Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2021 – 10:05 pm GMT

PDB ID	:	6ZDF
Title	:	Structure of the catalytic domain of human endo-alpha-mannosidase MANEA in complex with HEPES
Authors	:	Sobala, L.F.; Fernandes, P.Z.; Hakki, Z.; Thompson, A.J.; Howe, J.D.; Hill, M.; Zitzmann, N.; Davies, S.; Stamataki, Z.; Butters, T.D.; Alonzi, D.S.; Williams, S.J.; Davies, G.J.
Deposited on	:	2020-06-14
Resolution	:	3.00 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 ①) were used in the production of this report:

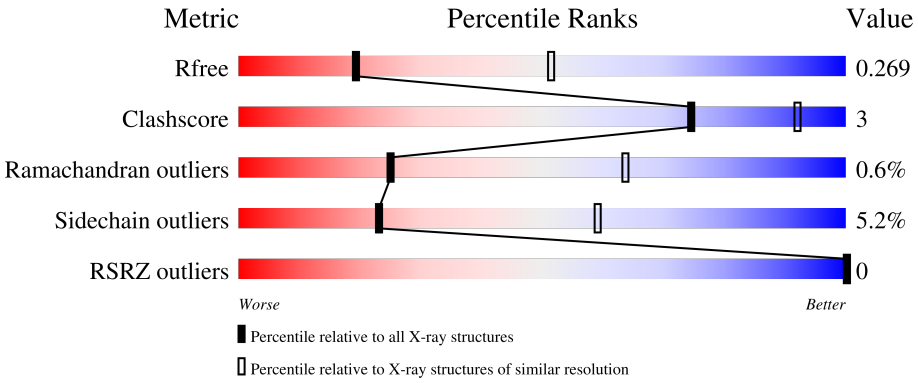
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	382	81% 12% 7%
1	B	382	81% 13% 7%
1	C	382	82% 12% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9038 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 Glycoprotein endo-alpha-1,2-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2947	1899	499	544	5			
1	B	357	Total	C	N	O	S	0	0	0
			2950	1901	499	545	5			
1	C	358	Total	C	N	O	S	0	0	0
			2956	1905	499	546	6			

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	MET	-	initiating methionine	UNP Q5SRI9
A	82	ASN	-	expression tag	UNP Q5SRI9
A	83	HIS	-	expression tag	UNP Q5SRI9
A	84	LYS	-	expression tag	UNP Q5SRI9
A	85	VAL	-	expression tag	UNP Q5SRI9
A	86	HIS	-	expression tag	UNP Q5SRI9
A	87	HIS	-	expression tag	UNP Q5SRI9
A	88	HIS	-	expression tag	UNP Q5SRI9
A	89	HIS	-	expression tag	UNP Q5SRI9
A	90	HIS	-	expression tag	UNP Q5SRI9
A	91	HIS	-	expression tag	UNP Q5SRI9
A	92	ILE	-	expression tag	UNP Q5SRI9
A	93	GLU	-	expression tag	UNP Q5SRI9
A	94	GLY	-	expression tag	UNP Q5SRI9
A	95	ARG	-	expression tag	UNP Q5SRI9
A	96	HIS	-	expression tag	UNP Q5SRI9
A	97	MET	-	expression tag	UNP Q5SRI9
B	81	MET	-	initiating methionine	UNP Q5SRI9
B	82	ASN	-	expression tag	UNP Q5SRI9
B	83	HIS	-	expression tag	UNP Q5SRI9
B	84	LYS	-	expression tag	UNP Q5SRI9
B	85	VAL	-	expression tag	UNP Q5SRI9
B	86	HIS	-	expression tag	UNP Q5SRI9

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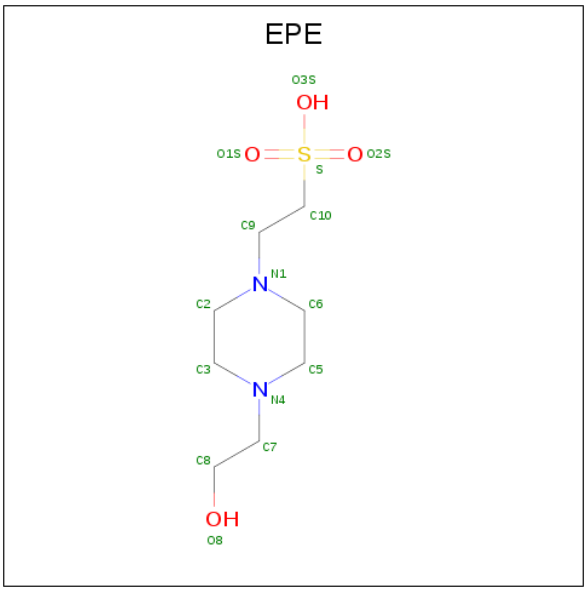
Chain	Residue	Modelled	Actual	Comment	Reference
B	87	HIS	-	expression tag	UNP Q5SRI9
B	88	HIS	-	expression tag	UNP Q5SRI9
B	89	HIS	-	expression tag	UNP Q5SRI9
B	90	HIS	-	expression tag	UNP Q5SRI9
B	91	HIS	-	expression tag	UNP Q5SRI9
B	92	ILE	-	expression tag	UNP Q5SRI9
B	93	GLU	-	expression tag	UNP Q5SRI9
B	94	GLY	-	expression tag	UNP Q5SRI9
B	95	ARG	-	expression tag	UNP Q5SRI9
B	96	HIS	-	expression tag	UNP Q5SRI9
B	97	MET	-	expression tag	UNP Q5SRI9
C	81	MET	-	initiating methionine	UNP Q5SRI9
C	82	ASN	-	expression tag	UNP Q5SRI9
C	83	HIS	-	expression tag	UNP Q5SRI9
C	84	LYS	-	expression tag	UNP Q5SRI9
C	85	VAL	-	expression tag	UNP Q5SRI9
C	86	HIS	-	expression tag	UNP Q5SRI9
C	87	HIS	-	expression tag	UNP Q5SRI9
C	88	HIS	-	expression tag	UNP Q5SRI9
C	89	HIS	-	expression tag	UNP Q5SRI9
C	90	HIS	-	expression tag	UNP Q5SRI9
C	91	HIS	-	expression tag	UNP Q5SRI9
C	92	ILE	-	expression tag	UNP Q5SRI9
C	93	GLU	-	expression tag	UNP Q5SRI9
C	94	GLY	-	expression tag	UNP Q5SRI9
C	95	ARG	-	expression tag	UNP Q5SRI9
C	96	HIS	-	expression tag	UNP Q5SRI9
C	97	MET	-	expression tag	UNP Q5SRI9

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

- Molecule 3 is water.

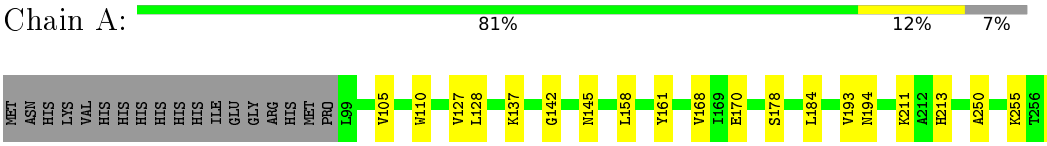
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	48	Total O 48 48	0	0
3	B	40	Total O 40 40	0	0
3	C	52	Total O 52 52	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

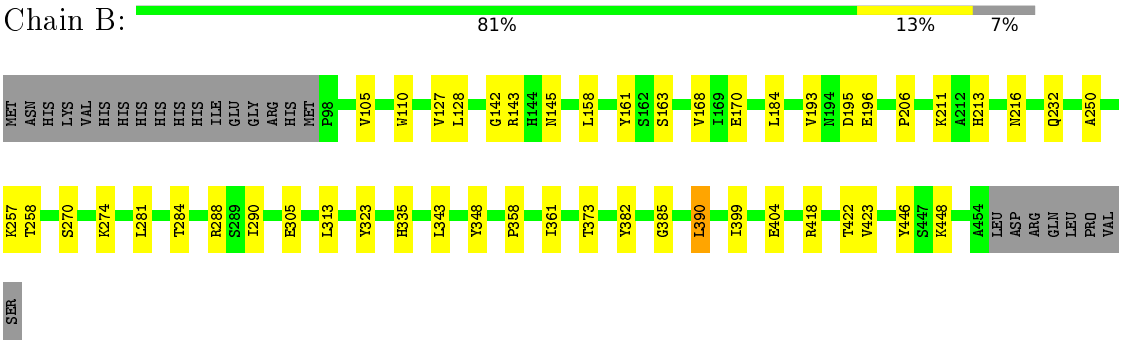
- Molecule 1: Glycoprotein endo-alpha-1,2-mannosidase

Chain A:



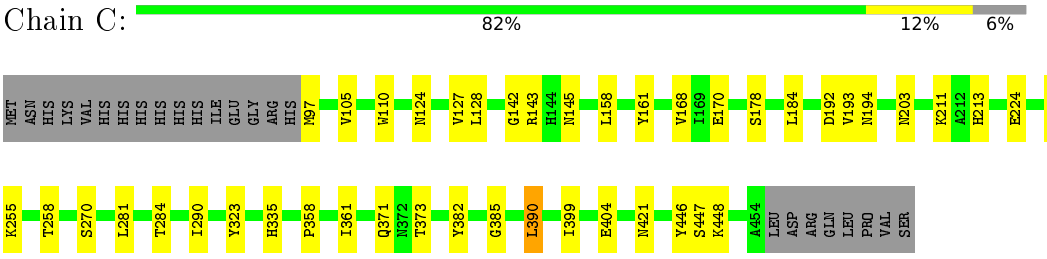
- Molecule 1: Glycoprotein endo-alpha-1,2-mannosidase

Chain B:



- Molecule 1: Glycoprotein endo-alpha-1,2-mannosidase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	144.25Å 144.25Å 139.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.20 – 3.00 102.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (102.20-3.00) 100.0 (102.00-3.00)	Depositor EDS
R_{merge}	0.58	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.215 , 0.269 0.215 , 0.269	Depositor DCC
R_{free} test set	1429 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 28.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.068 for -h,-l,-k 0.047 for l,-k,h	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	9038	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: 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	0.58	0/3047	0.74	0/4151
1	B	0.56	0/3051	0.72	0/4158
1	C	0.56	0/3057	0.73	1/4167 (0.0%)
All	All	0.56	0/9155	0.73	1/12476 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	421	ASN	CB-CA-C	-5.98	98.44	110.40

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	2947	0	2806	18	0
1	B	2950	0	2803	21	0
1	C	2956	0	2804	20	0
2	A	15	0	18	0	0
2	B	15	0	17	1	0
2	C	15	0	18	2	0
3	A	48	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	40	0	0	1	0
3	C	52	0	0	0	0
All	All	9038	0	8466	56	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 3.

All (56) 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:390:LEU:HD11	1:B:446:TYR:HB2	1.77	0.67
1:A:390:LEU:HD11	1:A:446:TYR:HB2	1.76	0.66
1:C:224:GLU:OE1	2:C:501:EPE:H52	1.95	0.66
1:C:390:LEU:HD11	1:C:446:TYR:HB2	1.79	0.64
1:A:326:THR:HG23	1:A:374:ARG:HD3	1.78	0.64
1:A:213:HIS:HB2	1:A:250:ALA:HB2	1.83	0.59
1:C:213:HIS:HB2	1:C:250:ALA:HB2	1.84	0.59
1:B:213:HIS:HB2	1:B:250:ALA:HB2	1.85	0.58
1:A:380:LYS:HE3	1:A:384:ILE:HD11	1.86	0.56
1:A:358:PRO:HA	1:A:382:TYR:HB2	1.87	0.56
1:B:358:PRO:HA	1:B:382:TYR:HB2	1.89	0.55
1:A:335:HIS:CE1	1:A:385:GLY:HA2	2.43	0.54
1:C:358:PRO:HA	1:C:382:TYR:HB2	1.90	0.54
1:B:335:HIS:CE1	1:B:385:GLY:HA2	2.45	0.50
1:C:335:HIS:CE1	1:C:385:GLY:HA2	2.47	0.50
1:B:232:GLN:HG2	1:B:288:ARG:CZ	2.43	0.49
1:B:418:ARG:HG2	1:B:423:VAL:HG22	1.94	0.49
1:A:335:HIS:HE1	1:A:385:GLY:HA2	1.78	0.48
1:B:105:VAL:HG23	1:B:399:ILE:HB	1.96	0.47
1:A:161:TYR:HB2	1:A:168:VAL:HG21	1.97	0.47
1:B:213:HIS:HD2	1:C:228:ASN:HD21	1.62	0.47
1:A:361:ILE:HB	1:A:373:THR:HG23	1.98	0.46
1:B:335:HIS:HE1	1:B:385:GLY:HA2	1.81	0.46
1:C:105:VAL:HG23	1:C:399:ILE:HB	1.98	0.45
1:B:313:LEU:HD21	1:B:348:TYR:HB3	1.99	0.45
1:B:361:ILE:HB	1:B:373:THR:HG23	1.98	0.45
1:C:170:GLU:HG2	1:C:211:LYS:HD2	1.98	0.45
1:A:105:VAL:HG23	1:A:399:ILE:HB	1.98	0.45
1:C:361:ILE:HB	1:C:373:THR:HG23	1.98	0.45
1:B:127:VAL:HG23	1:B:142:GLY:O	2.18	0.44
1:C:161:TYR:HB2	1:C:168:VAL:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:SER:HB3	3:B:619:HOH:O	2.17	0.44
1:B:281:LEU:O	1:B:290:ILE:HG13	2.18	0.44
1:B:161:TYR:HB2	1:B:168:VAL:HG21	1.99	0.43
1:A:127:VAL:HG23	1:A:142:GLY:O	2.18	0.43
1:B:170:GLU:HG2	1:B:211:LYS:HD2	2.00	0.43
1:C:281:LEU:O	1:C:290:ILE:HG13	2.18	0.43
1:A:170:GLU:HG3	1:A:211:LYS:HD2	2.01	0.43
1:A:281:LEU:O	1:A:290:ILE:HG13	2.19	0.42
1:C:158:LEU:HD13	1:C:168:VAL:HG22	2.01	0.42
1:B:158:LEU:HD13	1:B:168:VAL:HG22	2.00	0.42
1:A:414:ALA:HB1	3:A:616:HOH:O	2.18	0.42
1:B:213:HIS:CD2	1:C:228:ASN:HD21	2.38	0.42
1:C:224:GLU:OE1	2:C:501:EPE:H71	2.19	0.42
1:C:335:HIS:HE1	1:C:385:GLY:HA2	1.84	0.41
1:A:158:LEU:HD13	1:A:168:VAL:HG22	2.02	0.41
1:B:206:PRO:HG2	1:C:192:ASP:HB2	2.01	0.41
1:B:127:VAL:O	1:B:127:VAL:HG12	2.21	0.41
1:C:127:VAL:HG23	1:C:142:GLY:O	2.20	0.41
1:C:448:LYS:HB3	1:C:448:LYS:HE3	1.92	0.41
1:C:124:ASN:OD1	1:C:143:ARG:HD3	2.20	0.41
1:A:274:LYS:HE3	1:A:274:LYS:HB3	1.88	0.40
1:A:300:ILE:HG21	1:A:353:ILE:HD12	2.02	0.40
1:C:127:VAL:HG12	1:C:127:VAL:O	2.21	0.40
1:A:127:VAL:O	1:A:127:VAL:HG12	2.21	0.40
1:B:195:ASP:HB2	2:B:501:EPE:H101	2.03	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	354/382 (93%)	340 (96%)	12 (3%)	2 (1%)	25 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	355/382 (93%)	341 (96%)	12 (3%)	2 (1%)	25 64
1	C	356/382 (93%)	342 (96%)	12 (3%)	2 (1%)	25 64
All	All	1065/1146 (93%)	1023 (96%)	36 (3%)	6 (1%)	25 64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	TYR
1	B	323	TYR
1	C	323	TYR
1	A	128	LEU
1	B	128	LEU
1	C	128	LEU

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	318/345 (92%)	302 (95%)	16 (5%)	24 60
1	B	318/345 (92%)	300 (94%)	18 (6%)	20 56
1	C	318/345 (92%)	302 (95%)	16 (5%)	24 60
All	All	954/1035 (92%)	904 (95%)	50 (5%)	23 59

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	TRP
1	A	137	LYS
1	A	145	ASN
1	A	178	SER
1	A	184	LEU
1	A	193	VAL
1	A	194	ASN
1	A	255	LYS

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Mol	Chain	Res	Type
1	A	257	LYS
1	A	258	THR
1	A	270	SER
1	A	284	THR
1	A	306	GLU
1	A	371	GLN
1	A	390	LEU
1	A	404	GLU
1	B	110	TRP
1	B	143	ARG
1	B	145	ASN
1	B	184	LEU
1	B	193	VAL
1	B	196	GLU
1	B	216	ASN
1	B	257	LYS
1	B	258	THR
1	B	270	SER
1	B	274	LYS
1	B	284	THR
1	B	305	GLU
1	B	343	LEU
1	B	390	LEU
1	B	404	GLU
1	B	422	THR
1	B	448	LYS
1	C	97	MET
1	C	110	TRP
1	C	145	ASN
1	C	178	SER
1	C	184	LEU
1	C	193	VAL
1	C	194	ASN
1	C	203	ASN
1	C	255	LYS
1	C	258	THR
1	C	270	SER
1	C	284	THR
1	C	371	GLN
1	C	390	LEU
1	C	404	GLU
1	C	447	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	ASN
1	A	260	ASN
1	A	335	HIS
1	B	124	ASN
1	B	213	HIS
1	B	216	ASN
1	B	232	GLN
1	B	335	HIS
1	C	213	HIS
1	C	335	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EPE	A	501	-	15,15,15	1.93	1 (6%)	18,20,20	2.26	7 (38%)
2	EPE	B	501	-	15,15,15	2.08	1 (6%)	18,20,20	2.00	7 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EPE	C	501	-	15,15,15	1.96	1 (6%)	18,20,20	1.83	8 (44%)

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	501	-	-	4/9/19/19	0/1/1/1
2	EPE	B	501	-	-	8/9/19/19	0/1/1/1
2	EPE	C	501	-	-	2/9/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	EPE	C10-S	-7.74	1.66	1.77
2	C	501	EPE	C10-S	-7.30	1.67	1.77
2	A	501	EPE	C10-S	-7.00	1.67	1.77

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	EPE	O2S-S-C10	4.63	112.49	106.92
2	A	501	EPE	O3S-S-C10	3.95	112.16	105.77
2	B	501	EPE	O2S-S-C10	3.85	111.55	106.92
2	A	501	EPE	C6-N1-C2	3.79	117.37	108.83
2	B	501	EPE	O1S-S-C10	3.52	111.16	106.92
2	B	501	EPE	C2-C3-N4	-3.28	103.92	110.64
2	C	501	EPE	O3S-S-C10	3.03	110.67	105.77
2	A	501	EPE	C2-C3-N4	-2.94	104.61	110.64
2	C	501	EPE	O1S-S-C10	2.84	110.33	106.92
2	C	501	EPE	C2-C3-N4	-2.80	104.90	110.64
2	B	501	EPE	C6-C5-N4	-2.57	105.37	110.64
2	C	501	EPE	C7-N4-C5	-2.53	104.76	111.23
2	A	501	EPE	O1S-S-C10	-2.51	103.89	106.92
2	A	501	EPE	C5-C6-N1	2.50	115.78	110.64
2	C	501	EPE	C3-C2-N1	-2.34	105.85	110.64
2	C	501	EPE	O8-C8-C7	-2.29	101.69	111.19
2	A	501	EPE	C9-N1-C2	-2.28	105.39	111.23
2	B	501	EPE	O3S-S-C10	2.17	109.28	105.77
2	C	501	EPE	C5-C6-N1	-2.14	106.24	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	EPE	C8-C7-N4	-2.13	105.75	113.40
2	B	501	EPE	C6-N1-C2	2.11	113.58	108.83
2	C	501	EPE	O3S-S-O2S	-2.00	106.38	111.27

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	EPE	S-C10-C9-N1
2	B	501	EPE	C9-C10-S-O2S
2	A	501	EPE	C8-C7-N4-C5
2	C	501	EPE	N4-C7-C8-O8
2	B	501	EPE	C9-C10-S-O3S
2	B	501	EPE	N4-C7-C8-O8
2	B	501	EPE	C10-C9-N1-C2
2	B	501	EPE	C10-C9-N1-C6
2	B	501	EPE	C9-C10-S-O1S
2	A	501	EPE	C10-C9-N1-C2
2	B	501	EPE	C8-C7-N4-C3
2	B	501	EPE	C8-C7-N4-C5
2	C	501	EPE	C8-C7-N4-C3
2	A	501	EPE	C9-C10-S-O1S

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	EPE	1	0
2	C	501	EPE	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, 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	356/382 (93%)	-0.32	0	100	100	29, 47, 72, 109	0
1	B	357/382 (93%)	-0.37	0	100	100	27, 47, 71, 98	0
1	C	358/382 (93%)	-0.32	0	100	100	29, 47, 70, 92	0
All	All	1071/1146 (93%)	-0.34	0	100	100	27, 47, 71, 109	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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
2	EPE	B	501	15/15	0.94	0.21	50,63,67,77	0
2	EPE	C	501	15/15	0.96	0.24	39,42,55,55	0
2	EPE	A	501	15/15	0.98	0.19	37,45,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.