WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 02:22 PM EDT

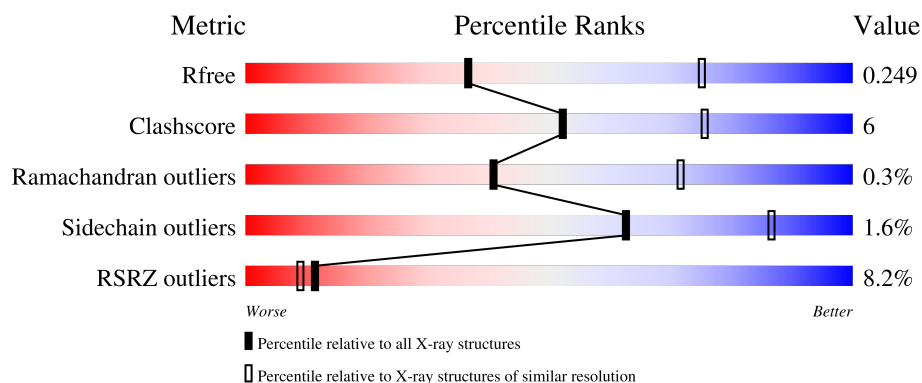|		
PDB ID	:	6G0K
Title	:	Crystal structure of Enterococcus faecium D63r Penicillin-Binding protein 5 (PBP5fm)
Authors	:	Sauvage, E.; El Gachi, M.; Herman, R.; Kerff, F.; Charlier, P.
Deposited on	:	2018-03-19
Resolution	:	2.90 Å(reported)

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 2.90 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	Percentile Ranks	Value
Rfree		0.249
Clashscore		6
Ramachandran outliers		0.3%
Sidechain outliers		1.6%
RSRZ outliers		8.2%

Worse *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	649	10% / 84% / 12% / · ·
1	B	649	7% / 82% / 11% / · 6%
1	C	649	7% / 80% / 11% / 8%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 27340 atoms, of which 13208 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 Low affinity penicillin-binding protein 5 (PBP5).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	629	Total	C	H	N	O	S	0	0	0
			9208	3004	4411	793	987	13			
1	B	609	Total	C	H	N	O	S	0	0	0
			9084	2927	4416	771	957	13			
1	C	595	Total	C	H	N	O	S	0	0	0
			8943	2858	4381	756	935	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	MET	-	initiating methionine	UNP Q47759
A	33	GLY	-	expression tag	UNP Q47759
A	679	LEU	-	expression tag	UNP Q47759
A	680	GLU	-	expression tag	UNP Q47759
B	32	MET	-	initiating methionine	UNP Q47759
B	33	GLY	-	expression tag	UNP Q47759
B	679	LEU	-	expression tag	UNP Q47759
B	680	GLU	-	expression tag	UNP Q47759
C	32	MET	-	initiating methionine	UNP Q47759
C	33	GLY	-	expression tag	UNP Q47759
C	679	LEU	-	expression tag	UNP Q47759
C	680	GLU	-	expression tag	UNP Q47759

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

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2

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

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PDB

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| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0

3 Residue-property plots ⓘ

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.
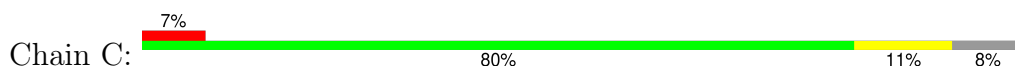
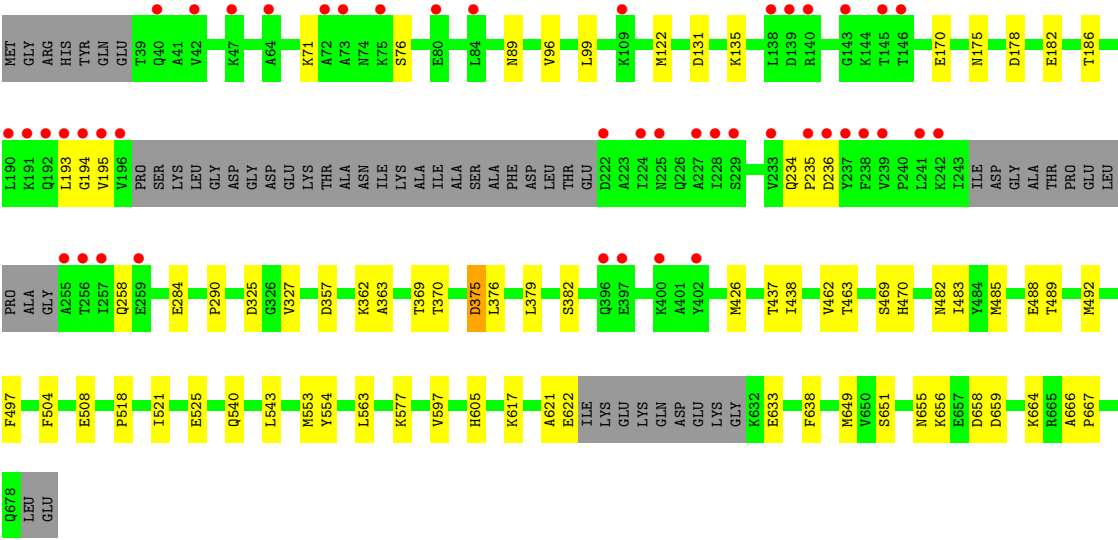- Molecule 1: Low affinity penicillin-binding protein 5 (PBP5)

- Molecule 1: Low affinity penicillin-binding protein 5 (PBP5)
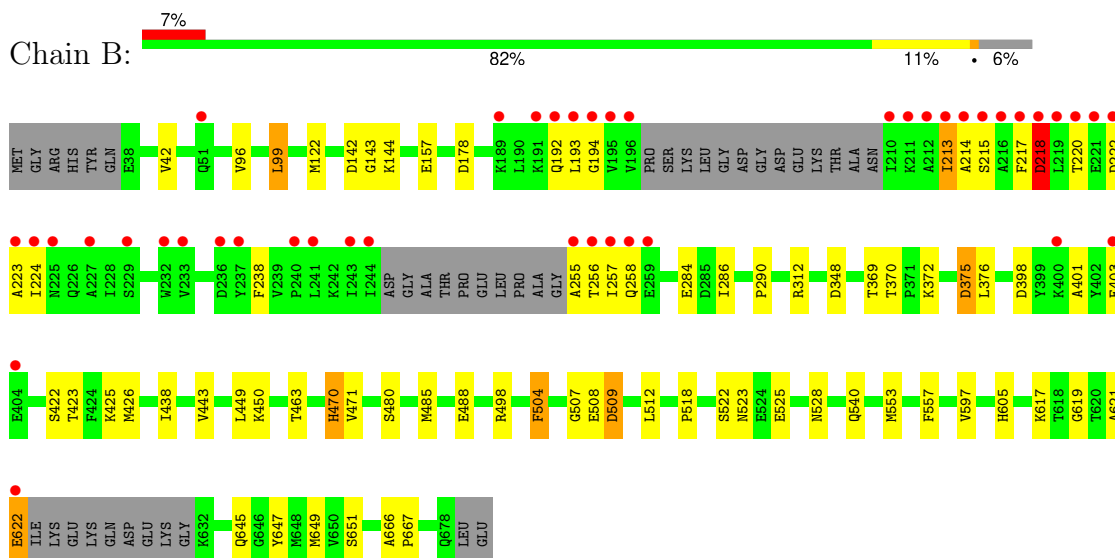
- Molecule 1: Low affinity penicillin-binding protein 5 (PBP5)

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	79.84Å 128.85Å 236.25Å 90.00° 93.88° 90.00°	Depositor
Resolution (Å)	47.14 – 2.90 47.14 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.14-2.90) 99.9 (47.14-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.43 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.198 , 0.247 0.201 , 0.249	Depositor DCC
R_{free} test set	2689 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	46.5	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 36.4	EDS
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	27340	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.72	0/4872	0.79	4/6593 (0.1%)
1	B	0.76	5/4738 (0.1%)	0.80	4/6405 (0.1%)
1	C	0.71	3/4631 (0.1%)	0.80	2/6260 (0.0%)
All	All	0.73	8/14241 (0.1%)	0.80	10/19258 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	284	GLU	CG-CD	6.71	1.62	1.51
1	C	182	GLU	CG-CD	6.30	1.61	1.51
1	B	157	GLU	CG-CD	6.00	1.60	1.51
1	B	42	VAL	CB-CG2	-5.43	1.41	1.52
1	B	403	GLU	CG-CD	5.40	1.60	1.51
1	C	525	GLU	CG-CD	5.35	1.59	1.51
1	B	647	TYR	CE1-CZ	-5.22	1.31	1.38
1	B	622	GLU	CG-CD	5.13	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	357	ASP	CB-CG-OD1	6.12	123.81	118.30
1	C	357	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	B	312	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	B	509	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	464	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	312	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	99	LEU	CA-CB-CG	5.32	127.53	115.30
1	B	512	LEU	CA-CB-CG	5.30	127.48	115.30
1	A	204	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	312	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

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	4797	4411	4733	55	0
1	B	4668	4416	4611	53	0
1	C	4562	4381	4502	53	0
2	A	35	0	0	0	0
2	B	35	0	0	0	0
2	C	35	0	0	0	0
All	All	14132	13208	13846	154	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 6.

All (154) 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:C:234:GLN:HB3	1:C:235:PRO:HD2	1.61	0.82
1:B:214:ALA:HB2	1:B:224:ILE:HD12	1.63	0.79
1:A:211:LYS:HD3	1:A:221:GLU:OE2	1.83	0.79
1:B:213:ILE:HG21	1:B:255:ALA:CB	2.14	0.78
1:B:214:ALA:HB2	1:B:224:ILE:CD1	2.14	0.78
1:B:213:ILE:HG21	1:B:255:ALA:HB2	1.70	0.74
1:A:426:MET:HE1	1:A:617:LYS:HB3	1.72	0.71
1:C:492:MET:HE1	1:C:497:PHE:CD1	2.26	0.70
1:B:193:LEU:HA	1:B:257:ILE:HG22	1.74	0.69
1:C:438:ILE:HD11	1:C:485:MET:HE1	1.75	0.68
1:B:99:LEU:HD13	1:B:122:MET:HB3	1.74	0.68
1:A:508:GLU:O	1:A:518:PRO:HB3	1.97	0.65
1:A:437:THR:HG21	1:A:492:MET:HB2	1.80	0.64
1:B:438:ILE:HD11	1:B:485:MET:HE1	1.80	0.62
1:C:426:MET:HE1	1:C:617:LYS:HB3	1.81	0.62
1:A:390:MET:HE3	1:C:327:VAL:HG21	1.82	0.61
1:C:508:GLU:O	1:C:518:PRO:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ALA:O	1:A:249:PRO:HD3	2.02	0.60
1:A:529:SER:HB3	1:A:532:LEU:H	1.67	0.60
1:A:200:LEU:HD23	1:A:206:LYS:HG3	1.82	0.60
1:A:456:SER:O	1:B:290:PRO:HB2	2.02	0.59
1:A:206:LYS:O	1:A:210:ILE:HG13	2.02	0.59
1:A:489:THR:HA	1:A:492:MET:HE2	1.84	0.58
1:B:438:ILE:CD1	1:B:485:MET:HE1	2.33	0.58
1:B:217:PHE:O	1:B:218:ASP:HB2	2.02	0.57
1:C:99:LEU:HD13	1:C:122:MET:HB3	1.86	0.57
1:C:96:VAL:HG13	1:C:122:MET:HE3	1.85	0.57
1:B:142:ASP:O	1:B:144:LYS:N	2.37	0.56
1:B:540:GLN:NE2	1:B:621:ALA:HA	2.19	0.56
1:B:425:LYS:NZ	1:B:480:SER:OG	2.36	0.56
1:A:655:ASN:O	1:A:655:ASN:ND2	2.39	0.56
1:A:309:LYS:HB2	1:B:528:ASN:HA	1.87	0.56
1:C:666:ALA:N	1:C:667:PRO:CD	2.69	0.55
1:A:193:LEU:HA	1:A:257:ILE:HG22	1.88	0.54
1:B:99:LEU:CD1	1:B:122:MET:HB3	2.37	0.53
1:B:238:PHE:HE1	1:B:256:THR:O	1.91	0.53
1:B:96:VAL:HG13	1:B:122:MET:HE3	1.90	0.53
1:B:284:GLU:OE1	1:B:284:GLU:N	2.37	0.53
1:B:372:LYS:HD2	1:B:645:GLN:HB2	1.90	0.52
1:C:426:MET:CE	1:C:617:LYS:HB3	2.38	0.52
1:A:535:ASP:HA	1:A:538:TYR:CE1	2.45	0.52
1:B:443:VAL:HG11	1:B:470:HIS:CD2	2.45	0.52
1:C:426:MET:HE2	1:C:617:LYS:HG2	1.91	0.52
1:A:211:LYS:HD3	1:A:221:GLU:CD	2.29	0.52
1:B:426:MET:HE1	1:B:617:LYS:HB3	1.92	0.52
1:C:96:VAL:CG2	1:C:122:MET:HE1	2.40	0.51
1:B:193:LEU:HD13	1:B:257:ILE:CG2	2.40	0.51
1:B:426:MET:HG3	1:B:557:PHE:CE2	2.45	0.51
1:A:208:ALA:O	1:A:211:LYS:HB2	2.11	0.51
1:B:214:ALA:HB2	1:B:224:ILE:HD11	1.93	0.51
1:C:438:ILE:HG12	1:C:488:GLU:OE1	2.11	0.51
1:A:234:GLN:HG2	1:A:237:TYR:CE2	2.46	0.51
1:B:504:PHE:CD2	1:B:553:MET:HG2	2.45	0.51
1:B:649:MET:CE	1:B:651:SER:HB2	2.41	0.50
1:C:96:VAL:HG22	1:C:122:MET:HE1	1.94	0.50
1:A:443:VAL:HG11	1:A:470:HIS:ND1	2.27	0.49
1:A:213:ILE:CG2	1:A:252:PRO:HB2	2.42	0.49
1:B:370:THR:OG1	1:B:375:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:469:SER:OG	1:C:470:HIS:HD2	1.95	0.49
1:C:175:ASN:OD1	1:C:186:THR:HA	2.12	0.49
1:C:376:LEU:HD22	1:C:379:LEU:HD21	1.94	0.49
1:C:666:ALA:N	1:C:667:PRO:HD3	2.28	0.49
1:B:597:VAL:O	1:B:605:HIS:HA	2.13	0.49
1:C:659:ASP:O	1:C:664:LYS:NZ	2.31	0.49
1:C:438:ILE:CD1	1:C:485:MET:HE1	2.42	0.48
1:A:205:GLU:HB3	1:A:209:ASN:OD1	2.13	0.48
1:A:568:LEU:O	1:A:568:LEU:HG	2.12	0.48
1:B:423:THR:O	1:B:426:MET:HE3	2.14	0.48
1:C:234:GLN:HB3	1:C:235:PRO:CD	2.38	0.48
1:C:426:MET:HE2	1:C:617:LYS:CB	2.43	0.48
1:C:99:LEU:CD1	1:C:122:MET:HB3	2.43	0.48
1:A:336:GLU:OE2	1:C:258:GLN:OE1	2.32	0.48
1:A:213:ILE:HG22	1:A:252:PRO:HG2	1.96	0.47
1:B:449:LEU:O	1:B:463:THR:HA	2.14	0.47
1:A:141:ASN:O	1:A:142:ASP:HB2	2.13	0.47
1:B:540:GLN:HE22	1:B:621:ALA:HA	1.80	0.47
1:A:460:TYR:HD2	1:A:531:ILE:HG21	1.80	0.47
1:B:192:GLN:O	1:B:192:GLN:HG3	2.15	0.47
1:B:369:THR:HG22	1:B:376:LEU:HD23	1.95	0.47
1:A:423:THR:O	1:A:426:MET:HE3	2.15	0.47
1:B:220:THR:HG22	1:B:222:ASP:HB2	1.96	0.47
1:A:213:ILE:HG22	1:A:252:PRO:HB2	1.96	0.47
1:B:426:MET:HG3	1:B:557:PHE:HE2	1.79	0.47
1:A:287:ASP:OD2	1:C:89:ASN:ND2	2.49	0.46
1:A:649:MET:CE	1:A:651:SER:HB2	2.45	0.46
1:B:450:LYS:HG2	1:B:463:THR:HG22	1.97	0.46
1:A:424:PHE:HE1	1:A:553:MET:HE1	1.81	0.45
1:A:520:GLN:NE2	1:A:523:ASN:OD1	2.49	0.45
1:C:426:MET:CE	1:C:617:LYS:CB	2.94	0.45
1:C:504:PHE:O	1:C:577:LYS:NZ	2.50	0.45
1:A:389:LYS:HB3	1:A:394:ILE:HB	1.99	0.45
1:B:348:ASP:OD1	1:B:348:ASP:C	2.55	0.45
1:A:438:ILE:HG12	1:A:488:GLU:OE1	2.17	0.45
1:B:422:SER:OG	1:B:619:GLY:HA2	2.17	0.45
1:B:438:ILE:HG12	1:B:488:GLU:OE1	2.17	0.44
1:C:234:GLN:CB	1:C:235:PRO:HD2	2.40	0.44
1:B:213:ILE:H	1:B:213:ILE:HG12	1.66	0.44
1:C:362:LYS:O	1:C:382:SER:HB3	2.16	0.44
1:B:470:HIS:C	1:B:471:VAL:HG23	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:563:LEU:C	1:C:563:LEU:HD23	2.38	0.44
1:A:426:MET:CE	1:A:617:LYS:HB3	2.44	0.44
1:C:462:VAL:HG11	1:C:483:ILE:HA	1.99	0.44
1:A:666:ALA:N	1:A:667:PRO:CD	2.81	0.44
1:C:370:THR:OG1	1:C:375:ASP:HB2	2.18	0.44
1:C:489:THR:HA	1:C:492:MET:HE2	2.00	0.44
1:C:369:THR:HG22	1:C:376:LEU:HD23	1.99	0.43
1:B:666:ALA:N	1:B:667:PRO:CD	2.80	0.43
1:B:286:ILE:HG23	1:B:290:PRO:HA	1.99	0.43
1:A:219:LEU:HD11	1:A:224:ILE:HD11	2.00	0.43
1:A:469:SER:OG	1:A:470:HIS:HD2	2.01	0.43
1:B:508:GLU:O	1:B:518:PRO:HB3	2.18	0.43
1:A:195:VAL:HG11	1:A:213:ILE:HD12	2.00	0.43
1:B:498:ARG:NH2	1:B:522:SER:OG	2.50	0.43
1:C:597:VAL:O	1:C:605:HIS:HA	2.19	0.43
1:C:504:PHE:CD2	1:C:553:MET:HG2	2.54	0.43
1:A:197:PRO:HD2	1:A:235:PRO:O	2.19	0.43
1:C:131:ASP:O	1:C:131:ASP:OD1	2.37	0.43
1:C:96:VAL:HG22	1:C:122:MET:CE	2.48	0.42
1:A:613:PRO:HG2	1:A:641:ASN:HD21	1.84	0.42
1:B:220:THR:O	1:B:223:ALA:N	2.52	0.42
1:C:71:LYS:HA	1:C:76:SER:O	2.19	0.42
1:C:649:MET:CE	1:C:651:SER:HB2	2.49	0.42
1:A:198:SER:C	1:A:200:LEU:H	2.22	0.42
1:A:269:GLU:HA	1:A:272:ALA:HB2	2.01	0.42
1:B:426:MET:CE	1:B:617:LYS:HB3	2.49	0.42
1:A:234:GLN:CG	1:A:237:TYR:CE2	3.02	0.42
1:A:300:ARG:NE	1:C:325:ASP:O	2.52	0.41
1:A:597:VAL:O	1:A:605:HIS:HD2	2.02	0.41
1:A:263:ARG:HB3	1:A:391:THR:HG21	2.02	0.41
1:A:370:THR:OG1	1:A:375:ASP:HB2	2.20	0.41
1:C:193:LEU:HD12	1:C:194:GLY:H	1.85	0.41
1:C:633:GLU:O	1:C:655:ASN:HA	2.20	0.41
1:C:633:GLU:HG3	1:C:656:LYS:HG2	2.03	0.41
1:C:437:THR:HG21	1:C:492:MET:HB2	2.01	0.41
1:A:193:LEU:HB2	1:A:244:ILE:HD11	2.02	0.41
1:A:509:ASP:HB2	1:B:507:GLY:CA	2.50	0.41
1:C:540:GLN:HE22	1:C:621:ALA:HA	1.84	0.41
1:A:613:PRO:HG2	1:A:641:ASN:ND2	2.36	0.41
1:C:363:ALA:HA	1:C:382:SER:O	2.21	0.41
1:C:492:MET:HE3	1:C:497:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:MET:O	1:A:556:VAL:HG22	2.21	0.41
1:B:523:ASN:OD1	1:B:523:ASN:N	2.54	0.41
1:C:463:THR:O	1:C:482:ASN:HB2	2.21	0.41
1:C:521:ILE:HA	1:C:543:LEU:HD23	2.03	0.41
1:A:520:GLN:NE2	1:A:544:LEU:HD12	2.37	0.40
1:A:522:SER:C	1:A:524:GLU:H	2.24	0.40
1:B:398:ASP:O	1:B:401:ALA:HB3	2.22	0.40
1:C:554:TYR:HB3	1:C:638:PHE:CE1	2.55	0.40
1:A:563:LEU:C	1:A:563:LEU:HD23	2.41	0.40
1:B:194:GLY:HA3	1:B:238:PHE:CZ	2.56	0.40
1:B:540:GLN:HE22	1:B:622:GLU:H	1.69	0.40
1:B:649:MET:HE3	1:B:651:SER:HB2	2.03	0.40
1:C:622:GLU:OE2	1:C:633:GLU:HB3	2.21	0.40
1:C:96:VAL:HG13	1:C:122:MET:CE	2.48	0.40

There are no symmetry-related clashes.

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	625/649 (96%)	587 (94%)	36 (6%)	2 (0%)	41	71
1	B	601/649 (93%)	576 (96%)	22 (4%)	3 (0%)	29	61
1	C	587/649 (90%)	563 (96%)	24 (4%)	0	100	100
All	All	1813/1947 (93%)	1726 (95%)	82 (4%)	5 (0%)	41	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	218	ASP
1	B	143	GLY
1	A	252	PRO

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Mol	Chain	Res	Type
1	B	504	PHE
1	A	199	LYS

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	519/537 (97%)	512 (99%)	7 (1%)	69	90
1	B	506/537 (94%)	497 (98%)	9 (2%)	59	85
1	C	495/537 (92%)	487 (98%)	8 (2%)	62	86
All	All	1520/1611 (94%)	1496 (98%)	24 (2%)	62	86

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	ASP
1	A	220	THR
1	A	245	ASP
1	A	375	ASP
1	A	469	SER
1	A	524	GLU
1	A	529	SER
1	B	178	ASP
1	B	213	ILE
1	B	215	SER
1	B	218	ASP
1	B	258	GLN
1	B	375	ASP
1	B	470	HIS
1	B	509	ASP
1	B	525	GLU
1	C	135	LYS
1	C	170	GLU
1	C	178	ASP
1	C	195	VAL

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Mol	Chain	Res	Type
1	C	236	ASP
1	C	290	PRO
1	C	375	ASP
1	C	658	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	470	HIS
1	A	605	HIS
1	B	540	GLN
1	C	470	HIS

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 ⓘ

21 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	706	-	4,4,4	0.42	0	6,6,6	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	707	-	4,4,4	0.34	0	6,6,6	0.34	0
2	SO4	B	702	-	4,4,4	0.39	0	6,6,6	0.44	0
2	SO4	B	703	-	4,4,4	0.46	0	6,6,6	0.39	0
2	SO4	A	706	-	4,4,4	0.31	0	6,6,6	0.49	0
2	SO4	C	705	-	4,4,4	0.45	0	6,6,6	0.41	0
2	SO4	A	701	-	4,4,4	0.20	0	6,6,6	1.09	0
2	SO4	C	702	-	4,4,4	0.28	0	6,6,6	0.51	0
2	SO4	A	707	-	4,4,4	0.29	0	6,6,6	0.24	0
2	SO4	C	706	-	4,4,4	0.41	0	6,6,6	0.49	0
2	SO4	C	703	-	4,4,4	0.33	0	6,6,6	0.35	0
2	SO4	C	707	-	4,4,4	0.28	0	6,6,6	0.44	0
2	SO4	B	701	-	4,4,4	0.41	0	6,6,6	1.08	0
2	SO4	C	704	-	4,4,4	0.46	0	6,6,6	0.46	0
2	SO4	A	705	-	4,4,4	0.39	0	6,6,6	0.19	0
2	SO4	B	704	-	4,4,4	0.41	0	6,6,6	0.73	0
2	SO4	B	705	-	4,4,4	0.45	0	6,6,6	0.51	0
2	SO4	A	703	-	4,4,4	0.37	0	6,6,6	0.19	0
2	SO4	C	701	-	4,4,4	0.31	0	6,6,6	0.70	0
2	SO4	A	702	-	4,4,4	0.39	0	6,6,6	0.29	0
2	SO4	A	704	-	4,4,4	0.30	0	6,6,6	0.49	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 ⓘ

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, 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(Å²)	Q<0.9
1	A	629/649 (96%)	0.56	62 (9%)	7	5	24, 43, 96, 129	0
1	B	609/649 (93%)	0.51	43 (7%)	16	12	24, 41, 94, 126	0
1	C	595/649 (91%)	0.46	45 (7%)	13	10	28, 46, 83, 120	0
All	All	1833/1947 (94%)	0.51	150 (8%)	11	9	24, 43, 91, 129	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	ALA	9.2
1	B	213	ILE	8.9
1	A	254	GLY	8.5
1	B	195	VAL	8.0
1	A	250	GLU	7.9
1	A	202	ASP	7.6
1	B	193	LEU	7.4
1	C	224	ILE	6.9
1	B	217	PHE	6.6
1	A	251	LEU	6.5
1	B	221	GLU	6.5
1	B	244	ILE	6.3
1	B	224	ILE	6.3
1	A	212	ALA	6.2
1	A	197	PRO	6.2
1	A	210	ILE	6.2
1	A	217	PHE	6.1
1	B	255	ALA	6.0
1	B	216	ALA	5.9
1	A	200	LEU	5.8
1	B	211	LYS	5.6
1	C	195	VAL	5.6
1	C	236	ASP	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	213	ILE	5.4
1	A	204	ASP	5.2
1	B	225	ASN	5.2
1	A	203	GLY	5.2
1	A	198	SER	5.2
1	A	207	THR	5.1
1	B	219	LEU	5.1
1	B	241	LEU	5.0
1	B	210	ILE	5.0
1	B	218	ASP	5.0
1	C	256	THR	4.9
1	A	201	GLY	4.9
1	A	196	VAL	4.9
1	C	241	LEU	4.8
1	A	255	ALA	4.7
1	A	211	LYS	4.7
1	B	257	ILE	4.5
1	C	255	ALA	4.5
1	A	206	LYS	4.5
1	A	247	ALA	4.4
1	A	195	VAL	4.4
1	A	223	ALA	4.3
1	A	216	ALA	4.2
1	A	248	THR	4.2
1	B	236	ASP	4.1
1	B	215	SER	4.0
1	A	199	LYS	3.9
1	A	228	ILE	3.9
1	B	237	TYR	3.9
1	C	193	LEU	3.8
1	C	225	ASN	3.8
1	B	194	GLY	3.8
1	A	253	ALA	3.7
1	B	259	GLU	3.6
1	B	256	THR	3.6
1	B	192	GLN	3.6
1	B	220	THR	3.6
1	A	236	ASP	3.5
1	A	215	SER	3.5
1	A	244	ILE	3.4
1	B	240	PRO	3.4
1	C	190	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	249	PRO	3.4
1	A	193	LEU	3.3
1	A	221	GLU	3.3
1	C	235	PRO	3.3
1	C	109	LYS	3.2
1	B	227	ALA	3.2
1	A	209	ASN	3.2
1	B	400	LYS	3.1
1	C	237	TYR	3.1
1	B	191	LYS	3.1
1	C	191	LYS	3.1
1	C	139	ASP	3.1
1	A	256	THR	3.0
1	B	232	TRP	3.0
1	C	397	GLU	3.0
1	C	396	GLN	3.0
1	A	219	LEU	3.0
1	C	145	THR	2.9
1	A	233	VAL	2.9
1	C	227	ALA	2.9
1	B	243	ILE	2.8
1	C	140	ARG	2.8
1	B	233	VAL	2.8
1	C	196	VAL	2.8
1	B	214	ALA	2.8
1	C	192	GLN	2.8
1	A	222	ASP	2.8
1	A	460	TYR	2.8
1	A	73	ALA	2.7
1	A	257	ILE	2.7
1	B	223	ALA	2.7
1	C	146	THR	2.7
1	A	74	ASN	2.7
1	C	73	ALA	2.7
1	B	222	ASP	2.7
1	C	222	ASP	2.7
1	C	80	GLU	2.7
1	A	205	GLU	2.6
1	B	403	GLU	2.6
1	C	239	VAL	2.6
1	B	258	GLN	2.6
1	A	225	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	218	ASP	2.6
1	A	397	GLU	2.5
1	A	224	ILE	2.5
1	A	208	ALA	2.5
1	A	145	THR	2.5
1	C	233	VAL	2.5
1	B	404	GLU	2.5
1	B	189	LYS	2.5
1	C	242	LYS	2.5
1	C	40	GLN	2.4
1	A	191	LYS	2.4
1	C	64	ALA	2.4
1	A	226	GLN	2.4
1	C	138	LEU	2.4
1	A	214	ALA	2.3
1	A	259	GLU	2.3
1	C	194	GLY	2.3
1	B	51	GLN	2.3
1	C	402	TYR	2.3
1	B	196	VAL	2.2
1	C	75	LYS	2.2
1	C	143	GLY	2.2
1	C	47	LYS	2.2
1	A	70	LYS	2.2
1	C	257	ILE	2.1
1	A	220	THR	2.1
1	C	72	ALA	2.1
1	A	449	LEU	2.1
1	A	246	GLY	2.1
1	C	84	LEU	2.1
1	C	228	ILE	2.1
1	C	259	GLU	2.0
1	C	238	PHE	2.0
1	B	229	SER	2.0
1	C	229	SER	2.0
1	C	42	VAL	2.0
1	A	192	GLN	2.0
1	A	404	GLU	2.0
1	B	622	GLU	2.0
1	A	260	VAL	2.0
1	A	234	GLN	2.0
1	A	240	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	400	LYS	2.0

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 ⓘ

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(Å^2)	Q<0.9
2	SO4	B	706	5/5	0.64	0.37	76,76,82,99	0
2	SO4	B	704	5/5	0.80	0.20	66,71,93,96	0
2	SO4	C	702	5/5	0.82	0.27	83,85,102,107	0
2	SO4	C	706	5/5	0.84	0.29	76,77,84,98	0
2	SO4	C	707	5/5	0.84	0.32	80,83,99,108	0
2	SO4	B	707	5/5	0.85	0.21	67,69,76,91	0
2	SO4	A	706	5/5	0.87	0.35	58,62,74,82	0
2	SO4	C	705	5/5	0.89	0.17	53,54,71,86	0
2	SO4	B	703	5/5	0.90	0.26	54,54,67,85	0
2	SO4	B	701	5/5	0.90	0.14	55,60,64,71	0
2	SO4	B	705	5/5	0.90	0.17	52,52,62,83	0
2	SO4	A	707	5/5	0.92	0.29	66,70,82,91	0
2	SO4	A	705	5/5	0.92	0.27	54,55,70,84	0
2	SO4	B	702	5/5	0.92	0.18	61,67,77,79	0
2	SO4	A	703	5/5	0.93	0.20	59,63,79,81	0
2	SO4	A	701	5/5	0.93	0.19	49,51,57,58	0
2	SO4	A	702	5/5	0.93	0.40	66,69,77,83	0
2	SO4	C	703	5/5	0.94	0.17	61,61,87,88	0
2	SO4	C	701	5/5	0.94	0.17	52,52,61,61	0
2	SO4	C	704	5/5	0.95	0.12	58,60,63,78	0
2	SO4	A	704	5/5	0.96	0.11	59,66,75,83	0

6.5 Other polymers (i)

There are no such residues in this entry.