



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2017 – 04:19 PM EST

PDB ID : 5H7N  
Title : Crystal structure of human NLRP12-PYD with a MBP tag  
Authors : Jin, T.C.; Xiao, T.S.  
Deposited on : 2016-11-19  
Resolution : 1.85 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

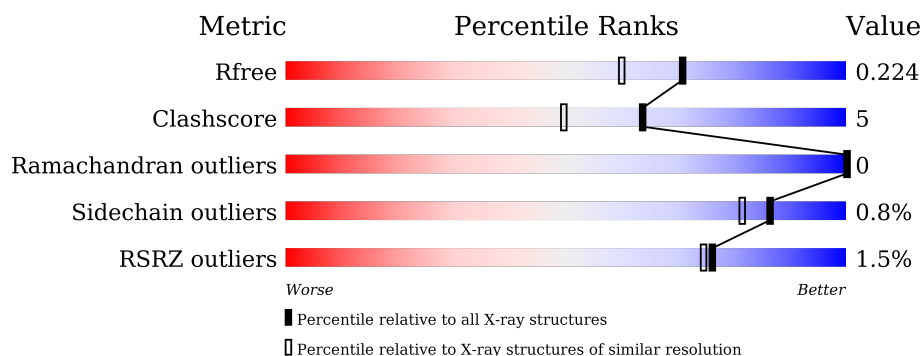
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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. 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	478	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 1px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; bottom: 0; left: 85%; width: 10%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; bottom: 0; left: 95%; width: 5%; height: 10px; background-color: grey;"></div> </div> <div> <span style="margin-right: 100px;">85%</span> <span>10%</span> <span style="margin-left: 10px;">.</span> </div> </div>
1	B	478	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 1px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; bottom: 0; left: 86%; width: 10%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; bottom: 0; left: 95%; width: 5%; height: 10px; background-color: grey;"></div> </div> <div> <span style="margin-right: 100px;">86%</span> <span>9%</span> <span style="margin-left: 10px;">..</span> </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	502	-	-	-	X
4	EDO	A	504	-	-	-	X
4	EDO	A	507	-	-	-	X
4	EDO	B	504	-	-	-	X
4	EDO	B	507	-	-	-	X
4	EDO	B	508	-	-	X	X

## 2 Entry composition [i](#)

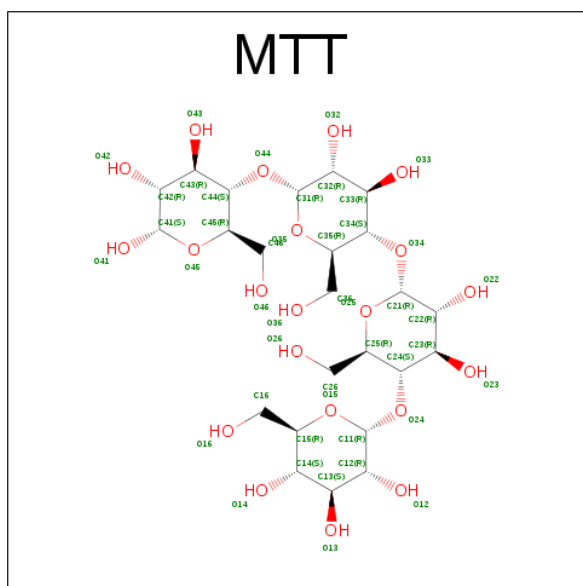
There are 6 unique types of molecules in this entry. The entry contains 7687 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NLRP12-PYD with MBP tag.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	2	0
			3556	2289	587	671	9			
1	B	460	Total	C	N	O	S	0	3	0
			3585	2309	590	677	9			

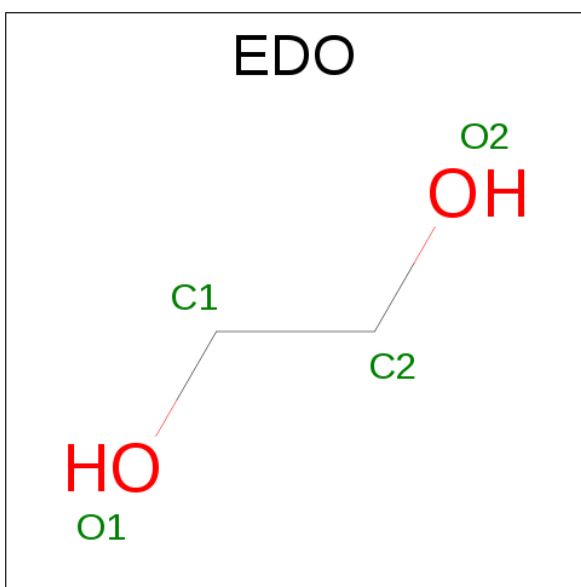
- Molecule 2 is MALTOTETRAOSE (three-letter code: MTT) (formula: C<sub>24</sub>H<sub>42</sub>O<sub>21</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

- Molecule 5 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
5	B	1	Total	C	O	0	0
			7	4	3		

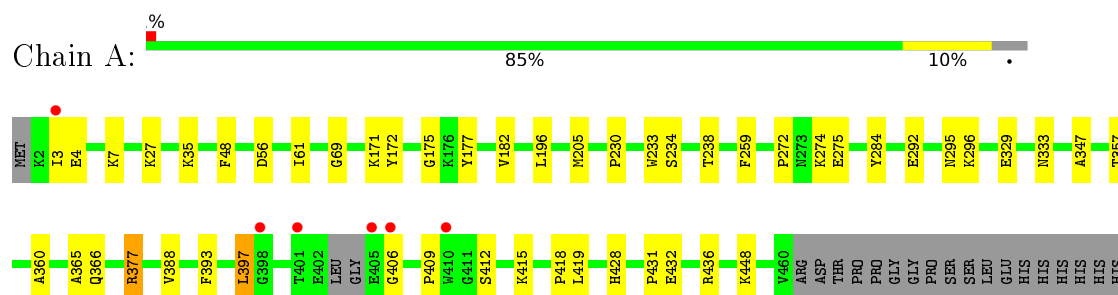
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	207	Total 207	O 207	0	0
6	B	191	Total 191	O 191	0	0

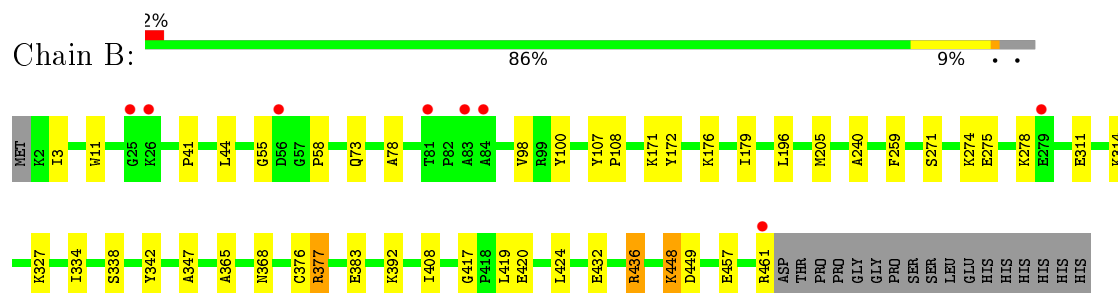
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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: NLRP12-PYD with MBP tag



- Molecule 1: NLRP12-PYD with MBP tag





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.54Å 104.55Å 110.94Å 90.00° 98.95° 90.00°	Depositor
Resolution (Å)	47.18 – 1.85 47.18 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.18-1.85) 91.0 (47.18-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.93 (at 1.84Å)	Xtriage
Refinement program	PHENIX (dev_2481: ???)	Depositor
R, $R_{free}$	0.179 , 0.224 0.177 , 0.224	Depositor DCC
$R_{free}$ test set	1915 reflections (2.51%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7687	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, SO4, MTT, EDO

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	0.67	0/3645	0.73	3/4945 (0.1%)
1	B	0.68	1/3678 (0.0%)	0.74	2/4991 (0.0%)
All	All	0.67	1/7323 (0.0%)	0.74	5/9936 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	376	CYS	CB-SG	-6.05	1.72	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	A	377	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	B	377	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	436	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	397	LEU	CA-CB-CG	-5.87	101.80	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	240	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	3556	0	3541	36	0
1	B	3585	0	3574	39	0
2	A	45	0	42	0	0
2	B	45	0	42	0	0
3	A	10	0	0	1	0
3	B	5	0	0	0	0
4	A	16	0	24	9	0
4	B	20	0	30	8	1
5	B	7	0	10	0	0
6	A	207	0	0	5	0
6	B	191	0	0	6	0
All	All	7687	0	7263	76	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 5.

All (76) 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)
4:B:507:EDO:H11	6:B:681:HOH:O	1.74	0.86
1:A:406:GLY:O	1:A:428:HIS:NE2	2.12	0.81
1:A:357:THR:HG23	1:A:360:ALA:H	1.49	0.77
1:B:179:ILE:HD11	1:B:377:ARG:HD2	1.67	0.76
1:A:366:GLN:NE2	6:A:601:HOH:O	2.15	0.74
1:A:4:GLU:OE1	1:A:7:LYS:HD3	1.89	0.73
1:B:3:ILE:H	1:B:3:ILE:HD12	1.55	0.71
1:A:275:GLU:H	4:A:507:EDO:H21	1.57	0.70
1:B:436:ARG:HH22	4:B:508:EDO:C2	2.04	0.69
1:A:377:ARG:HD2	6:A:731:HOH:O	1.94	0.68
1:A:432:GLU:OE2	1:A:436:ARG:NH2	2.28	0.67
1:A:388:VAL:HG11	6:B:778:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LEU:HB3	4:A:506:EDO:H12	1.81	0.63
1:A:329:GLU:OE2	4:A:505:EDO:H21	1.99	0.63
1:B:419:LEU:HB3	4:B:503:EDO:H12	1.81	0.62
1:B:3:ILE:N	1:B:3:ILE:HD12	2.15	0.62
1:B:271:SER:O	1:B:274:LYS:NZ	2.33	0.61
1:B:73:GLN:HG2	1:B:100:TYR:HE2	1.66	0.60
1:B:436:ARG:HH22	4:B:508:EDO:H22	1.67	0.58
1:B:73:GLN:HG2	1:B:100:TYR:CE2	2.39	0.58
1:A:448:LYS:NZ	3:A:503:SO4:O4	2.37	0.57
1:A:419:LEU:H	4:A:506:EDO:H11	1.70	0.56
1:B:436:ARG:HH22	4:B:508:EDO:H21	1.68	0.56
1:A:177:TYR:HE1	4:A:505:EDO:H11	1.71	0.55
1:B:448:LYS:HD2	1:B:449:ASP:N	2.21	0.55
4:A:504:EDO:O2	6:A:602:HOH:O	2.18	0.55
1:B:98:VAL:HG21	1:B:108:PRO:HD3	1.89	0.54
1:A:347:ALA:HB2	1:A:365:ALA:HB2	1.90	0.54
1:B:436:ARG:NH2	4:B:508:EDO:H21	2.23	0.54
1:A:69:GLY:HA3	1:A:333:ASN:O	2.08	0.53
1:A:48:PHE:CG	1:A:61:ILE:HD12	2.42	0.53
1:B:196:LEU:HD12	1:B:205:MET:HE1	1.91	0.53
1:B:176:LYS:HZ1	1:B:457:GLU:CD	2.12	0.52
1:B:408:ILE:HG21	1:B:424[B]:LEU:HD21	1.91	0.52
1:A:3:ILE:HG13	1:A:56:ASP:HA	1.92	0.51
1:A:7:LYS:HD2	1:A:35:LYS:HE3	1.93	0.51
1:A:274:LYS:HB2	4:A:507:EDO:H12	1.94	0.49
1:B:368:ASN:HB3	6:B:780:HOH:O	2.12	0.49
1:A:388:VAL:HG13	1:B:383:GLU:HB3	1.95	0.49
1:B:73:GLN:HG3	1:B:100:TYR:OH	2.12	0.49
1:A:418:PRO:HD2	4:A:506:EDO:H11	1.96	0.48
1:A:234:SER:O	1:A:238:THR:HG23	2.14	0.48
1:B:41:PRO:HG2	1:B:44:LEU:HB3	1.96	0.48
1:B:107:TYR:OH	1:B:278:LYS:HG3	2.13	0.48
1:A:295:ASN:HD22	1:A:296:LYS:NZ	2.12	0.47
1:A:296:LYS:HA	1:A:296:LYS:HD3	1.62	0.47
1:B:327:LYS:NZ	6:B:607:HOH:O	2.48	0.47
1:A:182:VAL:O	1:A:366:GLN:NE2	2.49	0.46
1:A:172:TYR:OH	1:A:175:GLY:HA2	2.16	0.46
1:B:338:SER:HB2	6:B:740:HOH:O	2.15	0.46
1:A:409:PRO:HG2	1:A:412:SER:OG	2.16	0.46
1:B:417:GLY:C	4:B:503:EDO:H11	2.37	0.46
1:B:275:GLU:H	1:B:275:GLU:CD	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ILE:CD1	1:B:3:ILE:H	2.26	0.45
1:A:292:GLU:O	1:A:296:LYS:HG2	2.17	0.44
1:B:196:LEU:CD1	1:B:205:MET:HE1	2.47	0.44
1:B:420:GLU:H	4:B:503:EDO:H12	1.83	0.44
1:A:27:LYS:HD3	1:A:284:TYR:CD2	2.53	0.43
1:A:196:LEU:HD12	1:A:205:MET:HE1	2.00	0.43
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.53	0.43
1:A:27:LYS:HD3	1:A:284:TYR:CE2	2.54	0.43
1:A:275:GLU:N	4:A:507:EDO:H21	2.28	0.43
1:B:338:SER:O	1:B:342:TYR:CD2	2.73	0.42
1:B:176:LYS:NZ	1:B:457:GLU:OE2	2.51	0.42
1:B:171:LYS:HD2	1:B:172:TYR:N	2.35	0.42
1:B:3:ILE:CD1	1:B:55:GLY:O	2.67	0.42
1:A:431:PRO:HD2	6:A:765:HOH:O	2.20	0.42
1:A:393:PHE:CE1	1:A:397:LEU:HD13	2.55	0.41
1:B:311:GLU:O	1:B:314:LYS:HG2	2.20	0.41
1:B:347:ALA:HB2	1:B:365:ALA:HB2	2.02	0.41
1:B:432:GLU:HG3	6:B:743:HOH:O	2.19	0.41
6:A:745:HOH:O	1:B:392:LYS:HE3	2.20	0.41
1:B:334:ILE:HG21	1:B:334:ILE:HD13	1.85	0.41
1:B:78:ALA:HB2	1:B:274:LYS:HE3	2.03	0.41
1:B:11:TRP:CD2	1:B:58:PRO:HG3	2.56	0.40
1:A:3:ILE:CG2	1:A:272:PRO:HD3	2.52	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)
4:B:507:EDO:O1	4:B:508:EDO:O1[2_8512]	2.08	0.12

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	455/478 (95%)	444 (98%)	11 (2%)	0	100	100
1	B	461/478 (96%)	453 (98%)	8 (2%)	0	100	100
All	All	916/956 (96%)	897 (98%)	19 (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	361/377 (96%)	358 (99%)	3 (1%)	86	81
1	B	364/377 (97%)	361 (99%)	3 (1%)	86	81
All	All	725/754 (96%)	719 (99%)	6 (1%)	86	81

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	LYS
1	A	259	PHE
1	A	415	LYS
1	B	259	PHE
1	B	448	LYS
1	B	461	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	ASN
1	A	366	GLN
1	B	254	GLN

### 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 ⓘ

15 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	MTT	A	501	-	48,48,48	1.84	10 (20%)	71,71,71	1.22	4 (5%)
3	SO4	A	502	-	4,4,4	0.33	0	6,6,6	0.38	0
3	SO4	A	503	-	4,4,4	0.12	0	6,6,6	0.11	0
4	EDO	A	504	-	3,3,3	0.65	0	2,2,2	0.29	0
4	EDO	A	505	-	3,3,3	1.03	0	2,2,2	0.71	0
4	EDO	A	506	-	3,3,3	0.42	0	2,2,2	0.66	0
4	EDO	A	507	-	3,3,3	0.64	0	2,2,2	1.05	0
2	MTT	B	501	-	48,48,48	1.97	14 (29%)	71,71,71	1.39	9 (12%)
3	SO4	B	502	-	4,4,4	0.35	0	6,6,6	0.53	0
4	EDO	B	503	-	3,3,3	0.33	0	2,2,2	0.75	0
4	EDO	B	504	-	3,3,3	0.58	0	2,2,2	0.32	0
4	EDO	B	505	-	3,3,3	0.53	0	2,2,2	0.39	0
5	PEG	B	506	-	6,6,6	0.53	0	5,5,5	0.48	0
4	EDO	B	507	-	3,3,3	0.59	0	2,2,2	0.10	0
4	EDO	B	508	-	3,3,3	0.77	0	2,2,2	0.79	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	MTT	A	501	-	-	0/20/100/100	0/4/4/4
3	SO4	A	502	-	-	0/0/0/0	0/0/0/0
3	SO4	A	503	-	-	0/0/0/0	0/0/0/0
4	EDO	A	504	-	-	0/1/1/1	0/0/0/0
4	EDO	A	505	-	-	0/1/1/1	0/0/0/0
4	EDO	A	506	-	-	0/1/1/1	0/0/0/0
4	EDO	A	507	-	-	0/1/1/1	0/0/0/0
2	MTT	B	501	-	-	0/20/100/100	0/4/4/4
3	SO4	B	502	-	-	0/0/0/0	0/0/0/0
4	EDO	B	503	-	-	0/1/1/1	0/0/0/0
4	EDO	B	504	-	-	0/1/1/1	0/0/0/0
4	EDO	B	505	-	-	0/1/1/1	0/0/0/0
5	PEG	B	506	-	-	0/4/4/4	0/0/0/0
4	EDO	B	507	-	-	0/1/1/1	0/0/0/0
4	EDO	B	508	-	-	0/1/1/1	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	MTT	C16-C15	-3.36	1.40	1.51
2	A	501	MTT	C16-C15	-3.20	1.40	1.51
2	A	501	MTT	C26-C25	-2.87	1.41	1.51
2	B	501	MTT	C36-C35	-2.75	1.42	1.51
2	B	501	MTT	C26-C25	-2.74	1.42	1.51
2	A	501	MTT	C36-C35	-2.71	1.42	1.51
2	B	501	MTT	C41-C42	-2.46	1.47	1.52
2	A	501	MTT	O42-C42	2.08	1.47	1.43
2	B	501	MTT	O12-C12	2.10	1.47	1.43
2	B	501	MTT	O25-C21	2.37	1.47	1.41
2	A	501	MTT	O15-C11	2.41	1.48	1.41
2	B	501	MTT	C34-C35	2.49	1.59	1.52
2	B	501	MTT	O42-C42	2.58	1.49	1.43
2	A	501	MTT	O33-C33	2.88	1.49	1.43
2	B	501	MTT	O15-C11	3.21	1.50	1.41
2	B	501	MTT	O33-C33	3.24	1.50	1.43
2	B	501	MTT	O25-C25	3.50	1.53	1.44
2	A	501	MTT	O35-C35	3.56	1.53	1.44
2	A	501	MTT	O25-C25	3.96	1.54	1.44
2	A	501	MTT	O45-C45	4.19	1.54	1.44
2	B	501	MTT	O35-C35	4.25	1.55	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	MTT	O45-C45	4.35	1.55	1.44
2	A	501	MTT	O15-C15	4.83	1.56	1.44
2	B	501	MTT	O15-C15	5.06	1.57	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	MTT	O43-C43-C42	-3.70	102.02	110.36
2	B	501	MTT	O34-C34-C35	-3.47	100.08	109.33
2	B	501	MTT	O44-C31-O35	-3.17	102.43	110.69
2	A	501	MTT	O15-C15-C14	-3.10	103.75	109.67
2	B	501	MTT	O24-C24-C25	-3.10	101.08	109.33
2	B	501	MTT	O32-C32-C31	-2.87	103.64	110.01
2	A	501	MTT	O35-C35-C34	-2.87	103.66	109.78
2	A	501	MTT	O13-C13-C12	-2.22	105.34	110.36
2	B	501	MTT	O42-C42-C41	-2.17	104.98	109.74
2	B	501	MTT	O41-C41-O45	-2.16	104.30	110.33
2	B	501	MTT	O43-C43-C44	-2.04	105.06	109.89
2	B	501	MTT	C11-C12-C13	2.00	113.95	109.98
2	A	501	MTT	C22-C23-C24	2.55	115.25	109.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	SO4	1	0
4	A	504	EDO	1	0
4	A	505	EDO	2	0
4	A	506	EDO	3	0
4	A	507	EDO	3	0
4	B	503	EDO	3	0
4	B	507	EDO	1	1
4	B	508	EDO	4	1

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	457/478 (95%)	-0.10	6 (1%) 79 78	29, 43, 64, 98	0
1	B	460/478 (96%)	-0.03	8 (1%) 73 71	26, 43, 71, 91	0
All	All	917/956 (95%)	-0.06	14 (1%) 76 74	26, 43, 68, 98	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	406	GLY	6.3
1	A	3	ILE	3.7
1	A	410	TRP	3.4
1	B	83	ALA	3.0
1	A	405	GLU	2.9
1	B	81	THR	2.9
1	A	398	GLY	2.4
1	B	56	ASP	2.3
1	B	461	ARG	2.3
1	B	84	ALA	2.2
1	B	26	LYS	2.2
1	B	25	GLY	2.1
1	A	401	THR	2.1
1	B	279	GLU	2.1

### 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 ⓘ

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<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	B	507	4/4	0.66	0.41	28.64	50,73,83,84	0
4	EDO	B	508	4/4	0.59	0.47	21.48	72,87,91,93	0
3	SO4	A	502	5/5	0.85	0.32	9.27	76,76,93,110	0
4	EDO	A	507	4/4	0.83	0.12	3.75	40,47,54,55	0
4	EDO	A	504	4/4	0.90	0.20	3.60	48,49,56,63	0
4	EDO	B	504	4/4	0.92	0.15	3.19	53,58,69,74	0
4	EDO	A	505	4/4	0.81	0.16	1.78	47,50,56,61	0
2	MTT	A	501	45/45	0.95	0.12	0.76	26,36,66,69	0
4	EDO	A	506	4/4	0.91	0.13	0.57	51,61,65,66	0
2	MTT	B	501	45/45	0.96	0.10	-0.15	29,38,70,74	0
5	PEG	B	506	7/7	0.86	0.10	-0.26	57,59,66,79	0
3	SO4	B	502	5/5	0.97	0.07	-3.15	60,74,78,79	0
3	SO4	A	503	5/5	0.95	0.15	-	79,85,91,94	0
4	EDO	B	503	4/4	0.96	0.10	-	45,50,62,63	0
4	EDO	B	505	4/4	0.80	0.14	-	57,59,66,66	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.