



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2025 – 01:37 pm BST

PDB ID : 9RWD / pdb\_00009rwd  
Title : High-resolution structure of human SHMT2 with covalently bound PLP (internal aldimine)  
Authors : Warlich, A.; Ruszkowski, M.; Nawrot, D.  
Deposited on : 2025-07-09  
Resolution : 1.30 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

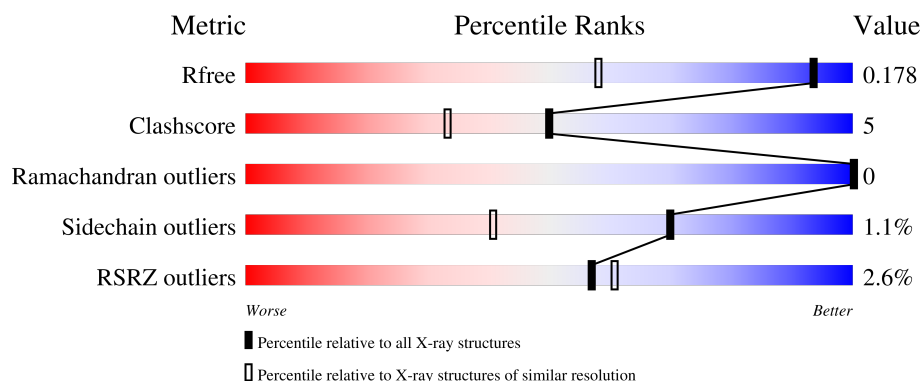
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.30 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))
$R_{free}$	164625	1387 (1.30-1.30)
Clashscore	180529	1497 (1.30-1.30)
Ramachandran outliers	177936	1455 (1.30-1.30)
Sidechain outliers	177891	1455 (1.30-1.30)
RSRZ outliers	164620	1384 (1.30-1.30)

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  $\geq 3$ , 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	476	<div> <div>2%</div> <div>87% 8% 5%</div> </div>
1	B	476	<div> <div>3%</div> <div>86% 10% .</div> </div>
1	C	476	<div> <div>3%</div> <div>84% 10% 5%</div> </div>
1	D	476	<div> <div>2%</div> <div>86% 9% 5%</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
2	EDO	A	601	-	-	X	-
2	EDO	D	602	-	-	X	-
4	PEG	D	604	-	-	X	-

## 2 Entry composition [i](#)

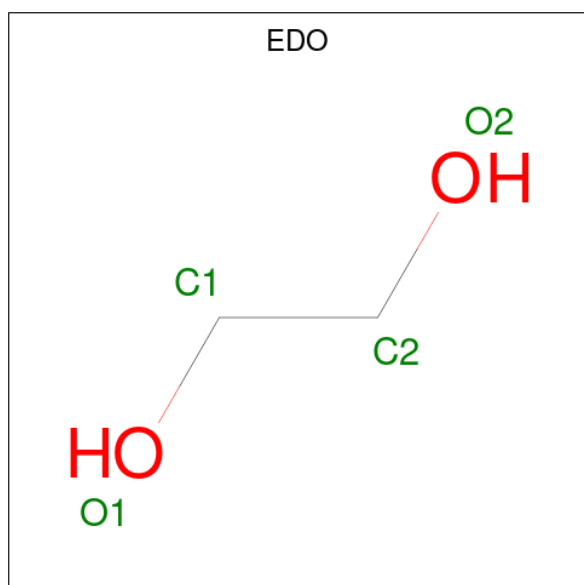
There are 6 unique types of molecules in this entry. The entry contains 16687 atoms, of which 148 are hydrogens and 0 are deuteriums.

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 Serine hydroxymethyltransferase, mitochondrial.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	453	Total	C	H	N	O	P	S		0	4	0
			3584	2256	8	639	664	1	16				
1	B	461	Total	C	H	N	O	P	S		0	4	0
			3638	2287	8	649	677	1	16				
1	C	452	Total	C	H	N	O	P	S		0	3	0
			3571	2245	8	638	663	1	16				
1	D	453	Total	C	H	N	O	P	S		0	2	0
			3571	2246	8	636	664	1	16				

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			4	2	2			
2	A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Na 1	0	0
5	B	1	Total 1	Na 1	0	0
5	C	1	Total 1	Na 1	0	0
5	D	1	Total 1	Na 1	0	0


- Molecule 6 is water.

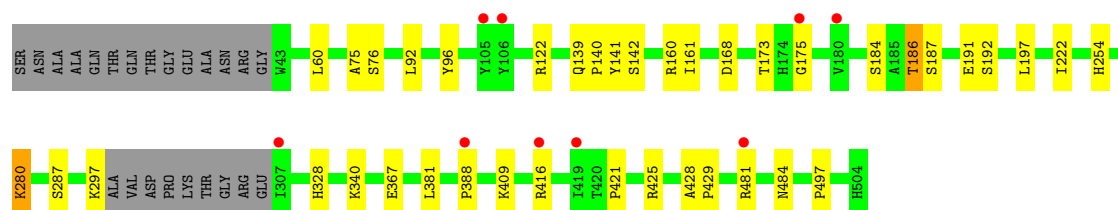
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	582	Total 582	O 582	0	0
6	B	573	Total 573	O 573	0	0
6	C	502	Total 502	O 502	0	0
6	D	456	Total 456	O 456	0	0

### 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.

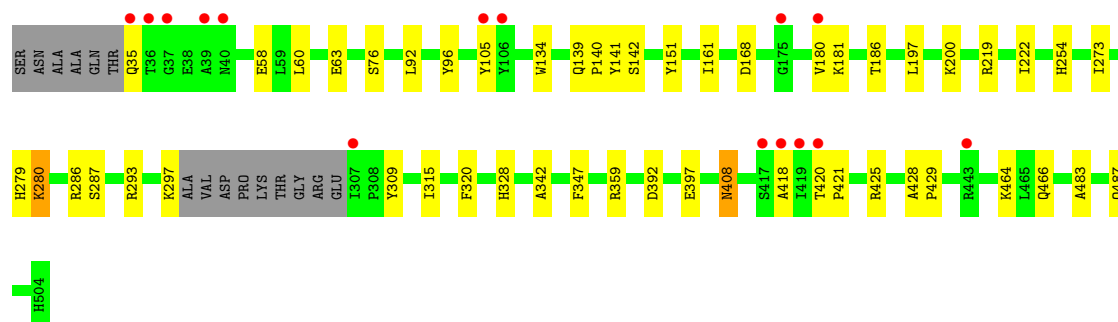
- Molecule 1: Serine hydroxymethyltransferase, mitochondrial

Chain A: 




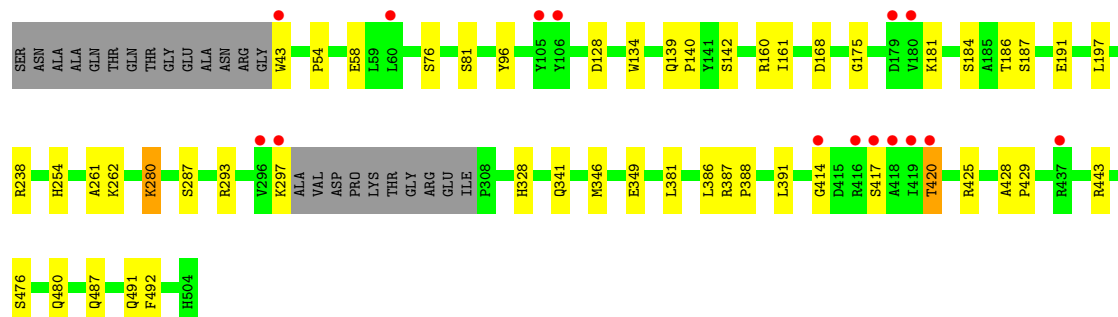
- Molecule 1: Serine hydroxymethyltransferase, mitochondrial

Chain B: 



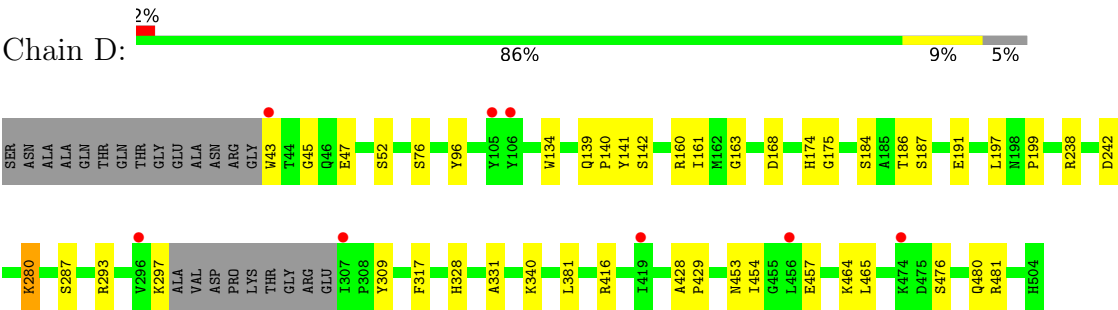
- Molecule 1: Serine hydroxymethyltransferase, mitochondrial

Chain C: 





● Molecule 1: Serine hydroxymethyltransferase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.18Å 125.57Å 135.14Å 90.00° 93.67° 90.00°	Depositor
Resolution (Å)	59.06 – 1.30 59.06 – 1.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (59.06-1.30) 97.7 (59.06-1.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 1.30Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.145 , 0.178 0.145 , 0.178	Depositor DCC
$R_{free}$ test set	1001 reflections (0.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.3	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	16687	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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, LLP, NA, EDO, TRS

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	0.23	0/3634	0.46	0/4912
1	B	0.22	0/3688	0.45	0/4985
1	C	0.20	0/3618	0.43	0/4889
1	D	0.18	0/3615	0.42	0/4887
All	All	0.21	0/14555	0.44	0/19673

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 [i](#)

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	3576	8	3576	35	0
1	B	3630	8	3625	37	0
1	C	3563	8	3555	42	0
1	D	3563	8	3552	41	0
2	A	16	18	24	4	0
2	B	20	30	30	3	0
2	C	20	30	30	7	0
2	D	12	18	18	7	0
3	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	7	10	10	1	0
4	D	7	10	10	8	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	582	0	0	7	0
6	B	573	0	0	6	0
6	C	502	0	0	5	0
6	D	456	0	0	1	0
All	All	16539	148	14442	151	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (151) 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:464:LYS:HD3	1:B:466:GLN:H	1.21	1.02
1:A:161[A]:ILE:HD11	1:A:222:ILE:HD11	1.48	0.95
1:C:184:SER:OG	1:C:186[B]:THR:HG22	1.67	0.92
1:D:184:SER:OG	1:D:186[B]:THR:HG22	1.70	0.92
1:A:184:SER:OG	1:A:186[A]:THR:HG22	1.70	0.89
1:A:497:PRO:HD3	4:A:606:PEG:H41	1.55	0.89
1:D:175:GLY:HA2	1:D:186[B]:THR:HG23	1.57	0.85
1:C:175:GLY:HA2	1:C:186[B]:THR:HG23	1.58	0.84
1:A:75:ALA:HB3	1:A:425[B]:ARG:HH11	1.46	0.80
1:C:43:TRP:HE1	2:C:604:EDO:H21	1.50	0.77
1:D:43:TRP:HE1	4:D:604:PEG:H32	1.51	0.75
1:D:141:TYR:HA	2:D:602:EDO:H22	1.67	0.74
1:C:54:PRO:O	1:C:58:GLU:HG2	1.87	0.74
1:B:35:GLN:HG2	6:B:1059:HOH:O	1.88	0.72
1:D:47:GLU:HB2	4:D:604:PEG:H21	1.72	0.70
1:C:81:SER:HB2	4:D:604:PEG:C1	2.21	0.70
1:B:483:ALA:O	1:B:487:GLN:HG3	1.90	0.70
1:D:184:SER:HG	1:D:186[B]:THR:HG22	1.53	0.70
1:A:175:GLY:HA2	1:A:186[A]:THR:HG23	1.75	0.69
1:B:328:HIS:HB2	2:B:601:EDO:H12	1.75	0.68
1:D:464:LYS:HE3	1:D:465:LEU:H	1.58	0.67
1:C:184:SER:HG	1:C:186[B]:THR:HG22	1.62	0.65
1:B:464:LYS:HD3	1:B:466:GLN:N	2.02	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ARG:HD2	6:B:864:HOH:O	1.96	0.64
1:D:199:PRO:HD3	2:D:603:EDO:H11	1.80	0.64
1:B:464:LYS:HG2	6:B:1065:HOH:O	1.97	0.64
1:D:287:SER:HA	2:D:602:EDO:H11	1.79	0.63
1:B:425:ARG:HD3	6:B:944:HOH:O	1.99	0.62
1:A:161[A]:ILE:CD1	1:A:222:ILE:HD11	2.25	0.62
1:A:141:TYR:HA	2:A:601:EDO:H22	1.81	0.61
1:B:408:ASN:OD1	1:B:425:ARG:HB3	2.00	0.61
1:D:45:GLY:HA2	4:D:604:PEG:H12	1.81	0.61
1:D:161:ILE:HD11	1:D:186[A]:THR:HG22	1.81	0.61
1:B:273:ILE:HD12	1:B:315[B]:ILE:HD11	1.82	0.60
1:A:328:HIS:HB2	2:A:601:EDO:H21	1.83	0.60
1:C:261:ALA:C	1:C:262:LYS:HD2	2.27	0.60
1:C:81:SER:HB2	4:D:604:PEG:H11	1.83	0.59
1:C:417:SER:HB2	1:C:420:THR:HG23	1.84	0.59
1:B:464:LYS:CD	1:B:466:GLN:H	2.08	0.59
1:C:161:ILE:HD11	1:C:186[A]:THR:HG22	1.85	0.58
1:A:173:THR:O	1:A:186[B]:THR:HG21	2.04	0.57
1:B:392:ASP:CG	1:B:420:THR:HG23	2.29	0.57
1:D:238:ARG:HD3	1:D:238:ARG:O	2.05	0.57
1:A:388:PRO:HB2	6:A:714:HOH:O	2.04	0.57
1:D:43:TRP:HE1	4:D:604:PEG:C3	2.18	0.56
1:D:328:HIS:HB2	2:D:602:EDO:H21	1.86	0.56
1:D:340:LYS:HE3	6:D:1100:HOH:O	2.04	0.56
1:D:175:GLY:CA	1:D:186[B]:THR:HG23	2.35	0.56
1:C:328:HIS:HB2	2:C:603:EDO:H12	1.89	0.55
1:D:174:HIS:O	2:D:601:EDO:H22	2.06	0.55
1:C:297:LYS:HA	6:C:1063:HOH:O	2.07	0.55
1:A:161[A]:ILE:HD11	1:A:222:ILE:CD1	2.31	0.55
1:A:175:GLY:HA2	1:A:186[B]:THR:OG1	2.07	0.54
1:C:262:LYS:HE3	6:C:702:HOH:O	2.07	0.54
1:D:175:GLY:O	1:D:187[A]:SER:OG	2.26	0.54
1:A:287:SER:HA	2:A:601:EDO:H11	1.90	0.54
1:A:92:LEU:HD11	1:B:60:LEU:CD2	2.38	0.53
1:A:75:ALA:HB3	1:A:425[B]:ARG:NH1	2.19	0.53
1:C:491:GLN:O	2:C:602:EDO:H12	2.09	0.52
1:B:464:LYS:HD2	1:B:466:GLN:HG2	1.90	0.52
1:B:219:ARG:HG2	6:B:856:HOH:O	2.10	0.52
1:C:175:GLY:HA2	1:C:186[B]:THR:CG2	2.36	0.52
1:B:58:GLU:HG2	6:B:1076:HOH:O	2.10	0.51
1:C:128:ASP:OD2	1:C:262:LYS:HE3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:ARG:HD2	1:C:492:PHE:CE1	2.45	0.51
1:B:76:SER:HB2	1:B:280:LLP:HE3	1.92	0.50
1:C:175:GLY:CA	1:C:186[B]:THR:HG23	2.36	0.50
1:D:52:SER:HB2	4:D:604:PEG:H42	1.93	0.50
1:C:487:GLN:O	1:C:491:GLN:HG3	2.12	0.50
1:C:387:ARG:NH2	1:C:414:GLY:HA3	2.27	0.50
1:A:425[A]:ARG:HD3	6:A:744:HOH:O	2.11	0.49
1:A:297:LYS:HE3	6:A:1129:HOH:O	2.13	0.49
1:A:484:ASN:HB3	6:A:704:HOH:O	2.12	0.48
1:B:151:TYR:HE2	1:B:186[A]:THR:HG21	1.78	0.48
1:D:428:ALA:N	1:D:429:PRO:CD	2.77	0.48
1:D:175:GLY:HA2	1:D:186[B]:THR:CG2	2.37	0.47
1:A:367:GLU:HG3	6:A:955:HOH:O	2.13	0.47
1:C:161:ILE:HD11	1:C:186[A]:THR:CG2	2.45	0.47
1:C:428:ALA:N	1:C:429:PRO:CD	2.78	0.47
1:D:297:LYS:HA	1:D:309:TYR:CE2	2.49	0.47
1:B:420:THR:HG22	1:B:420:THR:O	2.15	0.47
1:D:76:SER:HB2	1:D:280:LLP:HE3	1.96	0.47
1:C:43:TRP:HE1	2:C:604:EDO:C2	2.24	0.47
1:C:386:LEU:HB3	1:C:391:LEU:O	2.15	0.46
1:B:141:TYR:HA	2:B:601:EDO:H11	1.98	0.46
1:D:161:ILE:HD11	1:D:186[A]:THR:CG2	2.44	0.46
1:D:453:ASN:O	1:D:457:GLU:HG3	2.16	0.46
1:A:481:ARG:NH1	6:A:704:HOH:O	2.49	0.45
1:D:238:ARG:HD2	1:D:242:ASP:OD2	2.16	0.45
1:D:454:ILE:CD1	1:D:481:ARG:HG2	2.47	0.45
1:C:287:SER:OG	2:C:603:EDO:C2	2.65	0.45
1:B:180:VAL:O	1:B:181:LYS:HB3	2.17	0.45
1:B:287:SER:OG	2:B:601:EDO:C2	2.64	0.45
1:A:287:SER:OG	2:A:601:EDO:C1	2.65	0.44
1:C:387:ARG:HB2	1:C:388:PRO:HD3	1.98	0.44
1:C:341:GLN:NE2	4:D:604:PEG:H31	2.32	0.44
1:C:346:MET:HG3	1:D:43:TRP:HB2	1.98	0.44
1:A:76:SER:HB2	1:A:280:LLP:HE3	2.00	0.44
1:B:428:ALA:N	1:B:429:PRO:CD	2.80	0.44
1:B:105:TYR:HE1	1:B:320:PHE:HE2	1.66	0.44
1:D:139:GLN:N	1:D:140:PRO:CD	2.81	0.44
1:B:392:ASP:CB	1:B:420:THR:HG23	2.48	0.44
1:C:139:GLN:N	1:C:140:PRO:CD	2.80	0.43
1:A:60:LEU:CD2	1:B:92:LEU:HD11	2.48	0.43
1:C:76:SER:HB2	1:C:280:LLP:HE3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:603:EDO:C1	6:C:735:HOH:O	2.66	0.43
1:B:464:LYS:CD	1:B:466:GLN:HG2	2.49	0.43
1:C:181:LYS:HE2	1:D:317:PHE:CZ	2.53	0.43
1:C:425[A]:ARG:HG2	6:C:732:HOH:O	2.18	0.43
1:D:476:SER:O	1:D:480:GLN:HG3	2.18	0.43
1:A:160:ARG:HA	1:A:191:GLU:O	2.18	0.43
1:D:161:ILE:CD1	1:D:186[A]:THR:CG2	2.96	0.43
1:A:92:LEU:HD23	1:B:63:GLU:HG2	2.00	0.43
1:D:163:GLY:H	2:D:601:EDO:H21	1.83	0.43
1:A:175:GLY:O	1:A:192:SER:OG	2.35	0.43
1:A:425[B]:ARG:HG2	6:A:731:HOH:O	2.19	0.43
1:B:35:GLN:O	1:B:35:GLN:HG3	2.19	0.43
1:D:168:ASP:HB3	1:D:197:LEU:HG	2.01	0.43
1:D:381:LEU:HD12	1:D:381:LEU:C	2.44	0.43
1:C:417:SER:HB2	1:C:420:THR:CG2	2.48	0.42
1:A:428:ALA:N	1:A:429:PRO:CD	2.82	0.42
1:D:160:ARG:HA	1:D:191:GLU:O	2.19	0.42
1:C:175:GLY:O	1:C:187[B]:SER:OG	2.37	0.42
1:A:168:ASP:HB3	1:A:197:LEU:HG	2.02	0.42
1:C:381:LEU:C	1:C:381:LEU:HD12	2.44	0.42
1:D:464:LYS:HE3	1:D:465:LEU:N	2.31	0.42
1:A:416:ARG:HD2	1:A:416:ARG:N	2.34	0.42
1:C:43:TRP:NE1	2:C:604:EDO:H21	2.26	0.42
1:D:134:TRP:CZ2	1:D:293:ARG:HD3	2.55	0.42
1:A:175:GLY:O	1:A:187[A]:SER:OG	2.38	0.42
1:D:416:ARG:HB3	1:D:416:ARG:NH1	2.35	0.42
1:A:122:ARG:CZ	1:A:340:LYS:HD2	2.50	0.41
1:B:161[B]:ILE:CG2	1:B:222:ILE:HD11	2.49	0.41
1:C:238:ARG:O	1:C:238:ARG:HD3	2.19	0.41
1:D:428:ALA:N	1:D:429:PRO:HD3	2.35	0.41
1:C:134:TRP:CZ2	1:C:293:ARG:HD3	2.56	0.41
1:A:139:GLN:N	1:A:140:PRO:CD	2.83	0.41
1:B:297:LYS:HG3	1:B:309:TYR:CE1	2.55	0.41
1:A:409:LYS:HB2	1:A:421:PRO:HG2	2.03	0.41
1:C:160:ARG:HA	1:C:191:GLU:O	2.21	0.41
1:C:168:ASP:HB3	1:C:197:LEU:HG	2.02	0.41
1:C:476:SER:O	1:C:480:GLN:HG3	2.21	0.41
1:B:342:ALA:HA	1:B:347:PHE:CG	2.55	0.41
1:B:279:HIS:ND1	1:B:286:ARG:HA	2.36	0.41
1:B:418:ALA:O	1:B:421:PRO:HD3	2.21	0.41
1:D:331:ALA:HB1	2:D:602:EDO:H12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:TRP:CZ2	1:B:293:ARG:HD3	2.56	0.40
1:B:139:GLN:N	1:B:140:PRO:CD	2.84	0.40
1:B:168:ASP:HB3	1:B:197:LEU:HG	2.03	0.40
1:A:381:LEU:HD12	1:A:381:LEU:C	2.46	0.40
1:C:349:GLU:HG2	6:C:1182:HOH:O	2.20	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	452/476 (95%)	438 (97%)	14 (3%)	0	100	100
1	B	460/476 (97%)	447 (97%)	13 (3%)	0	100	100
1	C	450/476 (94%)	439 (98%)	11 (2%)	0	100	100
1	D	450/476 (94%)	439 (98%)	11 (2%)	0	100	100
All	All	1812/1904 (95%)	1763 (97%)	49 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	377/389 (97%)	372 (99%)	5 (1%)	65	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	382/389 (98%)	376 (98%)	6 (2%)	58	25
1	C	375/389 (96%)	371 (99%)	4 (1%)	70	41
1	D	375/389 (96%)	373 (100%)	2 (0%)	86	67
All	All	1509/1556 (97%)	1492 (99%)	17 (1%)	70	41

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	TYR
1	A	142	SER
1	A	186[A]	THR
1	A	186[B]	THR
1	A	254	HIS
1	B	96	TYR
1	B	142	SER
1	B	200	LYS
1	B	254	HIS
1	B	397	GLU
1	B	408	ASN
1	C	96	TYR
1	C	142	SER
1	C	254	HIS
1	C	420	THR
1	D	96	TYR
1	D	142	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	156	GLN
1	A	329	ASN
1	B	270	HIS
1	B	329	ASN
1	C	270	HIS
1	C	329	ASN
1	C	480	GLN
1	C	487	GLN
1	D	156	GLN
1	D	329	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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
1	LLP	C	280	1	23,24,25	1.12	1 (4%)	25,32,34	1.45	4 (16%)
1	LLP	D	280	1	23,24,25	1.05	1 (4%)	25,32,34	1.59	4 (16%)
1	LLP	B	280	1	23,24,25	1.04	1 (4%)	25,32,34	1.60	5 (20%)
1	LLP	A	280	1	23,24,25	1.06	1 (4%)	25,32,34	1.67	5 (20%)

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
1	LLP	C	280	1	-	4/16/17/19	0/1/1/1
1	LLP	D	280	1	-	4/16/17/19	0/1/1/1
1	LLP	B	280	1	-	5/16/17/19	0/1/1/1
1	LLP	A	280	1	-	5/16/17/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	280	LLP	P-OP4	3.68	1.72	1.60
1	D	280	LLP	P-OP4	3.55	1.71	1.60
1	B	280	LLP	P-OP4	3.48	1.71	1.60
1	A	280	LLP	P-OP4	3.45	1.71	1.60

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	280	LLP	OP4-C5'-C5	4.36	117.66	109.35
1	B	280	LLP	OP4-C5'-C5	4.33	117.59	109.35
1	A	280	LLP	OP4-C5'-C5	3.94	116.87	109.35
1	D	280	LLP	OP4-C5'-C5	3.86	116.71	109.35
1	D	280	LLP	CE-NZ-C4'	3.62	130.03	118.90
1	A	280	LLP	C5'-C5-C6	-3.59	113.46	119.37
1	B	280	LLP	CE-NZ-C4'	3.17	128.62	118.90
1	D	280	LLP	C5'-C5-C6	-3.12	114.23	119.37
1	A	280	LLP	CE-NZ-C4'	3.11	128.46	118.90
1	B	280	LLP	C5'-C5-C6	-2.79	114.79	119.37
1	C	280	LLP	CE-NZ-C4'	2.67	127.10	118.90
1	D	280	LLP	C4-C4'-NZ	-2.40	113.28	124.31
1	A	280	LLP	C4-C4'-NZ	-2.34	113.54	124.31
1	C	280	LLP	C4-C4'-NZ	-2.31	113.71	124.31
1	B	280	LLP	OP4-P-OP1	-2.30	100.02	106.47
1	A	280	LLP	OP2-P-OP4	-2.10	101.14	106.73
1	B	280	LLP	C4-C4'-NZ	-2.07	114.82	124.31
1	C	280	LLP	C5'-C5-C6	-2.02	116.05	119.37

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	LLP	O-C-CA-CB
1	B	280	LLP	O-C-CA-CB
1	C	280	LLP	O-C-CA-CB
1	D	280	LLP	O-C-CA-CB
1	C	280	LLP	CG-CD-CE-NZ
1	D	280	LLP	CG-CD-CE-NZ
1	B	280	LLP	C6-C5-C5'-OP4
1	B	280	LLP	CG-CD-CE-NZ
1	C	280	LLP	CD-CE-NZ-C4'
1	D	280	LLP	CD-CE-NZ-C4'
1	A	280	LLP	CG-CD-CE-NZ
1	A	280	LLP	C5'-OP4-P-OP1
1	D	280	LLP	C3-C4-C4'-NZ
1	A	280	LLP	CD-CE-NZ-C4'
1	B	280	LLP	CD-CE-NZ-C4'
1	A	280	LLP	C3-C4-C4'-NZ
1	C	280	LLP	C3-C4-C4'-NZ
1	B	280	LLP	C3-C4-C4'-NZ

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	280	LLP	1	0
1	D	280	LLP	1	0
1	B	280	LLP	1	0
1	A	280	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	EDO	A	601	-	3,3,3	0.29	0	2,2,2	0.36	0
2	EDO	D	601	-	3,3,3	0.32	0	2,2,2	0.47	0
2	EDO	A	603	-	3,3,3	0.27	0	2,2,2	0.48	0
2	EDO	B	603	-	3,3,3	0.26	0	2,2,2	0.54	0
4	PEG	D	604	-	6,6,6	0.24	0	5,5,5	0.16	0
2	EDO	C	603	-	3,3,3	0.27	0	2,2,2	0.25	0
2	EDO	D	603	-	3,3,3	0.27	0	2,2,2	0.49	0
4	PEG	A	606	-	6,6,6	0.24	0	5,5,5	0.50	0
2	EDO	C	605	-	3,3,3	0.27	0	2,2,2	0.30	0
2	EDO	B	601	-	3,3,3	0.28	0	2,2,2	0.50	0
2	EDO	C	604	-	3,3,3	0.27	0	2,2,2	0.49	0
2	EDO	C	601	-	3,3,3	0.30	0	2,2,2	0.37	0
2	EDO	B	602	-	3,3,3	0.28	0	2,2,2	0.21	0
2	EDO	B	604	-	3,3,3	0.25	0	2,2,2	0.48	0
2	EDO	B	605	-	3,3,3	0.30	0	2,2,2	0.35	0
2	EDO	A	604	-	3,3,3	0.31	0	2,2,2	0.06	0
2	EDO	C	602	-	3,3,3	0.25	0	2,2,2	0.45	0
2	EDO	A	602	-	3,3,3	0.28	0	2,2,2	0.40	0
2	EDO	D	602	-	3,3,3	0.27	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	TRS	A	605	-	7,7,7	0.34	0	9,9,9	0.74	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	EDO	A	601	-	-	0/1/1/1	-
2	EDO	D	601	-	-	0/1/1/1	-
2	EDO	A	603	-	-	0/1/1/1	-
2	EDO	B	603	-	-	0/1/1/1	-
4	PEG	D	604	-	-	4/4/4/4	-
2	EDO	C	603	-	-	0/1/1/1	-
2	EDO	D	603	-	-	0/1/1/1	-
4	PEG	A	606	-	-	2/4/4/4	-
2	EDO	C	605	-	-	0/1/1/1	-
2	EDO	B	601	-	-	0/1/1/1	-
2	EDO	C	604	-	-	0/1/1/1	-
2	EDO	C	601	-	-	0/1/1/1	-
2	EDO	B	602	-	-	0/1/1/1	-
2	EDO	B	604	-	-	0/1/1/1	-
2	EDO	B	605	-	-	1/1/1/1	-
2	EDO	A	604	-	-	0/1/1/1	-
2	EDO	C	602	-	-	1/1/1/1	-
2	EDO	A	602	-	-	1/1/1/1	-
2	EDO	D	602	-	-	0/1/1/1	-
3	TRS	A	605	-	-	0/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	606	PEG	O2-C3-C4-O4
4	D	604	PEG	O2-C3-C4-O4
2	A	602	EDO	O1-C1-C2-O2
2	B	605	EDO	O1-C1-C2-O2
2	C	602	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	D	604	PEG	O1-C1-C2-O2
4	A	606	PEG	O1-C1-C2-O2
4	D	604	PEG	C4-C3-O2-C2
4	D	604	PEG	C1-C2-O2-C3

There are no ring outliers.

10 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	EDO	4	0
2	D	601	EDO	2	0
4	D	604	PEG	8	0
2	C	603	EDO	3	0
2	D	603	EDO	1	0
4	A	606	PEG	1	0
2	B	601	EDO	3	0
2	C	604	EDO	3	0
2	C	602	EDO	1	0
2	D	602	EDO	4	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 [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	452/476 (94%)	-0.25	9 (1%) 64 69	7, 14, 32, 57	4 (0%)
1	B	460/476 (96%)	-0.13	15 (3%) 49 53	8, 15, 31, 59	4 (0%)
1	C	451/476 (94%)	-0.04	15 (3%) 49 53	8, 17, 34, 66	3 (0%)
1	D	452/476 (94%)	0.11	8 (1%) 67 71	8, 19, 39, 56	2 (0%)
All	All	1815/1904 (95%)	-0.08	47 (2%) 57 61	7, 16, 34, 66	13 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	419	ILE	5.6
1	B	105	TYR	5.1
1	B	420	THR	5.1
1	B	419	ILE	5.0
1	C	418	ALA	4.4
1	B	180	VAL	4.3
1	D	307	ILE	4.1
1	A	106	TYR	4.0
1	C	180	VAL	3.9
1	D	105	TYR	3.9
1	C	417	SER	3.8
1	A	105	TYR	3.6
1	D	106	TYR	3.5
1	C	420	THR	3.4
1	B	175	GLY	3.3
1	A	180	VAL	3.3
1	C	105	TYR	3.3
1	B	106	TYR	3.1
1	C	296	VAL	3.0
1	B	36	THR	3.0
1	B	307	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	416	ARG	2.9
1	B	418	ALA	2.9
1	D	419	ILE	2.9
1	B	37	GLY	2.8
1	B	35	GLN	2.7
1	A	419	ILE	2.6
1	B	40	ASN	2.6
1	D	296	VAL	2.5
1	C	297	LYS	2.5
1	C	43	TRP	2.4
1	A	388	PRO	2.4
1	A	416	ARG	2.4
1	D	43	TRP	2.3
1	C	106	TYR	2.3
1	B	417	SER	2.3
1	A	175	GLY	2.3
1	A	307	ILE	2.2
1	B	443	ARG	2.2
1	C	437	ARG	2.2
1	A	481	ARG	2.1
1	D	474	LYS	2.1
1	C	179	ASP	2.1
1	C	414	GLY	2.1
1	C	60	LEU	2.1
1	D	456	LEU	2.0
1	B	39	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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( $\text{\AA}^2$ )	Q<0.9
1	LLP	A	280	24/25	0.98	0.06	10,12,18,21	0
1	LLP	B	280	24/25	0.98	0.06	10,14,19,23	0
1	LLP	C	280	24/25	0.98	0.06	12,16,21,24	0
1	LLP	D	280	24/25	0.98	0.06	13,17,22,25	0



### 6.3 Carbohydrates ⓘ

There are no oligosaccharides 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<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
2	EDO	D	601	4/4	0.77	0.16	28,35,35,43	0
4	PEG	A	606	7/7	0.81	0.19	61,73,80,81	0
2	EDO	C	603	4/4	0.82	0.19	53,64,65,66	0
2	EDO	B	601	4/4	0.85	0.16	40,48,51,54	0
2	EDO	C	602	4/4	0.86	0.17	50,60,63,64	0
4	PEG	D	604	7/7	0.88	0.14	31,44,54,55	0
2	EDO	A	602	4/4	0.89	0.14	23,35,40,44	0
5	NA	D	605	1/1	0.89	0.11	47,47,47,47	0
2	EDO	D	602	4/4	0.90	0.13	48,58,59,60	0
2	EDO	A	601	4/4	0.92	0.13	34,36,37,37	0
2	EDO	C	605	4/4	0.92	0.10	33,39,40,40	0
3	TRS	A	605	8/8	0.92	0.09	24,25,27,27	0
2	EDO	A	603	4/4	0.93	0.09	31,37,40,41	0
2	EDO	D	603	4/4	0.93	0.11	42,50,53,53	0
2	EDO	C	604	4/4	0.93	0.10	30,36,43,43	0
2	EDO	B	603	4/4	0.94	0.09	30,36,38,38	0
2	EDO	A	604	4/4	0.94	0.09	22,31,36,41	0
2	EDO	B	604	4/4	0.95	0.08	36,43,45,45	0
2	EDO	B	605	4/4	0.96	0.07	23,28,33,33	0
2	EDO	B	602	4/4	0.96	0.07	17,25,30,34	0
2	EDO	C	601	4/4	0.97	0.07	21,30,35,36	0
5	NA	A	607	1/1	0.98	0.07	37,37,37,37	0
5	NA	C	606	1/1	0.99	0.03	30,30,30,30	0
5	NA	B	606	1/1	1.00	0.02	26,26,26,26	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.