



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:36 pm BST

PDB ID : 6OK1  
Title : Ltp2-ChsH2(DUF35) aldolase  
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Deposited on : 2019-04-12  
Resolution : 1.70 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](mailto: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.

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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

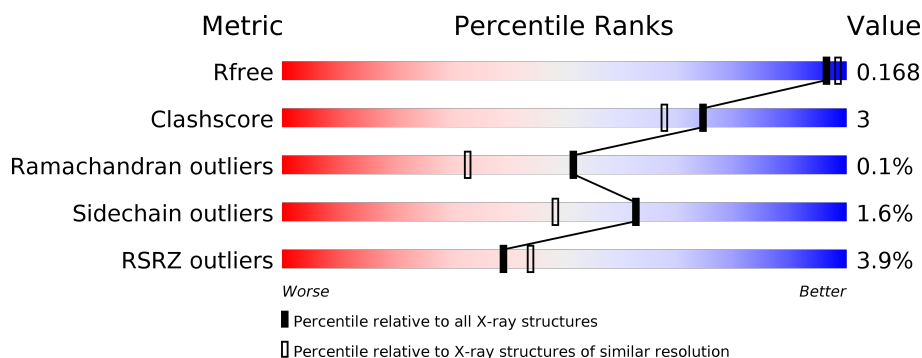
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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  $\geq 3$ , 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	403	<div> <div>0%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>5%</div> </div> </div>
1	C	403	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>5%</div> </div> </div>
2	B	133	<div> <div>7%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>•</div> </div> </div>
2	D	133	<div> <div>14%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>•</div> <div>5%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	C	502	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 16716 atoms, of which 7853 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 Lipid-transfer protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	382	Total	C	H	N	O	S	0	13	0
			5783	1839	2860	506	561	17			
1	C	382	Total	C	H	N	O	S	0	14	0
			5809	1843	2880	512	558	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	LYS	-	expression tag	UNP D1AB74
A	393	LEU	-	expression tag	UNP D1AB74
A	394	ARG	-	expression tag	UNP D1AB74
A	395	SER	-	expression tag	UNP D1AB74
A	396	LEU	-	expression tag	UNP D1AB74
A	397	GLU	-	expression tag	UNP D1AB74
A	398	HIS	-	expression tag	UNP D1AB74
A	399	HIS	-	expression tag	UNP D1AB74
A	400	HIS	-	expression tag	UNP D1AB74
A	401	HIS	-	expression tag	UNP D1AB74
A	402	HIS	-	expression tag	UNP D1AB74
A	403	HIS	-	expression tag	UNP D1AB74
C	392	LYS	-	expression tag	UNP D1AB74
C	393	LEU	-	expression tag	UNP D1AB74
C	394	ARG	-	expression tag	UNP D1AB74
C	395	SER	-	expression tag	UNP D1AB74
C	396	LEU	-	expression tag	UNP D1AB74
C	397	GLU	-	expression tag	UNP D1AB74
C	398	HIS	-	expression tag	UNP D1AB74
C	399	HIS	-	expression tag	UNP D1AB74
C	400	HIS	-	expression tag	UNP D1AB74
C	401	HIS	-	expression tag	UNP D1AB74
C	402	HIS	-	expression tag	UNP D1AB74
C	403	HIS	-	expression tag	UNP D1AB74

- Molecule 2 is a protein called ChsH2(DUF35).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	131	Total	C	H	N	O	S	0	10	0
			2110	682	1046	183	190	9			
2	D	127	Total	C	H	N	O	S	0	3	0
			2006	650	996	176	177	7			

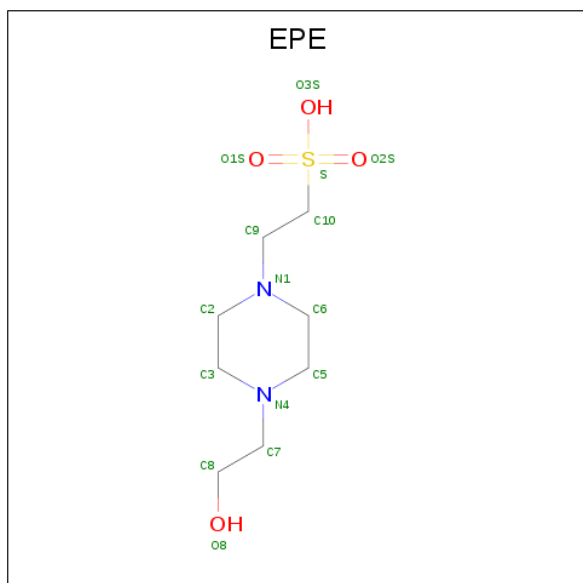
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	187	MET	-	initiating methionine	UNP D1AB77
D	187	MET	-	initiating methionine	UNP D1AB77

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

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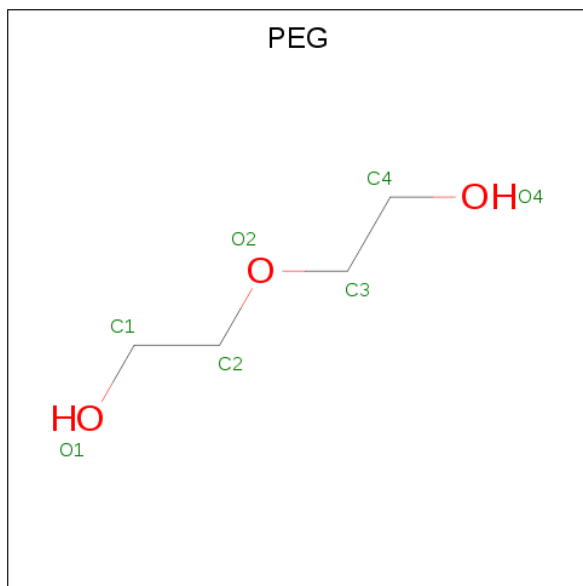
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
4	D	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Cl	0	0
			4	4		
5	D	1	Total	Cl	0	0
			1	1		
5	C	2	Total	Cl	0	0
			2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			17	4	10	3		
6	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 1	Zn 1	0	0
7	D	1	Total 1	Zn 1	0	0

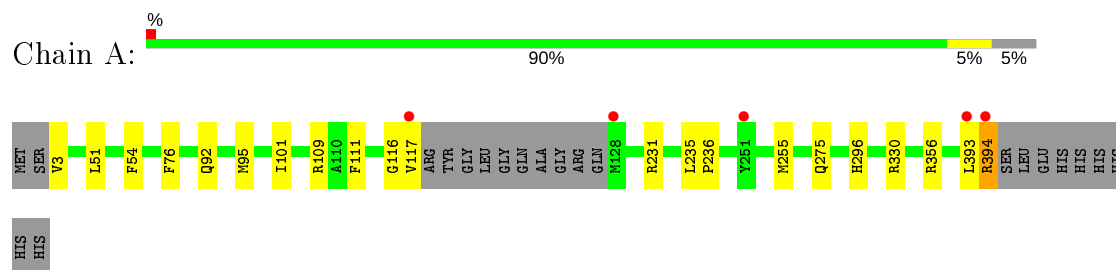
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	327	Total 327	O 327	0	0
8	B	139	Total 139	O 139	0	0
8	C	338	Total 338	O 338	0	0
8	D	63	Total 63	O 63	0	0

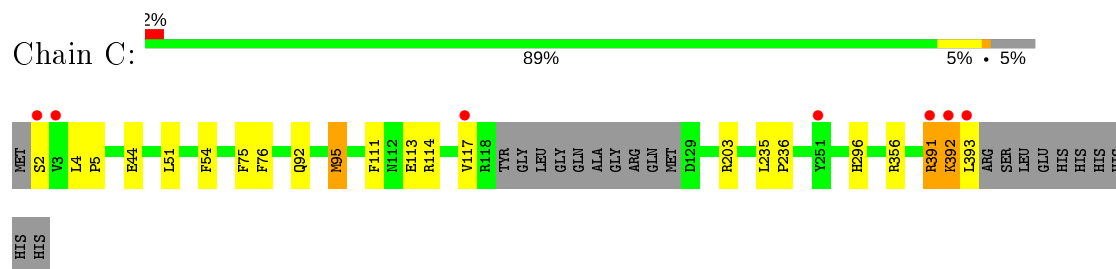
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

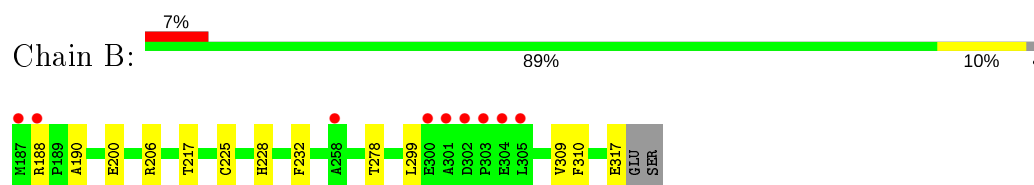
- Molecule 1: Lipid-transfer protein



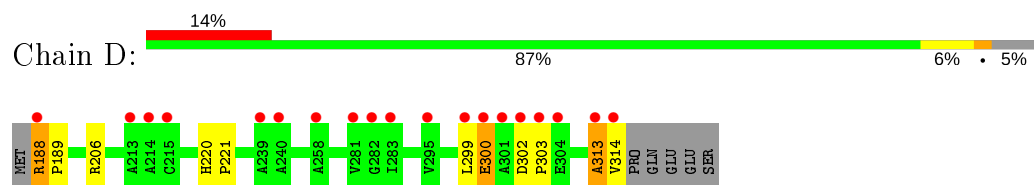
- Molecule 1: Lipid-transfer protein



- Molecule 2: ChsH2(DUF35)



- Molecule 2: ChsH2(DUF35)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.68Å 110.56Å 120.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.83 – 1.70 45.74 – 1.47	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.83-1.70) 99.9 (45.74-1.47)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 1.47Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.144 , 0.168 0.144 , 0.168	Depositor DCC
$R_{free}$ test set	10340 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 51.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	16716	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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

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	0.45	0/3022	0.65	1/4106 (0.0%)
1	C	0.44	0/3031	0.67	6/4118 (0.1%)
2	B	0.44	0/1144	0.63	0/1570
2	D	0.35	0/1051	0.59	0/1441
All	All	0.43	0/8248	0.65	7/11235 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	D	0	2
All	All	0	4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	356	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	A	356	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	C	95[A]	MET	CG-SD-CE	5.92	109.67	100.20
1	C	95[B]	MET	CG-SD-CE	5.92	109.67	100.20
1	C	54	PHE	CB-CG-CD2	-5.58	116.89	120.80
1	C	54	PHE	CB-CG-CD1	5.56	124.69	120.80
1	C	356	ARG	NE-CZ-NH2	5.50	123.05	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	393	LEU	Peptide
1	C	391	ARG	Peptide
2	D	300	GLU	Peptide
2	D	313	ALA	Peptide

## 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	2923	2860	2861	16	0
1	C	2929	2880	2880	19	0
2	B	1064	1046	1006	8	0
2	D	1010	996	996	8	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	15	17	17	0	0
4	B	15	17	17	0	0
4	D	15	17	17	0	0
5	A	4	0	0	2	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
6	A	7	10	10	0	0
6	C	7	10	10	2	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	A	327	0	0	4	0
8	B	139	0	0	3	1
8	C	338	0	0	10	1
8	D	63	0	0	4	0
All	All	8863	7853	7814	50	1

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 (50) 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:3:VAL:N	1:C:2:SER:HG	1.39	1.20
5:A:505:CL:CL	8:A:856:HOH:O	2.00	1.16
2:D:206[A]:ARG:NH2	8:D:501:HOH:O	2.03	0.90
2:B:200:GLU:OE2	8:B:501:HOH:O	1.93	0.84
2:B:317:GLU:OE1	8:B:502:HOH:O	1.97	0.81
1:A:92:GLN:HA	1:A:95[B]:MET:HE2	1.62	0.80
1:A:255[A]:MET:HE3	8:A:809:HOH:O	1.83	0.77
1:C:2:SER:OG	8:C:602:HOH:O	2.08	0.70
6:C:504:PEG:O1	8:C:601:HOH:O	2.02	0.64
6:C:504:PEG:H32	8:C:867:HOH:O	1.99	0.62
1:C:92:GLN:HA	1:C:95[A]:MET:CE	2.30	0.62
1:A:255[B]:MET:HE1	8:A:873:HOH:O	1.99	0.61
1:C:92:GLN:HA	1:C:95[A]:MET:HE3	1.81	0.61
1:A:3:VAL:N	1:C:2:SER:OG	2.22	0.59
1:C:44[A]:GLU:OE1	8:C:604:HOH:O	2.17	0.58
1:C:113:GLU:OE1	8:C:603:HOH:O	2.17	0.57
2:B:206:ARG:NH2	8:B:505:HOH:O	2.38	0.56
1:A:3:VAL:N	8:C:602:HOH:O	2.43	0.51
1:C:114:ARG:CZ	8:C:608:HOH:O	2.57	0.50
2:D:188:ARG:CD	8:D:506:HOH:O	2.62	0.48
2:D:313:ALA:O	2:D:314:VAL:CG2	2.64	0.46
1:A:101[A]:ILE:CD1	1:C:95[A]:MET:SD	3.04	0.45
1:C:114:ARG:NE	8:C:608:HOH:O	2.49	0.45
1:A:275[B]:GLN:HG2	8:A:860:HOH:O	2.15	0.45
5:A:503:CL:CL	2:B:190:ALA:N	2.85	0.45
1:C:51:LEU:O	1:C:76:PHE:HA	2.17	0.45
2:D:188:ARG:HD3	8:D:506:HOH:O	2.16	0.45
1:A:116:GLY:O	1:A:117:VAL:C	2.54	0.44
2:D:188:ARG:NE	8:D:506:HOH:O	2.51	0.44
1:A:394:ARG:HA	1:A:394:ARG:NE	2.33	0.43
1:A:51:LEU:O	1:A:76:PHE:HA	2.18	0.43
1:C:393:LEU:N	1:C:393:LEU:HD12	2.33	0.43
1:C:391:ARG:O	1:C:392:LYS:HB2	2.18	0.43
2:B:225[B]:CYS:HB3	2:B:232:PHE:CE2	2.54	0.43
1:C:235:LEU:HB3	1:C:236:PRO:CD	2.49	0.43
1:A:54:PHE:CG	1:A:109:ARG:HD3	2.54	0.42
1:C:391:ARG:O	1:C:392:LYS:CB	2.66	0.42
2:D:220:HIS:HA	2:D:221:PRO:C	2.40	0.42
1:A:394:ARG:HE	1:A:394:ARG:HA	1.83	0.42
1:C:203:ARG:NH1	8:C:605:HOH:O	2.21	0.42
1:C:114:ARG:NH2	8:C:608:HOH:O	2.52	0.42
1:A:92:GLN:HA	1:A:95[B]:MET:CE	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:302:ASP:HB2	2:D:303:PRO:HD2	2.02	0.41
2:B:278[B]:THR:HG21	2:B:310:PHE:HD1	1.84	0.41
1:A:95[A]:MET:HE1	1:C:75:PHE:HE1	1.86	0.41
1:A:235:LEU:HB3	1:A:236:PRO:CD	2.51	0.41
2:B:217:THR:HG21	2:B:228:HIS:CD2	2.56	0.41
2:B:309[B]:VAL:HG12	2:B:310:PHE:N	2.36	0.40
1:C:4:LEU:HB3	1:C:5:PRO:HD3	2.02	0.40
2:D:188:ARG:HA	2:D:189:PRO:HD3	1.96	0.40

All (1) 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)
8:B:594:HOH:O	8:C:734:HOH:O[4_445]	2.01	0.19

## 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	391/403 (97%)	376 (96%)	15 (4%)	0	100	100
1	C	392/403 (97%)	379 (97%)	12 (3%)	1 (0%)	41	24
2	B	139/133 (104%)	137 (99%)	2 (1%)	0	100	100
2	D	128/133 (96%)	125 (98%)	3 (2%)	0	100	100
All	All	1050/1072 (98%)	1017 (97%)	32 (3%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	392	LYS

### 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	301/305 (99%)	295 (98%)	6 (2%)	55	38
1	C	302/305 (99%)	299 (99%)	3 (1%)	76	67
2	B	120/112 (107%)	118 (98%)	2 (2%)	60	46
2	D	109/112 (97%)	106 (97%)	3 (3%)	43	25
All	All	832/834 (100%)	818 (98%)	14 (2%)	62	46

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	PHE
1	A	231[A]	ARG
1	A	231[B]	ARG
1	A	296	HIS
1	A	330	ARG
1	A	394	ARG
2	B	188	ARG
2	B	299	LEU
1	C	111	PHE
1	C	117	VAL
1	C	296	HIS
2	D	188	ARG
2	D	299	LEU
2	D	300	GLU

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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 11 are monoatomic - leaving 5 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	EPE	A	502	-	15,15,15	0.95	1 (6%)	18,20,20	1.96	5 (27%)
4	EPE	D	402	-	15,15,15	0.87	1 (6%)	18,20,20	1.76	5 (27%)
6	PEG	A	507	-	6,6,6	0.53	0	5,5,5	0.34	0
6	PEG	C	504	-	6,6,6	0.53	0	5,5,5	0.41	0
4	EPE	B	402	-	15,15,15	0.73	1 (6%)	18,20,20	1.91	4 (22%)

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
4	EPE	A	502	-	-	3/9/19/19	0/1/1/1
4	EPE	D	402	-	-	0/9/19/19	0/1/1/1
6	PEG	A	507	-	-	2/4/4/4	-
6	PEG	C	504	-	-	1/4/4/4	-
4	EPE	B	402	-	-	5/9/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	EPE	C10-S	3.42	1.82	1.77
4	D	402	EPE	C10-S	2.73	1.81	1.77
4	B	402	EPE	C10-S	2.31	1.80	1.77

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	EPE	C5-N4-C3	4.84	119.72	108.83
4	B	402	EPE	O2S-S-C10	4.71	112.58	106.92
4	B	402	EPE	C5-N4-C3	4.37	118.66	108.83
4	D	402	EPE	C7-N4-C5	3.36	119.83	111.23
4	A	502	EPE	O3S-S-C10	3.24	111.02	105.77
4	D	402	EPE	C7-N4-C3	3.23	119.49	111.23
4	B	402	EPE	C7-N4-C3	3.21	119.45	111.23
4	A	502	EPE	C6-C5-N4	2.83	116.45	110.64
4	D	402	EPE	O1S-S-C10	2.78	110.26	106.92
4	B	402	EPE	C7-N4-C5	2.68	118.10	111.23
4	D	402	EPE	C5-N4-C3	2.36	114.15	108.83
4	A	502	EPE	C7-N4-C3	2.22	116.90	111.23
4	D	402	EPE	O3S-S-C10	2.19	109.32	105.77
4	A	502	EPE	C2-C3-N4	2.08	114.91	110.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	EPE	C10-C9-N1-C6
6	C	504	PEG	O1-C1-C2-O2
4	B	402	EPE	N4-C7-C8-O8
6	A	507	PEG	O1-C1-C2-O2
4	A	502	EPE	C10-C9-N1-C2
4	B	402	EPE	C10-C9-N1-C2
6	A	507	PEG	C4-C3-O2-C2
4	B	402	EPE	C10-C9-N1-C6
4	A	502	EPE	C8-C7-N4-C5
4	B	402	EPE	C9-C10-S-O3S
4	B	402	EPE	C8-C7-N4-C5

There are no ring outliers.

1 monomer is involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	504	PEG	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	382/403 (94%)	-0.45	5 (1%) 77 81	18, 26, 45, 118	0
1	C	382/403 (94%)	-0.29	7 (1%) 68 72	18, 25, 43, 135	0
2	B	131/133 (98%)	-0.12	9 (6%) 16 19	19, 26, 70, 112	0
2	D	127/133 (95%)	0.54	19 (14%) 2 2	25, 41, 79, 137	0
All	All	1022/1072 (95%)	-0.23	40 (3%) 39 44	18, 27, 58, 137	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	393	LEU	11.1
2	D	301	ALA	6.7
2	B	303	PRO	6.6
2	D	303	PRO	6.5
1	A	394	ARG	5.4
2	B	258	ALA	5.4
1	C	392	LYS	5.4
2	B	304	GLU	5.3
2	B	187	MET	5.2
2	B	301	ALA	4.9
1	A	117	VAL	4.9
2	B	188	ARG	4.7
1	A	393	LEU	4.6
2	D	258	ALA	4.6
1	A	128	MET	3.8
1	A	251[A]	TYR	3.8
1	C	3	VAL	3.7
2	D	302	ASP	3.7
2	B	302	ASP	3.5
2	D	304	GLU	3.4
2	B	305	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	213	ALA	3.3
1	C	391	ARG	3.1
2	D	281	VAL	3.1
1	C	2	SER	3.0
2	D	313	ALA	3.0
2	D	214	ALA	3.0
2	D	299	LEU	3.0
2	D	300	GLU	2.9
2	D	240	ALA	2.7
2	D	314	VAL	2.6
2	D	282	GLY	2.6
2	D	188	ARG	2.5
2	B	300	GLU	2.5
2	D	283	ILE	2.5
1	C	251[A]	TYR	2.4
2	D	215	CYS	2.2
1	C	117	VAL	2.1
2	D	239	ALA	2.1
2	D	295	VAL	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	CL	A	506	1/1	0.62	0.17	82,82,82,82	0
4	EPE	A	502	15/15	0.66	0.26	66,80,84,86	0
6	PEG	C	504	7/7	0.75	0.12	55,66,68,68	0
5	CL	A	505	1/1	0.76	0.07	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EPE	D	402	15/15	0.77	0.28	75,90,97,98	0
6	PEG	A	507	7/7	0.77	0.20	60,72,75,75	0
5	CL	C	502	1/1	0.78	0.43	90,90,90,90	0
4	EPE	B	402	15/15	0.85	0.24	59,71,77,80	0
5	CL	C	503	1/1	0.89	0.11	73,73,73,73	0
5	CL	A	504	1/1	0.90	0.23	69,69,69,69	0
5	CL	D	403	1/1	0.93	0.07	73,73,73,73	0
5	CL	A	503	1/1	0.98	0.22	49,49,49,49	0
3	NA	A	501	1/1	0.99	0.04	27,27,27,27	0
3	NA	C	501	1/1	1.00	0.05	24,24,24,24	0
7	ZN	B	401	1/1	1.00	0.06	27,27,27,27	0
7	ZN	D	401	1/1	1.00	0.03	36,36,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.