



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:07 PM UTC

PDB ID : 6CN7 / pdb_00006cn7
Title : The structure of aerobactin synthetase IucC from a hypervirulent pathotype of *Klebsiella pneumoniae*
Authors : Bailey, D.C.; Rice, M.R.; Gulick, A.M.
Deposited on : 2018-03-07
Resolution : 2.45 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

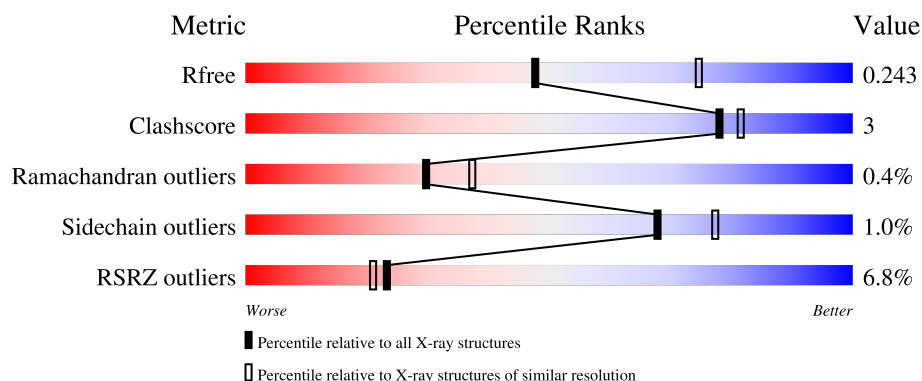
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	579	5% 87% 7% 6%
1	B	579	4% 89% • 6%
1	C	579	7% 87% 7% • 6%
1	D	579	8% 87% 7% 6%
1	E	579	8% 87% 6% 7%

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Mol	Chain	Length	Quality of chain
1	F	579	
1	G	579	
1	H	579	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33602 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 Aerobactin synthase IucC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4254	2735	735	761	23			
1	B	543	Total	C	N	O	S	0	0	0
			4185	2694	722	746	23			
1	C	547	Total	C	N	O	S	0	0	0
			4182	2700	716	743	23			
1	D	542	Total	C	N	O	S	0	0	0
			4205	2704	726	752	23			
1	E	539	Total	C	N	O	S	0	1	0
			4094	2641	705	726	22			
1	F	540	Total	C	N	O	S	0	0	0
			4074	2631	694	726	23			
1	G	542	Total	C	N	O	S	0	0	0
			4206	2711	726	746	23			
1	H	544	Total	C	N	O	S	0	0	0
			4130	2665	711	731	23			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q6U605
A	0	HIS	-	expression tag	UNP Q6U605
A	182	GLY	SER	engineered mutation	UNP Q6U605
A	183	SER	GLU	engineered mutation	UNP Q6U605
A	185	THR	ASP	engineered mutation	UNP Q6U605
A	187	GLY	GLN	engineered mutation	UNP Q6U605
A	188	THR	GLN	engineered mutation	UNP Q6U605
B	-1	GLY	-	expression tag	UNP Q6U605
B	0	HIS	-	expression tag	UNP Q6U605
B	182	GLY	SER	engineered mutation	UNP Q6U605
B	183	SER	GLU	engineered mutation	UNP Q6U605
B	185	THR	ASP	engineered mutation	UNP Q6U605
B	187	GLY	GLN	engineered mutation	UNP Q6U605

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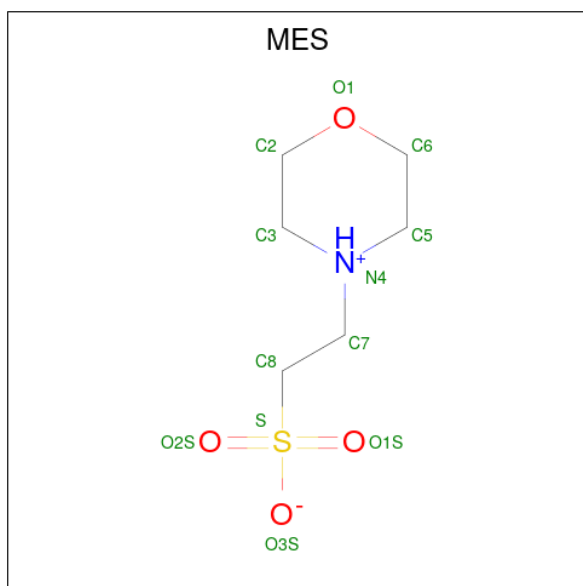
Chain	Residue	Modelled	Actual	Comment	Reference
B	188	THR	GLN	engineered mutation	UNP Q6U605
C	-1	GLY	-	expression tag	UNP Q6U605
C	0	HIS	-	expression tag	UNP Q6U605
C	182	GLY	SER	engineered mutation	UNP Q6U605
C	183	SER	GLU	engineered mutation	UNP Q6U605
C	185	THR	ASP	engineered mutation	UNP Q6U605
C	187	GLY	GLN	engineered mutation	UNP Q6U605
C	188	THR	GLN	engineered mutation	UNP Q6U605
D	-1	GLY	-	expression tag	UNP Q6U605
D	0	HIS	-	expression tag	UNP Q6U605
D	182	GLY	SER	engineered mutation	UNP Q6U605
D	183	SER	GLU	engineered mutation	UNP Q6U605
D	185	THR	ASP	engineered mutation	UNP Q6U605
D	187	GLY	GLN	engineered mutation	UNP Q6U605
D	188	THR	GLN	engineered mutation	UNP Q6U605
E	-1	GLY	-	expression tag	UNP Q6U605
E	0	HIS	-	expression tag	UNP Q6U605
E	182	GLY	SER	engineered mutation	UNP Q6U605
E	183	SER	GLU	engineered mutation	UNP Q6U605
E	185	THR	ASP	engineered mutation	UNP Q6U605
E	187	GLY	GLN	engineered mutation	UNP Q6U605
E	188	THR	GLN	engineered mutation	UNP Q6U605
F	-1	GLY	-	expression tag	UNP Q6U605
F	0	HIS	-	expression tag	UNP Q6U605
F	182	GLY	SER	engineered mutation	UNP Q6U605
F	183	SER	GLU	engineered mutation	UNP Q6U605
F	185	THR	ASP	engineered mutation	UNP Q6U605
F	187	GLY	GLN	engineered mutation	UNP Q6U605
F	188	THR	GLN	engineered mutation	UNP Q6U605
G	-1	GLY	-	expression tag	UNP Q6U605
G	0	HIS	-	expression tag	UNP Q6U605
G	182	GLY	SER	engineered mutation	UNP Q6U605
G	183	SER	GLU	engineered mutation	UNP Q6U605
G	185	THR	ASP	engineered mutation	UNP Q6U605
G	187	GLY	GLN	engineered mutation	UNP Q6U605
G	188	THR	GLN	engineered mutation	UNP Q6U605
H	-1	GLY	-	expression tag	UNP Q6U605
H	0	HIS	-	expression tag	UNP Q6U605
H	182	GLY	SER	engineered mutation	UNP Q6U605
H	183	SER	GLU	engineered mutation	UNP Q6U605
H	185	THR	ASP	engineered mutation	UNP Q6U605
H	187	GLY	GLN	engineered mutation	UNP Q6U605

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Chain	Residue	Modelled	Actual	Comment	Reference
H	188	THR	GLN	engineered mutation	UNP Q6U605

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total	O	0	0
			49	49		
3	B	45	Total	O	0	0
			45	45		
3	C	35	Total	O	0	0
			35	35		
3	D	49	Total	O	0	0
			49	49		
3	E	16	Total	O	0	0
			16	16		
3	F	18	Total	O	0	0
			18	18		

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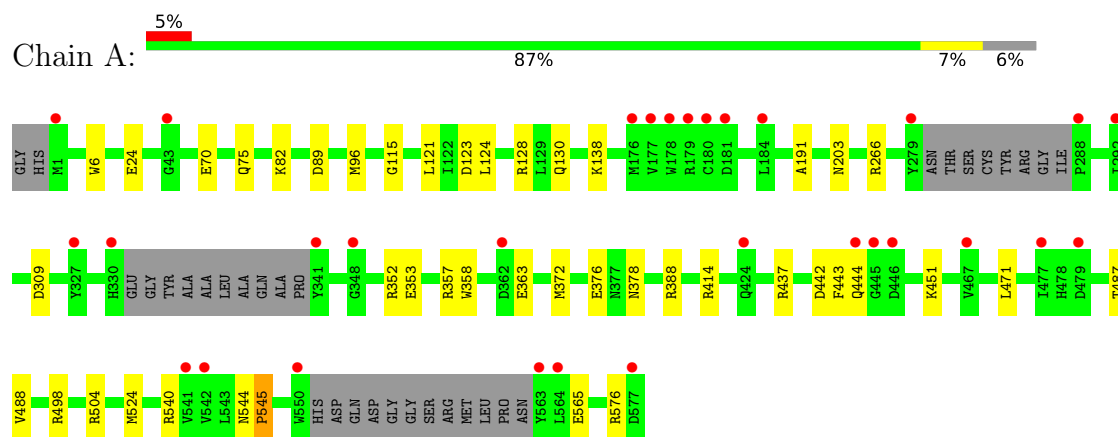
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	21	Total	O	0	0
			21	21		
3	H	15	Total	O	0	0
			15	15		

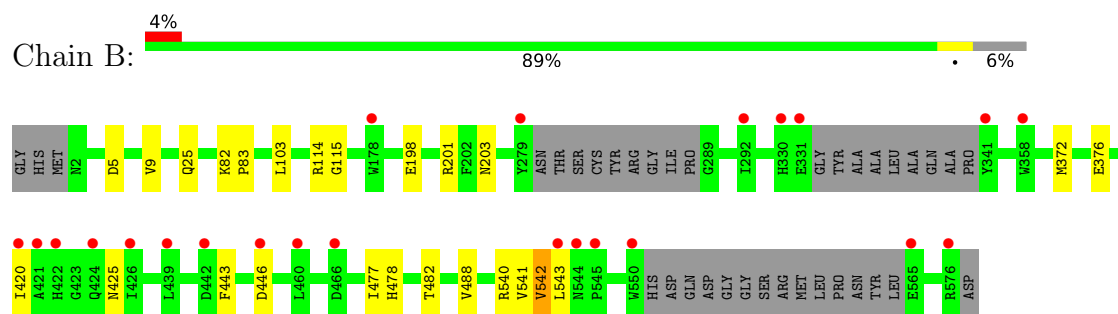
3 Residue-property plots [i](#)

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.

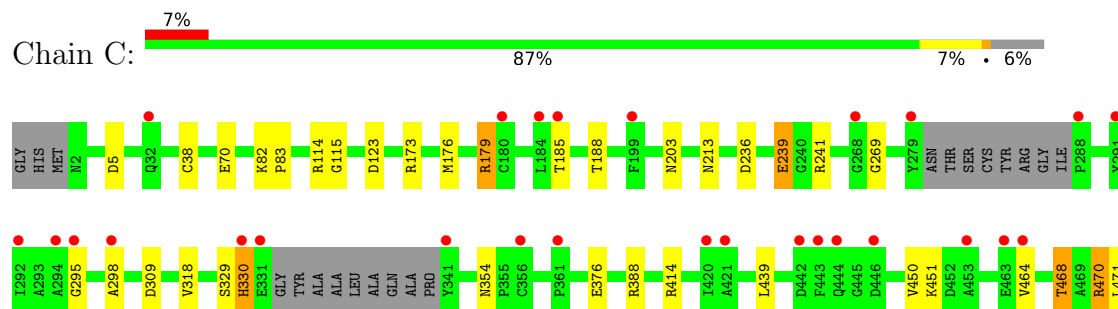
- Molecule 1: Aerobactin synthase IucC

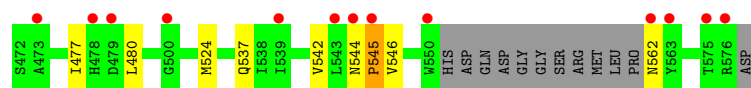


- Molecule 1: Aerobactin synthase IucC

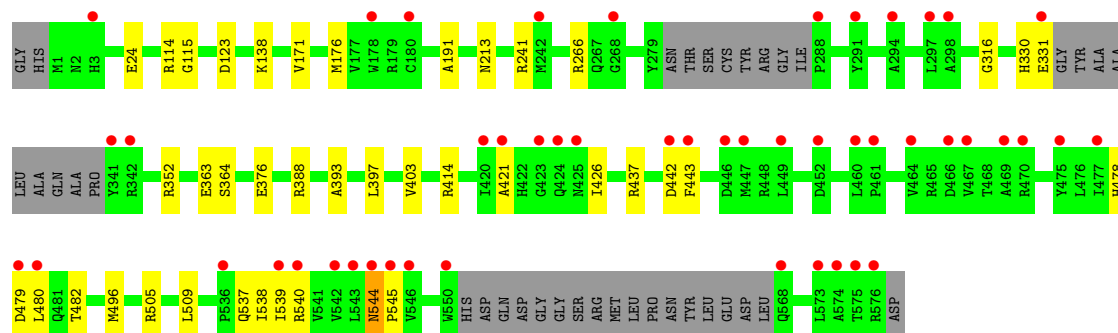
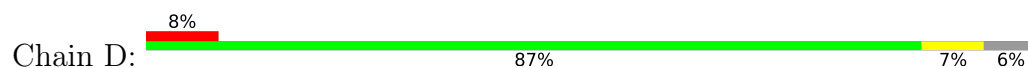


- Molecule 1: Aerobactin synthase IucC

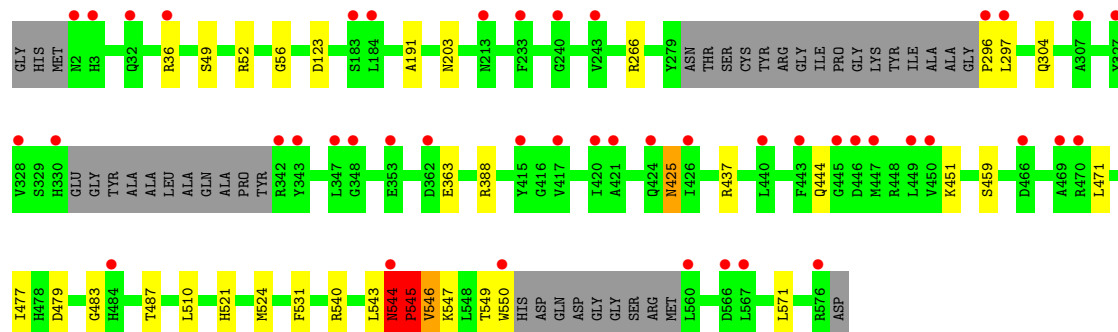
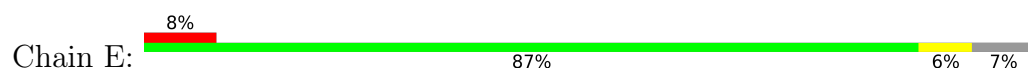




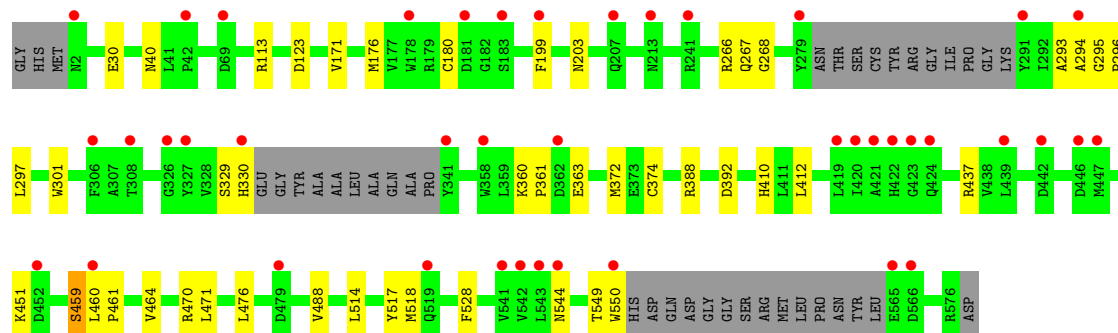
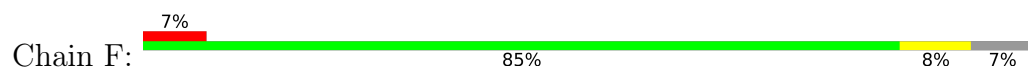
• Molecule 1: Aerobactin synthase IucC



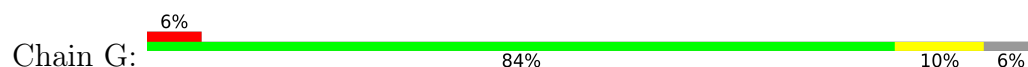
• Molecule 1: Aerobactin synthase IucC

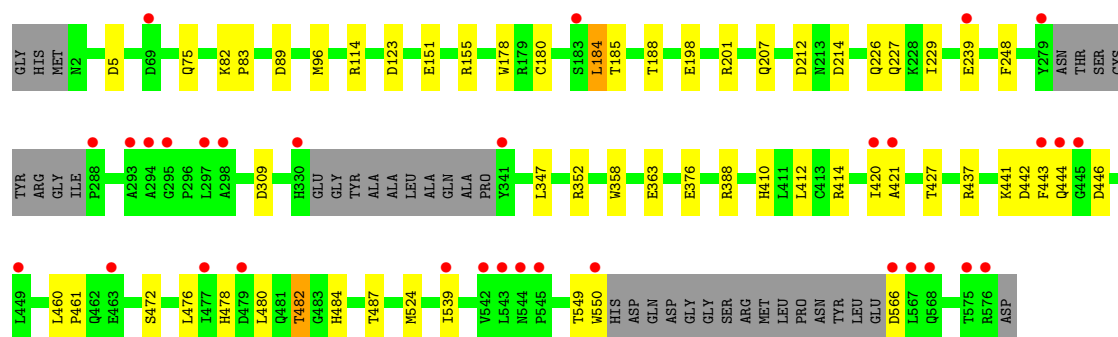


• Molecule 1: Aerobactin synthase IucC

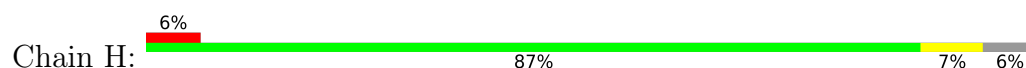
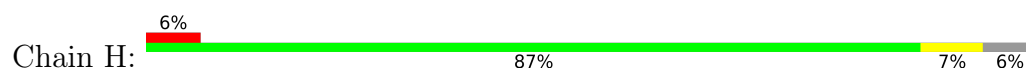


• Molecule 1: Aerobactin synthase IucC

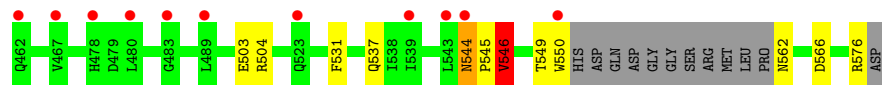
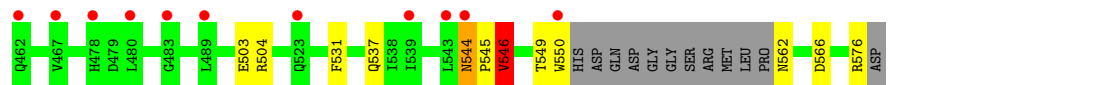
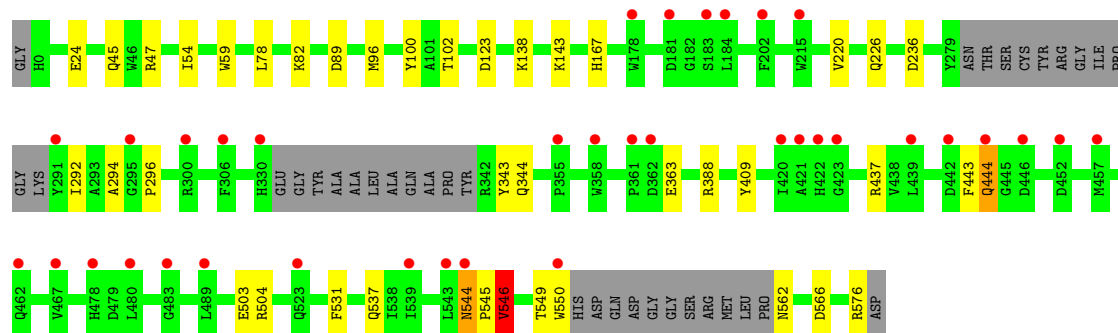




● Molecule 1: Aerobactin synthase IucC



Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	124.02Å 197.69Å 130.38Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	58.07 – 2.45 58.07 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (58.07-2.45) 95.1 (58.07-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.213 , 0.240 0.219 , 0.243	Depositor DCC
R_{free} test set	10530 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33602	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES

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	0.20	1/4358 (0.0%)	0.29	0/5938
1	B	0.11	0/4289	0.30	0/5851
1	C	0.16	0/4287	0.30	0/5852
1	D	0.13	0/4312	0.31	0/5881
1	E	0.26	5/4200 (0.1%)	0.34	4/5742 (0.1%)
1	F	0.11	0/4178	0.30	0/5712
1	G	0.16	0/4314	0.32	0/5882
1	H	0.13	0/4237	0.31	0/5792
All	All	0.16	6/34175 (0.0%)	0.31	4/46650 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	546	VAL	CA-C	-5.96	1.45	1.52
1	E	546	VAL	CA-CB	-5.92	1.48	1.54
1	E	546	VAL	C-O	-5.81	1.16	1.24
1	A	130	GLN	C-O	-5.71	1.17	1.24
1	E	543	LEU	CA-C	-5.21	1.46	1.52
1	E	544	ASN	CA-C	-5.00	1.46	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	545	PRO	N-CA-C	-6.11	99.88	112.47
1	E	546	VAL	CB-CA-C	-5.25	104.03	111.28
1	E	544	ASN	CA-C-N	-5.05	113.52	119.84
1	E	544	ASN	C-N-CA	-5.05	113.52	119.84

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	4254	0	4113	23	0
1	B	4185	0	4009	13	0
1	C	4182	0	3985	24	0
1	D	4205	0	4038	22	0
1	E	4094	0	3844	17	0
1	F	4074	0	3809	24	0
1	G	4206	0	4043	36	0
1	H	4130	0	3876	25	0
2	A	12	0	13	0	0
2	G	12	0	13	0	0
3	A	49	0	0	1	1
3	B	45	0	0	0	0
3	C	35	0	0	1	0
3	D	49	0	0	2	1
3	E	16	0	0	0	0
3	F	18	0	0	0	0
3	G	21	0	0	0	0
3	H	15	0	0	0	0
All	All	33602	0	31743	181	1

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 3.

All (181) 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:70:GLU:OE2	3:A:701:HOH:O	1.87	0.91
1:D:115:GLY:N	1:D:376:GLU:OE1	2.03	0.91
1:B:115:GLY:N	1:B:376:GLU:OE2	2.09	0.86
1:F:293:ALA:O	1:F:295:GLY:N	2.09	0.84
1:G:358:TRP:O	1:G:437:ARG:NH2	2.10	0.84
1:F:199:PHE:O	1:F:203:ASN:ND2	2.11	0.83
1:C:537:GLN:OE1	1:C:537:GLN:N	2.13	0.82
1:A:115:GLY:N	1:A:376:GLU:OE2	2.14	0.79
1:C:309:ASP:OD1	1:C:414:ARG:NH1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:537:GLN:N	1:H:537:GLN:OE1	2.19	0.74
1:A:378:ASN:O	1:A:498:ARG:NH1	2.20	0.74
1:H:363:GLU:OE2	1:H:437:ARG:NH1	2.22	0.71
1:G:352:ARG:NH1	1:G:442:ASP:OD1	2.23	0.70
1:H:409:TYR:OH	1:H:531:PHE:O	2.10	0.70
1:D:24:GLU:OE2	1:D:138:LYS:NZ	2.23	0.69
1:G:5:ASP:OD2	1:G:114:ARG:NH2	2.25	0.69
1:D:241:ARG:NH1	1:D:331:GLU:O	2.27	0.68
1:E:549:THR:O	1:E:550:TRP:HB2	1.94	0.68
1:F:301:TRP:NE1	1:F:459:SER:O	2.27	0.67
1:H:504:ARG:NH2	1:H:576:ARG:O	2.28	0.66
1:H:45:GLN:OE1	1:H:47:ARG:NH1	2.28	0.66
1:C:115:GLY:N	1:C:376:GLU:OE1	2.29	0.65
1:G:363:GLU:OE1	1:G:437:ARG:NH1	2.29	0.65
1:G:82:LYS:NZ	1:G:89:ASP:OD1	2.21	0.64
1:C:179:ARG:O	1:C:179:ARG:NE	2.30	0.64
1:E:123:ASP:OD1	1:E:388:ARG:NH1	2.30	0.63
1:G:549:THR:O	1:G:550:TRP:HB2	1.98	0.63
1:D:414:ARG:NH1	3:D:602:HOH:O	2.31	0.63
1:F:363:GLU:OE2	1:F:437:ARG:NH1	2.32	0.62
1:F:123:ASP:OD1	1:F:388:ARG:NH1	2.29	0.62
1:F:461:PRO:O	1:F:464:VAL:N	2.32	0.62
1:D:123:ASP:OD1	1:D:388:ARG:NH1	2.31	0.60
1:A:363:GLU:OE2	1:A:437:ARG:NH1	2.34	0.60
1:E:191:ALA:O	1:E:266:ARG:NH2	2.35	0.60
1:H:544:ASN:CB	1:H:545:PRO:HD2	2.32	0.59
1:D:364:SER:OG	3:D:601:HOH:O	2.16	0.59
1:G:478:HIS:NE2	1:G:539:ILE:HB	2.18	0.59
1:C:329:SER:O	1:C:330:HIS:CB	2.50	0.59
1:E:363:GLU:OE2	1:E:437:ARG:NH1	2.36	0.59
1:F:295:GLY:N	1:F:296:PRO:CD	2.66	0.59
1:D:191:ALA:O	1:D:266:ARG:NH2	2.32	0.57
1:G:309:ASP:OD1	1:G:414:ARG:NH1	2.37	0.57
1:D:352:ARG:NH2	1:D:442:ASP:OD1	2.39	0.56
1:C:451:LYS:N	1:C:471:LEU:O	2.39	0.55
1:G:460:LEU:HD12	1:G:461:PRO:HD2	1.88	0.55
1:C:464:VAL:O	1:C:468:THR:HG22	2.06	0.55
1:E:544:ASN:CB	1:E:545:PRO:CD	2.84	0.55
1:A:504:ARG:NH2	1:A:576:ARG:O	2.38	0.54
1:C:5:ASP:OD2	1:C:114:ARG:NH2	2.40	0.54
1:G:198:GLU:OE1	1:G:201:ARG:NH2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:544:ASN:CB	1:D:545:PRO:HD2	2.37	0.54
1:G:75:GLN:HG2	1:G:96:MET:HE1	1.90	0.54
1:D:363:GLU:OE2	1:D:437:ARG:NH1	2.42	0.53
1:F:451:LYS:N	1:F:471:LEU:O	2.41	0.53
1:B:5:ASP:OD2	1:B:114:ARG:NH2	2.42	0.53
1:F:514:LEU:O	1:F:518:MET:HG3	2.09	0.53
1:F:266:ARG:O	1:F:268:GLY:N	2.42	0.53
1:H:24:GLU:OE2	1:H:138:LYS:NZ	2.35	0.53
1:A:124:LEU:HD23	1:A:128:ARG:HG3	1.91	0.52
1:G:123:ASP:CG	1:G:388:ARG:HH22	2.17	0.52
1:A:544:ASN:O	1:A:545:PRO:C	2.52	0.52
1:H:123:ASP:OD1	1:H:388:ARG:NH1	2.39	0.52
1:F:297:LEU:O	1:F:301:TRP:HB2	2.09	0.52
1:A:82:LYS:NZ	1:A:89:ASP:OD1	2.31	0.52
1:E:544:ASN:CB	1:E:545:PRO:HD3	2.40	0.52
1:C:477:ILE:O	1:C:480:LEU:N	2.38	0.52
1:E:451:LYS:N	1:E:471:LEU:O	2.39	0.51
1:A:191:ALA:O	1:A:266:ARG:NH2	2.31	0.51
1:C:123:ASP:CG	1:C:388:ARG:HH22	2.18	0.51
1:B:114:ARG:HA	1:B:376:GLU:OE2	2.10	0.51
1:F:412:LEU:HD11	1:F:476:LEU:HD23	1.91	0.51
1:A:123:ASP:OD1	1:A:388:ARG:NH1	2.37	0.51
1:E:36[B]:ARG:NH2	1:E:49:SER:OG	2.44	0.51
1:F:410:HIS:ND1	1:F:517:TYR:OH	2.44	0.50
1:G:420:ILE:CB	1:G:446:ASP:CB	2.89	0.50
1:A:121:LEU:HA	1:A:124:LEU:HD13	1.93	0.50
1:G:427:THR:OG1	1:G:441:LYS:CE	2.60	0.50
1:H:82:LYS:NZ	1:H:89:ASP:OD1	2.34	0.50
1:A:24:GLU:OE2	1:A:138:LYS:NZ	2.39	0.49
1:D:330:HIS:O	1:D:331:GLU:C	2.55	0.49
1:E:521:HIS:HB3	1:E:524:MET:HE3	1.94	0.49
1:F:392:ASP:N	1:F:392:ASP:OD1	2.45	0.49
1:G:185:THR:HG23	1:G:188:THR:H	1.77	0.48
1:E:425:ASN:OD1	1:E:425:ASN:N	2.39	0.48
1:H:294:ALA:C	1:H:296:PRO:HD3	2.38	0.48
1:G:151:GLU:OE2	1:G:155:ARG:NH2	2.47	0.48
1:B:25:GLN:OE1	1:B:540:ARG:NH1	2.47	0.48
1:A:352:ARG:NH1	1:A:442:ASP:OD1	2.47	0.48
1:B:478:HIS:O	1:B:482:THR:N	2.47	0.48
1:F:549:THR:O	1:F:550:TRP:HB2	2.14	0.47
1:B:541:VAL:O	1:B:542:VAL:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:MET:HE2	1:B:488:VAL:HA	1.97	0.47
1:C:450:VAL:O	1:C:470:ARG:NE	2.47	0.47
1:G:421:ALA:HB3	1:G:484:HIS:HB2	1.96	0.47
1:F:360:LYS:CB	1:F:361:PRO:CD	2.93	0.46
1:G:114:ARG:HA	1:G:376:GLU:OE2	2.15	0.46
1:A:75:GLN:HG2	1:A:96:MET:HE1	1.98	0.46
1:H:236:ASP:OD2	1:H:343:TYR:OH	2.26	0.46
1:F:329:SER:O	1:F:330:HIS:C	2.58	0.46
1:F:372:MET:HE2	1:F:488:VAL:HA	1.97	0.46
1:F:549:THR:O	1:F:550:TRP:CB	2.64	0.46
1:E:477:ILE:HD11	1:E:531:PHE:HB3	1.98	0.45
1:C:414:ARG:HE	1:C:524:MET:CE	2.29	0.45
1:D:114:ARG:HA	1:D:376:GLU:OE1	2.17	0.45
1:E:296:PRO:O	1:E:297:LEU:CB	2.65	0.45
1:H:54:ILE:N	1:H:503:GLU:OE1	2.41	0.45
1:H:443:PHE:O	1:H:444:GLN:CB	2.64	0.45
1:G:212:ASP:OD1	1:G:214:ASP:HB2	2.17	0.45
1:C:451:LYS:HA	1:C:470:ARG:HD3	1.98	0.45
1:C:318:VAL:HB	1:C:439:LEU:HG	1.99	0.45
1:G:443:PHE:O	1:G:444:GLN:C	2.60	0.44
1:C:173:ARG:NE	1:C:213:ASN:O	2.35	0.44
1:B:198:GLU:OE1	1:B:201:ARG:NH2	2.46	0.44
1:E:52:ARG:NH1	1:E:56:GLY:O	2.49	0.44
1:H:544:ASN:CB	1:H:545:PRO:CD	2.96	0.43
1:D:478:HIS:C	1:D:480:LEU:N	2.75	0.43
1:G:239:GLU:OE2	1:H:100:TYR:OH	2.18	0.43
1:B:541:VAL:O	1:B:543:LEU:N	2.51	0.43
1:G:427:THR:OG1	1:G:441:LYS:HE3	2.18	0.43
1:F:518:MET:CE	1:F:528:PHE:HB3	2.49	0.43
1:A:309:ASP:OD2	1:A:414:ARG:NH1	2.51	0.43
1:C:82:LYS:HB3	1:C:83:PRO:HD3	2.01	0.43
1:G:184:LEU:HD23	1:G:185:THR:N	2.34	0.43
1:H:59:TRP:HZ2	1:H:503:GLU:OE2	2.02	0.43
1:C:185:THR:HG23	1:C:188:THR:H	1.84	0.43
1:D:171:VAL:HB	1:D:176:MET:HE2	2.01	0.43
1:B:420:ILE:HG23	1:B:425:ASN:ND2	2.33	0.43
1:C:542:VAL:CB	1:C:562:ASN:C	2.92	0.43
1:C:544:ASN:N	1:C:545:PRO:CD	2.82	0.43
1:H:167:HIS:O	1:H:220:VAL:N	2.48	0.43
1:C:203:ASN:OD1	3:C:601:HOH:O	2.21	0.42
1:D:403:VAL:HG13	1:D:437:ARG:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:123:ASP:CG	1:H:388:ARG:HH22	2.26	0.42
1:H:549:THR:HG22	1:H:550:TRP:N	2.34	0.42
1:A:372:MET:HE2	1:A:488:VAL:HA	2.02	0.42
1:G:226:GLN:NE2	1:H:226:GLN:OE1	2.52	0.42
1:A:414:ARG:HD2	1:A:524:MET:HE2	2.00	0.42
1:E:487:THR:O	1:E:487:THR:HG22	2.19	0.42
1:G:201:ARG:NH1	1:G:248:PHE:CE1	2.88	0.42
1:A:487:THR:HG22	1:A:487:THR:O	2.19	0.42
1:B:9:VAL:HG12	1:B:103:LEU:HD22	2.01	0.42
1:D:478:HIS:O	1:D:480:LEU:N	2.52	0.42
1:F:113:ARG:NH1	1:F:374:CYS:O	2.53	0.42
1:D:478:HIS:O	1:D:482:THR:N	2.53	0.42
1:G:226:GLN:NE2	1:G:227:GLN:OE1	2.45	0.42
1:G:412:LEU:HD11	1:G:476:LEU:HD23	2.00	0.42
1:C:295:GLY:O	1:C:298:ALA:N	2.46	0.42
1:G:460:LEU:HD12	1:G:461:PRO:CD	2.50	0.42
1:F:30:GLU:OE2	1:F:40:ASN:OD1	2.38	0.42
1:G:410:HIS:HE1	1:G:524:MET:HE1	1.85	0.42
1:G:566:ASP:OD1	1:G:566:ASP:N	2.53	0.42
1:E:546:VAL:HG12	1:E:547:LYS:N	2.35	0.41
1:D:421:ALA:HB1	1:D:426:ILE:HD11	2.03	0.41
1:H:102:THR:HA	1:H:143:LYS:HB2	2.02	0.41
1:H:544:ASN:C	1:H:546:VAL:H	2.28	0.41
1:A:353:GLU:OE2	1:A:358:TRP:NE1	2.52	0.41
1:G:82:LYS:HB3	1:G:83:PRO:HD3	2.02	0.41
1:B:420:ILE:HG21	1:B:446:ASP:CB	2.51	0.41
1:E:510:LEU:HD23	1:E:571:LEU:HD11	2.03	0.41
1:F:460:LEU:O	1:F:461:PRO:C	2.64	0.41
1:G:478:HIS:C	1:G:480:LEU:N	2.78	0.41
1:D:397:LEU:HD11	1:D:496:MET:SD	2.60	0.41
1:G:478:HIS:O	1:G:482:THR:N	2.54	0.41
1:D:393:ALA:O	1:D:397:LEU:HD13	2.21	0.41
1:D:505:ARG:CZ	1:D:509:LEU:HD11	2.51	0.41
1:E:479:ASP:O	1:E:483:GLY:N	2.48	0.41
1:G:229:ILE:HD13	1:G:347:LEU:HD21	2.02	0.41
1:C:236:ASP:OD1	1:C:241:ARG:NH2	2.44	0.40
1:C:269:GLY:HA2	1:C:354:ASN:HB3	2.03	0.40
1:F:171:VAL:HB	1:F:176:MET:CE	2.51	0.40
1:H:292:ILE:CB	1:H:344:GLN:OE1	2.69	0.40
1:A:540:ARG:NH1	1:A:565:GLU:HG3	2.36	0.40
1:B:82:LYS:HB3	1:B:83:PRO:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:178:TRP:NE1	1:G:180:CYS:HB2	2.36	0.40
1:H:78:LEU:HD23	1:H:96:MET:HE2	2.03	0.40
1:G:487:THR:O	1:G:487:THR:HG22	2.22	0.40
1:H:537:GLN:HB2	1:H:566:ASP:HB3	2.03	0.40
1:A:6:TRP:CZ2	1:C:239:GLU:HG3	2.57	0.40
1:A:451:LYS:N	1:A:471:LEU:O	2.50	0.40
1:A:540:ARG:HD2	1:A:565:GLU:HG3	2.03	0.40
1:D:316:GLY:O	1:D:437:ARG:HD2	2.22	0.40

All (1) 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)
3:A:745:HOH:O	3:D:620:HOH:O[2_556]	2.07	0.13

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	539/579 (93%)	521 (97%)	16 (3%)	2 (0%)	30	37
1	B	535/579 (92%)	517 (97%)	17 (3%)	1 (0%)	43	54
1	C	539/579 (93%)	524 (97%)	13 (2%)	2 (0%)	30	37
1	D	534/579 (92%)	515 (96%)	15 (3%)	4 (1%)	18	24
1	E	532/579 (92%)	520 (98%)	9 (2%)	3 (1%)	21	27
1	F	532/579 (92%)	507 (95%)	22 (4%)	3 (1%)	21	27
1	G	534/579 (92%)	523 (98%)	11 (2%)	0	100	100
1	H	536/579 (93%)	517 (96%)	16 (3%)	3 (1%)	21	27
All	All	4281/4632 (92%)	4144 (97%)	119 (3%)	18 (0%)	30	37

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	444	GLN
1	B	542	VAL
1	C	330	HIS
1	D	443	PHE
1	E	444	GLN
1	F	294	ALA
1	H	444	GLN
1	H	544	ASN
1	H	546	VAL
1	D	479	ASP
1	D	544	ASN
1	F	267	GLN
1	A	545	PRO
1	C	545	PRO
1	E	544	ASN
1	F	544	ASN
1	D	539	ILE
1	E	545	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	426/487 (88%)	423 (99%)	3 (1%)	76	84
1	B	413/487 (85%)	410 (99%)	3 (1%)	76	84
1	C	406/487 (83%)	398 (98%)	8 (2%)	48	63
1	D	420/487 (86%)	416 (99%)	4 (1%)	68	77
1	E	392/487 (80%)	387 (99%)	5 (1%)	61	73
1	F	385/487 (79%)	382 (99%)	3 (1%)	73	83
1	G	417/487 (86%)	413 (99%)	4 (1%)	68	77
1	H	393/487 (81%)	391 (100%)	2 (0%)	81	87
All	All	3252/3896 (84%)	3220 (99%)	32 (1%)	68	77

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	357	ARG
1	A	443	PHE
1	B	203	ASN
1	B	443	PHE
1	B	477	ILE
1	C	38	CYS
1	C	70	GLU
1	C	176	MET
1	C	179	ARG
1	C	239	GLU
1	C	468	THR
1	C	470	ARG
1	C	546	VAL
1	D	213	ASN
1	D	537	GLN
1	D	538	ILE
1	D	540	ARG
1	E	203	ASN
1	E	304	GLN
1	E	425	ASN
1	E	459	SER
1	E	540	ARG
1	F	180	CYS
1	F	459	SER
1	F	470	ARG
1	G	184	LEU
1	G	207	GLN
1	G	472	SER
1	G	482	THR
1	H	546	VAL
1	H	562	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	45	GLN
1	A	256	GLN
1	A	478	HIS
1	B	436	GLN

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Mol	Chain	Res	Type
1	B	481	GLN
1	C	379	GLN
1	C	484	HIS
1	D	436	GLN
1	D	484	HIS
1	E	478	HIS
1	F	537	GLN
1	G	209	ASN
1	G	226	GLN
1	G	436	GLN
1	H	436	GLN
1	H	484	HIS

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](#)

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	MES	A	600	-	12,12,12	2.31	1 (8%)	15,16,16	1.36	2 (13%)
2	MES	G	600	-	12,12,12	2.32	1 (8%)	15,16,16	1.41	2 (13%)

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	MES	A	600	-	-	2/6/14/14	0/1/1/1
2	MES	G	600	-	-	0/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	600	MES	C8-S	-7.74	1.66	1.77
2	A	600	MES	C8-S	-7.73	1.66	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	600	MES	C6-C5-N4	-2.88	105.74	110.12
2	A	600	MES	C5-N4-C3	2.36	113.93	108.84
2	A	600	MES	C6-C5-N4	-2.00	107.08	110.12
2	G	600	MES	O2S-S-C8	2.00	109.75	106.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	MES	C8-C7-N4-C3
2	A	600	MES	C8-C7-N4-C5

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, 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	547/579 (94%)	0.32	30 (5%)	30	28	37, 60, 93, 107	0
1	B	543/579 (93%)	0.36	23 (4%)	40	40	38, 67, 95, 110	0
1	C	547/579 (94%)	0.56	40 (7%)	21	18	38, 74, 103, 119	0
1	D	542/579 (93%)	0.45	49 (9%)	15	13	34, 66, 100, 120	0
1	E	539/579 (93%)	0.71	45 (8%)	17	15	38, 80, 113, 130	1 (0%)
1	F	540/579 (93%)	0.77	42 (7%)	19	16	56, 85, 111, 119	0
1	G	542/579 (93%)	0.53	32 (5%)	28	25	48, 73, 98, 115	0
1	H	544/579 (93%)	0.65	36 (6%)	24	22	47, 82, 110, 123	0
All	All	4344/4632 (93%)	0.54	297 (6%)	23	21	34, 74, 105, 130	1 (0%)

All (297) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	421	ALA	6.5
1	A	550	TRP	5.6
1	D	420	ILE	5.2
1	F	550	TRP	5.2
1	D	576	ARG	5.1
1	E	550	TRP	4.9
1	G	288	PRO	4.9
1	D	479	ASP	4.8
1	D	542	VAL	4.4
1	H	421	ALA	4.4
1	G	445	GLY	4.4
1	H	550	TRP	4.4
1	E	420	ILE	4.3
1	D	443	PHE	4.3
1	D	421	ALA	4.3
1	F	294	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	330	HIS	4.2
1	B	292	ILE	4.2
1	G	550	TRP	4.2
1	G	576	ARG	4.1
1	F	306	PHE	4.1
1	C	550	TRP	4.1
1	C	562	ASN	4.1
1	E	445	GLY	4.1
1	F	2	ASN	4.1
1	G	444	GLN	4.0
1	F	421	ALA	4.0
1	E	449	LEU	4.0
1	E	447	MET	3.9
1	F	178	TRP	3.8
1	C	341	TYR	3.8
1	B	341	TYR	3.8
1	D	268	GLY	3.7
1	B	330	HIS	3.7
1	B	544	ASN	3.7
1	G	443	PHE	3.7
1	A	180	CYS	3.7
1	A	564	LEU	3.7
1	E	2	ASN	3.7
1	D	341	TYR	3.7
1	E	327	TYR	3.7
1	D	288	PRO	3.6
1	F	213	ASN	3.6
1	G	543	LEU	3.6
1	C	543	LEU	3.6
1	D	550	TRP	3.5
1	D	424	GLN	3.5
1	E	560	LEU	3.5
1	E	296	PRO	3.5
1	C	479	ASP	3.4
1	D	180	CYS	3.4
1	C	446	ASP	3.4
1	A	577	ASP	3.4
1	F	543	LEU	3.4
1	G	239	GLU	3.4
1	A	330	HIS	3.3
1	E	544	ASN	3.3
1	G	297	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	575	THR	3.3
1	E	330	HIS	3.3
1	A	563	TYR	3.2
1	C	544	ASN	3.2
1	F	327	TYR	3.2
1	D	467	VAL	3.2
1	B	422	HIS	3.2
1	C	288	PRO	3.2
1	G	341	TYR	3.2
1	F	424	GLN	3.2
1	E	446	ASP	3.2
1	B	545	PRO	3.2
1	C	361	PRO	3.2
1	H	480	LEU	3.2
1	A	181	ASP	3.1
1	D	546	VAL	3.1
1	F	279	TYR	3.1
1	B	421	ALA	3.1
1	D	447	MET	3.1
1	D	544	ASN	3.1
1	G	542	VAL	3.1
1	H	467	VAL	3.1
1	C	292	ILE	3.1
1	A	424	GLN	3.1
1	D	442	ASP	3.1
1	E	233	PHE	3.1
1	H	202	PHE	3.1
1	E	328	VAL	3.1
1	C	291	TYR	3.0
1	C	184	LEU	3.0
1	F	565	GLU	3.0
1	E	343	TYR	3.0
1	D	425	ASN	3.0
1	H	544	ASN	3.0
1	A	1	MET	3.0
1	E	469	ALA	3.0
1	F	291	TYR	3.0
1	E	443	PHE	3.0
1	H	330	HIS	2.9
1	A	327	TYR	2.9
1	D	543	LEU	2.9
1	A	43	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	295	GLY	2.9
1	A	362	ASP	2.9
1	A	279	TYR	2.9
1	G	479	ASP	2.9
1	D	297	LEU	2.9
1	C	444	GLN	2.9
1	E	484	HIS	2.8
1	B	446	ASP	2.8
1	B	426	ILE	2.8
1	D	480	LEU	2.8
1	B	331	GLU	2.8
1	H	446	ASP	2.8
1	F	422	HIS	2.8
1	H	442	ASP	2.8
1	G	420	ILE	2.8
1	F	544	ASN	2.8
1	A	541	VAL	2.8
1	H	362	ASP	2.8
1	C	539	ILE	2.7
1	B	178	TRP	2.7
1	G	449	LEU	2.7
1	F	199	PHE	2.7
1	E	213	ASN	2.7
1	F	423	GLY	2.7
1	H	420	ILE	2.7
1	H	355	PRO	2.7
1	E	183	SER	2.7
1	D	470	ARG	2.7
1	F	69	ASP	2.7
1	E	347	LEU	2.7
1	B	550	TRP	2.7
1	F	308	THR	2.7
1	D	446	ASP	2.6
1	B	420	ILE	2.6
1	C	576	ARG	2.6
1	C	185	THR	2.6
1	F	341	TYR	2.6
1	G	330	HIS	2.6
1	H	422	HIS	2.6
1	F	452	ASP	2.6
1	A	542	VAL	2.6
1	D	178	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	442	ASP	2.6
1	E	362	ASP	2.6
1	H	423	GLY	2.6
1	A	176	MET	2.6
1	G	567	LEU	2.6
1	D	461	PRO	2.6
1	E	566	ASP	2.6
1	D	464	VAL	2.6
1	E	424	GLN	2.6
1	H	462	GLN	2.6
1	G	575	THR	2.6
1	A	446	ASP	2.5
1	A	479	ASP	2.5
1	B	466	ASP	2.5
1	C	442	ASP	2.5
1	C	545	PRO	2.5
1	H	483	GLY	2.5
1	D	294	ALA	2.5
1	F	183	SER	2.5
1	C	279	TYR	2.5
1	A	288	PRO	2.5
1	F	420	ILE	2.5
1	B	543	LEU	2.5
1	E	184	LEU	2.5
1	G	568	GLN	2.5
1	B	279	TYR	2.5
1	B	460	LEU	2.5
1	D	469	ALA	2.5
1	E	470	ARG	2.5
1	G	421	ALA	2.5
1	G	295	GLY	2.5
1	H	452	ASP	2.5
1	H	184	LEU	2.5
1	E	3	HIS	2.5
1	D	298	ALA	2.5
1	D	536	PRO	2.4
1	D	475	TYR	2.4
1	F	566	ASP	2.4
1	D	3	HIS	2.4
1	D	242	MET	2.4
1	A	292	ILE	2.4
1	H	543	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	576	ARG	2.4
1	F	479	ASP	2.4
1	E	36[A]	ARG	2.4
1	A	178	TRP	2.4
1	C	294	ALA	2.4
1	H	178	TRP	2.4
1	H	361	PRO	2.4
1	H	295	GLY	2.4
1	D	460	LEU	2.4
1	F	419	LEU	2.4
1	A	341	TYR	2.4
1	F	542	VAL	2.4
1	C	331	GLU	2.4
1	E	450	VAL	2.3
1	F	541	VAL	2.3
1	A	179	ARG	2.3
1	E	297	LEU	2.3
1	F	442	ASP	2.3
1	G	279	TYR	2.3
1	D	331	GLU	2.3
1	G	293	ALA	2.3
1	H	489	LEU	2.3
1	D	342	ARG	2.3
1	C	268	GLY	2.3
1	D	423	GLY	2.3
1	F	519	GLN	2.3
1	D	477	ILE	2.3
1	F	439	LEU	2.3
1	C	563	TYR	2.3
1	C	500	GLY	2.2
1	E	32	GLN	2.2
1	H	444	GLN	2.2
1	D	539	ILE	2.2
1	H	358	TRP	2.2
1	B	565	GLU	2.2
1	C	464	VAL	2.2
1	H	300	ARG	2.2
1	D	574	ALA	2.2
1	G	294	ALA	2.2
1	A	477	ILE	2.2
1	G	477	ILE	2.2
1	D	466	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	69	ASP	2.2
1	G	566	ASP	2.2
1	H	181	ASP	2.2
1	C	32	GLN	2.2
1	C	478	HIS	2.2
1	H	478	HIS	2.2
1	A	184	LEU	2.2
1	H	439	LEU	2.2
1	H	183	SER	2.2
1	H	215	TRP	2.2
1	E	243	VAL	2.2
1	C	330	HIS	2.2
1	G	183	SER	2.2
1	F	181	ASP	2.2
1	G	463	GLU	2.2
1	H	306	PHE	2.2
1	A	348	GLY	2.1
1	D	291	TYR	2.1
1	H	291	TYR	2.1
1	D	540	ARG	2.1
1	D	545	PRO	2.1
1	C	199	PHE	2.1
1	C	421	ALA	2.1
1	A	445	GLY	2.1
1	B	439	LEU	2.1
1	E	567	LEU	2.1
1	E	426	ILE	2.1
1	H	539	ILE	2.1
1	C	463	GLU	2.1
1	E	466	ASP	2.1
1	F	447	MET	2.1
1	D	449	LEU	2.1
1	D	573	LEU	2.1
1	E	440	LEU	2.1
1	C	575	THR	2.1
1	E	342	ARG	2.1
1	E	576	ARG	2.1
1	G	539	ILE	2.1
1	F	362	ASP	2.1
1	G	545	PRO	2.1
1	A	177	VAL	2.1
1	C	443	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	417	VAL	2.1
1	C	453	ALA	2.1
1	E	307	ALA	2.1
1	G	544	ASN	2.1
1	E	348	GLY	2.1
1	E	353	GLU	2.1
1	D	452	ASP	2.1
1	F	446	ASP	2.1
1	H	457	MET	2.1
1	A	444	GLN	2.0
1	B	424	GLN	2.0
1	D	568	GLN	2.0
1	F	207	GLN	2.0
1	H	523	GLN	2.0
1	G	298	ALA	2.0
1	F	460	LEU	2.0
1	F	358	TRP	2.0
1	E	415	TYR	2.0
1	C	180	CYS	2.0
1	C	356	CYS	2.0
1	A	467	VAL	2.0
1	F	241	ARG	2.0
1	C	298	ALA	2.0
1	C	473	ALA	2.0
1	E	240	GLY	2.0
1	F	326	GLY	2.0
1	C	420	ILE	2.0
1	B	358	TRP	2.0
1	F	42	PRO	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 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	MES	A	600	12/12	0.85	0.16	86,88,95,96	0
2	MES	G	600	12/12	0.85	0.16	99,102,112,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.