Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 10:46 AM EST

PDB ID	:	8SM3
Title	:	Structure of Bacillus cereus VD045 Gabija GajA-GajB Complex
Authors	:	Antine, S.P.; Mooney, S.E.; Johnson, A.G.; Kranzusch, P.J.
Deposited on	:	2023-04-25
Resolution	:	3.00 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:

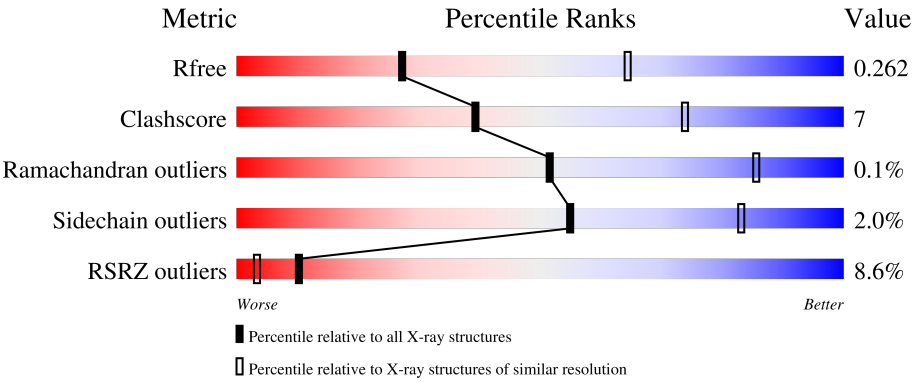
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	588	6% 75% 18% 7%
2	B	493	11% 77% 23%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8506 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 Endonuclease GajA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	548	4483	2877	738	855	13	0	0	0

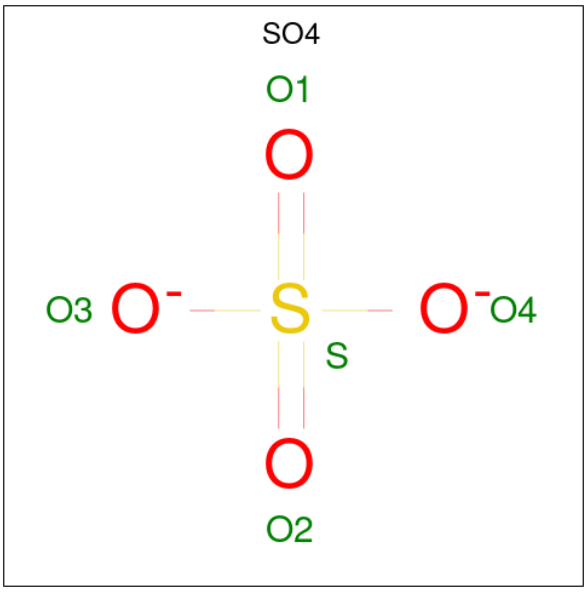
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP J8H9C1
A	-8	SER	-	expression tag	UNP J8H9C1
A	-7	GLY	-	expression tag	UNP J8H9C1
A	-6	SER	-	expression tag	UNP J8H9C1
A	-5	GLY	-	expression tag	UNP J8H9C1
A	-4	SER	-	expression tag	UNP J8H9C1
A	-3	GLY	-	expression tag	UNP J8H9C1
A	-2	SER	-	expression tag	UNP J8H9C1
A	-1	GLY	-	expression tag	UNP J8H9C1
A	0	SER	-	expression tag	UNP J8H9C1
A	1	SER	-	expression tag	UNP J8H9C1

- Molecule 2 is a protein called Gabija protein GajB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	493	4018	2574	664	770	10	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



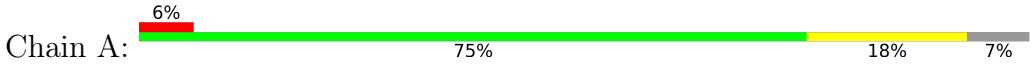
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

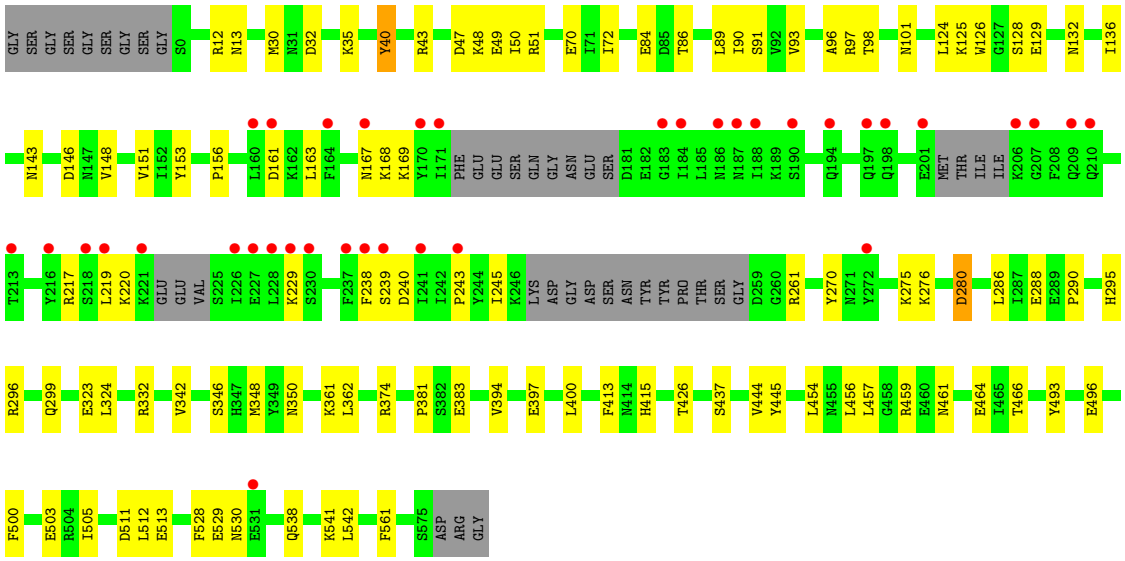
3 Residue-property plots (i)

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: Endonuclease GajA

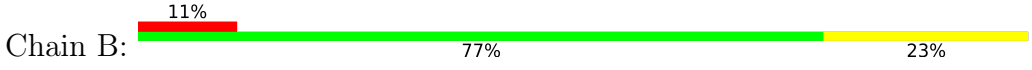
Chain A:

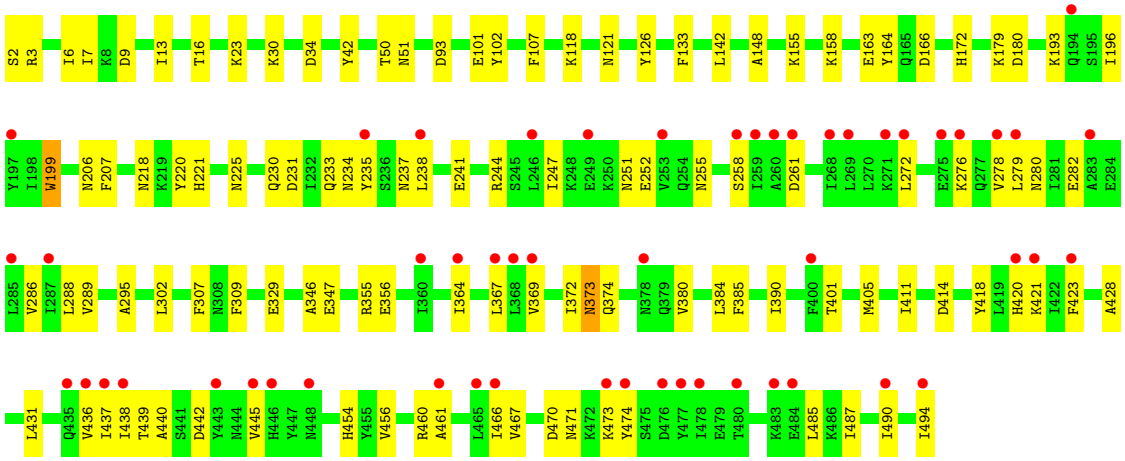




• Molecule 2: Gabija protein GajB

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	215.79Å 215.79Å 173.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.24 – 3.00 49.24 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.24-3.00) 99.9 (49.24-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.237 , 0.266 0.234 , 0.262	Depositor DCC
R_{free} test set	2000 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å^2)	91.4	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 80.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8506	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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	0.25	0/4555	0.44	0/6107
2	B	0.24	0/4087	0.43	0/5513
All	All	0.25	0/8642	0.44	0/11620

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	4483	0	4542	57	0
2	B	4018	0	4041	71	0
3	A	5	0	0	1	0
All	All	8506	0	8583	126	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 7.

All (126) 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:454:HIS:HE2	2:B:474:TYR:HH	1.19	0.88
2:B:101:GLU:OE2	2:B:355:ARG:NH2	2.24	0.69
1:A:290:PRO:HG2	1:A:324:LEU:HD21	1.75	0.68
1:A:444:VAL:HG12	1:A:466:THR:HG22	1.75	0.67
2:B:278:VAL:HG23	2:B:279:LEU:HD12	1.78	0.66
2:B:372:ILE:O	2:B:373:ASN:ND2	2.29	0.65
1:A:12:ARG:HH12	1:A:40:TYR:HD2	1.45	0.65
2:B:374:GLN:HG3	2:B:401:THR:HG21	1.80	0.64
2:B:230:GLN:O	2:B:234:ASN:ND2	2.31	0.63
2:B:289:VAL:HG21	2:B:295:ALA:HB2	1.79	0.63
1:A:163:LEU:O	1:A:167:ASN:ND2	2.33	0.61
2:B:364:ILE:HD11	2:B:384:LEU:HD13	1.82	0.61
1:A:84:GLU:OE2	2:B:42:TYR:OH	2.11	0.61
1:A:381:PRO:HG2	1:A:542:LEU:HD21	1.84	0.60
2:B:276:LYS:HG3	2:B:494:ILE:HD13	1.85	0.59
2:B:280:ASN:HD21	2:B:282:GLU:HB2	1.68	0.59
2:B:272:LEU:HB3	2:B:279:LEU:HD13	1.85	0.59
1:A:500:PHE:HB3	1:A:505:ILE:HB	1.86	0.58
1:A:383:GLU:HG3	1:A:512:LEU:HD22	1.85	0.58
1:A:296:ARG:HG3	1:A:323:GLU:HG2	1.86	0.57
2:B:164:TYR:OH	2:B:172:HIS:ND1	2.32	0.57
2:B:418:TYR:O	2:B:421:LYS:NZ	2.37	0.57
1:A:168:LYS:NZ	1:A:239:SER:O	2.38	0.57
1:A:245:ILE:HD13	1:A:261:ARG:HH22	1.70	0.57
1:A:125:LYS:NZ	3:A:601:SO4:O1	2.36	0.56
2:B:329:GLU:HG3	2:B:347:GLU:HG2	1.88	0.55
2:B:288:LEU:HD21	2:B:423:PHE:CE2	2.41	0.55
1:A:280:ASP:OD1	1:A:280:ASP:N	2.38	0.55
2:B:437:ILE:HG12	2:B:466:ILE:HB	1.88	0.55
2:B:225:ASN:O	2:B:233:GLN:NE2	2.41	0.54
1:A:48:LYS:NZ	1:A:49:GLU:OE2	2.41	0.54
2:B:34:ASP:OD2	2:B:158:LYS:HE3	2.07	0.53
2:B:23:LYS:HE3	2:B:163:GLU:OE2	2.09	0.53
2:B:279:LEU:HD11	2:B:466:ILE:HG13	1.90	0.53
1:A:153:TYR:OH	1:A:288:GLU:OE1	2.23	0.52
2:B:234:ASN:HA	2:B:247:ILE:HG21	1.90	0.52
2:B:50:THR:OG1	2:B:346:ALA:O	2.28	0.51
1:A:93:VAL:HG13	1:A:96:ALA:HB3	1.93	0.51
2:B:411:ILE:HA	2:B:414:ASP:HB2	1.91	0.51
2:B:241:GLU:HA	2:B:244:ARG:HD2	1.93	0.51
2:B:121:ASN:O	2:B:121:ASN:ND2	2.43	0.50
1:A:169:LYS:HD3	1:A:238:PHE:HE2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ASN:HB3	2:B:490:ILE:HD11	1.92	0.50
1:A:413:PHE:HB2	1:A:456:LEU:HD21	1.93	0.49
2:B:471:ASN:HD21	2:B:473:LYS:HB2	1.77	0.49
1:A:43:ARG:HB3	1:A:50:ILE:HG21	1.94	0.49
1:A:457:LEU:HB3	1:A:459:ARG:NH1	2.27	0.49
1:A:511:ASP:OD2	1:A:538:GLN:NE2	2.45	0.49
2:B:93:ASP:HB3	2:B:118:LYS:HE3	1.95	0.49
2:B:286:VAL:HA	2:B:421:LYS:O	2.13	0.49
1:A:129:GLU:HB2	1:A:132:ASN:OD1	2.13	0.49
1:A:156:PRO:HG3	1:A:288:GLU:O	2.13	0.49
2:B:166:ASP:HB3	2:B:199:TRP:HB3	1.95	0.49
1:A:93:VAL:HG11	1:A:97:ARG:HG3	1.93	0.48
2:B:102:TYR:N	2:B:356:GLU:OE2	2.44	0.48
2:B:485:LEU:HB2	2:B:487:ILE:HG12	1.95	0.48
1:A:528:PHE:C	1:A:530:ASN:H	2.17	0.48
2:B:231:ASP:HB2	2:B:255:ASN:HB2	1.95	0.48
2:B:16:THR:OG1	2:B:221:HIS:ND1	2.46	0.48
2:B:445:VAL:HG21	2:B:474:TYR:HA	1.95	0.48
1:A:32:ASP:HA	1:A:35:LYS:HZ3	1.78	0.48
1:A:503:GLU:HB3	1:A:505:ILE:HG12	1.94	0.47
2:B:401:THR:O	2:B:405:MET:HG2	2.13	0.47
2:B:423:PHE:CD2	2:B:428:ALA:HB3	2.48	0.47
1:A:13:ASN:HB2	1:A:342:VAL:HG21	1.96	0.47
2:B:276:LYS:HE3	2:B:494:ILE:HG23	1.96	0.47
1:A:151:VAL:HG13	1:A:286:LEU:HD13	1.96	0.47
1:A:275:LYS:HD2	1:A:276:LYS:HD3	1.97	0.47
1:A:374:ARG:HG2	1:A:426:THR:HB	1.97	0.47
1:A:32:ASP:OD1	1:A:35:LYS:NZ	2.47	0.46
2:B:436:VAL:HB	2:B:461:ALA:HB2	1.96	0.46
2:B:439:THR:OG1	2:B:442:ASP:OD2	2.34	0.46
1:A:124:LEU:HB3	1:A:136:ILE:HD12	1.97	0.46
2:B:107:PHE:HZ	2:B:133:PHE:CG	2.33	0.46
2:B:456:VAL:O	2:B:460:ARG:HG2	2.15	0.46
1:A:89:LEU:HD13	1:A:148:VAL:HG11	1.99	0.45
1:A:397:GLU:HA	1:A:400:LEU:HD13	1.98	0.45
2:B:179:LYS:NZ	2:B:180:ASP:OD1	2.34	0.45
2:B:261:ASP:OD1	2:B:261:ASP:N	2.50	0.45
1:A:454:LEU:HD22	1:A:459:ARG:HD2	1.98	0.45
2:B:2:SER:OG	2:B:3:ARG:N	2.50	0.45
2:B:258:SER:HA	2:B:467:VAL:O	2.18	0.44
2:B:280:ASN:ND2	2:B:282:GLU:HB2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:HA	1:A:128:SER:HB2	1.99	0.44
2:B:288:LEU:HB2	2:B:438:ILE:HG22	2.00	0.44
2:B:440:ALA:HB3	2:B:470:ASP:H	1.83	0.44
1:A:91:SER:HB2	2:B:155:LYS:HD2	2.00	0.43
1:A:383:GLU:OE1	1:A:383:GLU:N	2.46	0.43
2:B:206:ASN:OD1	2:B:207:PHE:N	2.51	0.43
1:A:13:ASN:OD1	1:A:13:ASN:N	2.51	0.43
1:A:161:ASP:OD1	1:A:243:PRO:HD2	2.19	0.43
1:A:240:ASP:N	1:A:240:ASP:OD1	2.51	0.43
2:B:288:LEU:HD21	2:B:423:PHE:CZ	2.53	0.43
2:B:431:LEU:H	2:B:431:LEU:HD23	1.83	0.43
2:B:367:LEU:HG	2:B:380:VAL:HG11	2.00	0.43
1:A:47:ASP:HB3	1:A:50:ILE:HG22	2.00	0.43
1:A:51:ARG:NH2	1:A:146:ASP:OD1	2.49	0.43
1:A:70:GLU:HG2	1:A:72:ILE:HD11	2.00	0.43
1:A:394:VAL:HG11	1:A:561:PHE:CG	2.54	0.43
2:B:251:ASN:OD1	2:B:252:GLU:N	2.52	0.43
1:A:98:THR:HG23	1:A:101:ASN:H	1.82	0.43
1:A:332:ARG:NH1	1:A:348:MET:HB2	2.34	0.42
1:A:86:THR:O	1:A:90:ILE:HG12	2.19	0.42
1:A:219:LEU:HD23	1:A:220:LYS:HB2	2.02	0.42
1:A:513:GLU:OE2	1:A:541:LYS:HE3	2.19	0.42
1:A:332:ARG:HE	1:A:346:SER:HB2	1.85	0.42
1:A:437:SER:HB3	1:A:445:TYR:HE1	1.84	0.42
1:A:362:LEU:HD21	1:A:415:HIS:CD2	2.55	0.41
2:B:309:PHE:CE1	2:B:420:HIS:HB3	2.56	0.41
2:B:2:SER:O	2:B:6:ILE:HG13	2.20	0.41
2:B:233:GLN:O	2:B:237:ASN:ND2	2.29	0.41
2:B:286:VAL:HG23	2:B:436:VAL:HG22	2.01	0.41
1:A:124:LEU:HD12	1:A:143:ASN:HD21	1.86	0.41
2:B:9:ASP:HB3	2:B:13:ILE:HD11	2.02	0.41
2:B:142:LEU:HD23	2:B:148:ALA:HB1	2.02	0.41
1:A:295:HIS:O	1:A:299:GLN:HG3	2.21	0.41
1:A:493:TYR:HD1	1:A:496:GLU:HG3	1.86	0.41
2:B:235:TYR:HA	2:B:238:LEU:HD23	2.02	0.41
2:B:247:ILE:H	2:B:247:ILE:HG13	1.66	0.41
2:B:302:LEU:HB3	2:B:307:PHE:HB2	2.02	0.41
2:B:385:PHE:HB3	2:B:390:ILE:O	2.21	0.41
2:B:7:ILE:O	2:B:30:LYS:NZ	2.52	0.41
2:B:6:ILE:HG12	2:B:220:TYR:CD1	2.55	0.40
2:B:471:ASN:ND2	2:B:473:LYS:HB2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:LEU:HD23	2:B:288:LEU:HA	1.67	0.40
2:B:490:ILE:HD12	2:B:490:ILE:HA	1.92	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	538/588 (92%)	513 (95%)	24 (4%)	1 (0%)	47 82
2	B	491/493 (100%)	475 (97%)	16 (3%)	0	100 100
All	All	1029/1081 (95%)	988 (96%)	40 (4%)	1 (0%)	51 85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	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	503/534 (94%)	492 (98%)	11 (2%)	52 81
2	B	447/447 (100%)	439 (98%)	8 (2%)	59 85
All	All	950/981 (97%)	931 (98%)	19 (2%)	55 83

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	MET
1	A	40	TYR
1	A	126	TRP
1	A	217	ARG
1	A	270	TYR
1	A	280	ASP
1	A	350	ASN
1	A	361	LYS
1	A	461	ASN
1	A	464	GLU
1	A	529	GLU
2	B	51	ASN
2	B	126	TYR
2	B	193	LYS
2	B	196	ILE
2	B	199	TRP
2	B	218	ASN
2	B	369	VAL
2	B	373	ASN

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

Mol	Chain	Res	Type
1	A	167	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
3	SO4	A	601	-	4,4,4	0.13	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	548/588 (93%)	0.29	37 (6%)	17	5	60, 94, 208, 236	0
2	B	493/493 (100%)	0.50	53 (10%)	5	2	76, 147, 228, 303	0
All	All	1041/1081 (96%)	0.39	90 (8%)	10	3	60, 120, 214, 303	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	PHE	11.9
1	A	171	ILE	6.3
2	B	490	ILE	6.2
1	A	167	ASN	6.2
1	A	209	GLN	5.8
2	B	364	ILE	5.7
1	A	241	ILE	5.6
2	B	260	ALA	5.6
1	A	238	PHE	5.5
1	A	206	LYS	5.5
2	B	279	LEU	5.5
1	A	210	GLN	5.4
2	B	438	ILE	5.1
2	B	197	TYR	5.1
2	B	272	LEU	5.0
2	B	423	PHE	4.8
2	B	246	LEU	4.7
2	B	446	HIS	4.7
2	B	367	LEU	4.4
2	B	474	TYR	4.4
2	B	261	ASP	4.3
2	B	360	ILE	4.3
1	A	207	GLY	4.3
2	B	465	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	259	ILE	4.2
1	A	226	ILE	4.1
2	B	477	TYR	4.0
2	B	369	VAL	4.0
2	B	253	VAL	3.9
1	A	227	GLU	3.9
1	A	198	GLN	3.9
1	A	164	PHE	3.8
2	B	368	LEU	3.7
1	A	161	ASP	3.7
1	A	190	SER	3.6
2	B	278	VAL	3.6
2	B	435	GLN	3.5
1	A	219	LEU	3.5
1	A	228	LEU	3.5
2	B	466	ILE	3.4
2	B	461	ALA	3.4
2	B	285	LEU	3.4
1	A	239	SER	3.3
2	B	269	LEU	3.3
1	A	213	THR	3.3
1	A	531	GLU	3.3
2	B	484	GLU	3.2
2	B	235	TYR	3.2
1	A	188	ILE	3.2
1	A	183	GLY	3.2
2	B	271	LYS	3.2
1	A	194	GLN	3.2
1	A	216	TYR	3.1
1	A	187	ASN	3.1
2	B	478	ILE	3.0
2	B	494	ILE	2.9
2	B	287	ILE	2.9
2	B	445	VAL	2.8
1	A	197	GLN	2.8
2	B	275	GLU	2.8
2	B	258	SER	2.7
2	B	476	ASP	2.7
2	B	283	ALA	2.7
1	A	186	ASN	2.7
2	B	400	PHE	2.7
2	B	378	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	483	LYS	2.6
2	B	420	HIS	2.6
2	B	276	LYS	2.6
2	B	480	THR	2.6
1	A	170	TYR	2.6
2	B	443	TYR	2.5
1	A	184	ILE	2.5
2	B	437	ILE	2.5
1	A	229	LYS	2.5
2	B	268	ILE	2.4
2	B	194	GLN	2.4
2	B	436	VAL	2.4
2	B	421	LYS	2.3
2	B	448	ASN	2.3
1	A	243	PRO	2.3
2	B	473	LYS	2.3
1	A	272	TYR	2.2
1	A	160	LEU	2.2
1	A	230	SER	2.2
2	B	249	GLU	2.2
1	A	218	SER	2.1
2	B	238	LEU	2.1
1	A	221	LYS	2.0
1	A	201	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 monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
3	SO4	A	601	5/5	0.89	0.29	113,119,141,371	0

6.5 Other polymers (i)

There are no such residues in this entry.