIS:O	1:B:75:SER:N	2.44	0.43
1:B:471:ARG:HD2	1:B:475:TYR:CE1	2.53	0.43
1:B:223:VAL:N	1:B:412:LEU:O	2.39	0.42
1:B:607:HIS:CG	1:B:608:PRO:HD2	2.55	0.42
1:A:604:LEU:HB3	1:A:613:THR:HG21	2.01	0.42
1:B:261:ASP:OD2	1:B:310:HIS:NE2	2.50	0.42
1:B:80:ASN:OD1	1:B:89:SER:CA	2.68	0.42
1:B:508:ILE:CG2	1:B:509:ASP:N	2.83	0.41
1:B:213:VAL:HG11	1:B:235:ASN:HD22	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASP:N	1:A:202:ASP:OD1	2.49	0.41
1:A:569:ARG:NH1	1:A:599:GLU:OE1	2.54	0.41
1:A:116:GLU:OE2	1:A:143:ARG:NH2	2.50	0.41
1:B:604:LEU:O	1:B:610:ILE:CD1	2.69	0.41
1:B:294:TYR:OH	1:B:545:ARG:NH2	2.54	0.41
1:A:485:GLU:N	1:A:485:GLU:OE1	2.53	0.41
1:A:70:ILE:N	1:A:70:ILE:HD12	2.36	0.41
1:A:69:ILE:HG22	1:A:103:ILE:HG13	2.03	0.41
1:B:114:VAL:HG11	1:B:144:GLU:HG3	2.03	0.41
1:A:239:ASN:OD1	1:A:275:LYS:HE3	2.21	0.40
1:B:38:GLN:OE1	1:B:38:GLN:N	2.54	0.40
1:B:481:TYR:C	1:B:489:MET:HG2	2.42	0.40
1:B:71:ASN:HB2	1:B:103:ILE:HD11	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:ILE:O	1:B:682:GLN:NE2[3_765]	2.06	0.14
1:A:220:VAL:O	1:A:341:ARG:HH22[5_535]	1.51	0.09

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	681/776 (88%)	660 (97%)	20 (3%)	1 (0%)	56	87
1	B	683/776 (88%)	654 (96%)	28 (4%)	1 (0%)	56	87
All	All	1364/1552 (88%)	1314 (96%)	48 (4%)	2 (0%)	56	87

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	488	ILE
1	A	488	ILE

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	583/666 (88%)	583 (100%)	0	100 100
1	B	583/666 (88%)	578 (99%)	5 (1%)	84 96
All	All	1166/1332 (88%)	1161 (100%)	5 (0%)	93 98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	80	ASN
1	B	442	THR
1	B	472	ASN
1	B	606	ASN
1	B	612	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	235	ASN
1	B	450	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	801	-	4,4,4	0.23	0	6,6,6	0.05	0
2	SO4	B	801	-	4,4,4	0.24	0	6,6,6	0.08	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	801	-	-	0/0/0/0	0/0/0/0
2	SO4	B	801	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	683/776 (88%)	0.48	35 (5%) 32 21	73, 117, 177, 194	0
1	B	685/776 (88%)	0.71	68 (9%) 9 4	86, 148, 192, 233	0
All	All	1368/1552 (88%)	0.60	103 (7%) 17 9	73, 139, 183, 233	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ARG	6.3
1	B	655	ILE	6.1
1	B	646	LEU	5.9
1	B	589	LYS	5.8
1	A	37	ALA	5.3
1	B	659	PHE	5.0
1	B	197	GLY	4.8
1	B	654	MET	4.6
1	B	593	TYR	4.6
1	B	652	ASP	4.4
1	B	656	PRO	4.4
1	B	590	ILE	4.3
1	B	657	THR	4.3
1	A	42	LEU	4.2
1	B	650	LEU	4.1
1	B	592	GLY	4.0
1	B	591	ARG	3.8
1	A	57	LEU	3.8
1	B	624	ARG	3.7
1	B	603	PHE	3.6
1	B	584	LEU	3.6
1	A	196	ARG	3.6
1	B	595	ILE	3.5
1	B	636	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	599	GLU	3.4
1	B	649	ASP	3.3
1	B	609	LEU	3.3
1	B	634	PRO	3.3
1	B	196	ARG	3.3
1	B	13	LYS	3.3
1	B	642	LEU	3.2
1	B	631	TYR	3.2
1	A	683	ALA	3.2
1	A	34	LYS	3.2
1	A	48	ILE	3.1
1	A	654	MET	3.1
1	A	197	GLY	3.1
1	A	226	GLY	3.1
1	B	629	GLY	3.1
1	A	620	GLN	3.1
1	A	627	LEU	3.0
1	B	176	LEU	3.0
1	B	522	LEU	3.0
1	B	235	ASN	3.0
1	A	10	PHE	3.0
1	B	604	LEU	3.0
1	A	609	LEU	2.9
1	B	620	GLN	2.9
1	A	36	HIS	2.9
1	B	651	PRO	2.9
1	B	600	ILE	2.9
1	A	228	SER	2.8
1	B	198	GLU	2.8
1	A	32	GLN	2.8
1	B	199	LYS	2.7
1	A	35	VAL	2.7
1	A	17	VAL	2.7
1	B	541	GLY	2.7
1	A	372	CYS	2.7
1	B	484	THR	2.7
1	B	625	LYS	2.7
1	B	338	HIS	2.7
1	A	4	ILE	2.6
1	B	653	TYR	2.6
1	A	126	LEU	2.6
1	B	637	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	596	GLU	2.5
1	B	419	ARG	2.5
1	A	38	GLN	2.5
1	A	61	ILE	2.4
1	A	13	LYS	2.4
1	A	60	GLU	2.4
1	A	486	CYS	2.4
1	B	635	GLU	2.4
1	A	68	ARG	2.4
1	B	645	TRP	2.3
1	B	456	PHE	2.3
1	B	663	LYS	2.2
1	B	208	LEU	2.2
1	B	514	LEU	2.2
1	B	201	ILE	2.2
1	B	289	GLY	2.2
1	B	565	ARG	2.2
1	B	588	VAL	2.2
1	B	304	LEU	2.1
1	A	18	VAL	2.1
1	A	626	TYR	2.1
1	B	55	TYR	2.1
1	B	626	TYR	2.1
1	A	632	VAL	2.1
1	B	388	LEU	2.1
1	B	648	ASN	2.1
1	B	18	VAL	2.1
1	A	550	ALA	2.1
1	A	290	GLU	2.1
1	B	259	MET	2.0
1	B	628	VAL	2.0
1	B	438	SER	2.0
1	B	393	PHE	2.0
1	B	676	ARG	2.0
1	B	317	ALA	2.0
1	B	318	CYS	2.0
1	A	33	GLU	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, 95^{th} 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	801	5/5	0.91	0.16	-0.19	143,151,164,166	0
2	SO4	B	801	5/5	0.90	0.14	-0.97	175,176,186,186	0

6.5 Other polymers (i)

There are no such residues in this entry.