



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:27 am BST

PDB ID : 6CL6
Title : Structure of *P. aeruginosa* R2 pyocin fiber PA0620 comprising C-terminal residues 323-691
Authors : Buth, S.A.; Shneider, M.M.; Leiman, P.G.
Deposited on : 2018-03-01
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

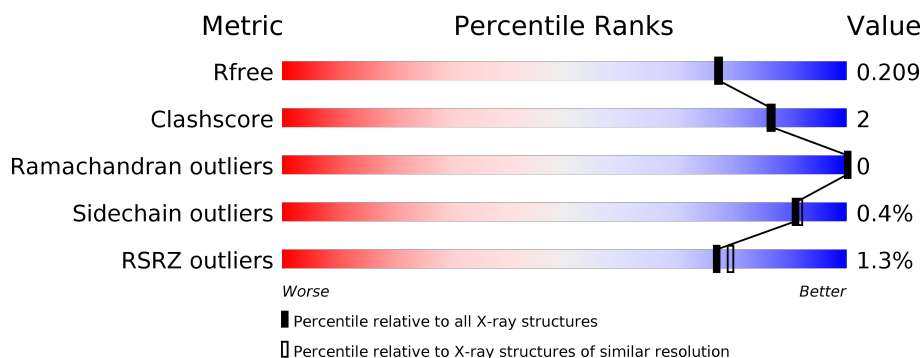
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	372	<div> <div>%</div> <div> <div></div> <div>94%</div> <div></div> </div> <div>• •</div> </div>
1	B	372	<div> <div>%</div> <div> <div></div> <div>94%</div> <div></div> </div> <div>• •</div> </div>
1	C	372	<div> <div>%</div> <div> <div></div> <div>95%</div> <div></div> </div> <div>• •</div> </div>
1	D	372	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div></div> </div> <div>• •</div> </div>
1	E	372	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> <div>•</div> </div>
1	F	372	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> <div>•</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36677 atoms, of which 15834 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 Tail fiber protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	364	Total	C	H	N	O	S	0	3	0
			5391	1759	2611	485	527	9			
1	B	364	Total	C	H	N	O	S	0	8	0
			5441	1773	2635	490	534	9			
1	C	364	Total	C	H	N	O	S	0	3	0
			5390	1758	2612	484	527	9			
1	D	364	Total	C	H	N	O	S	0	4	0
			5393	1759	2613	485	527	9			
1	E	364	Total	C	H	N	O	S	0	7	0
			5427	1769	2629	488	532	9			
1	F	364	Total	C	H	N	O	S	0	3	0
			5389	1758	2611	484	527	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	SER	-	cloning artifact	UNP G3XD71
A	321	GLY	-	cloning artifact	UNP G3XD71
A	322	SER	-	cloning artifact	UNP G3XD71
B	320	SER	-	cloning artifact	UNP G3XD71
B	321	GLY	-	cloning artifact	UNP G3XD71
B	322	SER	-	cloning artifact	UNP G3XD71
C	320	SER	-	cloning artifact	UNP G3XD71
C	321	GLY	-	cloning artifact	UNP G3XD71
C	322	SER	-	cloning artifact	UNP G3XD71
D	320	SER	-	cloning artifact	UNP G3XD71
D	321	GLY	-	cloning artifact	UNP G3XD71
D	322	SER	-	cloning artifact	UNP G3XD71
E	320	SER	-	cloning artifact	UNP G3XD71
E	321	GLY	-	cloning artifact	UNP G3XD71
E	322	SER	-	cloning artifact	UNP G3XD71
F	320	SER	-	cloning artifact	UNP G3XD71
F	321	GLY	-	cloning artifact	UNP G3XD71

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Chain	Residue	Modelled	Actual	Comment	Reference
F	322	SER	-	cloning artifact	UNP G3XD71

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0
4	A	2	Total Ca 2 2	0	0
4	D	2	Total Ca 2 2	0	0
4	E	1	Total Ca 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			8	2	4	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			8	2	4	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		
5	D	1	Total	C	H	O	0	0
			10	2	6	2		
5	D	1	Total	C	H	O	0	0
			9	2	5	2		
5	D	1	Total	C	H	O	0	0
			8	2	4	2		
5	E	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	H	O	0	0
			10	2	6	2		
5	E	1	Total	C	H	O	0	0
			10	2	6	2		
5	E	1	Total	C	H	O	0	0
			10	2	6	2		
5	E	1	Total	C	H	O	0	0
			8	2	4	2		
5	F	1	Total	C	H	O	0	0
			10	2	6	2		
5	F	1	Total	C	H	O	0	0
			10	2	6	2		
5	F	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	645	Total	O	0	0
			645	645		
6	B	664	Total	O	0	0
			664	664		
6	C	710	Total	O	0	0
			710	710		
6	D	691	Total	O	0	0
			691	691		
6	E	675	Total	O	0	0
			675	675		
6	F	640	Total	O	0	0
			640	640		

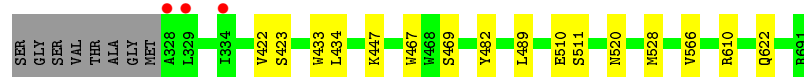
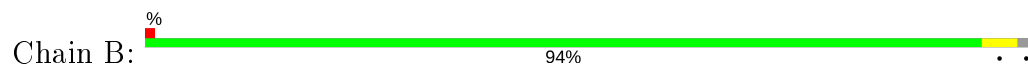
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Tail fiber protein



- Molecule 1: Tail fiber protein



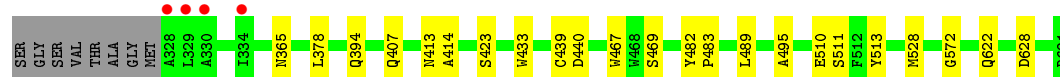
- Molecule 1: Tail fiber protein



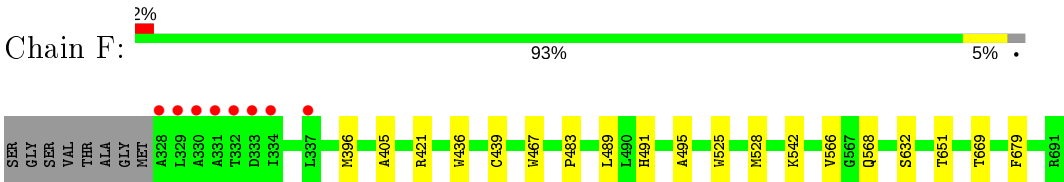
- Molecule 1: Tail fiber protein



- Molecule 1: Tail fiber protein



- Molecule 1: Tail fiber protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.32Å 126.95Å 432.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.96 – 1.90 49.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.96-1.90) 99.8 (49.96-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 1.90Å)	Xtriage
Refinement program	PHENIX (dev_3042: ???)	Depositor
R, R_{free}	0.160 , 0.208 0.158 , 0.209	Depositor DCC
R_{free} test set	3692 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36677	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3466e-03.*

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: MG, EDO, CA, FE

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	0.53	0/2867	0.60	0/3922
1	B	0.52	0/2904	0.60	0/3972
1	C	0.51	0/2865	0.61	0/3919
1	D	0.54	0/2873	0.60	0/3930
1	E	0.52	0/2896	0.60	0/3961
1	F	0.50	0/2865	0.60	0/3919
All	All	0.52	0/17270	0.60	0/23623

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2780	2611	2611	12	0
1	B	2806	2635	2620	13	0
1	C	2778	2612	2609	10	0
1	D	2780	2613	2606	12	0
1	E	2798	2629	2615	19	0
1	F	2778	2611	2609	14	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	E	1	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
5	A	12	16	16	0	0
5	B	16	22	22	2	0
5	C	12	18	18	1	0
5	D	12	15	16	1	0
5	E	20	28	28	3	0
5	F	16	24	24	0	0
6	A	645	0	0	6	12
6	B	664	0	0	3	8
6	C	710	0	0	6	13
6	D	691	0	0	3	9
6	E	675	0	0	7	9
6	F	640	0	0	5	11
All	All	20843	15834	15794	70	32

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 2.

All (70) 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:342:LEU:O	6:A:801:HOH:O	1.99	0.79
5:E:704:EDO:O1	6:E:801:HOH:O	2.05	0.71
1:B:520[B]:ASN:OD1	6:B:801:HOH:O	2.08	0.70
1:F:632:SER:O	6:F:801:HOH:O	2.13	0.67
1:A:448:GLU:OE1	6:A:802:HOH:O	2.14	0.65
5:C:701:EDO:O1	6:C:801:HOH:O	2.15	0.65
1:A:328:ALA:N	6:A:807:HOH:O	2.29	0.64
1:A:467:TRP:HE3	1:A:489:LEU:HD11	1.62	0.63
1:A:464:THR:HG23	6:A:1200:HOH:O	1.97	0.63
1:C:386:VAL:HG11	6:C:1079:HOH:O	1.99	0.63
1:C:443:GLY:N	6:C:803:HOH:O	2.21	0.63
1:E:365[B]:ASN:OD1	6:E:802:HOH:O	2.15	0.63
1:E:622[B]:GLN:NE2	6:E:804:HOH:O	2.34	0.60
1:A:647:TYR:CE2	1:A:687:GLU:HB2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:GLY:CA	6:C:803:HOH:O	2.55	0.54
1:D:647:TYR:CE2	1:D:687:GLU:HB2	2.43	0.54
1:A:467:TRP:CE3	1:A:489:LEU:HD11	2.43	0.52
1:C:448:GLU:OE2	6:C:802:HOH:O	2.17	0.50
1:D:374:VAL:HG22	6:D:1125:HOH:O	2.11	0.50
1:F:651:THR:O	6:F:802:HOH:O	2.20	0.50
1:B:423:SER:HB2	1:B:433:TRP:CD2	2.47	0.49
1:B:447:LYS:HE2	6:C:865:HOH:O	2.13	0.49
1:C:365:ASN:HA	1:C:378:LEU:O	2.12	0.49
1:E:483:PRO:HB2	1:E:513:TYR:CD2	2.47	0.49
1:E:378:LEU:HD23	6:E:1103:HOH:O	2.12	0.49
1:B:467:TRP:HE3	1:B:489:LEU:HD11	1.77	0.48
1:F:542:LYS:NZ	6:F:809:HOH:O	2.45	0.48
1:A:528:MET:HE2	1:B:528:MET:HE2	1.95	0.48
1:A:559:PRO:O	6:A:803:HOH:O	2.20	0.48
1:E:365[B]:ASN:ND2	6:E:815:HOH:O	2.46	0.48
1:E:482:TYR:HB2	5:E:704:EDO:H12	1.95	0.47
1:D:691:ARG:NH1	6:D:808:HOH:O	2.33	0.47
5:D:706:EDO:O1	1:E:628:ASP:OD2	2.32	0.47
1:A:439:CYS:HA	1:C:440:ASP:HA	1.96	0.46
1:D:440:ASP:HA	1:E:439:CYS:HA	1.98	0.46
1:E:467:TRP:HE3	1:E:489:LEU:HD11	1.80	0.45
1:B:482:TYR:HB2	5:B:703:EDO:H12	1.98	0.45
1:D:574:LEU:HA	1:F:566:VAL:HG11	1.97	0.45
1:A:622:GLN:HG2	6:A:1358:HOH:O	2.17	0.45
1:B:469:SER:HB2	1:C:495:ALA:HB1	1.98	0.45
1:D:528:MET:HE1	1:E:528:MET:HE2	1.98	0.45
1:F:421:ARG:HD3	1:F:436:TRP:CE2	2.53	0.44
1:E:394:GLN:O	1:E:407:GLN:HA	2.18	0.43
1:B:566:VAL:HG11	1:C:574:LEU:HA	1.99	0.43
1:E:413:ASN:O	1:E:414:ALA:HB3	2.18	0.43
1:D:423:SER:HB2	1:D:433:TRP:CD2	2.54	0.43
5:B:705:EDO:O1	1:C:659:ASP:OD1	2.36	0.42
1:E:622[B]:GLN:NE2	6:E:814:HOH:O	2.45	0.42
1:F:396:MET:O	1:F:405:ALA:HA	2.20	0.42
1:D:528:MET:HE2	1:F:528:MET:HE2	2.02	0.41
5:E:702:EDO:H22	6:E:1103:HOH:O	2.19	0.41
1:D:469:SER:HB2	1:E:495:ALA:HB1	2.01	0.41
1:F:467:TRP:HE3	1:F:489:LEU:HD11	1.85	0.41
1:E:469:SER:HB2	1:F:495:ALA:HB1	2.03	0.41
1:A:528:MET:HE2	1:B:528:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:568:GLN:NE2	6:F:817:HOH:O	2.49	0.41
1:F:483:PRO:HB3	1:F:525:TRP:CG	2.56	0.41
1:B:422:VAL:CG1	1:B:434:LEU:HD12	2.50	0.41
1:F:669:THR:OG1	6:F:803:HOH:O	2.22	0.41
1:F:467:TRP:HB3	1:F:491:HIS:CD2	2.55	0.41
1:C:554:PRO:HG2	1:C:557:PHE:CE2	2.56	0.41
1:D:566:VAL:HG22	1:E:572:GLY:HA3	2.03	0.41
1:E:440:ASP:HA	1:F:439:CYS:HA	2.03	0.41
1:E:423:SER:HB2	1:E:433:TRP:CD2	2.56	0.41
1:E:510:GLU:O	1:E:511:SER:HB2	2.20	0.41
1:B:622[B]:GLN:NE2	6:B:835:HOH:O	2.54	0.40
1:B:510:GLU:O	1:B:511:SER:HB2	2.21	0.40
1:B:610:ARG:NH2	6:B:837:HOH:O	2.54	0.40
1:D:328:ALA:N	6:D:837:HOH:O	2.54	0.40
1:D:467:TRP:HE3	1:D:489:LEU:HD11	1.86	0.40

All (32) 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)
6:A:1430:HOH:O	6:C:1373:HOH:O[4_465]	1.85	0.35
6:A:1165:HOH:O	6:F:1114:HOH:O[3_545]	1.93	0.27
6:A:1420:HOH:O	6:D:1457:HOH:O[3_645]	1.96	0.24
6:A:1337:HOH:O	6:E:1311:HOH:O[3_645]	1.97	0.23
6:B:1135:HOH:O	6:E:1185:HOH:O[4_475]	1.97	0.23
6:B:1135:HOH:O	6:E:1146:HOH:O[4_475]	1.97	0.23
6:A:1017:HOH:O	6:C:1317:HOH:O[4_465]	1.98	0.22
6:B:1307:HOH:O	6:E:968:HOH:O[4_475]	1.99	0.21
6:C:1008:HOH:O	6:E:804:HOH:O[3_545]	2.00	0.20
6:A:1242:HOH:O	6:C:932:HOH:O[4_465]	2.00	0.20
6:A:1430:HOH:O	6:C:1447:HOH:O[4_465]	2.03	0.17
6:B:801:HOH:O	6:F:1052:HOH:O[4_475]	2.03	0.17
6:C:1151:HOH:O	6:D:1162:HOH:O[3_545]	2.03	0.17
6:B:1281:HOH:O	6:D:1341:HOH:O[3_645]	2.06	0.14
6:D:1181:HOH:O	6:D:1224:HOH:O[4_475]	2.06	0.14
6:B:1182:HOH:O	6:E:843:HOH:O[4_475]	2.07	0.13
6:D:1344:HOH:O	6:E:1452:HOH:O[4_475]	2.07	0.13
6:A:1242:HOH:O	6:C:1142:HOH:O[4_465]	2.08	0.12
6:A:1344:HOH:O	6:E:1181:HOH:O[4_475]	2.09	0.11
6:C:1147:HOH:O	6:F:1238:HOH:O[3_545]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:813:HOH:O	6:F:1107:HOH:O[3_645]	2.10	0.10
6:A:1131:HOH:O	6:C:1243:HOH:O[4_465]	2.11	0.09
6:A:1140:HOH:O	6:F:809:HOH:O[3_645]	2.12	0.08
6:B:1180:HOH:O	6:D:1323:HOH:O[3_645]	2.12	0.08
6:A:1197:HOH:O	6:C:988:HOH:O[4_465]	2.13	0.07
6:C:1313:HOH:O	6:F:1089:HOH:O[3_545]	2.14	0.06
6:C:1230:HOH:O	6:F:832:HOH:O[3_545]	2.15	0.05
6:D:992:HOH:O	6:F:1121:HOH:O[4_475]	2.16	0.04
6:D:1163:HOH:O	6:F:1069:HOH:O[4_475]	2.18	0.02
6:D:990:HOH:O	6:F:1097:HOH:O[4_475]	2.18	0.02
6:F:1201:HOH:O	6:F:1375:HOH:O[2_584]	2.19	0.01
6:C:1019:HOH:O	6:E:842:HOH:O[3_545]	2.19	0.01

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	365/372 (98%)	352 (96%)	13 (4%)	0	100	100
1	B	370/372 (100%)	361 (98%)	9 (2%)	0	100	100
1	C	365/372 (98%)	356 (98%)	9 (2%)	0	100	100
1	D	366/372 (98%)	355 (97%)	11 (3%)	0	100	100
1	E	369/372 (99%)	358 (97%)	11 (3%)	0	100	100
1	F	365/372 (98%)	356 (98%)	9 (2%)	0	100	100
All	All	2200/2232 (99%)	2138 (97%)	62 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/284 (99%)	280 (99%)	2 (1%)	84	84
1	B	286/284 (101%)	286 (100%)	0	100	100
1	C	282/284 (99%)	281 (100%)	1 (0%)	91	91
1	D	283/284 (100%)	281 (99%)	2 (1%)	84	84
1	E	285/284 (100%)	285 (100%)	0	100	100
1	F	282/284 (99%)	281 (100%)	1 (0%)	91	91
All	All	1700/1704 (100%)	1694 (100%)	6 (0%)	91	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	568	GLN
1	A	679	PHE
1	C	679	PHE
1	D	568	GLN
1	D	679	PHE
1	F	679	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 10 are monoatomic - leaving 22 for Mogul analysis.

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	$\# Z > 2$
5	EDO	B	702	-	3,3,3	0.56	0	2,2,2	0.54	0
5	EDO	C	702	-	3,3,3	0.46	0	2,2,2	0.47	0
5	EDO	D	706	4	3,3,3	0.55	0	2,2,2	0.26	0
5	EDO	E	702	-	3,3,3	0.44	0	2,2,2	0.27	0
5	EDO	C	703	-	3,3,3	0.63	0	2,2,2	0.14	0
5	EDO	B	701	-	3,3,3	0.35	0	2,2,2	0.67	0
5	EDO	F	701	-	3,3,3	0.58	0	2,2,2	0.19	0
5	EDO	D	704	-	3,3,3	0.35	0	2,2,2	0.52	0
5	EDO	A	707	4	3,3,3	0.55	0	2,2,2	0.02	0
5	EDO	E	705	-	3,3,3	0.41	0	2,2,2	0.33	0
5	EDO	B	703	-	3,3,3	0.57	0	2,2,2	0.52	0
5	EDO	B	705	4	3,3,3	0.38	0	2,2,2	0.26	0
5	EDO	A	704	-	3,3,3	0.56	0	2,2,2	0.46	0
5	EDO	C	701	-	3,3,3	0.41	0	2,2,2	0.43	0
5	EDO	D	703	-	3,3,3	0.58	0	2,2,2	0.23	0
5	EDO	F	703	-	3,3,3	0.30	0	2,2,2	0.65	0
5	EDO	F	702	-	3,3,3	0.46	0	2,2,2	0.38	0
5	EDO	E	707	4	3,3,3	0.43	0	2,2,2	0.64	0
5	EDO	E	704	-	3,3,3	0.48	0	2,2,2	0.45	0
5	EDO	F	704	-	3,3,3	0.30	0	2,2,2	0.29	0
5	EDO	E	703	-	3,3,3	0.46	0	2,2,2	0.17	0
5	EDO	A	705	-	3,3,3	0.51	0	2,2,2	0.50	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	702	-	-	0/1/1/1	-
5	EDO	C	702	-	-	0/1/1/1	-
5	EDO	D	706	4	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	E	702	-	-	0/1/1/1	-
5	EDO	C	703	-	-	1/1/1/1	-
5	EDO	B	701	-	-	0/1/1/1	-
5	EDO	F	701	-	-	1/1/1/1	-
5	EDO	D	704	-	-	0/1/1/1	-
5	EDO	A	707	4	-	0/1/1/1	-
5	EDO	E	705	-	-	1/1/1/1	-
5	EDO	B	703	-	-	0/1/1/1	-
5	EDO	B	705	4	-	0/1/1/1	-
5	EDO	A	704	-	-	0/1/1/1	-
5	EDO	C	701	-	-	0/1/1/1	-
5	EDO	D	703	-	-	1/1/1/1	-
5	EDO	F	703	-	-	0/1/1/1	-
5	EDO	F	702	-	-	1/1/1/1	-
5	EDO	E	707	4	-	0/1/1/1	-
5	EDO	E	704	-	-	0/1/1/1	-
5	EDO	F	704	-	-	1/1/1/1	-
5	EDO	E	703	-	-	0/1/1/1	-
5	EDO	A	705	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	703	EDO	O1-C1-C2-O2
5	F	704	EDO	O1-C1-C2-O2
5	E	705	EDO	O1-C1-C2-O2
5	F	702	EDO	O1-C1-C2-O2
5	F	701	EDO	O1-C1-C2-O2
5	C	703	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	706	EDO	1	0
5	E	702	EDO	1	0
5	B	703	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	705	EDO	1	0
5	C	701	EDO	1	0
5	E	704	EDO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	364/372 (97%)	-0.35	4 (1%) 80 82	9, 19, 39, 83	0
1	B	364/372 (97%)	-0.47	3 (0%) 86 87	9, 19, 41, 70	0
1	C	364/372 (97%)	-0.37	3 (0%) 86 87	10, 21, 40, 68	0
1	D	364/372 (97%)	-0.29	7 (1%) 66 69	11, 21, 40, 70	0
1	E	364/372 (97%)	-0.30	4 (1%) 80 82	10, 19, 41, 62	0
1	F	364/372 (97%)	-0.33	8 (2%) 62 64	10, 21, 42, 71	0
All	All	2184/2232 (97%)	-0.35	29 (1%) 77 79	9, 20, 41, 83	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	329	LEU	5.9
1	D	328	ALA	5.1
1	E	328	ALA	4.5
1	C	328	ALA	4.3
1	E	329	LEU	4.2
1	F	328	ALA	3.7
1	A	328	ALA	3.5
1	C	329	LEU	3.4
1	F	332	THR	2.8
1	F	329	LEU	2.7
1	E	334	ILE	2.7
1	D	330	ALA	2.6
1	E	330	ALA	2.6
1	A	334	ILE	2.6
1	D	334	ILE	2.5
1	B	328	ALA	2.5
1	D	333	ASP	2.4
1	F	334	ILE	2.4
1	A	330	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	332	THR	2.3
1	F	331	ALA	2.3
1	F	337	LEU	2.3
1	C	334	ILE	2.2
1	B	329	LEU	2.2
1	F	333	ASP	2.1
1	A	331	ALA	2.1
1	D	331	ALA	2.1
1	F	330	ALA	2.1
1	B	334	ILE	2.1

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 carbohydrates 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
5	EDO	C	703	4/4	0.89	0.19	33,39,51,62	0
5	EDO	A	704	4/4	0.91	0.14	28,34,45,45	0
5	EDO	B	702	4/4	0.92	0.15	23,34,40,41	0
5	EDO	D	706	4/4	0.93	0.13	18,38,46,46	0
5	EDO	F	701	4/4	0.93	0.10	27,33,44,44	0
5	EDO	F	703	4/4	0.93	0.22	30,36,56,67	0
5	EDO	A	705	4/4	0.93	0.10	24,35,42,42	0
5	EDO	E	703	4/4	0.94	0.11	22,27,35,42	0
5	EDO	B	705	4/4	0.95	0.13	16,29,35,35	0
5	EDO	E	707	4/4	0.95	0.12	17,28,34,34	0
5	EDO	D	704	4/4	0.95	0.13	23,33,37,45	0
5	EDO	E	702	4/4	0.95	0.11	30,38,39,47	0
3	MG	A	702	1/1	0.95	0.06	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	B	703	4/4	0.95	0.17	21,37,44,48	0
5	EDO	F	704	4/4	0.96	0.12	15,25,39,39	0
5	EDO	A	707	4/4	0.96	0.09	17,35,42,42	0
5	EDO	B	701	4/4	0.96	0.09	18,28,34,40	0
5	EDO	D	703	4/4	0.96	0.11	28,35,49,49	0
5	EDO	E	704	4/4	0.96	0.14	25,32,43,52	0
5	EDO	E	705	4/4	0.97	0.07	15,30,51,51	0
5	EDO	F	702	4/4	0.97	0.09	18,26,49,49	0
5	EDO	C	701	4/4	0.97	0.12	29,34,42,51	0
5	EDO	C	702	4/4	0.98	0.13	19,28,42,48	0
3	MG	E	701	1/1	0.98	0.03	26,26,26,26	0
4	CA	B	704	1/1	0.99	0.06	19,19,19,19	0
4	CA	D	702	1/1	0.99	0.05	21,21,21,21	0
4	CA	D	705	1/1	0.99	0.08	18,18,18,18	0
4	CA	A	706	1/1	0.99	0.07	16,16,16,16	0
2	FE	A	701	1/1	1.00	0.05	40,40,40,40	0
4	CA	A	703	1/1	1.00	0.05	20,20,20,20	0
4	CA	E	706	1/1	1.00	0.04	21,21,21,21	0
2	FE	D	701	1/1	1.00	0.02	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.