



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:00 PM UTC

PDB ID : 5CPH / pdb_00005cph
Title : Crystal structure of the ATP binding domain of S. aureus GyrB complexed with a fragment
Authors : Andersen, O.A.; Barker, J.; Cheng, R.K.; Kahmann, J.; Felicetti, B.; Wood, M.; Scheich, C.; Mesleh, M.; Cross, J.B.; Zhang, J.; Yang, Q.; Lippa, B.; Ryan, M.D.
Deposited on : 2015-07-21
Resolution : 1.20 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

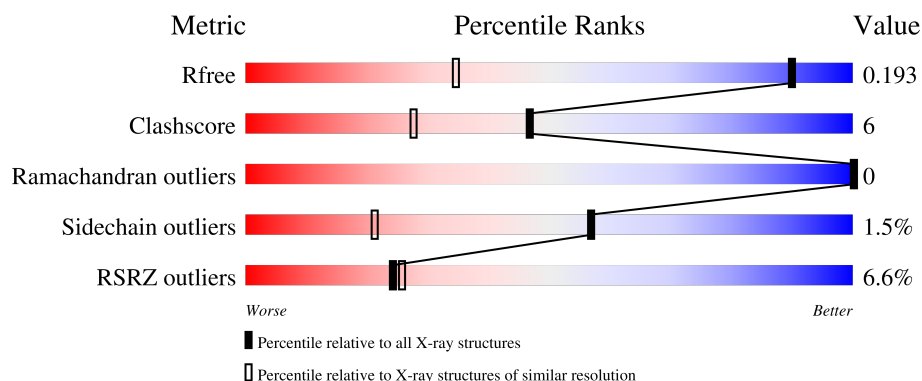
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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	212	4% 73% 15% • 9%
1	B	212	8% 68% 19% 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3704 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 gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	12	0
			1612	1015	277	318	2			
1	B	186	Total	C	N	O	S	0	4	0
			1518	954	261	302	1			

There are 50 discrepancies between the modelled and reference sequences:

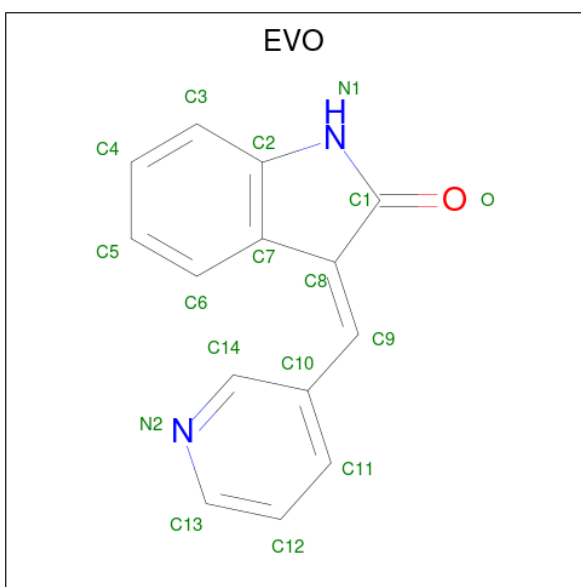
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P0A0K8
A	1	SER	-	expression tag	UNP P0A0K8
A	?	-	VAL	deletion	UNP P0A0K8
A	?	-	LEU	deletion	UNP P0A0K8
A	?	-	HIS	deletion	UNP P0A0K8
A	?	-	ALA	deletion	UNP P0A0K8
A	?	-	GLY	deletion	UNP P0A0K8
A	?	-	GLY	deletion	UNP P0A0K8
A	?	-	LYS	deletion	UNP P0A0K8
A	?	-	PHE	deletion	UNP P0A0K8
A	?	-	GLY	deletion	UNP P0A0K8
A	?	-	GLY	deletion	UNP P0A0K8
A	?	-	GLY	deletion	UNP P0A0K8
A	?	-	GLY	deletion	UNP P0A0K8
A	?	-	GLY	deletion	UNP P0A0K8
A	?	-	TYR	deletion	UNP P0A0K8
A	?	-	LYS	deletion	UNP P0A0K8
A	?	-	VAL	deletion	UNP P0A0K8
A	?	-	SER	deletion	UNP P0A0K8
A	?	-	GLY	deletion	UNP P0A0K8
A	?	-	GLY	deletion	UNP P0A0K8
A	?	-	LEU	deletion	UNP P0A0K8
A	?	-	HIS	deletion	UNP P0A0K8
A	?	-	GLY	deletion	UNP P0A0K8
A	?	-	VAL	deletion	UNP P0A0K8
A	?	-	GLY	deletion	UNP P0A0K8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P0A0K8
B	1	SER	-	expression tag	UNP P0A0K8
B	?	-	VAL	deletion	UNP P0A0K8
B	?	-	LEU	deletion	UNP P0A0K8
B	?	-	HIS	deletion	UNP P0A0K8
B	?	-	ALA	deletion	UNP P0A0K8
B	?	-	GLY	deletion	UNP P0A0K8
B	?	-	GLY	deletion	UNP P0A0K8
B	?	-	LYS	deletion	UNP P0A0K8
B	?	-	PHE	deletion	UNP P0A0K8
B	?	-	GLY	deletion	UNP P0A0K8
B	?	-	GLY	deletion	UNP P0A0K8
B	?	-	GLY	deletion	UNP P0A0K8
B	?	-	GLY	deletion	UNP P0A0K8
B	?	-	TYR	deletion	UNP P0A0K8
B	?	-	LYS	deletion	UNP P0A0K8
B	?	-	VAL	deletion	UNP P0A0K8
B	?	-	SER	deletion	UNP P0A0K8
B	?	-	GLY	deletion	UNP P0A0K8
B	?	-	GLY	deletion	UNP P0A0K8
B	?	-	LEU	deletion	UNP P0A0K8
B	?	-	HIS	deletion	UNP P0A0K8
B	?	-	GLY	deletion	UNP P0A0K8
B	?	-	VAL	deletion	UNP P0A0K8
B	?	-	GLY	deletion	UNP P0A0K8

- Molecule 2 is (3E)-3-(pyridin-3-ylmethyldene)-1,3-dihydro-2H-indol-2-one (CCD ID: EVO) (formula: C₁₄H₁₀N₂O).



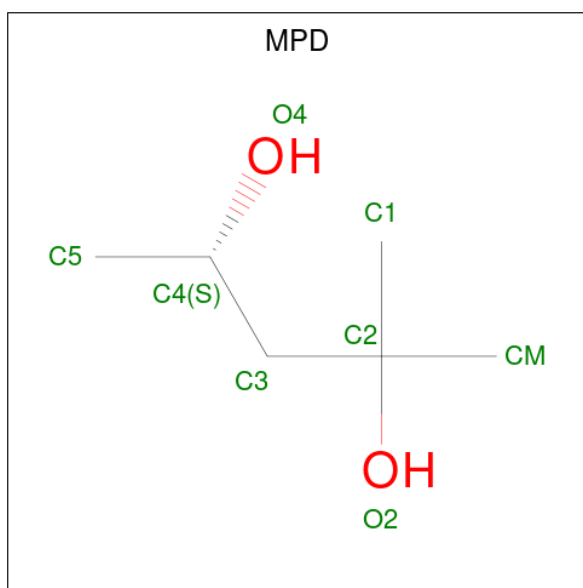
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	14	2	1		
2	B	1	Total	C	N	O	0	0
			17	14	2	1		

- Molecule 3 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is water.

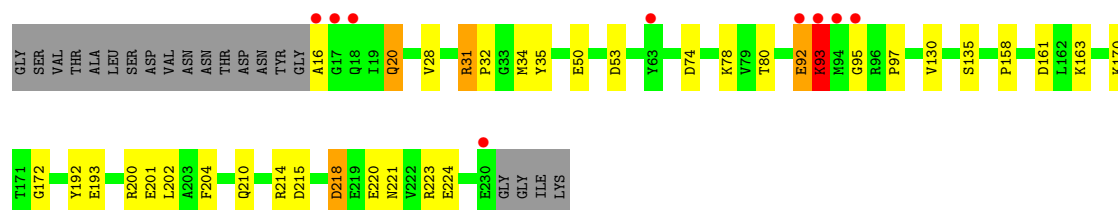
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	261	Total	O	0	0
			261	261		
5	B	261	Total	O	0	0
			261	261		

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.

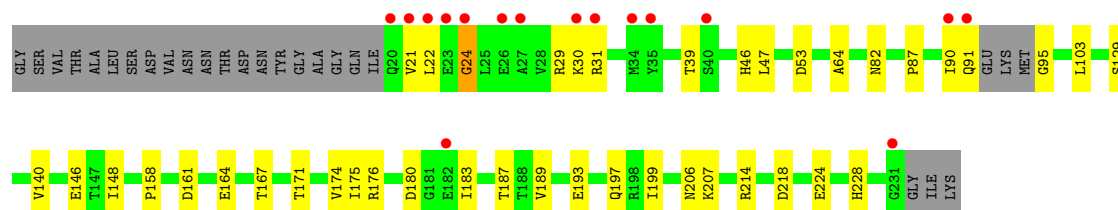
• Molecule 1: DNA gyrase subunit B

Chain A: 



• Molecule 1: DNA gyrase subunit B

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.85Å 55.68Å 51.57Å 90.00° 100.69° 90.00°	Depositor
Resolution (Å)	37.89 – 1.20 37.89 – 1.20	Depositor EDS
% Data completeness (in resolution range)	95.6 (37.89-1.20) 95.6 (37.89-1.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.172 , 0.194 0.171 , 0.193	Depositor DCC
R_{free} test set	5976 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3704	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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: MPD, SO4, EVO

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	1.83	30/1673 (1.8%)	1.38	8/2263 (0.4%)
1	B	1.85	21/1554 (1.4%)	1.37	7/2105 (0.3%)
All	All	1.84	51/3227 (1.6%)	1.37	15/4368 (0.3%)

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	PHE	C-N	-7.92	1.23	1.33
1	A	200	ARG	NE-CZ	-7.50	1.24	1.33
1	A	172	GLY	CA-C	-7.21	1.44	1.51
1	A	31	ARG	CA-C	-7.06	1.44	1.52
1	A	163	LYS	CA-CB	-7.05	1.36	1.53
1	B	214	ARG	NE-CZ	6.62	1.40	1.33
1	A	201	GLU	CA-CB	-6.53	1.43	1.53
1	A	224	GLU	N-CA	6.50	1.54	1.46
1	A	163	LYS	CB-CG	-6.48	1.33	1.52
1	A	224	GLU	CA-CB	-6.43	1.43	1.53
1	B	207	LYS	N-CA	-6.40	1.38	1.46
1	A	31	ARG	C-N	6.36	1.41	1.34
1	B	164	GLU	C-O	6.34	1.31	1.24
1	B	176	ARG	CA-CB	6.31	1.65	1.53
1	A	221	ASN	CA-CB	6.14	1.61	1.52
1	A	158	PRO	C-O	6.12	1.30	1.23
1	B	183	ILE	CA-C	6.09	1.60	1.52
1	B	158	PRO	C-O	6.08	1.30	1.23
1	B	148	ILE	C-O	6.02	1.30	1.24
1	A	214	ARG	CD-NE	-5.85	1.38	1.46
1	B	64	ALA	CA-CB	-5.83	1.44	1.53
1	A	78	LYS	CA-C	-5.70	1.46	1.52
1	B	87	PRO	C-O	5.68	1.30	1.23
1	A	170	LYS	CA-CB	-5.68	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	180	ASP	C-O	-5.67	1.17	1.24
1	B	129	SER	C-O	-5.64	1.17	1.24
1	A	202	LEU	C-O	5.62	1.30	1.24
1	B	90	ILE	N-CA	-5.60	1.39	1.46
1	A	161	ASP	N-CA	-5.50	1.39	1.45
1	A	221	ASN	N-CA	-5.48	1.40	1.46
1	B	183	ILE	N-CA	-5.46	1.39	1.46
1	A	215	ASP	C-O	5.40	1.30	1.24
1	A	35	TYR	C-O	-5.40	1.17	1.24
1	A	80	THR	C-O	5.39	1.30	1.24
1	B	218	ASP	CA-CB	-5.39	1.44	1.53
1	B	199	ILE	N-CA	-5.30	1.40	1.46
1	B	224	GLU	CA-C	-5.25	1.46	1.52
1	A	202	LEU	CA-C	-5.22	1.46	1.52
1	B	47	LEU	CA-CB	-5.22	1.45	1.53
1	B	206	ASN	CA-C	-5.21	1.46	1.53
1	B	228	HIS	CA-C	-5.10	1.48	1.53
1	A	32	PRO	C-O	-5.09	1.18	1.24
1	B	46	HIS	C-N	-5.08	1.27	1.33
1	A	218	ASP	C-O	5.07	1.29	1.23
1	A	218	ASP	CB-CG	5.06	1.64	1.52
1	A	95	GLY	CA-C	5.06	1.58	1.51
1	A	135	SER	CA-CB	-5.05	1.45	1.53
1	A	224	GLU	C-O	5.05	1.29	1.23
1	A	50[A]	GLU	C-O	5.02	1.30	1.24
1	A	50[B]	GLU	C-O	5.02	1.30	1.24
1	B	90	ILE	CA-C	-5.00	1.47	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	ASP	OD1-CG-OD2	7.26	140.33	122.90
1	B	21	VAL	N-CA-C	-7.11	104.84	111.45
1	A	202	LEU	O-C-N	-6.25	115.50	122.12
1	A	31	ARG	CA-C-O	6.20	127.61	121.29
1	B	24	GLY	O-C-N	6.08	128.09	122.19
1	A	93	LYS	N-CA-C	5.92	117.41	111.07
1	B	187	THR	O-C-N	5.81	129.99	123.48
1	B	29	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	B	189	VAL	CA-C-O	5.49	126.44	120.57
1	B	39	THR	O-C-N	5.35	128.76	122.34
1	A	221	ASN	N-CA-CB	5.29	120.11	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	PRO	CA-C-O	-5.21	115.40	121.34
1	A	200	ARG	NH1-CZ-NH2	5.20	126.06	119.30
1	B	180	ASP	O-C-N	5.17	129.54	122.82
1	A	200	ARG	NE-CZ-NH2	-5.05	114.65	119.20

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	1612	0	1611	15	1
1	B	1518	0	1492	20	1
2	A	17	0	10	1	0
2	B	17	0	10	3	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	B	8	0	14	1	0
5	A	261	0	0	6	2
5	B	261	0	0	10	2
All	All	3704	0	3137	36	4

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 6.

All (36) 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:53[B]:ASP:OD1	5:A:401:HOH:O	1.64	1.13
1:B:53[A]:ASP:OD2	5:B:401:HOH:O	1.72	1.06
1:B:53[B]:ASP:OD1	5:B:402:HOH:O	1.81	0.99
1:B:103:LEU:CD1	1:B:140[B]:VAL:HG21	1.95	0.96
1:A:220:GLU:OE1	5:A:402:HOH:O	1.92	0.86
1:A:193:GLU:OE2	1:A:223[B]:ARG:NH1	2.12	0.82
2:B:302:EVO:H10	2:B:302:EVO:H1	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:THR:OG1	5:B:403:HOH:O	1.90	0.82
1:A:53[B]:ASP:OD1	5:A:403:HOH:O	2.00	0.79
1:B:103:LEU:HD11	1:B:140[B]:VAL:HG21	1.68	0.73
1:B:140[B]:VAL:HG22	1:B:175:ILE:HD13	1.72	0.68
1:B:103:LEU:HD13	1:B:140[B]:VAL:HG21	1.75	0.68
1:A:210[B]:GLN:HG3	5:A:414:HOH:O	1.96	0.64
2:B:302:EVO:H1	2:B:302:EVO:C11	2.28	0.64
2:B:302:EVO:H10	2:B:302:EVO:C6	2.28	0.63
1:B:95:GLY:N	5:B:406:HOH:O	2.30	0.62
1:B:167[B]:THR:HG21	5:B:572:HOH:O	1.99	0.61
1:B:161:ASP:OD2	5:B:404:HOH:O	2.17	0.60
1:A:92:GLU:HG2	1:B:24:GLY:HA2	1.85	0.58
1:A:223[B]:ARG:HD3	5:A:451:HOH:O	2.02	0.58
1:B:140[B]:VAL:HG22	1:B:175:ILE:CD1	2.34	0.58
1:B:30:LYS:NZ	5:B:405:HOH:O	2.25	0.57
1:B:30:LYS:NZ	5:B:409:HOH:O	2.38	0.56
1:A:28:VAL:CG1	1:A:130[B]:VAL:HG23	2.41	0.51
1:A:218:ASP:OD2	5:A:404:HOH:O	2.20	0.47
1:A:93:LYS:HE3	1:B:31:ARG:HG3	1.96	0.46
1:A:28:VAL:HG11	1:A:130[B]:VAL:HG23	1.98	0.45
1:A:16:ALA:O	1:A:20:GLN:NE2	2.43	0.45
1:B:91:GLN:O	1:B:95:GLY:N	2.50	0.45
1:B:174:VAL:HG21	4:B:301:MPD:H53	1.98	0.44
2:A:301:EVO:H1	2:A:301:EVO:H10	1.98	0.44
1:B:82:ASN:O	5:B:403:HOH:O	2.21	0.44
1:A:31:ARG:HD3	1:A:34:MET:SD	2.57	0.43
1:B:193[B]:GLU:CG	5:B:543:HOH:O	2.65	0.43
1:A:93:LYS:HE3	1:B:31:ARG:HB2	2.02	0.42
1:A:192:TYR:CZ	1:A:223[B]:ARG:HD2	2.57	0.40

All (4) 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)
5:A:634:HOH:O	5:B:409:HOH:O[2_555]	1.84	0.36
5:A:622:HOH:O	5:A:622:HOH:O[2_555]	1.94	0.26
5:B:587:HOH:O	5:B:635:HOH:O[4_454]	1.97	0.23
1:A:74[B]:ASP:OD1	1:B:146:GLU:OE2[2_564]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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	202/212 (95%)	197 (98%)	5 (2%)	0	100	100
1	B	186/212 (88%)	183 (98%)	3 (2%)	0	100	100
All	All	388/424 (92%)	380 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	180/183 (98%)	177 (98%)	3 (2%)	53	18
1	B	167/183 (91%)	165 (99%)	2 (1%)	63	27
All	All	347/366 (95%)	342 (99%)	5 (1%)	57	24

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

Mol	Chain	Res	Type
1	A	20	GLN
1	A	92	GLU
1	A	93	LYS
1	B	22	LEU
1	B	197	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	B	145	ASN
1	B	210	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	EVO	A	301	-	19,19,19	2.39	5 (26%)	26,26,26	3.23	10 (38%)
2	EVO	B	302	-	19,19,19	4.11	9 (47%)	26,26,26	4.00	12 (46%)
4	MPD	B	301	-	7,7,7	2.24	2 (28%)	9,10,10	2.39	4 (44%)
3	SO4	A	302	-	4,4,4	0.62	0	6,6,6	0.29	0
3	SO4	B	303	-	4,4,4	0.63	0	6,6,6	0.72	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	EVO	A	301	-	-	0/4/16/16	0/3/3/3
2	EVO	B	302	-	-	0/4/16/16	0/3/3/3
4	MPD	B	301	-	-	2/5/5/5	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	EVO	C9-C8	12.53	1.53	1.34
2	A	301	EVO	C9-C8	6.78	1.44	1.34
2	B	302	EVO	O-C1	6.56	1.36	1.23
2	B	302	EVO	C7-C2	5.45	1.48	1.41
2	B	302	EVO	C1-N1	5.17	1.41	1.36
2	B	302	EVO	C4-C3	5.09	1.47	1.38
2	A	301	EVO	O-C1	4.95	1.33	1.23
4	B	301	MPD	CM-C2	-4.87	1.38	1.52
2	B	302	EVO	C7-C8	3.39	1.51	1.45
4	B	301	MPD	O2-C2	3.10	1.52	1.44
2	A	301	EVO	C8-C1	-3.02	1.46	1.50
2	A	301	EVO	C1-N1	2.69	1.38	1.36
2	B	302	EVO	C10-C9	2.68	1.51	1.46
2	A	301	EVO	C12-C11	2.34	1.42	1.38
2	B	302	EVO	C3-C2	2.33	1.43	1.39
2	B	302	EVO	C11-C10	2.13	1.43	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	EVO	O-C1-C8	-11.44	113.36	127.70
2	B	302	EVO	C3-C2-C7	-9.70	112.80	122.19
2	A	301	EVO	C2-N1-C1	-9.48	105.50	111.35
2	B	302	EVO	C8-C1-N1	7.21	110.86	106.91
2	B	302	EVO	O-C1-N1	5.95	135.78	126.30
2	A	301	EVO	C8-C1-N1	5.20	109.76	106.91
2	A	301	EVO	C2-C7-C8	-5.13	103.34	106.62
2	A	301	EVO	C7-C2-N1	5.12	114.00	108.23
2	B	302	EVO	C2-N1-C1	-4.64	108.49	111.35
2	B	302	EVO	C13-N2-C14	4.49	124.71	116.85
2	A	301	EVO	C11-C10-C14	4.36	121.56	117.07
2	A	301	EVO	C13-N2-C14	4.35	124.47	116.85
4	B	301	MPD	O2-C2-CM	-4.27	94.66	107.99
4	B	301	MPD	O2-C2-C1	4.04	120.59	107.99
2	A	301	EVO	C10-C14-N2	-3.88	116.92	124.00
2	A	301	EVO	C3-C2-C7	-3.78	118.53	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	EVO	C7-C8-C1	3.58	107.29	105.31
2	B	302	EVO	C6-C7-C2	3.15	122.10	118.84
2	B	302	EVO	C7-C8-C1	-3.14	103.58	105.31
2	B	302	EVO	C10-C14-N2	-3.10	118.34	124.00
2	B	302	EVO	C3-C2-N1	3.02	136.94	130.83
2	A	301	EVO	O-C1-C8	-2.67	124.35	127.70
4	B	301	MPD	O2-C2-C3	2.43	118.36	109.27
2	B	302	EVO	C4-C3-C2	2.30	123.36	118.69
4	B	301	MPD	CM-C2-C1	2.21	115.57	110.63
2	B	302	EVO	C12-C11-C10	2.21	123.22	120.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	MPD	C2-C3-C4-C5
4	B	301	MPD	C2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	EVO	1	0
2	B	302	EVO	3	0
4	B	301	MPD	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, 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	192/212 (90%)	0.25	9 (4%) 36 38	6, 13, 28, 66	12 (6%)
1	B	186/212 (87%)	0.41	16 (8%) 16 17	6, 13, 33, 62	4 (2%)
All	All	378/424 (89%)	0.33	25 (6%) 24 26	6, 13, 29, 66	16 (4%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	VAL	7.8
1	A	16	ALA	6.7
1	A	93	LYS	4.2
1	B	20	GLN	4.0
1	A	94	MET	3.7
1	B	22	LEU	3.5
1	B	27	ALA	3.3
1	A	230	GLU	3.2
1	B	35	TYR	3.1
1	A	92	GLU	3.1
1	B	31	ARG	2.9
1	B	90	ILE	2.9
1	B	40	SER	2.8
1	B	24	GLY	2.6
1	A	18	GLN	2.5
1	A	95	GLY	2.3
1	B	231	GLY	2.3
1	B	182	GLU	2.3
1	A	17	GLY	2.3
1	B	34	MET	2.2
1	B	23	GLU	2.2
1	B	26	GLU	2.2
1	B	30	LYS	2.1
1	B	91	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	63	TYR	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
2	EVO	B	302	17/17	0.77	0.15	20,24,34,35	17
3	SO4	A	302	5/5	0.86	0.12	29,40,44,48	5
3	SO4	B	303	5/5	0.86	0.12	28,31,44,46	5
4	MPD	B	301	8/8	0.88	0.11	15,24,29,30	0
2	EVO	A	301	17/17	0.92	0.09	15,18,24,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.