



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 09:01 PM UTC

PDB ID : 6U8T / pdb_00006u8t
Title : Crystal structure of YopT domain of Pasteurella Multocida PfhB2-toxin
Authors : Kumar, S.; Mattoo, S.
Deposited on : 2019-09-05
Resolution : 2.39 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

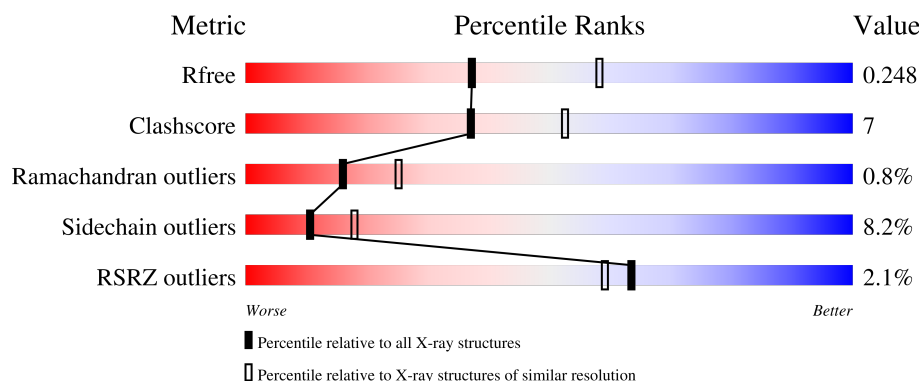
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	222	
1	B	222	
1	C	222	
1	D	222	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6914 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 PfhB2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	Se	0	0	0
			1639	1036	279	319	1	4			
1	C	219	Total	C	N	O	S	Se	0	0	0
			1706	1080	290	331	1	4			
1	B	221	Total	C	N	O	S	Se	0	0	0
			1726	1090	293	338	1	4			
1	D	203	Total	C	N	O	S	Se	0	0	0
			1583	1002	268	309	1	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3696	SER	-	expression tag	UNP Q9CPH9
A	3697	MSE	-	expression tag	UNP Q9CPH9
A	3698	ALA	-	expression tag	UNP Q9CPH9
A	3733	SER	CYS	engineered mutation	UNP Q9CPH9
C	3696	SER	-	expression tag	UNP Q9CPH9
C	3697	MSE	-	expression tag	UNP Q9CPH9
C	3698	ALA	-	expression tag	UNP Q9CPH9
C	3733	SER	CYS	engineered mutation	UNP Q9CPH9
B	3696	SER	-	expression tag	UNP Q9CPH9
B	3697	MSE	-	expression tag	UNP Q9CPH9
B	3698	ALA	-	expression tag	UNP Q9CPH9
B	3733	SER	CYS	engineered mutation	UNP Q9CPH9
D	3696	SER	-	expression tag	UNP Q9CPH9
D	3697	MSE	-	expression tag	UNP Q9CPH9
D	3698	ALA	-	expression tag	UNP Q9CPH9
D	3733	SER	CYS	engineered mutation	UNP Q9CPH9

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

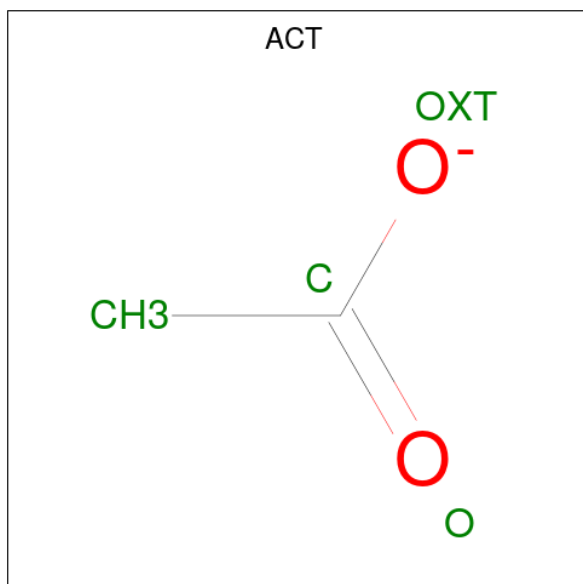
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is water.

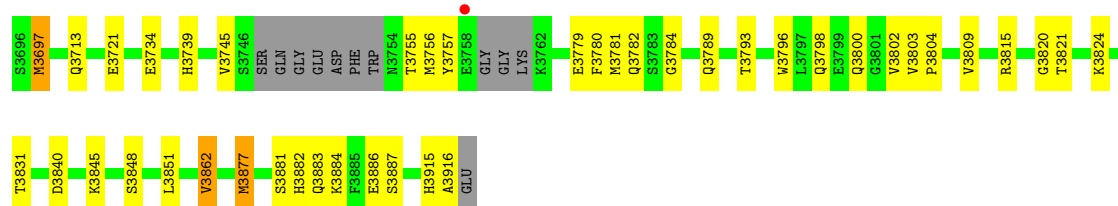
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	83	Total	O	0	0
			83	83		
5	C	22	Total	O	0	0
			22	22		
5	B	109	Total	O	0	0
			109	109		
5	D	27	Total	O	0	0
			27	27		

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.

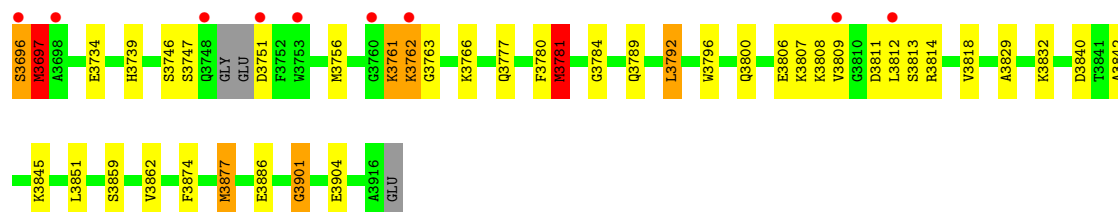
- Molecule 1: PfhB2

Chain A: 



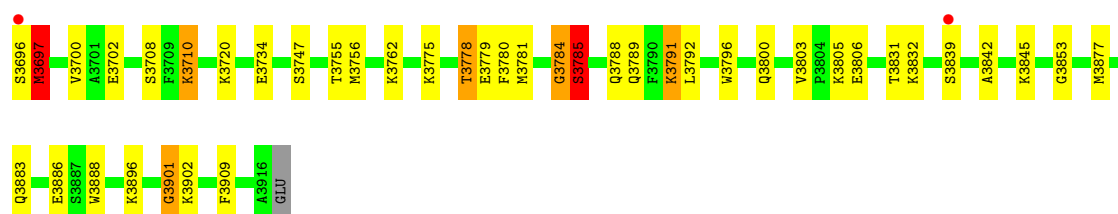
- Molecule 1: PfhB2

Chain C: 



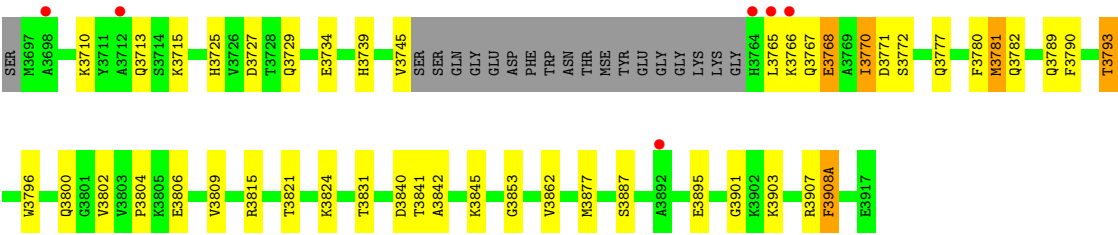
- Molecule 1: PfhB2

Chain B: 



- Molecule 1: PfhB2

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.65Å 62.96Å 164.34Å 90.00° 93.15° 90.00°	Depositor
Resolution (Å)	29.41 – 2.39 29.41 – 2.39	Depositor EDS
% Data completeness (in resolution range)	88.3 (29.41-2.39) 88.3 (29.41-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.45 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.199 , 0.245 0.208 , 0.248	Depositor DCC
R_{free} test set	1650 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6914	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: NA, ACT, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.06	0/1667	1.43	1/2232 (0.0%)
1	B	1.06	1/1759 (0.1%)	1.44	5/2356 (0.2%)
1	C	0.99	0/1738	1.42	6/2327 (0.3%)
1	D	1.00	0/1612	1.41	4/2162 (0.2%)
All	All	1.02	1/6776 (0.0%)	1.42	16/9077 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3803	VAL	N-CA	5.96	1.50	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3781	MSE	CG-SE-CE	11.70	124.67	98.92
1	A	3697	MSE	CG-SE-CE	11.67	124.59	98.92
1	B	3778	THR	CA-CB-OG1	-8.25	97.23	109.60
1	B	3756	MSE	CG-SE-CE	7.58	115.59	98.92
1	C	3901	GLY	CA-C-O	-6.83	117.12	122.52
1	D	3901	GLY	CA-C-O	-6.21	117.61	122.52
1	B	3697	MSE	CG-SE-CE	5.70	111.46	98.92
1	D	3781	MSE	CG-SE-CE	5.51	111.05	98.92
1	B	3755	THR	CA-CB-OG1	-5.37	101.54	109.60
1	C	3751	ASP	CA-C-N	5.32	127.67	120.38
1	C	3751	ASP	C-N-CA	5.32	127.67	120.38
1	B	3901	GLY	CA-C-O	-5.29	117.70	122.57
1	C	3766	LYS	CA-C-N	5.26	127.33	120.28
1	C	3766	LYS	C-N-CA	5.26	127.33	120.28
1	D	3715	LYS	CA-C-N	5.16	125.71	119.98
1	D	3715	LYS	C-N-CA	5.16	125.71	119.98

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	1639	0	1591	31	0
1	B	1726	0	1675	27	0
1	C	1706	0	1657	27	0
1	D	1583	0	1548	25	0
2	A	1	0	0	0	0
3	A	14	0	20	3	0
4	B	4	0	3	0	0
5	A	83	0	0	3	0
5	B	109	0	0	2	0
5	C	22	0	0	0	0
5	D	27	0	0	2	0
All	All	6914	0	6494	94	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (94) 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:3697:MSE:HE3	1:A:3877:MSE:CE	1.92	0.98
1:A:3697:MSE:HE3	1:A:3877:MSE:HE2	1.48	0.96
1:A:3824:LYS:HD3	1:B:3901:GLY:O	1.70	0.91
1:C:3762:LYS:HA	1:C:3762:LYS:HE2	1.52	0.88
1:D:3734:GLU:OE2	1:D:3793:THR:HG21	1.75	0.86
1:B:3697:MSE:HE1	1:B:3896:LYS:HE2	1.58	0.83
1:A:3697:MSE:HE3	1:A:3877:MSE:SE	2.31	0.80
1:B:3877:MSE:HE2	1:B:3888:TRP:CH2	2.16	0.80
1:D:3766:LYS:O	1:D:3770:ILE:HG23	1.81	0.80
1:C:3762:LYS:HA	1:C:3762:LYS:CE	2.12	0.78
1:C:3901:GLY:O	1:D:3824:LYS:HE2	1.87	0.75
1:B:3785:SER:HB3	1:B:3788:GLN:HE21	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3720:LYS:HD2	5:B:4181:HOH:O	1.89	0.73
1:B:3877:MSE:HE2	1:B:3888:TRP:HH2	1.53	0.72
1:C:3792:LEU:HD22	1:C:3792:LEU:O	1.91	0.71
1:B:3696:SER:HB3	1:B:3710:LYS:HG2	1.76	0.68
1:C:3829:ALA:O	1:C:3832:LYS:HG3	1.96	0.65
1:D:3739:HIS:HE1	1:D:3772:SER:OG	1.79	0.65
1:D:3777:GLN:O	1:D:3781:MSE:HG2	1.97	0.64
1:A:3697:MSE:CE	1:A:3877:MSE:SE	2.95	0.64
1:C:3777:GLN:O	1:C:3781:MSE:HG2	1.97	0.63
1:D:3745:VAL:CG2	1:D:3802:VAL:HG22	2.29	0.63
1:A:3745:VAL:O	1:A:3745:VAL:HG23	1.99	0.62
1:C:3739:HIS:C	1:C:3756:MSE:HE1	2.26	0.61
1:D:3768:GLU:HA	1:D:3768:GLU:OE2	2.00	0.61
1:A:3755:THR:HG22	1:A:3757:TYR:H	1.66	0.60
1:B:3696:SER:HB3	1:B:3710:LYS:CG	2.32	0.59
1:C:3812:LEU:HD12	1:C:3812:LEU:O	2.03	0.59
1:C:3809:VAL:HG12	1:C:3809:VAL:O	2.02	0.59
1:A:3739:HIS:HB3	1:A:3756:MSE:HE1	1.85	0.58
1:A:3779:GLU:HA	1:A:3782:GLN:HE21	1.69	0.58
1:B:3839:SER:HA	5:B:4198:HOH:O	2.02	0.57
1:A:3882:HIS:HD2	5:A:4172:HOH:O	1.88	0.57
1:B:3791:LYS:HA	1:B:3791:LYS:HE2	1.89	0.54
1:C:3792:LEU:HD22	1:C:3792:LEU:C	2.33	0.53
1:A:3734:GLU:HG2	1:A:3780:PHE:CE1	2.44	0.53
1:C:3886:GLU:HG3	1:D:3831:THR:HG21	1.91	0.53
1:A:3745:VAL:CG2	1:A:3802:VAL:HG22	2.39	0.52
1:C:3862:VAL:O	1:D:3842:ALA:HA	2.10	0.52
1:D:3734:GLU:HG2	1:D:3780:PHE:CE2	2.46	0.51
1:C:3696:SER:HB2	1:C:3874:PHE:HB3	1.93	0.51
1:C:3762:LYS:CE	1:C:3762:LYS:CA	2.85	0.51
1:B:3780:PHE:CE1	1:B:3789:GLN:HB3	2.46	0.50
1:A:3780:PHE:CE1	1:A:3789:GLN:HB3	2.47	0.50
1:B:3697:MSE:HE1	1:B:3896:LYS:CE	2.34	0.50
1:D:3727:ASP:OD2	1:D:3781:MSE:HE1	2.11	0.50
1:A:3798:GLN:NE2	5:A:4103:HOH:O	2.45	0.50
1:A:3884:LYS:HG3	3:A:4003:PEG:H12	1.93	0.49
1:C:3763:GLY:HA2	1:D:3710:LYS:O	2.12	0.49
1:C:3901:GLY:O	1:D:3824:LYS:CE	2.58	0.49
1:D:3780:PHE:CE2	1:D:3789:GLN:HB3	2.48	0.49
1:C:3780:PHE:CE2	1:C:3789:GLN:HB3	2.48	0.49
1:C:3808:LYS:HE2	1:C:3811:ASP:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3779:GLU:HB3	1:B:3792:LEU:HD11	1.95	0.49
1:D:3804:PRO:HB3	1:D:3815:ARG:NH2	2.29	0.48
1:A:3831:THR:HG21	1:B:3886:GLU:HG3	1.94	0.48
1:B:3784:GLY:O	1:B:3785:SER:HB3	2.14	0.48
1:A:3803:VAL:HG23	1:A:3803:VAL:O	2.13	0.47
1:A:3804:PRO:HB3	1:A:3815:ARG:NH2	2.29	0.47
1:C:3696:SER:N	1:C:3877:MSE:SE	2.97	0.47
1:D:3725:HIS:CE1	1:D:3729:GLN:HG3	2.49	0.47
1:C:3734:GLU:HG2	1:C:3780:PHE:CE2	2.50	0.46
1:B:3734:GLU:HG2	1:B:3780:PHE:CE1	2.50	0.46
1:A:3851:LEU:O	1:B:3853:GLY:HA3	2.14	0.46
1:A:3886:GLU:HG3	1:B:3831:THR:HG21	1.97	0.46
1:D:3907:ARG:N	5:D:4001:HOH:O	2.26	0.45
1:C:3842:ALA:HA	1:D:3862:VAL:O	2.17	0.45
1:C:3818:VAL:HG11	1:C:3832:LYS:NZ	2.31	0.45
1:A:3721:GLU:HG3	5:A:4176:HOH:O	2.17	0.45
1:B:3796:TRP:O	1:B:3800:GLN:HG2	2.17	0.45
1:D:3790:PHE:HA	1:D:3793:THR:CG2	2.47	0.44
1:B:3700:VAL:HG21	1:B:3877:MSE:HG2	1.98	0.44
1:B:3697:MSE:CE	1:B:3896:LYS:HD3	2.48	0.44
1:C:3697:MSE:CE	1:C:3874:PHE:CE1	3.01	0.43
1:A:3916:ALA:C	3:A:4002:PEG:O4	2.61	0.43
1:B:3697:MSE:CE	1:B:3896:LYS:HE2	2.39	0.43
1:A:3734:GLU:CG	1:A:3793:THR:HG21	2.49	0.43
1:A:3824:LYS:CD	1:B:3901:GLY:O	2.53	0.43
1:D:3907:ARG:O	1:D:3908(A):PHE:HB2	2.18	0.43
1:C:3780:PHE:CD1	1:C:3781:MSE:HE3	2.54	0.43
1:D:3796:TRP:O	1:D:3800:GLN:HG2	2.19	0.42
1:C:3761:LYS:HD3	1:C:3761:LYS:HA	1.70	0.42
1:A:3796:TRP:O	1:A:3800:GLN:HG2	2.19	0.42
1:C:3796:TRP:O	1:C:3800:GLN:HG2	2.20	0.41
1:C:3851:LEU:O	1:D:3853:GLY:HA3	2.20	0.41
1:D:3782:GLN:HE21	1:D:3782:GLN:HB2	1.70	0.41
1:A:3734:GLU:HG3	1:A:3793:THR:HG21	2.01	0.41
1:A:3820:GLY:HA3	1:B:3909:PHE:CE2	2.56	0.41
1:A:3862:VAL:O	1:B:3842:ALA:HA	2.20	0.41
1:A:3915:HIS:CE1	1:B:3805:LYS:HG2	2.55	0.41
1:D:3770:ILE:HG13	1:D:3771:ASP:N	2.36	0.40
1:D:3908(A):PHE:N	5:D:4001:HOH:O	2.22	0.40
1:A:3881:SER:OG	3:A:4003:PEG:C3	2.70	0.40
1:A:3848:SER:O	1:B:3909:PHE:HA	2.22	0.40

There are no symmetry-related clashes.

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	205/222 (92%)	200 (98%)	4 (2%)	1 (0%)	24	37
1	B	219/222 (99%)	211 (96%)	6 (3%)	2 (1%)	14	22
1	C	215/222 (97%)	204 (95%)	8 (4%)	3 (1%)	9	13
1	D	199/222 (90%)	194 (98%)	4 (2%)	1 (0%)	24	37
All	All	838/888 (94%)	809 (96%)	22 (3%)	7 (1%)	16	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3746	SER
1	B	3785	SER
1	C	3784	GLY
1	B	3784	GLY
1	A	3784	GLY
1	D	3908(A)	PHE
1	C	3697	MSE

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	174/181 (96%)	164 (94%)	10 (6%)	18	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	184/181 (102%)	168 (91%)	16 (9%)	9	16
1	C	181/181 (100%)	165 (91%)	16 (9%)	9	15
1	D	169/181 (93%)	153 (90%)	16 (10%)	8	13
All	All	708/724 (98%)	650 (92%)	58 (8%)	10	18

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3713	GLN
1	A	3781	MSE
1	A	3809	VAL
1	A	3821	THR
1	A	3840	ASP
1	A	3845	LYS
1	A	3862	VAL
1	A	3877	MSE
1	A	3883	GLN
1	A	3887	SER
1	C	3696	SER
1	C	3697	MSE
1	C	3747	SER
1	C	3761	LYS
1	C	3762	LYS
1	C	3781	MSE
1	C	3792	LEU
1	C	3806	GLU
1	C	3807	LYS
1	C	3813	SER
1	C	3814	ARG
1	C	3840	ASP
1	C	3845	LYS
1	C	3859	SER
1	C	3877	MSE
1	C	3904	GLU
1	B	3697	MSE
1	B	3702	GLU
1	B	3708	SER
1	B	3710	LYS
1	B	3747	SER
1	B	3762	LYS
1	B	3775	LYS

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Mol	Chain	Res	Type
1	B	3778	THR
1	B	3781	MSE
1	B	3785	SER
1	B	3791	LYS
1	B	3806	GLU
1	B	3832	LYS
1	B	3845	LYS
1	B	3883	GLN
1	B	3902	LYS
1	D	3713	GLN
1	D	3765	LEU
1	D	3767	GLN
1	D	3768	GLU
1	D	3770	ILE
1	D	3793	THR
1	D	3806	GLU
1	D	3809	VAL
1	D	3821	THR
1	D	3840	ASP
1	D	3841	THR
1	D	3845	LYS
1	D	3877	MSE
1	D	3887	SER
1	D	3895	GLU
1	D	3903	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3713	GLN
1	A	3729	GLN
1	A	3743	ASN
1	A	3764	HIS
1	A	3782	GLN
1	A	3850	ASN
1	A	3882	HIS
1	A	3915	HIS
1	C	3729	GLN
1	C	3754	ASN
1	C	3850	ASN
1	B	3729	GLN
1	B	3743	ASN

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Mol	Chain	Res	Type
1	B	3764	HIS
1	B	3788	GLN
1	B	3795	ASN
1	B	3798	GLN
1	D	3713	GLN
1	D	3725	HIS
1	D	3739	HIS
1	D	3767	GLN
1	D	3782	GLN
1	D	3910	ASN

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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
4	ACT	B	4001	-	3,3,3	1.09	0	3,3,3	0.79	0
3	PEG	A	4003	-	6,6,6	0.38	0	5,5,5	0.33	0
3	PEG	A	4002	-	6,6,6	0.18	0	5,5,5	0.15	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
3	PEG	A	4003	-	-	2/4/4/4	-
3	PEG	A	4002	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4003	PEG	O2-C3-C4-O4
3	A	4003	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4003	PEG	2	0
3	A	4002	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	207/222 (93%)	0.07	1 (0%) 87 85	12, 43, 82, 119	0
1	B	217/222 (97%)	0.03	2 (0%) 81 78	10, 36, 73, 86	0
1	C	215/222 (96%)	0.60	9 (4%) 40 36	36, 61, 90, 133	0
1	D	200/222 (90%)	0.46	6 (3%) 52 48	37, 56, 83, 116	0
All	All	839/888 (94%)	0.29	18 (2%) 63 59	10, 51, 83, 133	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3765	LEU	4.6
1	C	3760	GLY	4.0
1	D	3698	ALA	3.3
1	C	3698	ALA	3.1
1	A	3758	GLU	3.0
1	C	3751	ASP	2.9
1	C	3696	SER	2.9
1	C	3812	LEU	2.9
1	D	3764	HIS	2.8
1	C	3748	GLN	2.8
1	D	3712	ALA	2.5
1	C	3753	TRP	2.4
1	D	3892	ALA	2.3
1	B	3696	SER	2.3
1	C	3809	VAL	2.3
1	C	3762	LYS	2.2
1	D	3766	LYS	2.0
1	B	3839	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	B	4001	4/4	0.80	0.18	43,46,47,61	0
3	PEG	A	4002	7/7	0.84	0.15	49,60,65,74	0
3	PEG	A	4003	7/7	0.85	0.20	40,57,61,64	0
2	NA	A	4001	1/1	0.88	0.15	37,37,37,37	1

6.5 Other polymers [i](#)

There are no such residues in this entry.