Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2016 – 05:17 AM EDT

PDB ID	:	4ZNR
Title	:	Crystal structure of Dln1 complexed with Man(alpha1-3)Man
Authors	:	Jia, N.; Jiang, Y.L.; Cheng, W.; Wang, H.W.; Zhou, C.Z.; Chen, Y.
Deposited on	:	2015-05-05
Resolution	:	2.10 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
http://wwpdb.org/validation/2016/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:

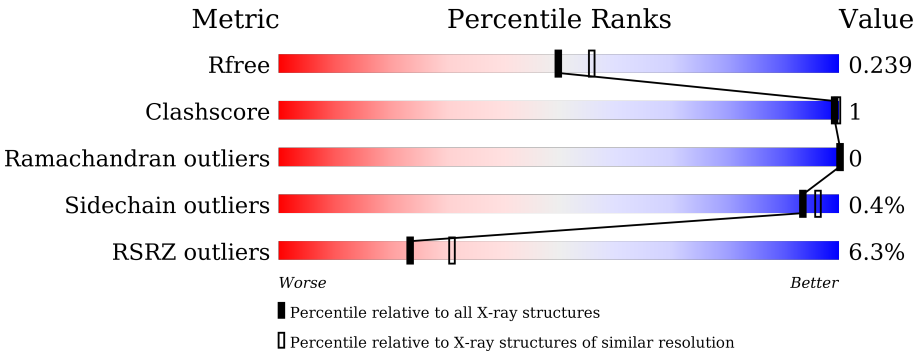
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	335	7%, 93%, • 5%
1	B	335	4%, 93%, • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	B	408	-	-	-	X
5	PGE	A	407	-	-	-	X
5	PGE	B	411	-	-	-	X
6	PG4	A	408	-	-	-	X
8	EPE	B	404	-	-	-	X
9	1PE	B	413	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5459 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 Natterin-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	2	0
			2444	1550	401	483	10			
1	B	318	Total	C	N	O	S	0	1	0
			2441	1548	400	483	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q5CZR5
A	-18	GLY	-	expression tag	UNP Q5CZR5
A	-17	SER	-	expression tag	UNP Q5CZR5
A	-16	SER	-	expression tag	UNP Q5CZR5
A	-15	HIS	-	expression tag	UNP Q5CZR5
A	-14	HIS	-	expression tag	UNP Q5CZR5
A	-13	HIS	-	expression tag	UNP Q5CZR5
A	-12	HIS	-	expression tag	UNP Q5CZR5
A	-11	HIS	-	expression tag	UNP Q5CZR5
A	-10	HIS	-	expression tag	UNP Q5CZR5
A	-9	SER	-	expression tag	UNP Q5CZR5
A	-8	SER	-	expression tag	UNP Q5CZR5
A	-7	GLY	-	expression tag	UNP Q5CZR5
A	-6	LEU	-	expression tag	UNP Q5CZR5
A	-5	VAL	-	expression tag	UNP Q5CZR5
A	-4	PRO	-	expression tag	UNP Q5CZR5
A	-3	ARG	-	expression tag	UNP Q5CZR5
A	-2	GLY	-	expression tag	UNP Q5CZR5
A	-1	SER	-	expression tag	UNP Q5CZR5
A	0	HIS	-	expression tag	UNP Q5CZR5
B	-19	MET	-	expression tag	UNP Q5CZR5
B	-18	GLY	-	expression tag	UNP Q5CZR5
B	-17	SER	-	expression tag	UNP Q5CZR5
B	-16	SER	-	expression tag	UNP Q5CZR5
B	-15	HIS	-	expression tag	UNP Q5CZR5

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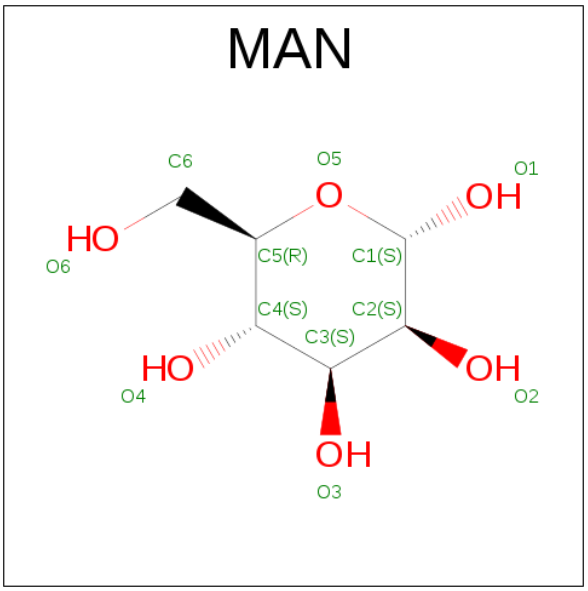
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q5CZR5
B	-13	HIS	-	expression tag	UNP Q5CZR5
B	-12	HIS	-	expression tag	UNP Q5CZR5
B	-11	HIS	-	expression tag	UNP Q5CZR5
B	-10	HIS	-	expression tag	UNP Q5CZR5
B	-9	SER	-	expression tag	UNP Q5CZR5
B	-8	SER	-	expression tag	UNP Q5CZR5
B	-7	GLY	-	expression tag	UNP Q5CZR5
B	-6	LEU	-	expression tag	UNP Q5CZR5
B	-5	VAL	-	expression tag	UNP Q5CZR5
B	-4	PRO	-	expression tag	UNP Q5CZR5
B	-3	ARG	-	expression tag	UNP Q5CZR5
B	-2	GLY	-	expression tag	UNP Q5CZR5
B	-1	SER	-	expression tag	UNP Q5CZR5
B	0	HIS	-	expression tag	UNP Q5CZR5

- Molecule 2 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).

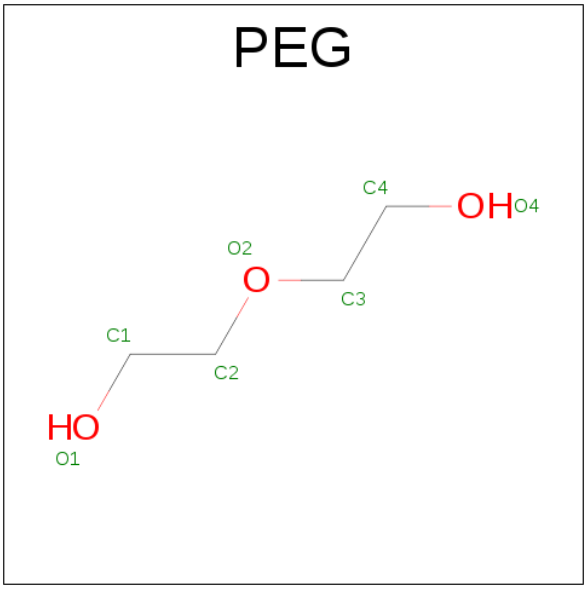


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	0
2	A	1	Total C O 11 6 5	0	0
2	B	1	Total C O 12 6 6	0	0
2	B	1	Total C O 11 6 5	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

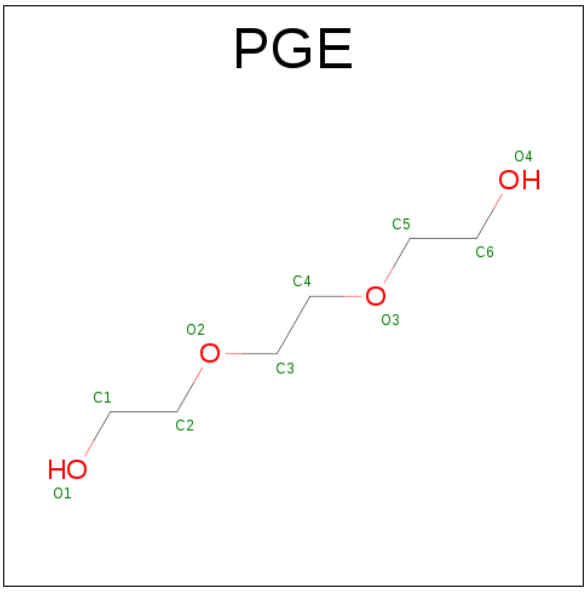
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



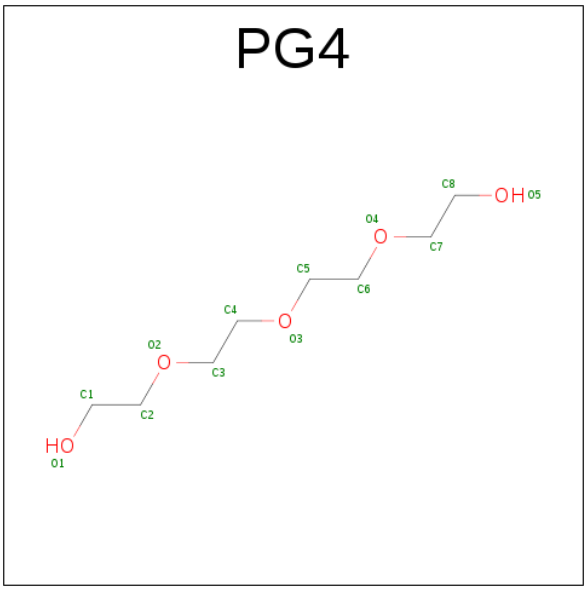
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



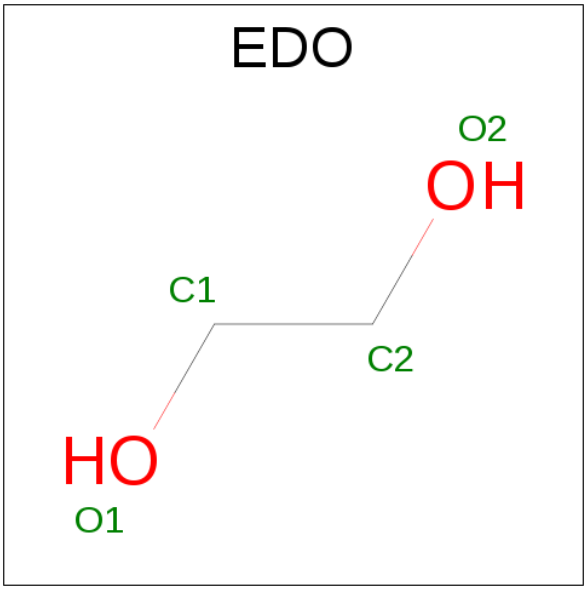
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 6 4	0	0
5	A	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



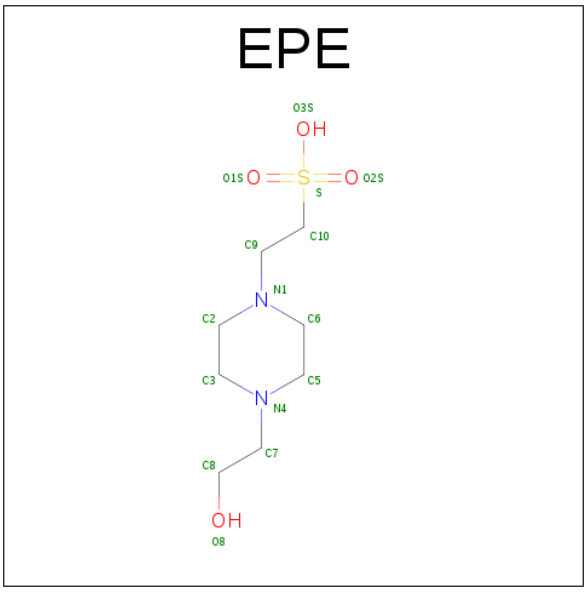
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 8 5	0	0
6	A	1	Total C O 13 8 5	0	0
6	B	1	Total C O 13 8 5	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



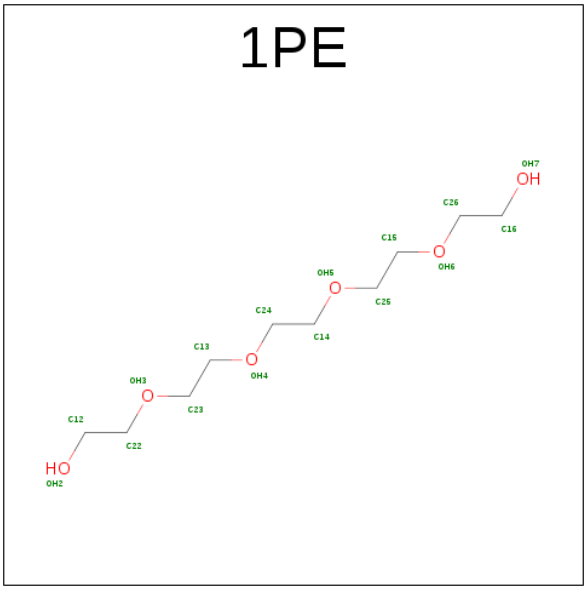
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0

- Molecule 8 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
8	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 9 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	O		0	0
			16	10	6			

- Molecule 10 is water.

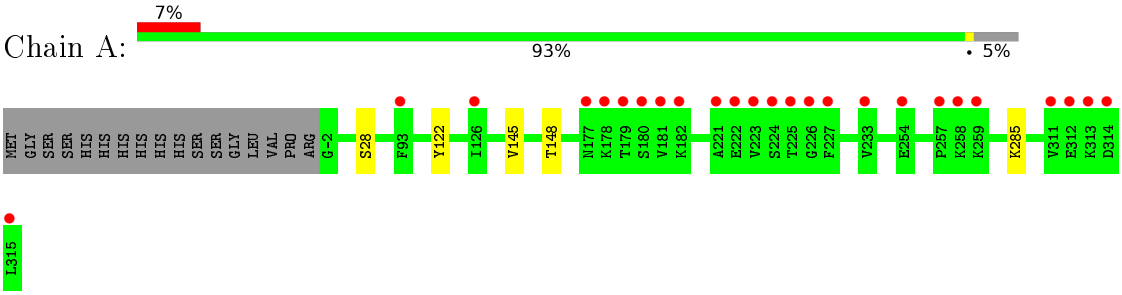
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	157	Total O 157 157	0	0
10	B	212	Total O 212 212	0	0

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 errors 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.

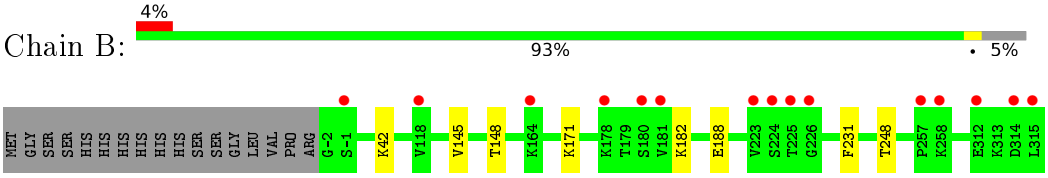
- Molecule 1: Natterin-like protein

Chain A:



- Molecule 1: Natterin-like protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.17Å 95.21Å 146.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.57 – 2.10 34.55 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.0 (34.57-2.10) 95.1 (34.55-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.26 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.207 , 0.241 0.208 , 0.239	Depositor DCC
R_{free} test set	2265 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.924	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	6 of 44992 reflections (0.013%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5459	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.90% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: EPE, PGE, CL, EDO, 1PE, PG4, PEG, MAN

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	0.33	0/2503	0.53	0/3388
1	B	0.34	0/2494	0.54	0/3375
All	All	0.33	0/4997	0.54	0/6763

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	2444	0	2409	3	0
1	B	2441	0	2401	4	0
2	A	23	0	21	0	0
2	B	23	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	14	0	20	0	0
4	B	21	0	30	0	0
5	A	20	0	28	0	0
5	B	20	0	28	0	0
6	A	26	0	36	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	13	0	18	0	0
7	A	4	0	6	0	0
7	B	8	0	12	0	0
8	B	15	0	18	0	0
9	B	16	0	22	0	0
10	A	157	0	0	0	0
10	B	212	0	0	1	0
All	All	5459	0	5070	6	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 1.

All (6) 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:B:171:LYS:NZ	1:B:188:GLU:O	2.44	0.48
1:A:285:LYS:HD2	1:B:248:THR:HB	1.99	0.45
1:B:145:VAL:HG11	1:B:148:THR:HG23	1.98	0.44
1:A:145:VAL:HG11	1:A:148:THR:HG23	2.00	0.43
1:A:28:SER:HB3	1:A:122:TYR:CZ	2.55	0.40
1:B:182:LYS:NZ	10:B:502:HOH:O	2.50	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	318/335 (95%)	314 (99%)	4 (1%)	0	100	100
1	B	317/335 (95%)	310 (98%)	7 (2%)	0	100	100
All	All	635/670 (95%)	624 (98%)	11 (2%)	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	273/286 (96%)	273 (100%)	0	100 100
1	B	272/286 (95%)	270 (99%)	2 (1%)	88 92
All	All	545/572 (95%)	543 (100%)	2 (0%)	93 96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	42	LYS
1	B	231	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 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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	MAN	A	401	2	12,12,12	2.09	3 (25%)	17,17,17	1.13	1 (5%)
2	MAN	A	402	2	11,11,12	2.19	4 (36%)	15,15,17	0.77	1 (6%)
4	PEG	A	404	-	6,6,6	0.52	0	5,5,5	0.24	0
4	PEG	A	405	-	6,6,6	0.53	0	5,5,5	0.32	0
5	PGE	A	406	-	9,9,9	0.50	0	8,8,8	0.20	0
5	PGE	A	407	-	9,9,9	0.50	0	8,8,8	0.17	0
6	PG4	A	408	-	12,12,12	0.51	0	11,11,11	0.15	0
6	PG4	A	409	-	12,12,12	0.51	0	11,11,11	0.22	0
7	EDO	A	410	-	3,3,3	0.47	0	2,2,2	0.32	0
2	MAN	B	401	2	12,12,12	2.12	3 (25%)	17,17,17	1.26	3 (17%)
2	MAN	B	402	2	11,11,12	2.14	3 (27%)	15,15,17	0.93	1 (6%)
8	EPE	B	404	-	15,15,15	1.93	1 (6%)	19,20,20	3.30	11 (57%)
7	EDO	B	405	-	3,3,3	0.42	0	2,2,2	0.33	0
7	EDO	B	406	-	3,3,3	0.43	0	2,2,2	0.30	0
4	PEG	B	407	-	6,6,6	0.48	0	5,5,5	0.21	0
4	PEG	B	408	-	6,6,6	0.50	0	5,5,5	0.59	0
4	PEG	B	409	-	6,6,6	0.52	0	5,5,5	0.21	0
5	PGE	B	410	-	9,9,9	0.51	0	8,8,8	0.20	0
5	PGE	B	411	-	9,9,9	0.47	0	8,8,8	0.36	0
6	PG4	B	412	-	12,12,12	0.51	0	11,11,11	0.16	0
9	1PE	B	413	-	15,15,15	0.53	0	14,14,14	0.22	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	MAN	A	401	2	-	0/2/22/22	0/1/1/1
2	MAN	A	402	2	-	0/2/19/22	0/1/1/1
4	PEG	A	404	-	-	0/4/4/4	0/0/0/0
4	PEG	A	405	-	-	0/4/4/4	0/0/0/0
5	PGE	A	406	-	-	0/7/7/7	0/0/0/0
5	PGE	A	407	-	-	0/7/7/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PG4	A	408	-	-	0/10/10/10	0/0/0/0
6	PG4	A	409	-	-	0/10/10/10	0/0/0/0
7	EDO	A	410	-	-	0/1/1/1	0/0/0/0
2	MAN	B	401	2	-	0/2/22/22	0/1/1/1
2	MAN	B	402	2	-	0/2/19/22	0/1/1/1
8	EPE	B	404	-	-	0/9/19/19	0/1/1/1
7	EDO	B	405	-	-	0/1/1/1	0/0/0/0
7	EDO	B	406	-	-	0/1/1/1	0/0/0/0
4	PEG	B	407	-	-	0/4/4/4	0/0/0/0
4	PEG	B	408	-	-	0/4/4/4	0/0/0/0
4	PEG	B	409	-	-	0/4/4/4	0/0/0/0
5	PGE	B	410	-	-	0/7/7/7	0/0/0/0
5	PGE	B	411	-	-	0/7/7/7	0/0/0/0
6	PG4	B	412	-	-	0/10/10/10	0/0/0/0
9	1PE	B	413	-	-	0/13/13/13	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	404	EPE	C10-S	-7.19	1.66	1.77
2	A	402	MAN	C2-C3	-5.02	1.45	1.52
2	B	402	MAN	C2-C3	-4.87	1.46	1.52
2	A	401	MAN	C3-C2	-4.07	1.41	1.52
2	A	401	MAN	C4-C3	-4.00	1.41	1.52
2	B	401	MAN	C4-C3	-3.95	1.41	1.52
2	B	401	MAN	C3-C2	-3.84	1.42	1.52
2	A	402	MAN	C4-C3	-3.57	1.42	1.52
2	B	402	MAN	C4-C3	-3.51	1.43	1.52
2	A	402	MAN	O5-C1	-2.06	1.40	1.43
2	A	402	MAN	O3-C3	2.35	1.48	1.43
2	B	402	MAN	O3-C3	2.36	1.48	1.43
2	A	401	MAN	O3-C3	3.55	1.51	1.43
2	B	401	MAN	O3-C3	3.86	1.52	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	404	EPE	C3-C2-N1	-4.84	101.22	110.65
8	B	404	EPE	C2-C3-N4	-2.80	105.20	110.65
8	B	404	EPE	C8-C7-N4	-2.22	104.76	113.44
2	A	402	MAN	O6-C6-C5	2.10	118.30	111.30
2	A	401	MAN	O6-C6-C5	2.17	118.55	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	MAN	O6-C6-C5	2.19	118.63	111.30
2	B	401	MAN	O5-C1-C2	2.22	113.89	110.00
2	B	402	MAN	C1-C2-C3	2.31	112.35	109.55
2	B	401	MAN	C1-C2-C3	2.60	114.94	110.68
8	B	404	EPE	C6-N1-C2	3.02	115.63	108.87
8	B	404	EPE	C7-N4-C3	3.09	117.98	111.25
8	B	404	EPE	O2S-S-C10	3.84	109.58	106.87
8	B	404	EPE	C7-N4-C5	4.27	120.55	111.25
8	B	404	EPE	C9-N1-C6	4.65	121.37	111.25
8	B	404	EPE	C9-N1-C2	5.37	122.95	111.25
8	B	404	EPE	O1S-S-C10	5.49	110.75	106.87
8	B	404	EPE	C5-N4-C3	5.62	121.44	108.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	318/335 (94%)	0.27	25 (7%)	15	21	20, 34, 71, 90	0
1	B	318/335 (94%)	0.13	15 (4%)	35	44	20, 32, 58, 84	0
All	All	636/670 (94%)	0.20	40 (6%)	23	31	20, 33, 65, 90	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	LEU	7.1
1	B	225	THR	6.0
1	A	223	VAL	5.9
1	A	224	SER	5.8
1	A	181	VAL	5.8
1	A	225	THR	5.0
1	B	224	SER	4.7
1	A	180	SER	4.7
1	A	226	GLY	4.4
1	A	233	VAL	4.2
1	B	181	VAL	4.2
1	A	182	LYS	4.2
1	B	223	VAL	4.1
1	B	315	LEU	4.0
1	A	178	LYS	3.6
1	A	179	THR	3.5
1	B	314	ASP	2.9
1	B	258	LYS	2.9
1	B	178	LYS	2.9
1	A	258	LYS	2.8
1	A	314	ASP	2.8
1	A	312	GLU	2.7
1	B	226	GLY	2.6
1	A	259	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	222	GLU	2.6
1	A	311	VAL	2.5
1	B	-1	SER	2.5
1	A	177	ASN	2.5
1	A	257	PRO	2.4
1	B	180	SER	2.4
1	A	93	PHE	2.3
1	A	313	LYS	2.2
1	A	254	GLU	2.2
1	A	221	ALA	2.2
1	A	126	ILE	2.1
1	B	312	GLU	2.1
1	B	164	LYS	2.1
1	B	118	VAL	2.0
1	A	227	PHE	2.0
1	B	257	PRO	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
8	EPE	B	404	15/15	0.81	0.33	14.99	56,61,67,69	5
9	1PE	B	413	16/16	0.76	0.19	6.71	49,55,64,64	0
4	PEG	B	408	7/7	0.85	0.16	4.92	54,57,58,60	0
6	PG4	A	408	13/13	0.79	0.20	4.21	44,48,49,51	0
5	PGE	A	407	10/10	0.89	0.15	2.27	51,52,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	PGE	B	411	10/10	0.89	0.13	2.10	49,50,52,55	0
4	PEG	A	405	7/7	0.73	0.19	1.87	65,66,66,67	0
4	PEG	A	404	7/7	0.68	0.17	1.74	54,55,56,56	0
5	PGE	B	410	10/10	0.83	0.17	1.46	44,48,49,49	0
5	PGE	A	406	10/10	0.88	0.12	1.42	45,46,49,50	0
6	PG4	A	409	13/13	0.75	0.16	0.94	49,50,53,53	0
7	EDO	A	410	4/4	0.75	0.12	0.74	57,57,57,57	0
4	PEG	B	409	7/7	0.79	0.21	0.53	67,70,72,72	0
7	EDO	B	406	4/4	0.80	0.13	0.46	56,57,57,58	0
2	MAN	B	402	11/12	0.92	0.12	0.28	33,36,39,42	0
6	PG4	B	412	13/13	0.87	0.14	-0.03	50,53,54,55	0
3	CL	A	403	1/1	0.98	0.07	-0.14	32,32,32,32	0
2	MAN	A	402	11/12	0.94	0.09	-0.69	34,35,38,41	0
3	CL	B	403	1/1	1.00	0.05	-1.98	30,30,30,30	0
2	MAN	A	401	12/12	0.79	0.37	-	47,58,62,63	0
4	PEG	B	407	7/7	0.71	0.21	-	59,59,61,62	0
7	EDO	B	405	4/4	0.84	0.27	-	58,59,59,59	0
2	MAN	B	401	12/12	0.78	0.41	-	47,60,65,69	0

6.5 Other polymers

There are no such residues in this entry.