Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 10:32 AM EDT

PDB ID	:	6CN7
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 (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 (i)) were used in the production of this report:

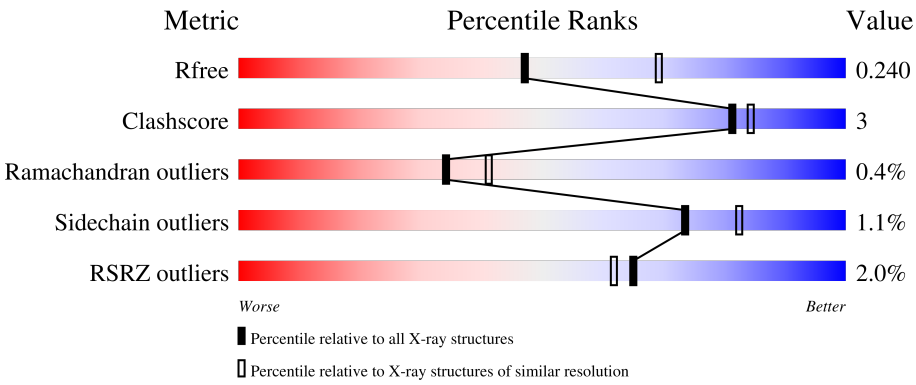
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	579	.% 88% 6% 6%
1	B	579	2% 89% • 6%
1	C	579	.% 87% 7% • 6%
1	D	579	2% 87% 7% 6%
1	E	579	3% 87% 5% 7%

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Mol	Chain	Length	Quality of chain
1	F	579	3% 85% 8% 7%
1	G	579	% 85% 9% 6%
1	H	579	2% 87% 7% 6%

2 Entry composition (i)

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

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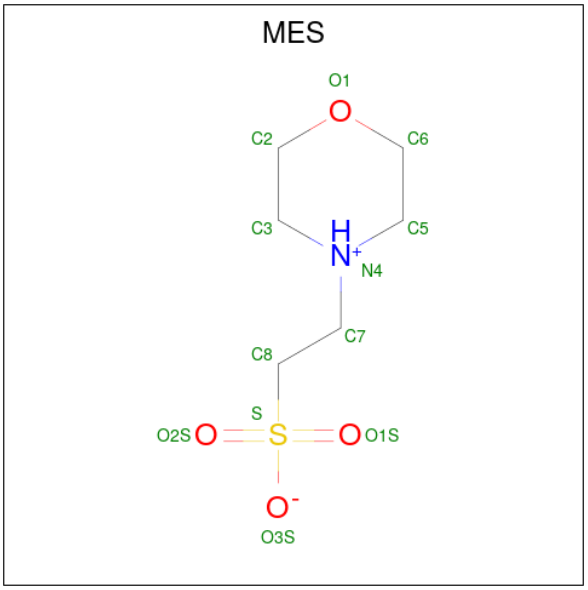
Chain	Residue	Modelled	Actual	Comment	Reference
H	188	THR	GLN	engineered mutation	UNP Q6U605

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



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

- Molecule 3 is water.

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

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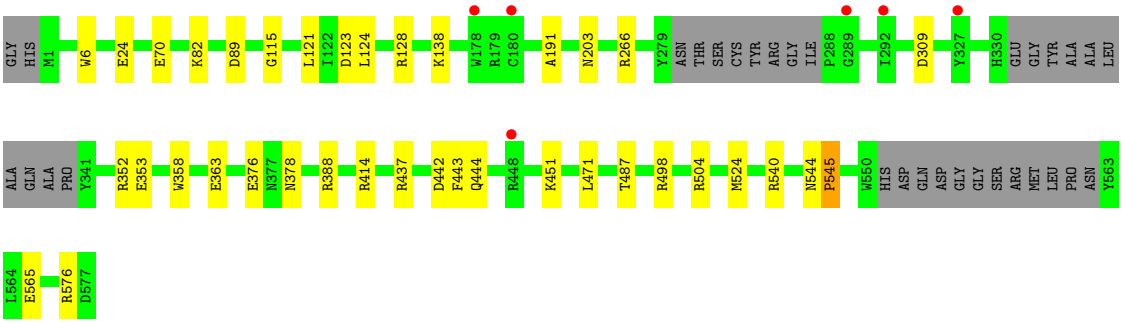
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	G	21	21	21	0	0
			Total	O		
3	H	15	15	15	0	0

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.

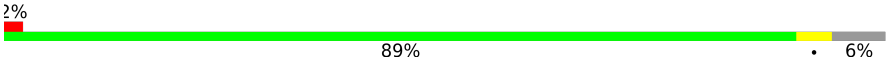
• Molecule 1: Aerobactin synthase IucC

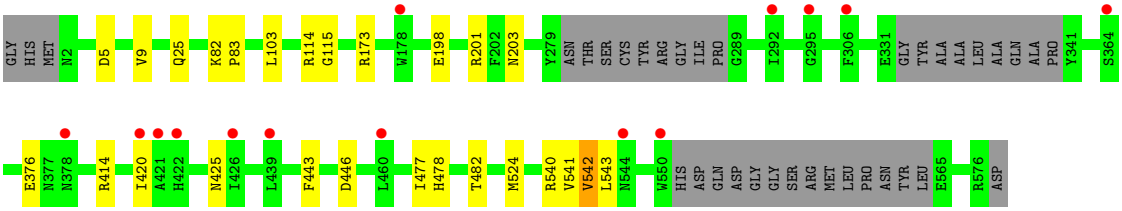
Chain A:



• Molecule 1: Aerobactin synthase IucC

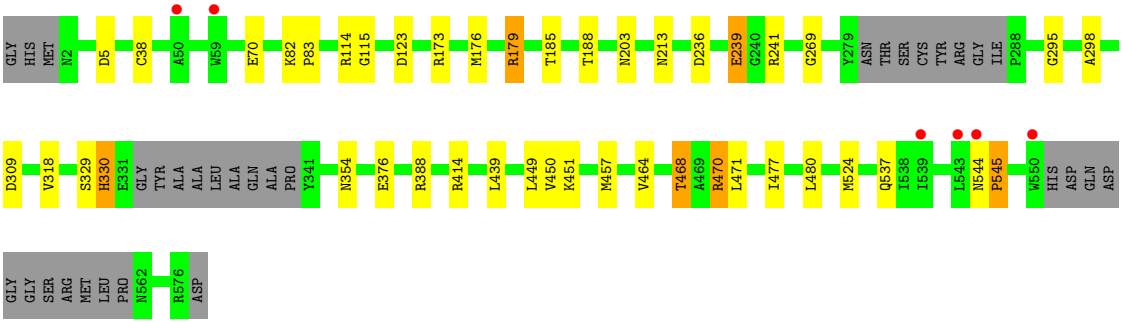
Chain B:





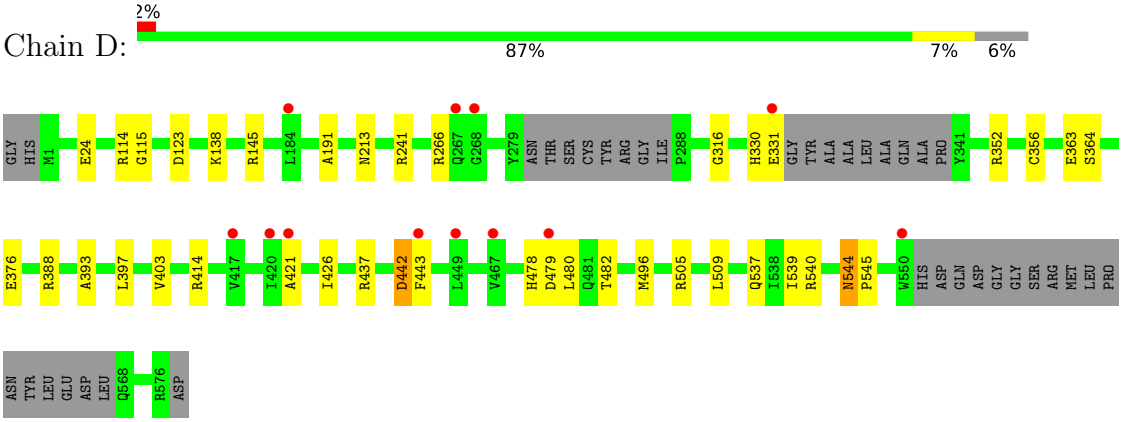
• Molecule 1: Aerobactin synthase IucC

Chain C:



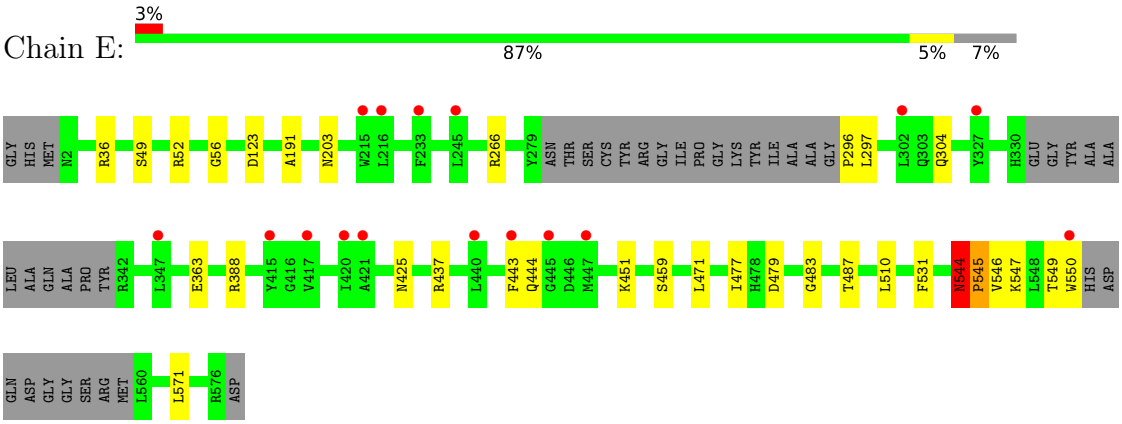
• Molecule 1: Aerobactin synthase IucC

Chain D:



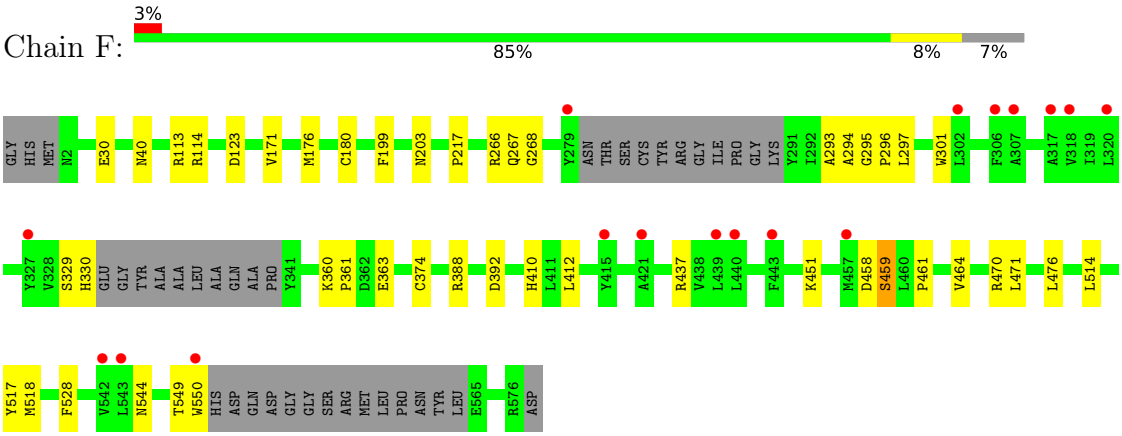
• Molecule 1: Aerobactin synthase IucC

Chain E:



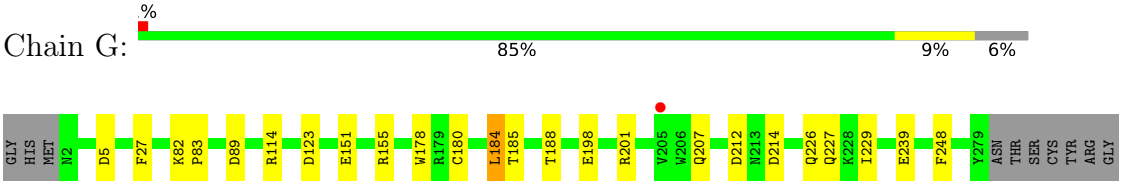
• Molecule 1: Aerobactin synthase IucC

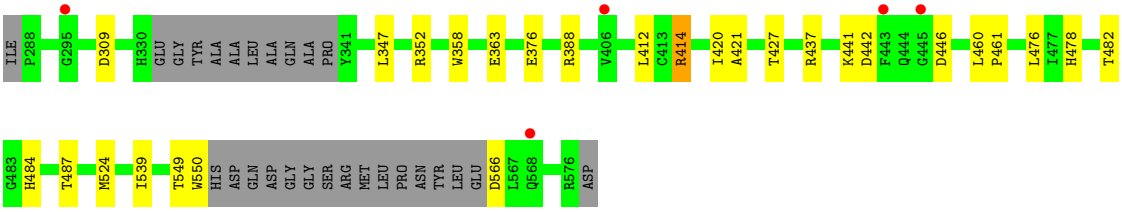
Chain F:



• Molecule 1: Aerobactin synthase IucC

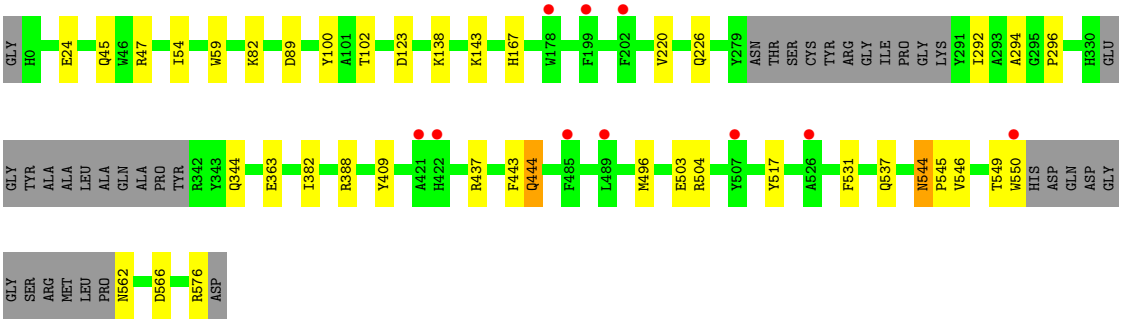
Chain G:





- Molecule 1: Aerobactin synthase IucC

Chain H:



4 Data and refinement statistics (i)

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 98.85 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (58.07-2.45) 95.1 (98.85-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.213 , 0.240 0.215 , 0.240	Depositor DCC
R_{free} test set	10530 reflections (4.88%)	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)	0.30 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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 (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	0.26	0/4358	0.42	0/5938
1	B	0.24	0/4289	0.42	0/5851
1	C	0.25	0/4287	0.42	0/5852
1	D	0.25	0/4312	0.42	0/5881
1	E	0.29	0/4200	0.43	1/5742 (0.0%)
1	F	0.24	0/4178	0.42	0/5712
1	G	0.27	0/4314	0.44	0/5882
1	H	0.25	0/4237	0.43	0/5792
All	All	0.26	0/34175	0.42	1/46650 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	544	ASN	C-N-CD	5.21	139.35	128.40

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	4254	0	4113	21	0
1	B	4185	0	4009	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4182	0	3985	24	0
1	D	4205	0	4038	21	0
1	E	4094	0	3844	16	0
1	F	4074	0	3809	22	0
1	G	4206	0	4043	33	0
1	H	4130	0	3876	22	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	169	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 (169) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:414:ARG:HD3	1:G:524:MET:HE1	1.89	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
1:D:544:ASN:CB	1:D:545:PRO:HD2	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:HD23	1:A:128:ARG:HG3	1.91	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: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: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:A:24:GLU:OE2	1:A:138:LYS:NZ	2.39	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:G:123:ASP:CG	1:G:388:ARG:HH22	2.17	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:A:544:ASN:O	1:A:545:PRO:C	2.52	0.47
1:F:549:THR:O	1:F:550:TRP:HB2	2.14	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:C:123:ASP:CG	1:C:388:ARG:HH22	2.18	0.46
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:330:HIS:O	1:D:331:GLU:C	2.55	0.45
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:294:ALA:C	1:H:296:PRO:HD3	2.38	0.44
1:H:544:ASN:CB	1:H:545:PRO:CD	2.96	0.43
1:A:414:ARG:HD3	1:A:524:MET:HE1	1.99	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:C:449:LEU:HD13	1:C:457:MET:HE3	2.01	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:B:414:ARG:HD2	1:B:524:MET:HE1	2.00	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:B:420:ILE:HG23	1:B:425:ASN:ND2	2.33	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
1:H:549:THR:HG22	1:H:550:TRP:N	2.34	0.42
1:G:226:GLN:NE2	1:H:226:GLN:OE1	2.52	0.42
1:E:487:THR:O	1:E:487:THR:HG22	2.19	0.42
1:B:541:VAL:O	1:B:542:VAL:C	2.58	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:566:ASP:OD1	1:G:566:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:546:VAL:HG12	1:E:547:LYS:N	2.35	0.41
1:F:329:SER:O	1:F:330:HIS:C	2.58	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: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: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:H:382:ILE:HG12	1:H:496:MET:HE3	2.03	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
1:G:178:TRP:NE1	1:G:180:CYS:HB2	2.36	0.40
1:D:478:HIS:C	1:D:480:LEU:N	2.75	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 (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	539/579 (93%)	521 (97%)	16 (3%)	2 (0%)	34	41
1	B	535/579 (92%)	517 (97%)	17 (3%)	1 (0%)	47	57
1	C	539/579 (93%)	524 (97%)	13 (2%)	2 (0%)	34	41
1	D	534/579 (92%)	515 (96%)	15 (3%)	4 (1%)	22	25
1	E	532/579 (92%)	520 (98%)	9 (2%)	3 (1%)	25	29
1	F	532/579 (92%)	507 (95%)	22 (4%)	3 (1%)	25	29
1	G	534/579 (92%)	523 (98%)	11 (2%)	0	100	100
1	H	536/579 (93%)	517 (96%)	16 (3%)	3 (1%)	25	29
All	All	4281/4632 (92%)	4144 (97%)	119 (3%)	18 (0%)	34	41

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

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Mol	Chain	Res	Type
1	E	545	PRO

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	426/487 (88%)	424 (100%)	2 (0%)	88 93
1	B	413/487 (85%)	409 (99%)	4 (1%)	76 84
1	C	406/487 (83%)	399 (98%)	7 (2%)	60 73
1	D	420/487 (86%)	414 (99%)	6 (1%)	67 77
1	E	392/487 (80%)	388 (99%)	4 (1%)	76 84
1	F	385/487 (79%)	379 (98%)	6 (2%)	62 74
1	G	417/487 (86%)	413 (99%)	4 (1%)	76 84
1	H	393/487 (81%)	391 (100%)	2 (0%)	88 93
All	All	3252/3896 (84%)	3217 (99%)	35 (1%)	73 82

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	443	PHE
1	B	173	ARG
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	D	145	ARG

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Mol	Chain	Res	Type
1	D	213	ASN
1	D	356	CYS
1	D	442	ASP
1	D	537	GLN
1	D	540	ARG
1	E	203	ASN
1	E	304	GLN
1	E	443	PHE
1	E	459	SER
1	F	114	ARG
1	F	180	CYS
1	F	217	PRO
1	F	458	ASP
1	F	459	SER
1	F	470	ARG
1	G	27	PHE
1	G	184	LEU
1	G	207	GLN
1	G	414	ARG
1	H	517	TYR
1	H	562	ASN

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

Mol	Chain	Res	Type
1	A	478	HIS
1	H	436	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 monosaccharides 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	2.26	1 (8%)	14,16,16	1.44	4 (28%)
2	MES	G	600	-	12,12,12	2.27	1 (8%)	14,16,16	1.55	3 (21%)

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	-7.57	1.66	1.77
2	A	600	MES	C8-S	-7.56	1.66	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	600	MES	C6-C5-N4	-2.88	105.74	110.10
2	G	600	MES	O2S-S-C8	2.36	109.75	106.92
2	G	600	MES	O3S-S-C8	2.30	109.48	105.77
2	A	600	MES	C5-N4-C3	2.27	113.93	108.83
2	A	600	MES	O2S-S-C8	2.24	109.61	106.92
2	A	600	MES	O3S-S-C8	2.18	109.29	105.77
2	A	600	MES	O1S-S-C8	2.14	109.49	106.92

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.14	6 (1%)	80	80	37, 60, 93, 107	0
1	B	543/579 (93%)	0.22	14 (2%)	56	52	38, 67, 95, 110	0
1	C	547/579 (94%)	0.14	6 (1%)	80	80	38, 74, 103, 119	0
1	D	542/579 (93%)	0.24	12 (2%)	62	58	34, 66, 100, 120	0
1	E	539/579 (93%)	0.19	16 (2%)	50	46	49, 80, 113, 130	0
1	F	540/579 (93%)	0.26	17 (3%)	49	45	56, 85, 111, 119	0
1	G	542/579 (93%)	0.10	6 (1%)	80	80	48, 73, 98, 115	0
1	H	544/579 (93%)	0.18	10 (1%)	68	65	47, 82, 110, 123	0
All	All	4344/4632 (93%)	0.18	87 (2%)	65	62	34, 74, 105, 130	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	543	LEU	8.2
1	E	421	ALA	7.2
1	E	445	GLY	6.7
1	F	306	PHE	6.3
1	B	292	ILE	5.9
1	B	544	ASN	5.5
1	F	302	LEU	4.5
1	C	544	ASN	4.5
1	H	421	ALA	4.2
1	B	420	ILE	4.0
1	E	417	VAL	3.8
1	F	415	TYR	3.7
1	F	307	ALA	3.7
1	F	320	LEU	3.6
1	H	550	TRP	3.6
1	F	421	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	543	LEU	3.5
1	B	421	ALA	3.5
1	F	550	TRP	3.4
1	E	447	MET	3.3
1	H	489	LEU	3.2
1	D	443	PHE	3.2
1	E	245	LEU	3.2
1	F	327	TYR	3.1
1	D	550	TRP	3.1
1	G	443	PHE	3.1
1	E	440	LEU	3.1
1	G	445	GLY	3.1
1	A	178	TRP	3.0
1	G	295	GLY	3.0
1	E	215	TRP	3.0
1	A	180	CYS	3.0
1	E	233	PHE	3.0
1	H	507	TYR	2.9
1	F	457	MET	2.9
1	B	295	GLY	2.8
1	D	268	GLY	2.8
1	E	443	PHE	2.8
1	F	317	ALA	2.8
1	H	526	ALA	2.8
1	F	318	VAL	2.8
1	F	542	VAL	2.8
1	H	178	TRP	2.7
1	D	479	ASP	2.7
1	B	426	ILE	2.7
1	D	421	ALA	2.7
1	E	347	LEU	2.6
1	B	178	TRP	2.6
1	C	50	ALA	2.6
1	G	568	GLN	2.6
1	C	539	ILE	2.5
1	E	415	TYR	2.5
1	A	327	TYR	2.5
1	C	550	TRP	2.5
1	B	439	LEU	2.4
1	B	364	SER	2.4
1	E	327	TYR	2.4
1	H	422	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	331	GLU	2.3
1	B	422	HIS	2.3
1	F	439	LEU	2.3
1	H	202	PHE	2.3
1	F	440	LEU	2.2
1	F	279	TYR	2.2
1	D	467	VAL	2.2
1	D	420	ILE	2.2
1	H	485	PHE	2.2
1	A	292	ILE	2.2
1	A	289	GLY	2.2
1	D	449	LEU	2.2
1	D	184	LEU	2.1
1	C	59	TRP	2.1
1	B	378	ASN	2.1
1	B	306	PHE	2.1
1	B	460	LEU	2.1
1	E	216	LEU	2.1
1	E	302	LEU	2.1
1	D	417	VAL	2.1
1	G	406	VAL	2.1
1	F	443	PHE	2.1
1	A	448	ARG	2.1
1	G	205	VAL	2.1
1	H	199	PHE	2.1
1	D	267	GLN	2.1
1	E	550	TRP	2.0
1	E	420	ILE	2.0
1	B	550	TRP	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, 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	MES	G	600	12/12	0.90	0.30	99,102,112,112	0
2	MES	A	600	12/12	0.92	0.34	86,88,95,96	0

6.5 Other polymers (i)

There are no such residues in this entry.