



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 7, 2025 – 10:15 am BST

PDB ID : 9QCY / pdb\_00009qcy  
Title : Crystal structure of Rhizobium etli L-asparaginase ReAV S80A mutant  
Authors : Pokrywka, K.; Grzechowiak, M.; Loch, J.I.; Ruszkowski, M.; Gilski, M.; Jaskolski, M.  
Deposited on : 2025-03-05  
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.

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	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

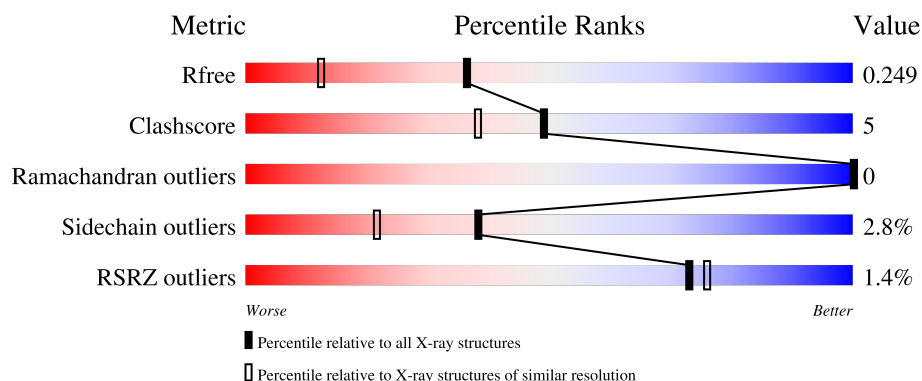
# 1 Overall quality at a glance

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))
$R_{free}$	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (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 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	373	<div> <div>2%</div> <div>85% 8% 6%</div> </div>
1	B	373	<div> <div>2%</div> <div>78% 15% 7%</div> </div>
1	C	373	<div> <div>2%</div> <div>79% 14% 7%</div> </div>
1	D	373	<div> <div>2%</div> <div>84% 9% 6%</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
4	EDO	B	402	-	-	X	-
4	EDO	B	407	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11594 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 L-asparaginase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	7	0
			2620	1619	482	498	21			
1	B	348	Total	C	N	O	S	0	10	0
			2637	1633	486	497	21			
1	C	348	Total	C	N	O	S	0	12	0
			2642	1639	484	497	22			
1	D	349	Total	C	N	O	S	0	7	0
			2625	1624	484	496	21			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q9RFN5
A	-4	ILE	-	expression tag	UNP Q9RFN5
A	-3	ASP	-	expression tag	UNP Q9RFN5
A	-2	PRO	-	expression tag	UNP Q9RFN5
A	-1	PHE	-	expression tag	UNP Q9RFN5
A	0	THR	-	expression tag	UNP Q9RFN5
A	80	ALA	SER	engineered mutation	UNP Q9RFN5
B	-5	GLY	-	expression tag	UNP Q9RFN5
B	-4	ILE	-	expression tag	UNP Q9RFN5
B	-3	ASP	-	expression tag	UNP Q9RFN5
B	-2	PRO	-	expression tag	UNP Q9RFN5
B	-1	PHE	-	expression tag	UNP Q9RFN5
B	0	THR	-	expression tag	UNP Q9RFN5
B	80	ALA	SER	engineered mutation	UNP Q9RFN5
C	-5	GLY	-	expression tag	UNP Q9RFN5
C	-4	ILE	-	expression tag	UNP Q9RFN5
C	-3	ASP	-	expression tag	UNP Q9RFN5
C	-2	PRO	-	expression tag	UNP Q9RFN5
C	-1	PHE	-	expression tag	UNP Q9RFN5
C	0	THR	-	expression tag	UNP Q9RFN5
C	80	ALA	SER	engineered mutation	UNP Q9RFN5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	GLY	-	expression tag	UNP Q9RFN5
D	-4	ILE	-	expression tag	UNP Q9RFN5
D	-3	ASP	-	expression tag	UNP Q9RFN5
D	-2	PRO	-	expression tag	UNP Q9RFN5
D	-1	PHE	-	expression tag	UNP Q9RFN5
D	0	THR	-	expression tag	UNP Q9RFN5
D	80	ALA	SER	engineered mutation	UNP Q9RFN5

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



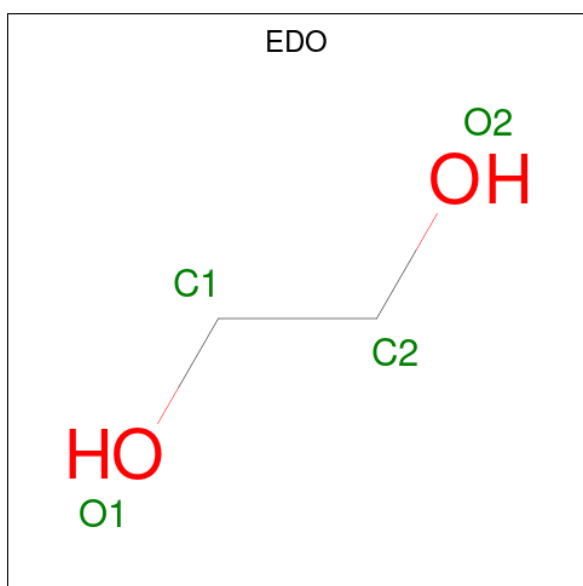
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



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		

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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	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		
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		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Cl 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	208	Total O 208 208	0	0
7	B	238	Total O 238 238	0	0
7	C	251	Total O 251 251	0	0

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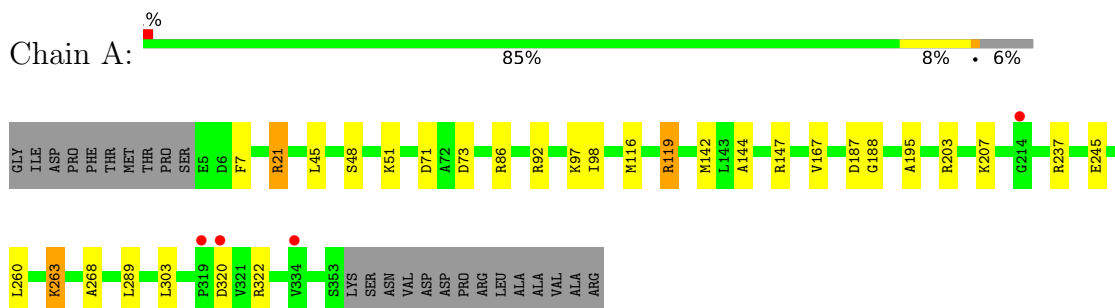
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	214	Total 214	O 214	0	0

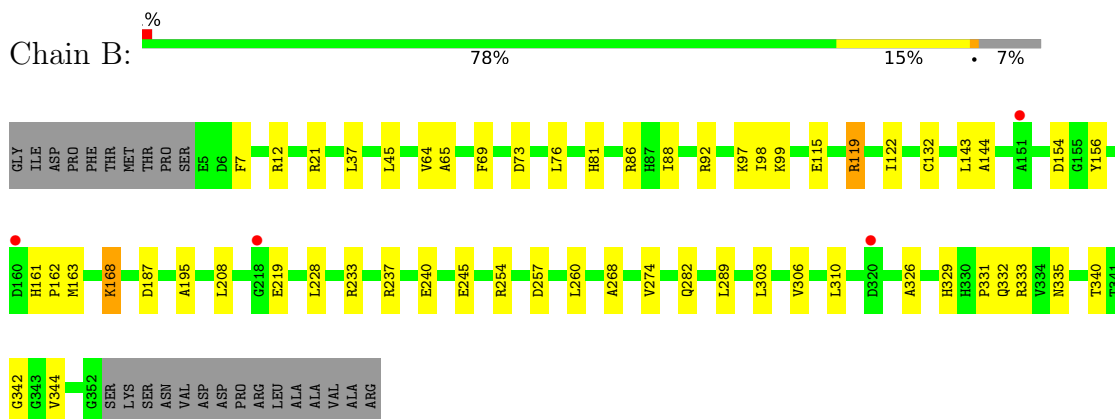
### 3 Residue-property plots

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.

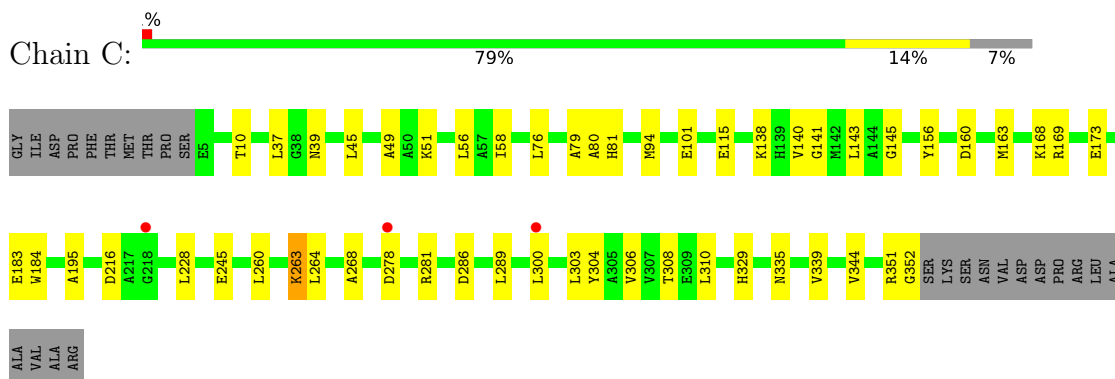
- Molecule 1: L-asparaginase II



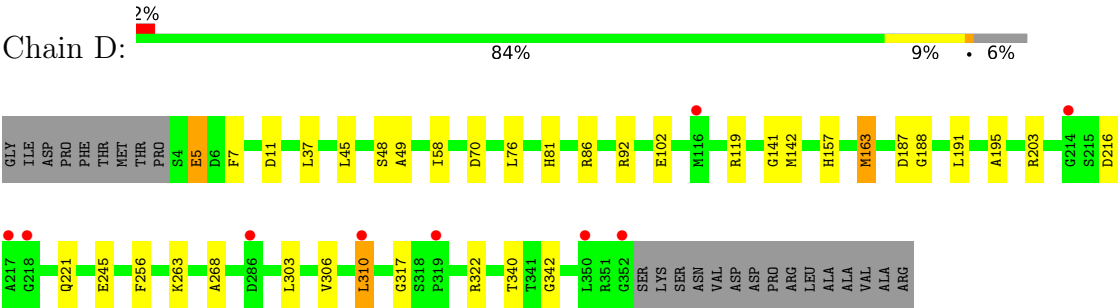
- Molecule 1: L-asparaginase II



- Molecule 1: L-asparaginase II



● Molecule 1: L-asparaginase II



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.06Å 91.48Å 104.31Å 90.00° 105.61° 90.00°	Depositor
Resolution (Å)	53.66 – 1.70 53.66 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (53.66-1.70) 99.4 (53.66-1.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 1.70Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.205 , 0.248 0.206 , 0.249	Depositor DCC
$R_{free}$ test set	152929 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtrriage
Anisotropy	0.559	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11594	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2770e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: SO4, CSD, CL, EDO, PEG, ZN

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	0.49	0/2677	0.65	0/3616
1	B	0.53	0/2703	0.70	0/3649
1	C	0.52	0/2716	0.69	2/3670 (0.1%)
1	D	0.51	2/2682 (0.1%)	0.68	2/3622 (0.1%)
All	All	0.51	2/10778 (0.0%)	0.68	4/14557 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	310[A]	LEU	C-O	5.72	1.30	1.24
1	D	310[B]	LEU	C-O	5.72	1.30	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	80	ALA	N-CA-C	-7.48	97.99	108.54
1	D	310[A]	LEU	CA-C-O	6.96	127.92	120.55
1	D	310[B]	LEU	CA-C-O	6.96	127.92	120.55
1	C	79	ALA	N-CA-C	5.36	118.80	110.17

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	2620	0	2604	19	0
1	B	2637	0	2638	40	0
1	C	2642	0	2640	31	0
1	D	2625	0	2617	24	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	7	0	10	1	0
3	D	7	0	10	1	0
4	A	16	0	24	2	0
4	B	48	0	72	14	0
4	C	32	0	48	8	0
4	D	24	0	36	6	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	C	1	0	0	0	0
7	A	208	0	0	3	0
7	B	238	0	0	5	0
7	C	251	0	0	3	0
7	D	214	0	0	2	0
All	All	11594	0	10699	114	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 (114) 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:D:203:ARG:HH22	4:D:403:EDO:H21	1.40	0.87
1:B:65:ALA:HA	4:B:404:EDO:H22	1.58	0.83
1:D:45:LEU:HD23	1:D:195:ALA:HB2	1.68	0.75
1:B:45:LEU:HD23	1:B:195:ALA:HB2	1.68	0.75
1:B:12:ARG:HH12	4:B:402:EDO:H22	1.53	0.74
1:B:329:HIS:ND1	4:B:408:EDO:H22	2.02	0.74
1:A:207:LYS:HG2	4:A:403:EDO:H12	1.70	0.74
1:A:45:LEU:HD23	1:A:195:ALA:HB2	1.69	0.74
1:C:45:LEU:HD23	1:C:195:ALA:HB2	1.76	0.68
1:C:286:ASP:O	4:C:409:EDO:H12	1.94	0.67
1:B:340:THR:HG23	4:B:407:EDO:H21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21[B]:ARG:NH2	7:B:504:HOH:O	2.32	0.63
1:C:10:THR:HG22	1:C:344[B]:VAL:HG22	1.80	0.63
1:B:333:ARG:H	4:B:407:EDO:H22	1.63	0.63
1:B:99:LYS:NZ	7:B:505:HOH:O	2.32	0.62
1:B:7:PHE:CE1	1:B:21[B]:ARG:HG3	2.34	0.62
1:B:333:ARG:H	4:B:407:EDO:C2	2.14	0.60
1:C:39:ASN:HD22	4:C:406:EDO:H12	1.66	0.60
1:D:317:GLY:O	1:D:322:ARG:NH1	2.35	0.60
1:B:64:VAL:HG12	4:B:404:EDO:H21	1.83	0.58
1:C:168:LYS:HD2	7:C:514:HOH:O	2.03	0.58
1:B:115:GLU:OE2	1:B:119:ARG:HD2	2.05	0.56
1:A:71:ASP:HB2	1:A:237:ARG:HH21	1.69	0.56
4:D:404:EDO:H22	7:D:619:HOH:O	2.04	0.56
1:C:49:ALA:HA	1:C:263:LYS:HG2	1.89	0.55
1:D:119:ARG:NH2	7:D:510:HOH:O	2.40	0.55
1:D:340:THR:CG2	4:D:405:EDO:H11	2.37	0.55
1:B:92:ARG:NH2	7:B:509:HOH:O	2.39	0.54
1:B:335:ASN:HB3	4:B:402:EDO:H21	1.88	0.54
1:A:7:PHE:CE2	1:A:21:ARG:HG2	2.42	0.54
1:C:278:ASP:OD1	1:C:281:ARG:NH2	2.41	0.54
1:C:184:TRP:HD1	4:C:402:EDO:H12	1.73	0.54
1:A:21:ARG:NH1	7:A:503:HOH:O	2.34	0.54
1:C:37:LEU:HD11	1:C:310[B]:LEU:HD21	1.90	0.53
1:C:308:THR:HG21	1:C:329:HIS:HB2	1.89	0.53
1:D:268:ALA:HA	1:D:303:LEU:HD22	1.91	0.53
1:B:12:ARG:HH12	4:B:402:EDO:C2	2.18	0.53
1:B:37:LEU:HD11	1:B:310[B]:LEU:HD21	1.91	0.53
1:A:119:ARG:HE	1:B:122:ILE:HD13	1.73	0.52
1:B:268:ALA:HA	1:B:303:LEU:HD22	1.90	0.52
1:C:58:ILE:HD13	1:C:141:GLY:HA3	1.92	0.52
1:D:163:MET:HA	1:D:163:MET:HE2	1.91	0.52
1:D:58:ILE:HD13	1:D:141:GLY:HA3	1.92	0.52
1:C:39:ASN:HD22	4:C:406:EDO:C1	2.23	0.51
1:D:37:LEU:HD11	1:D:310[B]:LEU:HD21	1.92	0.51
1:C:335:ASN:ND2	1:C:339[B]:VAL:HG22	2.25	0.51
1:D:221:GLN:HG2	4:D:406:EDO:H11	1.93	0.51
1:D:58:ILE:HD11	1:D:142[A]:MET:HE2	1.92	0.51
1:B:76:LEU:HD11	1:B:81:HIS:CD2	2.46	0.51
1:A:268:ALA:HA	1:A:303:LEU:HD22	1.92	0.50
1:C:335:ASN:HB2	1:D:188:GLY:HA2	1.93	0.50
1:A:188:GLY:HA2	1:B:335:ASN:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:LEU:HD11	1:D:81:HIS:CD2	2.47	0.49
1:C:169:ARG:O	1:C:173:GLU:HG3	2.13	0.49
1:C:168:LYS:HG2	1:C:184:TRP:CZ2	2.48	0.49
1:A:92:ARG:NH1	7:A:518:HOH:O	2.45	0.48
1:B:12:ARG:NH1	4:B:402:EDO:H22	2.25	0.48
1:C:56:LEU:HD22	1:C:228:LEU:HD21	1.94	0.48
1:A:322:ARG:NH2	7:A:519:HOH:O	2.47	0.48
1:B:168:LYS:HG2	7:B:535:HOH:O	2.13	0.48
1:C:173:GLU:HB3	4:C:405:EDO:H21	1.96	0.48
1:B:88[B]:ILE:HD12	1:B:132:CYS:HA	1.96	0.47
1:C:264:LEU:HD11	1:C:300:LEU:HD11	1.96	0.47
1:C:76:LEU:HD11	1:C:81:HIS:CD2	2.50	0.47
1:A:86:ARG:NH2	1:A:245:GLU:HG2	2.31	0.46
1:B:86:ARG:NH2	1:B:245:GLU:HG2	2.30	0.46
1:B:342:GLY:O	4:B:407:EDO:O1	2.32	0.46
1:C:268:ALA:HA	1:C:303:LEU:HD22	1.97	0.46
1:D:340:THR:HG21	4:D:405:EDO:H11	1.97	0.46
1:A:142[B]:MET:HE2	1:A:167:VAL:HG21	1.98	0.45
1:B:333:ARG:N	4:B:407:EDO:H22	2.28	0.45
1:D:86:ARG:NH2	1:D:245:GLU:HG2	2.32	0.45
1:D:306:VAL:O	1:D:310[B]:LEU:HG	2.17	0.45
1:B:73:ASP:OD2	1:B:97:LYS:NZ	2.50	0.45
1:B:143:LEU:HD21	1:B:156:TYR:CE2	2.52	0.45
1:D:48:SER:O	1:D:263:LYS:HE3	2.17	0.45
1:C:51:LYS:HE2	1:C:138:LYS:HE2	1.99	0.44
1:C:145:GLY:HA3	1:C:163[B]:MET:HE3	2.00	0.44
1:B:326:ALA:HA	4:B:408:EDO:H11	1.99	0.44
1:A:48[B]:SER:HG	1:A:51:LYS:HD2	1.81	0.44
1:D:5:GLU:HB2	1:D:7:PHE:HE2	1.82	0.44
1:A:147:ARG:HH21	4:A:405:EDO:H11	1.83	0.43
1:B:240:GLU:HB3	1:B:254:ARG:NH2	2.33	0.43
1:D:49:ALA:HA	1:D:263:LYS:HG2	1.99	0.43
1:D:157:HIS:HB2	1:D:191:LEU:HD23	1.99	0.43
1:A:203:ARG:HH12	3:A:402:PEG:H32	1.84	0.43
1:B:274:VAL:HB	1:B:289:LEU:HB3	2.01	0.43
1:D:70:ASP:HB2	4:D:404:EDO:H12	2.00	0.43
1:B:254:ARG:HD3	7:B:707:HOH:O	2.18	0.43
3:D:407:PEG:H32	3:D:407:PEG:H12	1.75	0.43
1:B:98:ILE:HG21	1:B:144:ALA:HB2	2.00	0.43
1:A:73:ASP:OD2	1:A:97:LYS:NZ	2.52	0.42
1:B:260:LEU:C	1:B:260:LEU:HD12	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:VAL:O	1:B:310[B]:LEU:HG	2.18	0.42
1:C:281:ARG:HD3	4:C:409:EDO:O1	2.19	0.42
1:A:260:LEU:C	1:A:260:LEU:HD12	2.44	0.42
1:C:143:LEU:HD21	1:C:156:TYR:CE2	2.54	0.42
1:D:256:PHE:CE2	1:D:317:GLY:HA3	2.55	0.42
1:B:331:PRO:HD2	1:B:344:VAL:HG21	2.01	0.42
1:D:92:ARG:NE	1:D:102[A]:GLU:OE2	2.28	0.42
1:B:163:MET:HE3	1:B:163:MET:HB3	1.76	0.42
1:A:98:ILE:HG21	1:A:144:ALA:HB2	2.02	0.42
1:A:263:LYS:HZ3	1:A:263:LYS:HG2	1.79	0.42
1:C:300:LEU:HG	1:C:304:TYR:CZ	2.55	0.41
1:D:11:ASP:O	1:D:342:GLY:HA3	2.20	0.41
1:B:208:LEU:HD23	1:B:228:LEU:HD22	2.02	0.41
1:B:161:HIS:CG	1:B:162:PRO:HD2	2.54	0.41
1:C:94:MET:HB3	1:C:140:VAL:HG11	2.01	0.41
1:C:260:LEU:C	1:C:260:LEU:HD12	2.44	0.41
1:C:245:GLU:O	4:C:407:EDO:H11	2.21	0.41
1:C:306:VAL:O	1:C:310[B]:LEU:HG	2.21	0.40
1:B:69:PHE:HB2	4:B:404:EDO:H11	2.02	0.40
4:C:402:EDO:H11	7:C:643:HOH:O	2.21	0.40
1:C:352:GLY:O	7:C:501:HOH:O	2.22	0.40

There are no symmetry-related clashes.

## 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	353/373 (95%)	345 (98%)	8 (2%)	0	100	100
1	B	355/373 (95%)	347 (98%)	8 (2%)	0	100	100
1	C	357/373 (96%)	348 (98%)	9 (2%)	0	100	100
1	D	353/373 (95%)	343 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1418/1492 (95%)	1383 (98%)	35 (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	268/281 (95%)	261 (97%)	7 (3%)	41	24
1	B	270/281 (96%)	259 (96%)	11 (4%)	26	10
1	C	272/281 (97%)	264 (97%)	8 (3%)	37	20
1	D	268/281 (95%)	264 (98%)	4 (2%)	60	47
All	All	1078/1124 (96%)	1048 (97%)	30 (3%)	38	21

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	116	MET
1	A	119	ARG
1	A	187	ASP
1	A	263	LYS
1	A	289	LEU
1	A	320	ASP
1	B	119	ARG
1	B	154	ASP
1	B	168	LYS
1	B	187	ASP
1	B	219	GLU
1	B	233[A]	ARG
1	B	233[B]	ARG
1	B	237	ARG
1	B	257	ASP
1	B	282	GLN

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Mol	Chain	Res	Type
1	B	332	GLN
1	C	101	GLU
1	C	115	GLU
1	C	160	ASP
1	C	183	GLU
1	C	216	ASP
1	C	263	LYS
1	C	289	LEU
1	C	351	ARG
1	D	5	GLU
1	D	163	MET
1	D	187	ASP
1	D	216	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	324	GLN
1	B	330	HIS
1	C	39	ASN
1	C	124	GLN
1	C	332	GLN

### 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	CSD	B	249	1	3,7,8	0.85	0	1,8,10	0.25	0
1	CSD	D	249	1	3,7,8	0.86	0	1,8,10	0.01	0
1	CSD	C	249	1	3,7,8	0.76	0	1,8,10	0.31	0
1	CSD	A	249	1	3,7,8	0.88	0	1,8,10	0.39	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
1	CSD	B	249	1	-	0/2/6/8	-
1	CSD	D	249	1	-	0/2/6/8	-
1	CSD	C	249	1	-	0/2/6/8	-
1	CSD	A	249	1	-	0/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 41 ligands modelled in this entry, 5 are monoatomic - leaving 36 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	EDO	B	405	-	3,3,3	0.49	0	2,2,2	0.50	0
4	EDO	C	408	-	3,3,3	0.47	0	2,2,2	0.63	0
4	EDO	B	410	-	3,3,3	0.51	0	2,2,2	0.21	0
2	SO4	A	401	-	4,4,4	0.33	0	6,6,6	0.54	0
4	EDO	B	406	-	3,3,3	0.39	0	2,2,2	0.75	0
4	EDO	A	405	-	3,3,3	0.26	0	2,2,2	1.11	0
4	EDO	C	404	-	3,3,3	0.38	0	2,2,2	0.45	0
4	EDO	D	406	-	3,3,3	0.49	0	2,2,2	0.26	0
4	EDO	C	402	-	3,3,3	0.33	0	2,2,2	0.55	0
4	EDO	D	404	-	3,3,3	0.50	0	2,2,2	0.48	0
4	EDO	C	409	-	3,3,3	0.48	0	2,2,2	0.17	0
4	EDO	D	405	-	3,3,3	0.42	0	2,2,2	0.31	0
4	EDO	B	404	-	3,3,3	0.64	0	2,2,2	0.29	0
4	EDO	B	402	-	3,3,3	0.40	0	2,2,2	0.54	0
4	EDO	D	402	-	3,3,3	0.61	0	2,2,2	0.13	0
4	EDO	B	408	-	3,3,3	0.56	0	2,2,2	0.32	0
3	PEG	D	407	-	6,6,6	0.45	0	5,5,5	0.25	0
3	PEG	A	402	-	6,6,6	0.20	0	5,5,5	0.19	0
4	EDO	C	406	-	3,3,3	0.43	0	2,2,2	0.49	0
4	EDO	B	407	-	3,3,3	0.34	0	2,2,2	0.73	0
4	EDO	A	404	-	3,3,3	0.57	0	2,2,2	0.21	0
4	EDO	B	409	-	3,3,3	0.44	0	2,2,2	0.51	0
4	EDO	A	403	-	3,3,3	0.55	0	2,2,2	0.24	0
4	EDO	B	411	-	3,3,3	0.47	0	2,2,2	0.59	0
4	EDO	B	413	-	3,3,3	0.55	0	2,2,2	0.63	0
4	EDO	D	409	-	3,3,3	0.11	0	2,2,2	0.13	0
2	SO4	C	401	-	4,4,4	0.12	0	6,6,6	0.41	0
2	SO4	B	401	-	4,4,4	0.24	0	6,6,6	0.34	0
2	SO4	D	401	-	4,4,4	0.19	0	6,6,6	0.35	0
4	EDO	C	403	-	3,3,3	0.58	0	2,2,2	0.17	0
4	EDO	B	412	-	3,3,3	0.65	0	2,2,2	0.41	0
4	EDO	B	403	-	3,3,3	0.55	0	2,2,2	0.09	0
4	EDO	C	405	-	3,3,3	0.37	0	2,2,2	0.84	0
4	EDO	C	407	-	3,3,3	0.40	0	2,2,2	0.66	0
4	EDO	D	403	-	3,3,3	0.47	0	2,2,2	0.35	0
4	EDO	A	406	-	3,3,3	0.58	0	2,2,2	0.40	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
4	EDO	B	405	-	-	0/1/1/1	-
4	EDO	C	408	-	-	0/1/1/1	-
4	EDO	B	410	-	-	0/1/1/1	-
4	EDO	B	406	-	-	0/1/1/1	-
4	EDO	A	405	-	-	0/1/1/1	-
4	EDO	C	404	-	-	0/1/1/1	-
4	EDO	D	406	-	-	0/1/1/1	-
4	EDO	C	402	-	-	0/1/1/1	-
4	EDO	D	404	-	-	0/1/1/1	-
4	EDO	C	409	-	-	0/1/1/1	-
4	EDO	D	405	-	-	0/1/1/1	-
4	EDO	B	404	-	-	0/1/1/1	-
4	EDO	B	402	-	-	0/1/1/1	-
4	EDO	D	402	-	-	0/1/1/1	-
4	EDO	B	408	-	-	0/1/1/1	-
3	PEG	D	407	-	-	2/4/4/4	-
3	PEG	A	402	-	-	1/4/4/4	-
4	EDO	C	406	-	-	0/1/1/1	-
4	EDO	B	407	-	-	0/1/1/1	-
4	EDO	A	404	-	-	0/1/1/1	-
4	EDO	B	409	-	-	0/1/1/1	-
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	B	411	-	-	0/1/1/1	-
4	EDO	B	413	-	-	0/1/1/1	-
4	EDO	D	409	-	-	0/1/1/1	-
4	EDO	C	403	-	-	0/1/1/1	-
4	EDO	B	412	-	-	0/1/1/1	-
4	EDO	B	403	-	-	0/1/1/1	-
4	EDO	C	405	-	-	0/1/1/1	-
4	EDO	C	407	-	-	0/1/1/1	-
4	EDO	D	403	-	-	0/1/1/1	-
4	EDO	A	406	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	407	PEG	O2-C3-C4-O4
3	D	407	PEG	C1-C2-O2-C3
3	A	402	PEG	C1-C2-O2-C3

There are no ring outliers.

17 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	EDO	1	0
4	D	406	EDO	1	0
4	C	402	EDO	2	0
4	D	404	EDO	2	0
4	C	409	EDO	2	0
4	D	405	EDO	2	0
4	B	404	EDO	3	0
4	B	402	EDO	4	0
4	B	408	EDO	2	0
3	D	407	PEG	1	0
3	A	402	PEG	1	0
4	C	406	EDO	2	0
4	B	407	EDO	5	0
4	A	403	EDO	1	0
4	C	405	EDO	1	0
4	C	407	EDO	1	0
4	D	403	EDO	1	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	348/373 (93%)	0.37	4 (1%) 77 80	15, 27, 40, 60	7 (2%)
1	B	347/373 (93%)	0.20	4 (1%) 76 79	11, 23, 36, 49	10 (2%)
1	C	347/373 (93%)	0.13	3 (0%) 81 83	11, 22, 35, 46	12 (3%)
1	D	348/373 (93%)	0.39	9 (2%) 57 60	11, 27, 41, 57	7 (2%)
All	All	1390/1492 (93%)	0.27	20 (1%) 73 76	11, 25, 39, 60	36 (2%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151	ALA	5.3
1	D	218	GLY	3.2
1	B	218	GLY	2.8
1	C	278	ASP	2.7
1	D	217	ALA	2.7
1	D	310[A]	LEU	2.6
1	A	320	ASP	2.5
1	B	160	ASP	2.5
1	A	214	GLY	2.4
1	A	319	PRO	2.4
1	D	319	PRO	2.4
1	D	350	LEU	2.4
1	D	214	GLY	2.3
1	C	300	LEU	2.2
1	C	218	GLY	2.2
1	D	352	GLY	2.2
1	A	334	VAL	2.1
1	D	116	MET	2.0
1	D	286	ASP	2.0
1	B	320	ASP	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(Å <sup>2</sup> )	Q<0.9
1	CSD	A	249	8/9	0.95	0.09	23,24,33,33	0
1	CSD	C	249	8/9	0.95	0.07	19,21,29,31	0
1	CSD	D	249	8/9	0.95	0.09	20,24,30,32	0
1	CSD	B	249	8/9	0.96	0.10	19,21,30,31	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
3	PEG	A	402	7/7	0.71	0.14	38,41,47,49	0
4	EDO	B	413	4/4	0.71	0.16	32,33,35,37	0
4	EDO	D	404	4/4	0.73	0.13	36,43,43,45	0
4	EDO	B	410	4/4	0.78	0.14	38,42,42,43	0
3	PEG	D	407	7/7	0.78	0.15	30,35,38,38	0
4	EDO	B	404	4/4	0.78	0.20	27,30,32,38	0
4	EDO	B	412	4/4	0.81	0.15	26,30,32,35	0
4	EDO	B	405	4/4	0.81	0.13	39,40,41,44	0
4	EDO	A	406	4/4	0.81	0.13	36,36,37,40	0
4	EDO	B	406	4/4	0.82	0.13	39,40,42,44	0
4	EDO	B	407	4/4	0.82	0.15	33,35,35,35	0
4	EDO	C	402	4/4	0.82	0.16	25,27,31,34	0
4	EDO	A	404	4/4	0.82	0.13	34,35,36,42	0
4	EDO	A	403	4/4	0.83	0.14	35,35,35,45	0
4	EDO	C	407	4/4	0.83	0.13	26,30,31,39	0
4	EDO	B	411	4/4	0.83	0.14	36,39,41,47	0
4	EDO	D	406	4/4	0.83	0.13	41,47,47,51	0
4	EDO	A	405	4/4	0.84	0.16	32,35,38,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	D	405	4/4	0.84	0.18	34,36,39,40	0
4	EDO	B	409	4/4	0.84	0.19	27,33,34,39	0
4	EDO	D	409	4/4	0.84	0.15	31,33,36,37	0
4	EDO	B	402	4/4	0.85	0.13	25,33,38,38	0
4	EDO	C	409	4/4	0.86	0.15	32,33,35,41	0
4	EDO	B	408	4/4	0.88	0.15	30,31,36,36	0
4	EDO	C	406	4/4	0.89	0.12	25,26,32,36	0
4	EDO	B	403	4/4	0.89	0.11	29,36,38,38	0
4	EDO	C	408	4/4	0.89	0.13	32,37,37,39	0
4	EDO	C	405	4/4	0.89	0.10	29,30,33,35	0
2	SO4	A	401	5/5	0.90	0.16	29,30,37,37	0
4	EDO	D	403	4/4	0.90	0.10	41,42,43,49	0
4	EDO	C	403	4/4	0.90	0.10	28,28,29,34	0
4	EDO	D	402	4/4	0.91	0.10	30,30,34,37	0
4	EDO	C	404	4/4	0.93	0.09	28,31,34,36	0
2	SO4	D	401	5/5	0.94	0.13	27,32,35,38	0
2	SO4	B	401	5/5	0.95	0.11	27,29,32,36	0
6	CL	C	411	1/1	0.96	0.07	52,52,52,52	0
2	SO4	C	401	5/5	0.97	0.10	29,29,31,33	0
5	ZN	C	410	1/1	0.99	0.04	19,19,19,19	0
5	ZN	D	408	1/1	0.99	0.03	23,23,23,23	0
5	ZN	A	407	1/1	0.99	0.04	23,23,23,23	0
5	ZN	B	414	1/1	1.00	0.04	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.