Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 10:03 PM JST

PDB ID	:	7BY5
Title	:	Tetanus neurotoxin mutant-(H233A/E234Q/H237A/Y375F)
Authors	:	Zhang, C.M.; Imoto, Y.; Fukuda, Y.; Yamashita, E.; Inoue, T.
Deposited on	:	2020-04-21
Resolution	:	2.27 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 (1)) were used in the production of this report:

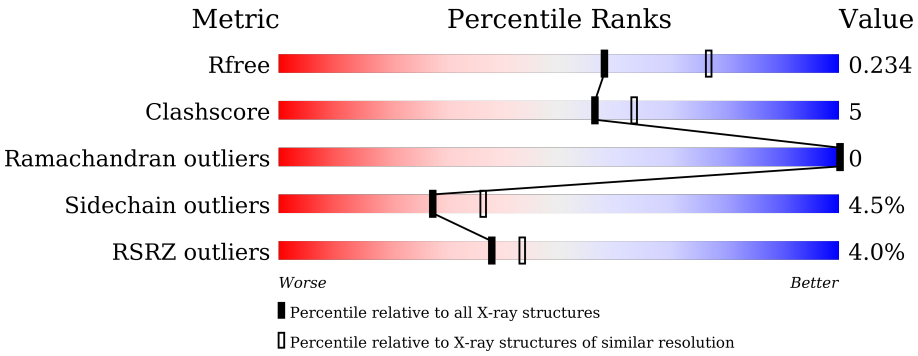
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	1322	4% 84% 12%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11306 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.

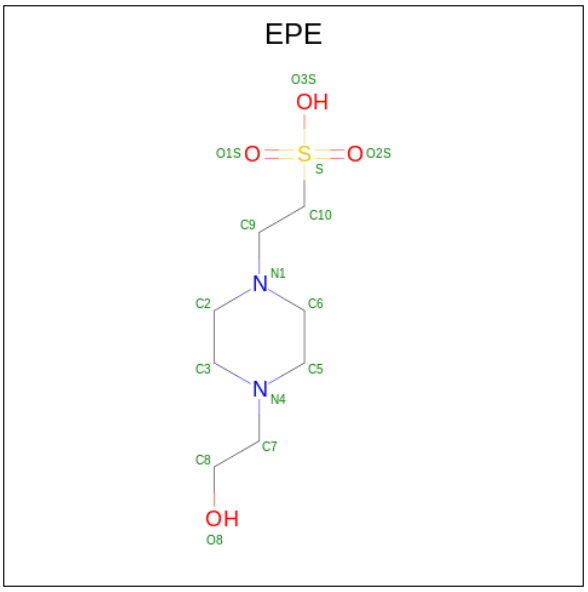
- Molecule 1 is a protein called Tetanus toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1286	10470	6706	1713	2017	34	0	10	0

There are 12 discrepancies between the modelled and reference sequences:

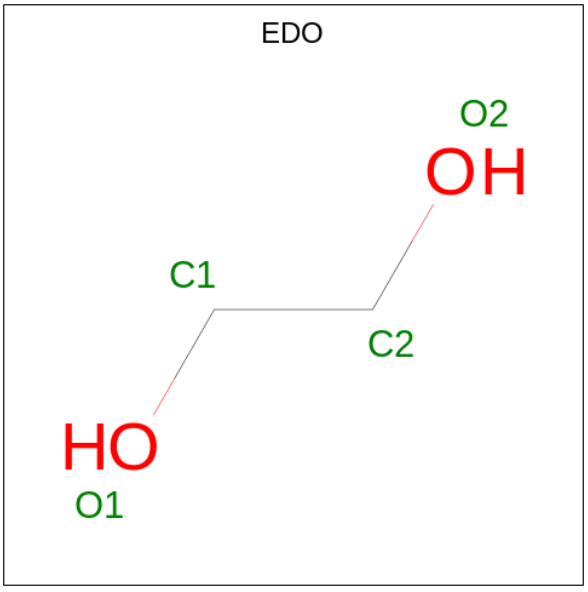
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	HIS	-	expression tag	UNP P04958
A	-5	HIS	-	expression tag	UNP P04958
A	-4	HIS	-	expression tag	UNP P04958
A	-3	HIS	-	expression tag	UNP P04958
A	-2	HIS	-	expression tag	UNP P04958
A	-1	HIS	-	expression tag	UNP P04958
A	0	HIS	-	expression tag	UNP P04958
A	1	MET	-	expression tag	UNP P04958
A	233	ALA	HIS	engineered mutation	UNP P04958
A	234	GLN	GLU	engineered mutation	UNP P04958
A	237	ALA	HIS	engineered mutation	UNP P04958
A	375	PHE	TYR	engineered mutation	UNP P04958

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Na 3 3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	772	Total O 785 785	0	14

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: Tetanus toxin

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	145.54Å 145.54Å 129.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.28 – 2.27 48.28 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.28-2.27) 99.1 (48.28-2.27)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.186 , 0.233 0.188 , 0.234	Depositor DCC
R_{free} test set	3663 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 68.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11306	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, NA, CL, EPE

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	0/10702	0.55	0/14493

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

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	10470	0	10405	105	0
2	A	15	0	18	4	0
3	A	32	0	48	1	0
4	A	3	0	0	0	0
5	A	1	0	0	0	0
6	A	785	0	0	4	0
All	All	11306	0	10471	105	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 5.

All (105) 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:138:ASN:HD21	1:A:532:VAL:H	1.05	0.97
1:A:127:LYS:NZ	1:A:311:SER:HB2	1.84	0.91
1:A:127:LYS:HZ1	1:A:311:SER:HB2	1.39	0.87
1:A:1246:ARG:NH2	1:A:1296:ASP:O	2.07	0.85
1:A:127:LYS:HG3	1:A:311:SER:O	1.78	0.84
1:A:187:ARG:HE	1:A:246:GLN:HE21	1.28	0.82
1:A:739[B]:TYR:HD2	1:A:743[B]:ARG:HH21	1.36	0.73
1:A:807:ASN:O	1:A:811:ASN:HB2	1.91	0.69
1:A:171:VAL:HG23	1:A:234:GLN:HE21	1.58	0.69
1:A:138:ASN:HD21	1:A:532:VAL:N	1.87	0.67
1:A:229:LEU:HD21	1:A:371:THR:HG22	1.75	0.67
1:A:646:ILE:HD12	1:A:741:MET:HG3	1.77	0.67
1:A:982:LYS:NZ	1:A:1069:ASN:HD22	1.92	0.66
1:A:982:LYS:HZ3	1:A:1069:ASN:HD22	1.45	0.64
1:A:127:LYS:CG	1:A:311:SER:O	2.46	0.63
1:A:569:SER:HA	1:A:592:ILE:HD11	1.80	0.62
1:A:229:LEU:CD2	1:A:371:THR:HG22	2.30	0.61
1:A:212:ASN:OD1	1:A:798:ARG:NH1	2.34	0.60
1:A:1033:PHE:H	1:A:1049:ASN:ND2	1.99	0.60
1:A:289:ASN:HD21	1:A:501:LYS:HB3	1.67	0.60
1:A:972:ASN:HD21	1:A:1078:ASN:H	1.48	0.59
1:A:958:VAL:HG12	1:A:1084:VAL:HG12	1.84	0.58
1:A:1023:PHE:CE2	1:A:1136:SER:HB2	2.40	0.57
1:A:1168:ARG:NH2	1:A:1315:ASP:O	2.37	0.57
1:A:319:ILE:HD12	1:A:319:ILE:N	2.20	0.57
1:A:138:ASN:ND2	1:A:532:VAL:H	1.88	0.56
1:A:543:LYS:HB3	2:A:1401:EPE:H32	1.86	0.56
1:A:357:GLY:HA3	1:A:512:ILE:HD11	1.88	0.56
1:A:972:ASN:ND2	1:A:1078:ASN:H	2.05	0.55
1:A:127:LYS:HZ2	1:A:311:SER:HB2	1.71	0.55
1:A:98:ILE:O	1:A:104:GLY:HA3	2.07	0.54
1:A:67:GLU:OE2	2:A:1401:EPE:H62	2.08	0.54
1:A:643:VAL:O	1:A:646:ILE:HG12	2.08	0.53
1:A:93:LYS:NZ	1:A:394:TYR:O	2.42	0.53
1:A:866:ASN:HD21	1:A:940:ASP:HB2	1.73	0.52
1:A:866:ASN:HA	1:A:902:PHE:HE1	1.76	0.51
1:A:1030:LYS:HB2	6:A:1790:HOH:O	2.10	0.51
1:A:839:ILE:HG22	1:A:843:GLU:HB3	1.93	0.51
1:A:217:THR:HG22	1:A:410:GLU:OE2	2.11	0.51
1:A:127:LYS:HA	1:A:311:SER:O	2.11	0.50
1:A:676:TYR:H	1:A:733:GLN:HE22	1.59	0.50
1:A:139:LEU:H	1:A:139:LEU:HD12	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LEU:HD21	1:A:371:THR:CG2	2.41	0.50
1:A:1170:TYR:CE1	1:A:1308:THR:HA	2.47	0.50
1:A:127:LYS:NZ	1:A:311:SER:CB	2.65	0.49
1:A:1171:ASN:HB2	6:A:1569:HOH:O	2.12	0.49
1:A:501:LYS:HB2	1:A:713[B]:GLU:OE1	2.12	0.49
1:A:320:ASP:HA	1:A:323:LYS:HB2	1.94	0.49
1:A:545:ASN:OD1	2:A:1401:EPE:H61	2.12	0.49
1:A:127:LYS:HG3	1:A:311:SER:C	2.33	0.49
1:A:289:ASN:ND2	1:A:501:LYS:HB3	2.26	0.49
1:A:265:TYR:CD1	2:A:1401:EPE:H21	2.49	0.48
1:A:39:ILE:HD11	1:A:92:VAL:HA	1.96	0.48
1:A:1240:MET:HA	1:A:1256:LYS:O	2.13	0.48
1:A:139:LEU:HD12	1:A:139:LEU:N	2.29	0.48
1:A:697:LYS:O	1:A:701:ILE:HG12	2.14	0.47
1:A:891:ILE:HG12	1:A:896:ILE:HG12	1.97	0.47
1:A:343:ASN:HD22	1:A:346:LYS:H	1.62	0.47
1:A:646:ILE:CD1	1:A:741:MET:HG3	2.44	0.47
1:A:991:TRP:HA	1:A:1003:THR:O	2.16	0.46
1:A:503:LEU:HD21	1:A:713[B]:GLU:HG3	1.96	0.46
1:A:884:SER:O	1:A:1092:PHE:HA	2.15	0.46
1:A:213:ILE:CG1	1:A:218:ILE:HG22	2.46	0.46
1:A:356:TYR:CE2	1:A:505:PHE:HB3	2.50	0.46
1:A:862:SER:HB3	6:A:1793:HOH:O	2.16	0.46
1:A:918:ILE:HG12	1:A:955:TRP:CD2	2.52	0.45
1:A:211:GLU:HG3	1:A:373:LEU:HD22	1.98	0.45
1:A:875:GLU:HB3	1:A:879:VAL:HG21	1.99	0.45
1:A:1132:PRO:CB	3:A:1407:EDO:H21	2.47	0.44
1:A:370:LYS:HB2	1:A:411:TYR:CG	2.52	0.44
1:A:319:ILE:N	1:A:319:ILE:CD1	2.81	0.44
1:A:866:ASN:HA	1:A:902:PHE:CE1	2.53	0.44
1:A:164:PRO:HG2	1:A:542:TYR:CZ	2.53	0.44
1:A:700:ILE:HG21	1:A:839:ILE:HD11	2.00	0.44
1:A:1195:PHE:CD1	1:A:1239:LYS:HE2	2.53	0.44
1:A:0:HIS:HE1	1:A:516:TYR:O	2.00	0.43
1:A:191:GLY:HA2	1:A:241:GLY:O	2.19	0.43
1:A:847:LEU:HD12	1:A:847:LEU:HA	1.84	0.43
1:A:818:LEU:HD12	1:A:818:LEU:HA	1.89	0.43
1:A:1033:PHE:H	1:A:1049:ASN:HD21	1.65	0.43
1:A:181:LYS:HD3	1:A:181:LYS:HA	1.90	0.42
1:A:981:LYS:HA	1:A:1067:ASP:HB2	2.01	0.42
1:A:343:ASN:HD21	1:A:345:ASP:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:SER:HA	1:A:902:PHE:O	2.19	0.42
1:A:1043:SER:HB2	1:A:1056:ALA:O	2.19	0.42
1:A:1072:LEU:HD12	1:A:1072:LEU:N	2.35	0.42
1:A:42:ARG:HD2	1:A:156:ASN:OD1	2.20	0.42
1:A:586:LEU:HD12	1:A:586:LEU:HA	1.85	0.42
1:A:1114:LEU:HD12	1:A:1190:VAL:HG12	2.02	0.42
1:A:1004:LEU:O	1:A:1011:VAL:HA	2.20	0.42
1:A:405:LYS:HB3	1:A:405:LYS:HE2	1.84	0.41
1:A:319:ILE:CD1	1:A:319:ILE:H	2.34	0.41
1:A:373:LEU:H	1:A:373:LEU:HD23	1.84	0.41
1:A:857:THR:HA	1:A:858:PRO:HD2	1.92	0.41
1:A:955:TRP:HB2	1:A:1087:ASP:HB3	2.03	0.41
1:A:213:ILE:HD13	1:A:791:ILE:HG12	2.03	0.41
1:A:1029:ASN:HB3	1:A:1118:TRP:CZ3	2.56	0.41
1:A:564:LEU:HD12	1:A:564:LEU:HA	1.86	0.41
1:A:1299:LEU:HD13	1:A:1301:CYS:SG	2.60	0.41
1:A:616:VAL:HA	1:A:619:ILE:HD12	2.02	0.40
1:A:966:LEU:HD12	1:A:966:LEU:HA	1.91	0.40
1:A:1173:LEU:HD12	1:A:1173:LEU:HA	1.85	0.40
1:A:1073:LYS:NZ	6:A:1545:HOH:O	2.54	0.40
1:A:1211:TYR:CD1	1:A:1223:ARG:HB3	2.56	0.40
1:A:1223:ARG:O	1:A:1285:ILE:HA	2.21	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	1290/1322 (98%)	1255 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1182/1205 (98%)	1129 (96%)	53 (4%)	27 36

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	8	PHE
1	A	82	SER
1	A	99	LYS
1	A	125	LEU
1	A	139	LEU
1	A	181	LYS
1	A	213	ILE
1	A	251	GLU
1	A	289	ASN
1	A	310	THR
1	A	311	SER
1	A	317	ILE
1	A	335	ASP
1	A	337	ASN
1	A	344	GLU
1	A	405	LYS
1	A	496	TYR
1	A	518	LEU
1	A	521	LYS
1	A	550	ILE
1	A	552	ILE
1	A	555	ILE
1	A	557	ASP
1	A	560	ILE
1	A	564	LEU
1	A	568	LYS
1	A	574	GLN
1	A	575	ARG
1	A	586	LEU

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Mol	Chain	Res	Type
1	A	673	LEU
1	A	761	LYS
1	A	769	GLU
1	A	776	ASN
1	A	811	ASN
1	A	815	LYS
1	A	818	LEU
1	A	843	GLU
1	A	845	LYS
1	A	847	LEU
1	A	848	GLU
1	A	853	LYS
1	A	857	THR
1	A	864	SER
1	A	865	LYS
1	A	882	LYS
1	A	929	GLU
1	A	1057	GLU
1	A	1059	THR
1	A	1135	SER
1	A	1167	ARG
1	A	1173	LEU
1	A	1246	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	16	ASN
1	A	138	ASN
1	A	234	GLN
1	A	246	GLN
1	A	289	ASN
1	A	297	ASN
1	A	343	ASN
1	A	504	ASN
1	A	526	ASN
1	A	567	GLN
1	A	605	GLN
1	A	625	ASN
1	A	629	GLN
1	A	696	GLN

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Mol	Chain	Res	Type
1	A	733	GLN
1	A	777	ASN
1	A	807	ASN
1	A	826	ASN
1	A	866	ASN
1	A	972	ASN
1	A	983	HIS
1	A	998	ASN
1	A	1049	ASN
1	A	1069	ASN
1	A	1216	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
2	EPE	A	1401	-	15,15,15	1.80	1 (6%)	18,20,20	1.62	4 (22%)
3	EDO	A	1407	-	3,3,3	0.09	0	2,2,2	0.31	0
3	EDO	A	1409	-	3,3,3	0.06	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	A	1405	-	3,3,3	0.17	0	2,2,2	0.36	0
3	EDO	A	1402	-	3,3,3	0.05	0	2,2,2	0.13	0
3	EDO	A	1408	-	3,3,3	0.11	0	2,2,2	0.32	0
3	EDO	A	1403	-	3,3,3	0.07	0	2,2,2	0.19	0
3	EDO	A	1404	-	3,3,3	0.08	0	2,2,2	0.13	0
3	EDO	A	1406	-	3,3,3	0.07	0	2,2,2	0.17	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
2	EPE	A	1401	-	-	2/9/19/19	0/1/1/1
3	EDO	A	1407	-	-	0/1/1/1	-
3	EDO	A	1409	-	-	0/1/1/1	-
3	EDO	A	1405	-	-	0/1/1/1	-
3	EDO	A	1402	-	-	0/1/1/1	-
3	EDO	A	1408	-	-	0/1/1/1	-
3	EDO	A	1403	-	-	1/1/1/1	-
3	EDO	A	1404	-	-	1/1/1/1	-
3	EDO	A	1406	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	EPE	C10-S	-6.56	1.68	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1401	EPE	O1S-S-C10	3.92	111.64	106.92
2	A	1401	EPE	O3S-S-C10	2.37	109.59	105.77
2	A	1401	EPE	C3-C2-N1	2.36	115.48	110.64
2	A	1401	EPE	C9-N1-C2	-2.12	105.81	111.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1404	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	1403	EDO	O1-C1-C2-O2
2	A	1401	EPE	C8-C7-N4-C5
2	A	1401	EPE	C8-C7-N4-C3

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	EPE	4	0
3	A	1407	EDO	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, 95^{th} 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	1286/1322 (97%)	0.00	52 (4%) 38 43	43, 56, 85, 122	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	125	LEU	10.5
1	A	441	LYS	6.5
1	A	338	GLY	5.9
1	A	1204	ASN	5.6
1	A	875	GLU	5.6
1	A	538	TYR	4.7
1	A	536	ILE	4.2
1	A	309	VAL	4.1
1	A	337	ASN	4.1
1	A	145	SER	4.0
1	A	866	ASN	3.9
1	A	126	ASP	3.9
1	A	124	LEU	3.9
1	A	146	GLY	3.5
1	A	310	THR	3.4
1	A	319	ILE	3.4
1	A	465	GLU	3.3
1	A	693	SER	3.1
1	A	308	GLN	3.1
1	A	320	ASP	3.0
1	A	216	LEU	3.0
1	A	842	THR	3.0
1	A	311	SER	2.8
1	A	777	ASN	2.8
1	A	571	THR	2.8
1	A	336	SER	2.8
1	A	770	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	467	CYS	2.8
1	A	215	SER	2.7
1	A	496	TYR	2.7
1	A	497	ASN	2.7
1	A	534	LYS	2.6
1	A	572	THR	2.6
1	A	841	ILE	2.6
1	A	321	SER	2.5
1	A	1202	TYR	2.5
1	A	307[A]	SER	2.5
1	A	466	LEU	2.5
1	A	143	ASP	2.3
1	A	142	GLN	2.3
1	A	404	SER	2.2
1	A	521	LYS	2.2
1	A	259	ILE	2.2
1	A	573	LEU	2.1
1	A	1182	PRO	2.1
1	A	522	ILE	2.1
1	A	773	ASP	2.1
1	A	0	HIS	2.1
1	A	1248	LEU	2.1
1	A	339	GLN	2.0
1	A	610	ILE	2.0
1	A	280	ALA	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, 95^{th} 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
4	NA	A	1410	1/1	0.56	0.36	83,83,83,83	0
3	EDO	A	1409	4/4	0.78	0.27	66,67,69,71	0
4	NA	A	1412	1/1	0.83	0.18	79,79,79,79	0
2	EPE	A	1401	15/15	0.87	0.22	74,85,101,103	0
3	EDO	A	1404	4/4	0.89	0.19	77,85,86,87	0
3	EDO	A	1407	4/4	0.91	0.18	52,54,56,61	0
3	EDO	A	1403	4/4	0.92	0.17	60,61,61,65	0
3	EDO	A	1406	4/4	0.93	0.19	53,54,54,57	0
3	EDO	A	1408	4/4	0.95	0.12	56,56,58,59	0
4	NA	A	1411	1/1	0.95	0.10	64,64,64,64	0
3	EDO	A	1405	4/4	0.95	0.08	51,53,57,57	0
5	CL	A	1413	1/1	0.96	0.31	90,90,90,90	0
3	EDO	A	1402	4/4	0.97	0.15	63,67,68,73	0

6.5 Other polymers (i)

There are no such residues in this entry.