



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:45 PM GMT

PDB ID : 3UT0  
Title : Crystal structure of exo-1,3/1,4-beta-glucanase (EXOP) from Pseudoal-  
teromonas sp. BB1  
Authors : Nakatani, Y.; Cutfield, S.M.; Cutfield, J.F.  
Deposited on : 2011-11-24  
Resolution : 2.30 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  
<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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

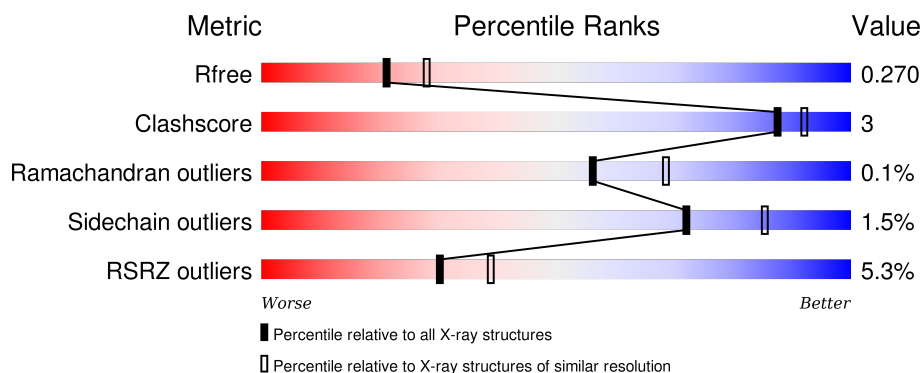
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 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	822	<div> <div>2%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	B	822	<div> <div>7%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	C	822	<div> <div>3%</div> <div>90%</div> <div>7%</div> <div>..</div> </div>
1	D	822	<div> <div>9%</div> <div>90%</div> <div>7%</div> <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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	B	902	-	-	-	X
3	NA	C	902	-	-	-	X
5	EDO	C	827	-	-	-	X
5	EDO	D	825	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25742 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 Exo-1,3/1,4-beta-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	804	Total	C	N	O	S	0	0	0
			6228	3929	1075	1203	21			
1	B	798	Total	C	N	O	S	0	0	0
			6181	3904	1067	1189	21			
1	C	798	Total	C	N	O	S	0	0	0
			6181	3904	1067	1189	21			
1	D	799	Total	C	N	O	S	0	0	0
			6190	3909	1068	1192	21			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP Q0QJA3
A	814	LEU	-	EXPRESSION TAG	UNP Q0QJA3
A	815	GLU	-	EXPRESSION TAG	UNP Q0QJA3
A	816	HIS	-	EXPRESSION TAG	UNP Q0QJA3
A	817	HIS	-	EXPRESSION TAG	UNP Q0QJA3
A	818	HIS	-	EXPRESSION TAG	UNP Q0QJA3
A	819	HIS	-	EXPRESSION TAG	UNP Q0QJA3
A	820	HIS	-	EXPRESSION TAG	UNP Q0QJA3
A	821	HIS	-	EXPRESSION TAG	UNP Q0QJA3
B	0	MET	-	EXPRESSION TAG	UNP Q0QJA3
B	814	LEU	-	EXPRESSION TAG	UNP Q0QJA3
B	815	GLU	-	EXPRESSION TAG	UNP Q0QJA3
B	816	HIS	-	EXPRESSION TAG	UNP Q0QJA3
B	817	HIS	-	EXPRESSION TAG	UNP Q0QJA3
B	818	HIS	-	EXPRESSION TAG	UNP Q0QJA3
B	819	HIS	-	EXPRESSION TAG	UNP Q0QJA3
B	820	HIS	-	EXPRESSION TAG	UNP Q0QJA3
B	821	HIS	-	EXPRESSION TAG	UNP Q0QJA3
C	0	MET	-	EXPRESSION TAG	UNP Q0QJA3
C	814	LEU	-	EXPRESSION TAG	UNP Q0QJA3
C	815	GLU	-	EXPRESSION TAG	UNP Q0QJA3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	816	HIS	-	EXPRESSION TAG	UNP Q0QJA3
C	817	HIS	-	EXPRESSION TAG	UNP Q0QJA3
C	818	HIS	-	EXPRESSION TAG	UNP Q0QJA3
C	819	HIS	-	EXPRESSION TAG	UNP Q0QJA3
C	820	HIS	-	EXPRESSION TAG	UNP Q0QJA3
C	821	HIS	-	EXPRESSION TAG	UNP Q0QJA3
D	0	MET	-	EXPRESSION TAG	UNP Q0QJA3
D	814	LEU	-	EXPRESSION TAG	UNP Q0QJA3
D	815	GLU	-	EXPRESSION TAG	UNP Q0QJA3
D	816	HIS	-	EXPRESSION TAG	UNP Q0QJA3
D	817	HIS	-	EXPRESSION TAG	UNP Q0QJA3
D	818	HIS	-	EXPRESSION TAG	UNP Q0QJA3
D	819	HIS	-	EXPRESSION TAG	UNP Q0QJA3
D	820	HIS	-	EXPRESSION TAG	UNP Q0QJA3
D	821	HIS	-	EXPRESSION TAG	UNP Q0QJA3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

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

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



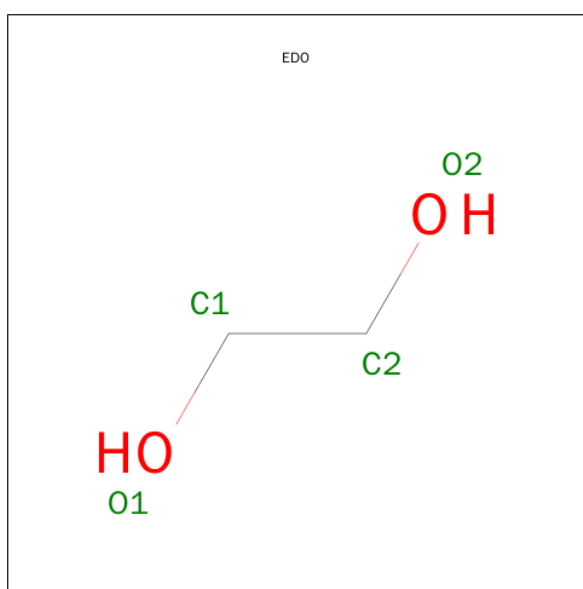
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total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

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

- Molecule 5 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
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 6 is water.

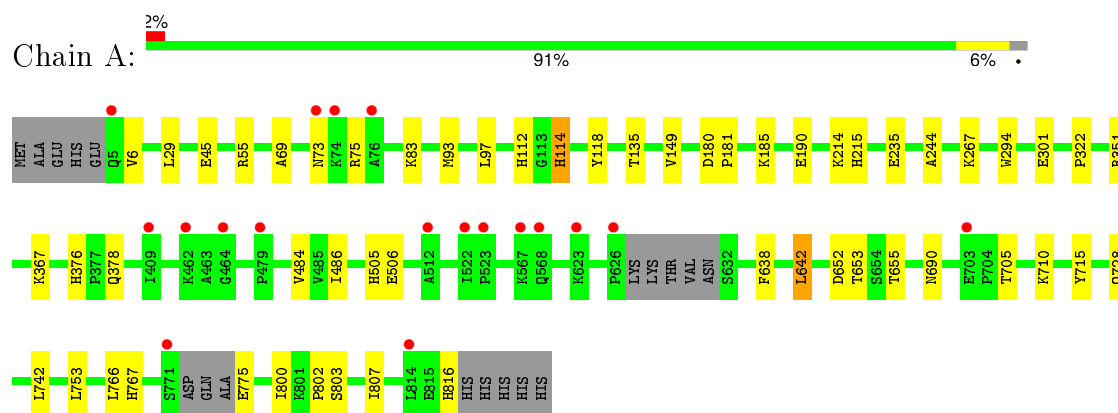
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	262	Total	O	0	0
			262	262		
6	B	283	Total	O	0	0
			283	283		
6	C	177	Total	O	0	0
			177	177		
6	D	106	Total	O	0	0
			106	106		



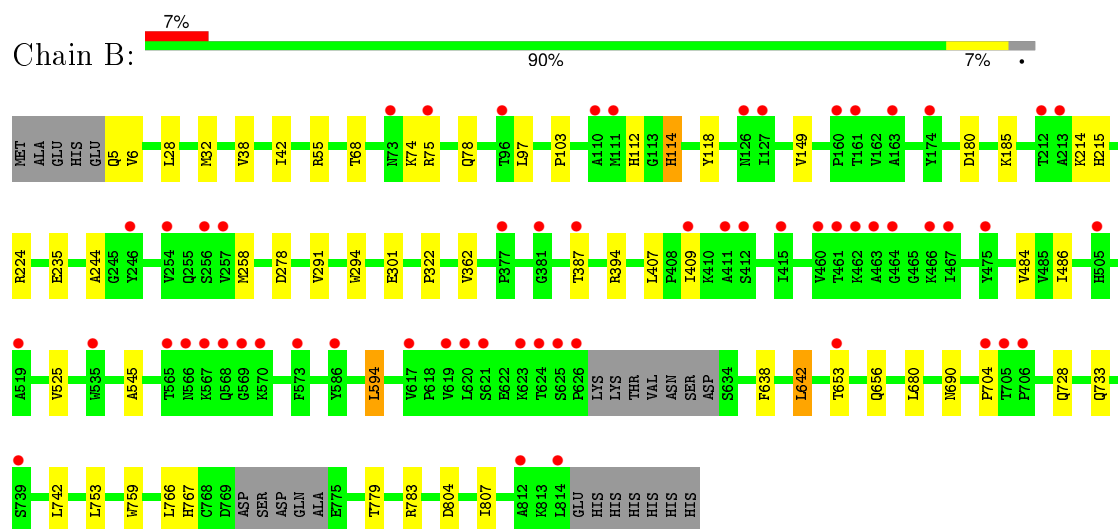
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

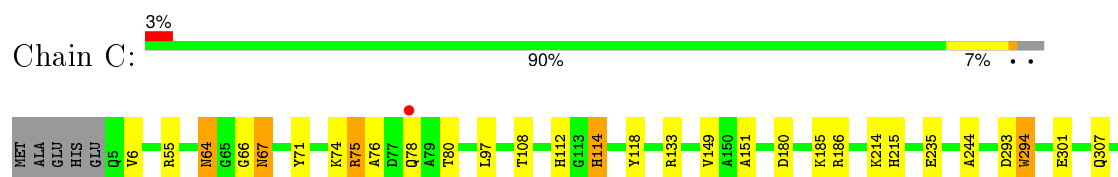
#### • Molecule 1: Exo-1,3/1,4-beta-glucanase

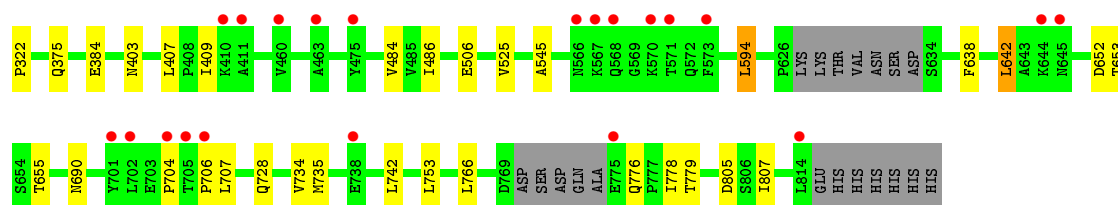


#### • Molecule 1: Exo-1,3/1,4-beta-glucanase

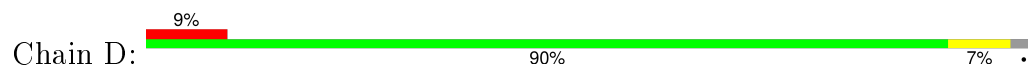


#### • Molecule 1: Exo-1,3/1,4-beta-glucanase





• Molecule 1: Exo-1,3/1,4-beta-glucanase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.91Å 257.82Å 85.61Å 90.00° 115.47° 90.00°	Depositor
Resolution (Å)	38.33 – 2.30 38.33 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (38.33-2.30) 97.8 (38.33-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.223 , 0.270 0.223 , 0.270	Depositor DCC
$R_{free}$ test set	7205 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.784	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.3	EDS
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 143332 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	25742	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, CA, SO4, 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	0.38	0/6362	0.59	0/8630
1	B	0.33	0/6314	0.50	0/8565
1	C	0.35	0/6314	0.52	0/8565
1	D	0.35	0/6323	0.51	0/8577
All	All	0.36	0/25313	0.53	0/34337

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	93	MET	Mainchain

### 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	6228	0	6088	32	0
1	B	6181	0	6057	36	0
1	C	6181	0	6057	37	0
1	D	6190	0	6063	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	25	0	0	0	0
4	B	25	0	0	0	0
4	C	25	0	0	1	0
4	D	15	0	0	0	0
5	A	12	0	18	0	0
5	B	8	0	12	1	0
5	C	8	0	12	0	0
5	D	8	0	12	1	0
6	A	262	0	0	3	0
6	B	283	0	0	7	0
6	C	177	0	0	7	0
6	D	106	0	0	2	0
All	All	25742	0	24319	130	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (130) 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:367:LYS:NZ	1:C:375:GLN:OE1	2.10	0.85
1:A:710:LYS:HE2	1:A:800:ILE:HD11	1.69	0.74
1:B:753:LEU:HD21	1:B:807:ILE:HG21	1.69	0.73
1:A:376:HIS:CE1	1:D:79:ALA:HB1	2.27	0.69
1:A:753:LEU:HD21	1:A:807:ILE:HG21	1.74	0.69
1:A:301:GLU:OE1	1:A:690:ASN:ND2	2.31	0.64
1:A:301:GLU:HG2	6:A:1048:HOH:O	1.96	0.64
1:D:753:LEU:HD21	1:D:807:ILE:HG21	1.82	0.61
1:C:301:GLU:HG2	6:C:895:HOH:O	2.00	0.60
1:A:378:GLN:HG3	1:D:367:LYS:NZ	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:GLN:NE2	6:B:1083:HOH:O	2.24	0.60
1:D:6:VAL:HG21	1:D:235:GLU:HB3	1.84	0.59
1:C:6:VAL:HG21	1:C:235:GLU:HB3	1.84	0.59
1:D:301:GLU:OE1	1:D:690:ASN:ND2	2.36	0.59
1:B:6:VAL:HG21	1:B:235:GLU:HB3	1.85	0.58
1:B:301:GLU:HG2	6:B:1042:HOH:O	2.04	0.58
1:B:704:PRO:HG3	1:B:779:THR:HG22	1.85	0.58
1:A:6:VAL:HG21	1:A:235:GLU:HB3	1.86	0.58
1:B:301:GLU:OE1	1:B:690:ASN:ND2	2.38	0.56
1:A:83:LYS:NZ	1:B:74:LYS:H	2.04	0.56
1:C:301:GLU:OE1	1:C:690:ASN:ND2	2.37	0.56
1:C:753:LEU:HD21	1:C:807:ILE:HG21	1.88	0.55
1:C:64:ASN:OD1	1:C:108:THR:OG1	2.21	0.55
1:B:394:ARG:HH21	5:B:828:EDO:H21	1.72	0.54
1:A:767:HIS:NE2	1:A:816:HIS:O	2.39	0.53
1:B:733:GLN:OE1	1:B:783:ARG:NH1	2.41	0.52
1:A:376:HIS:NE2	1:D:79:ALA:O	2.40	0.52
1:A:83:LYS:HZ3	1:B:74:LYS:H	1.58	0.51
1:B:75:ARG:HG2	1:B:118:TYR:CG	2.45	0.51
1:B:278:ASP:OD2	6:B:858:HOH:O	2.20	0.50
1:C:706:PRO:HA	1:C:776:GLN:O	2.11	0.50
1:C:78:GLN:HG3	1:C:151:ALA:O	2.12	0.49
1:D:185:LYS:HB2	1:D:244:ALA:HB1	1.94	0.49
1:D:114:HIS:CD2	1:D:149:VAL:HA	2.48	0.49
1:C:525:VAL:HG22	1:C:545:ALA:HB3	1.95	0.49
1:B:114:HIS:CD2	1:B:149:VAL:HA	2.48	0.49
1:C:75:ARG:HB3	1:C:118:TYR:CD2	2.48	0.49
1:A:715:TYR:CZ	1:A:802:PRO:HG3	2.48	0.49
1:C:735:MET:SD	1:C:778:ILE:HD13	2.53	0.48
1:A:75:ARG:HD3	1:A:118:TYR:CZ	2.49	0.48
1:D:99:GLY:HA2	6:D:854:HOH:O	2.14	0.48
1:C:742:LEU:HD23	1:C:766:LEU:HB3	1.96	0.48
1:D:726:PRO:HG2	6:D:928:HOH:O	2.14	0.48
1:C:185:LYS:HB2	1:C:244:ALA:HB1	1.96	0.48
1:B:185:LYS:HB2	1:B:244:ALA:HB1	1.96	0.47
1:D:715:TYR:CZ	1:D:802:PRO:HG3	2.50	0.47
1:A:505:HIS:HB2	6:A:1046:HOH:O	2.14	0.47
1:D:742:LEU:HD23	1:D:766:LEU:HB3	1.97	0.47
1:C:506:GLU:HB3	6:C:928:HOH:O	2.15	0.46
1:D:180:ASP:HB2	1:D:594:LEU:HD22	1.98	0.46
1:C:186:ARG:NH2	6:C:1000:HOH:O	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:HIS:CD2	1:A:149:VAL:HA	2.50	0.46
1:D:78:GLN:OE1	1:D:377:PRO:HB3	2.15	0.46
1:A:484:VAL:HG12	1:A:486:ILE:HG23	1.98	0.46
1:D:407:LEU:HD23	1:D:409:ILE:HG13	1.98	0.46
1:A:742:LEU:HD23	1:A:766:LEU:HB3	1.98	0.46
1:B:742:LEU:HD23	1:B:766:LEU:HB3	1.98	0.45
1:D:484:VAL:HG12	1:D:486:ILE:HG23	1.99	0.45
1:C:133:ARG:NE	4:C:824:SO4:O4	2.46	0.45
1:B:525:VAL:HG22	1:B:545:ALA:HB3	1.99	0.45
1:B:180:ASP:HB2	1:B:594:LEU:HD22	1.99	0.45
1:A:185:LYS:HB2	1:A:244:ALA:HB1	1.99	0.45
1:C:403:ASN:OD1	6:C:1002:HOH:O	2.21	0.45
1:C:407:LEU:HD23	1:C:409:ILE:HG13	1.98	0.45
1:B:387:THR:HG22	6:B:1022:HOH:O	2.17	0.45
1:B:55:ARG:HG2	1:B:97:LEU:HD12	1.99	0.45
1:A:45:GLU:HB2	1:A:322:PRO:HB3	1.99	0.45
1:B:484:VAL:HG12	1:B:486:ILE:HG23	1.99	0.44
1:A:753:LEU:CD2	1:A:807:ILE:HG21	2.45	0.44
1:C:114:HIS:CD2	1:C:149:VAL:HA	2.52	0.44
1:C:180:ASP:HB2	1:C:594:LEU:HD22	1.98	0.44
1:B:38:VAL:O	1:B:42:ILE:HG12	2.18	0.44
1:C:638:PHE:CD1	1:C:642:LEU:HD13	2.52	0.44
1:C:384:GLU:HB2	6:C:915:HOH:O	2.18	0.44
1:C:294:TRP:CE2	1:C:322:PRO:HG3	2.53	0.44
1:A:652:ASP:OD1	1:A:655:THR:OG1	2.30	0.44
1:A:135:THR:HB	1:A:190:GLU:HG3	1.99	0.44
1:A:638:PHE:CD1	1:A:642:LEU:HD13	2.53	0.44
1:C:55:ARG:HG2	1:C:97:LEU:HD12	2.01	0.43
1:D:258:MET:HA	1:D:291:VAL:O	2.18	0.43
1:B:407:LEU:HD23	1:B:409:ILE:HG13	1.99	0.43
1:B:75:ARG:HG2	1:B:118:TYR:CD2	2.53	0.43
1:C:484:VAL:HG12	1:C:486:ILE:HG23	2.01	0.43
1:C:76:ALA:HB1	1:C:80:THR:HB	2.00	0.43
1:B:5:GLN:N	6:B:1095:HOH:O	2.51	0.43
1:D:652:ASP:OD1	1:D:655:THR:OG1	2.29	0.43
1:B:638:PHE:CD1	1:B:642:LEU:HD13	2.53	0.43
1:C:66:GLY:O	1:C:67:ASN:HB2	2.19	0.43
1:C:293:ASP:OD1	1:C:294:TRP:N	2.45	0.43
1:A:180:ASP:OD1	1:A:181:PRO:HD2	2.19	0.43
1:B:214:LYS:HA	1:B:215:HIS:HA	1.86	0.42
1:A:29:LEU:HD11	1:A:351:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ARG:NH1	6:C:856:HOH:O	2.51	0.42
1:A:378:GLN:HG3	1:D:367:LYS:HZ2	1.84	0.42
1:D:680:LEU:HD13	1:D:759:TRP:CE2	2.54	0.42
1:C:214:LYS:HA	1:C:215:HIS:HA	1.88	0.42
1:D:75:ARG:H	1:D:75:ARG:HG2	1.70	0.42
1:D:75:ARG:HD2	1:D:118:TYR:CZ	2.55	0.42
1:D:294:TRP:CE2	1:D:322:PRO:HG3	2.55	0.42
1:A:69:ALA:HB3	1:A:73:ASN:O	2.19	0.42
1:B:74:LYS:HB3	1:B:74:LYS:HE2	1.83	0.42
1:D:293:ASP:OD1	1:D:294:TRP:N	2.46	0.42
1:C:704:PRO:HG3	1:C:779:THR:HG22	2.01	0.42
1:A:55:ARG:HG2	1:A:97:LEU:HD12	2.01	0.42
1:B:74:LYS:NZ	1:B:75:ARG:HH21	2.17	0.41
1:C:71:TYR:CD1	1:D:74:LYS:HB3	2.55	0.41
1:B:680:LEU:HD13	1:B:759:TRP:CE2	2.55	0.41
1:D:55:ARG:HG2	1:D:97:LEU:HD12	2.02	0.41
1:C:734:VAL:HG12	1:C:735:MET:HG2	2.02	0.41
1:A:294:TRP:CE2	1:A:322:PRO:HG3	2.55	0.41
1:A:506:GLU:HB3	6:A:961:HOH:O	2.20	0.41
1:D:214:LYS:HE3	1:D:214:LYS:HB2	1.90	0.41
1:D:28:LEU:O	1:D:32:MET:HG3	2.21	0.41
1:D:525:VAL:HG22	1:D:545:ALA:HB3	2.02	0.41
1:B:224:ARG:NH2	6:B:986:HOH:O	2.53	0.41
1:C:652:ASP:OD1	1:C:655:THR:OG1	2.33	0.41
1:B:28:LEU:O	1:B:32:MET:HG3	2.21	0.41
1:B:638:PHE:HD1	1:B:642:LEU:HD13	1.86	0.41
1:B:103:PRO:HB2	1:B:362:VAL:HB	2.02	0.41
1:D:239:ARG:HH22	5:D:826:EDO:H22	1.86	0.41
1:D:38:VAL:O	1:D:42:ILE:HG12	2.21	0.41
1:B:258:MET:HA	1:B:291:VAL:O	2.21	0.41
1:D:694:GLN:OE1	1:D:787:GLN:HG2	2.21	0.41
1:B:294:TRP:CE2	1:B:322:PRO:HG3	2.56	0.40
1:C:594:LEU:HD23	6:C:987:HOH:O	2.21	0.40
1:D:688:GLY:HA2	1:D:792:ALA:HA	2.02	0.40
1:C:707:LEU:HB2	1:C:778:ILE:CD1	2.52	0.40
1:B:767:HIS:NE2	6:B:1029:HOH:O	2.31	0.40
1:C:638:PHE:HD1	1:C:642:LEU:HD13	1.87	0.40
1:A:214:LYS:HA	1:A:215:HIS:HA	1.88	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	798/822 (97%)	766 (96%)	32 (4%)	0	100	100
1	B	792/822 (96%)	756 (96%)	36 (4%)	0	100	100
1	C	792/822 (96%)	757 (96%)	33 (4%)	2 (0%)	46	57
1	D	793/822 (96%)	760 (96%)	33 (4%)	0	100	100
All	All	3175/3288 (97%)	3039 (96%)	134 (4%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	67	ASN
1	C	294	TRP

### 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	664/680 (98%)	655 (99%)	9 (1%)	74	86
1	B	658/680 (97%)	649 (99%)	9 (1%)	74	86
1	C	658/680 (97%)	647 (98%)	11 (2%)	68	83
1	D	659/680 (97%)	648 (98%)	11 (2%)	68	83
All	All	2639/2720 (97%)	2599 (98%)	40 (2%)	72	85

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	114	HIS
1	A	267	LYS
1	A	642	LEU
1	A	653	THR
1	A	705	THR
1	A	728	GLN
1	A	775	GLU
1	A	803	SER
1	B	68	THR
1	B	78	GLN
1	B	112	HIS
1	B	114	HIS
1	B	594	LEU
1	B	642	LEU
1	B	653	THR
1	B	728	GLN
1	B	804	ASP
1	C	64	ASN
1	C	74	LYS
1	C	75	ARG
1	C	112	HIS
1	C	114	HIS
1	C	307	GLN
1	C	594	LEU
1	C	642	LEU
1	C	653	THR
1	C	728	GLN
1	C	805	ASP
1	D	68	THR
1	D	75	ARG
1	D	112	HIS
1	D	114	HIS
1	D	307	GLN
1	D	594	LEU
1	D	653	THR
1	D	728	GLN
1	D	782	LEU
1	D	800	ILE
1	D	806	SER

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 ⓘ

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 ⓘ

Of 35 ligands modelled in this entry, 8 are monoatomic - leaving 27 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	SO4	A	822	-	4,4,4	0.21	0	6,6,6	0.17	0
4	SO4	A	823	-	4,4,4	0.32	0	6,6,6	0.17	0
4	SO4	A	824	-	4,4,4	0.32	0	6,6,6	0.15	0
4	SO4	A	825	-	4,4,4	0.21	0	6,6,6	0.27	0
4	SO4	A	826	-	4,4,4	0.28	0	6,6,6	0.12	0
5	EDO	A	827	-	3,3,3	0.48	0	2,2,2	0.76	0
5	EDO	A	828	-	3,3,3	0.49	0	2,2,2	0.48	0
5	EDO	A	829	-	3,3,3	0.46	0	2,2,2	0.52	0
4	SO4	B	822	-	4,4,4	0.28	0	6,6,6	0.20	0
4	SO4	B	823	-	4,4,4	0.24	0	6,6,6	0.18	0
4	SO4	B	824	-	4,4,4	0.19	0	6,6,6	0.14	0
4	SO4	B	825	-	4,4,4	0.18	0	6,6,6	0.24	0
4	SO4	B	826	-	4,4,4	0.27	0	6,6,6	0.13	0
5	EDO	B	827	-	3,3,3	0.42	0	2,2,2	0.76	0
5	EDO	B	828	-	3,3,3	0.47	0	2,2,2	0.47	0
4	SO4	C	822	-	4,4,4	0.14	0	6,6,6	0.32	0
4	SO4	C	823	-	4,4,4	0.38	0	6,6,6	0.38	0
4	SO4	C	824	-	4,4,4	0.20	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	C	825	-	4,4,4	0.22	0	6,6,6	0.14	0
4	SO4	C	826	-	4,4,4	0.11	0	6,6,6	0.14	0
5	EDO	C	827	-	3,3,3	0.49	0	2,2,2	0.19	0
5	EDO	C	828	-	3,3,3	0.51	0	2,2,2	0.38	0
4	SO4	D	822	-	4,4,4	0.21	0	6,6,6	0.09	0
4	SO4	D	823	-	4,4,4	0.24	0	6,6,6	0.19	0
4	SO4	D	824	-	4,4,4	0.20	0	6,6,6	0.21	0
5	EDO	D	825	-	3,3,3	0.47	0	2,2,2	0.67	0
5	EDO	D	826	-	3,3,3	0.48	0	2,2,2	0.38	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	SO4	A	822	-	-	0/0/0/0	0/0/0/0
4	SO4	A	823	-	-	0/0/0/0	0/0/0/0
4	SO4	A	824	-	-	0/0/0/0	0/0/0/0
4	SO4	A	825	-	-	0/0/0/0	0/0/0/0
4	SO4	A	826	-	-	0/0/0/0	0/0/0/0
5	EDO	A	827	-	-	0/1/1/1	0/0/0/0
5	EDO	A	828	-	-	0/1/1/1	0/0/0/0
5	EDO	A	829	-	-	0/1/1/1	0/0/0/0
4	SO4	B	822	-	-	0/0/0/0	0/0/0/0
4	SO4	B	823	-	-	0/0/0/0	0/0/0/0
4	SO4	B	824	-	-	0/0/0/0	0/0/0/0
4	SO4	B	825	-	-	0/0/0/0	0/0/0/0
4	SO4	B	826	-	-	0/0/0/0	0/0/0/0
5	EDO	B	827	-	-	0/1/1/1	0/0/0/0
5	EDO	B	828	-	-	0/1/1/1	0/0/0/0
4	SO4	C	822	-	-	0/0/0/0	0/0/0/0
4	SO4	C	823	-	-	0/0/0/0	0/0/0/0
4	SO4	C	824	-	-	0/0/0/0	0/0/0/0
4	SO4	C	825	-	-	0/0/0/0	0/0/0/0
4	SO4	C	826	-	-	0/0/0/0	0/0/0/0
5	EDO	C	827	-	-	0/1/1/1	0/0/0/0
5	EDO	C	828	-	-	0/1/1/1	0/0/0/0
4	SO4	D	822	-	-	0/0/0/0	0/0/0/0
4	SO4	D	823	-	-	0/0/0/0	0/0/0/0
4	SO4	D	824	-	-	0/0/0/0	0/0/0/0
5	EDO	D	825	-	-	0/1/1/1	0/0/0/0
5	EDO	D	826	-	-	0/1/1/1	0/0/0/0

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	828	EDO	1	0
4	C	824	SO4	1	0
5	D	826	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	804/822 (97%)	0.07	18 (2%) 65 73	16, 38, 71, 98	48 (5%)
1	B	798/822 (97%)	0.37	58 (7%) 18 25	20, 43, 74, 90	50 (6%)
1	C	798/822 (97%)	0.10	22 (2%) 56 66	16, 40, 70, 92	40 (5%)
1	D	799/822 (97%)	0.50	71 (8%) 12 17	23, 43, 74, 91	51 (6%)
All	All	3199/3288 (97%)	0.26	169 (5%) 30 39	16, 41, 72, 98	189 (5%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	475	TYR	6.9
1	D	477	SER	6.2
1	B	814	LEU	5.8
1	D	415	ILE	5.7
1	B	624	THR	5.6
1	C	568	GLN	5.6
1	B	73	ASN	5.4
1	D	512	ALA	5.2
1	D	476	THR	4.9
1	D	464	GLY	4.7
1	B	626	PRO	4.7
1	D	625	SER	4.6
1	D	474	GLU	4.5
1	D	619	VAL	4.4
1	B	461	THR	4.4
1	B	111	MET	4.4
1	D	519	ALA	4.3
1	D	522	ILE	4.3
1	D	479	PRO	4.3
1	C	567	LYS	4.2
1	A	567	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	485	VAL	4.1
1	B	706	PRO	4.1
1	D	501	LEU	4.0
1	A	73	ASN	3.9
1	B	620	LEU	3.8
1	D	460	VAL	3.7
1	D	500	LEU	3.6
1	B	415	ILE	3.6
1	B	460	VAL	3.6
1	D	565	THR	3.6
1	D	101	ALA	3.6
1	A	462	LYS	3.6
1	B	623	LYS	3.6
1	C	775	GLU	3.5
1	C	571	THR	3.5
1	B	254	VAL	3.5
1	D	506	GLU	3.5
1	A	568	GLN	3.4
1	C	738	GLU	3.4
1	B	161	THR	3.3
1	A	522	ILE	3.3
1	C	411	ALA	3.3
1	A	74	LYS	3.3
1	D	467	ILE	3.3
1	C	705	THR	3.3
1	D	739	SER	3.2
1	B	411	ALA	3.2
1	B	619	VAL	3.2
1	B	463	ALA	3.2
1	B	381	GLY	3.2
1	D	776	GLN	3.2
1	D	453	PHE	3.2
1	B	96	THR	3.1
1	D	570	LYS	3.1
1	B	127	ILE	3.1
1	D	463	ALA	3.1
1	D	705	THR	3.1
1	B	617	VAL	3.1
1	C	475	TYR	3.1
1	D	711	PHE	3.1
1	B	812	ALA	3.0
1	B	570	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	464	GLY	3.0
1	B	569	GLY	3.0
1	B	412	SER	3.0
1	A	76	ALA	3.0
1	B	467	ILE	3.0
1	D	645	ASN	2.9
1	B	621	SER	2.9
1	D	505	HIS	2.9
1	C	463	ALA	2.9
1	B	535	TRP	2.9
1	D	439	THR	2.9
1	A	771	SER	2.9
1	B	739	SER	2.9
1	D	117	VAL	2.8
1	D	502	GLU	2.8
1	B	565	THR	2.8
1	B	625	SER	2.8
1	C	704	PRO	2.8
1	A	814	LEU	2.8
1	D	409	ILE	2.8
1	D	540	LEU	2.8
1	B	567	LYS	2.8
1	B	409	ILE	2.8
1	D	161	THR	2.8
1	A	703	GLU	2.8
1	D	777	PRO	2.7
1	B	126	ASN	2.7
1	D	815	GLU	2.7
1	D	478	LYS	2.7
1	B	213	ALA	2.7
1	D	368	PRO	2.7
1	B	653	THR	2.6
1	D	626	PRO	2.6
1	D	775	GLU	2.6
1	D	528	PHE	2.6
1	D	31	LYS	2.6
1	D	418	ALA	2.6
1	B	462	LYS	2.5
1	C	410	LYS	2.5
1	B	257	VAL	2.5
1	C	570	LYS	2.5
1	B	505	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	586	TYR	2.5
1	C	645	ASN	2.5
1	D	67	ASN	2.5
1	A	626	PRO	2.4
1	A	409	ILE	2.4
1	D	363	PHE	2.4
1	B	705	THR	2.4
1	C	566	ASN	2.4
1	B	568	GLN	2.4
1	D	414	ARG	2.4
1	D	118	TYR	2.4
1	B	387	THR	2.4
1	B	704	PRO	2.4
1	D	58	GLY	2.4
1	B	174	TYR	2.4
1	C	701	TYR	2.4
1	A	464	GLY	2.4
1	D	615	ILE	2.4
1	D	410	LYS	2.4
1	D	338	ALA	2.3
1	B	466	LYS	2.3
1	B	475	TYR	2.3
1	D	434	VAL	2.3
1	D	484	VAL	2.3
1	A	512	ALA	2.3
1	B	163	ALA	2.3
1	B	246	TYR	2.3
1	D	422	ALA	2.3
1	D	96	THR	2.3
1	C	644	LYS	2.3
1	B	566	ASN	2.3
1	D	535	TRP	2.3
1	D	462	LYS	2.2
1	C	78	GLN	2.2
1	C	814	LEU	2.2
1	D	412	SER	2.2
1	D	327	ALA	2.2
1	B	110	ALA	2.2
1	A	5	GLN	2.2
1	D	568	GLN	2.2
1	B	212	THR	2.1
1	D	257	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	519	ALA	2.1
1	A	523	PRO	2.1
1	C	460	VAL	2.1
1	D	51	VAL	2.1
1	D	551	LEU	2.1
1	D	569	GLY	2.1
1	C	706	PRO	2.1
1	B	256	SER	2.1
1	D	737	SER	2.1
1	C	702	LEU	2.1
1	D	119	GLY	2.1
1	D	553	GLY	2.1
1	C	573	PHE	2.1
1	D	637	LEU	2.1
1	D	738	GLU	2.1
1	B	75	ARG	2.1
1	A	479	PRO	2.1
1	B	160	PRO	2.0
1	D	127	ILE	2.0
1	A	623	LYS	2.0
1	B	377	PRO	2.0
1	B	573	PHE	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. 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( $\text{\AA}^2$ )	Q<0.9
5	EDO	C	827	4/4	0.81	0.23	5.90	51,54,59,59	0
3	NA	C	902	1/1	0.92	0.23	4.28	24,24,24,24	0
3	NA	B	902	1/1	0.92	0.20	2.60	24,24,24,24	0
5	EDO	D	825	4/4	0.92	0.30	2.15	57,60,65,65	0
4	SO4	A	823	5/5	0.98	0.24	2.00	32,50,61,82	0
3	NA	A	902	1/1	0.87	0.17	0.99	18,18,18,18	0
4	SO4	C	823	5/5	0.97	0.20	0.87	31,34,45,72	0
2	CA	C	901	1/1	0.97	0.14	0.13	31,31,31,31	0
4	SO4	A	826	5/5	0.97	0.10	-0.12	29,34,66,83	1
2	CA	B	901	1/1	0.95	0.14	-0.13	40,40,40,40	0
3	NA	D	902	1/1	0.94	0.12	-0.80	27,27,27,27	0
2	CA	A	901	1/1	0.93	0.12	-1.20	30,30,30,30	0
4	SO4	A	824	5/5	0.96	0.12	-1.38	26,31,42,43	5
4	SO4	B	826	5/5	0.98	0.08	-1.50	48,61,68,77	1
2	CA	D	901	1/1	0.93	0.09	-1.91	36,36,36,36	0
4	SO4	C	826	5/5	0.93	0.09	-2.20	59,64,81,85	0
5	EDO	B	827	4/4	0.94	0.28	-	51,54,57,58	0
5	EDO	B	828	4/4	0.93	0.10	-	30,42,66,67	0
4	SO4	A	825	5/5	0.94	0.21	-	19,33,50,52	4
5	EDO	A	828	4/4	0.85	0.10	-	44,60,63,64	0
4	SO4	D	822	5/5	0.97	0.12	-	45,52,64,66	1
5	EDO	D	826	4/4	0.92	0.09	-	46,46,53,56	0
4	SO4	C	825	5/5	0.92	0.11	-	28,28,44,47	5
4	SO4	A	822	5/5	0.97	0.13	-	43,67,84,90	0
4	SO4	C	824	5/5	0.93	0.10	-	61,65,79,81	1
5	EDO	A	827	4/4	0.94	0.14	-	31,32,39,58	0
4	SO4	D	824	5/5	0.95	0.23	-	40,55,84,90	1
4	SO4	D	823	5/5	0.95	0.13	-	52,55,65,68	0
4	SO4	B	823	5/5	0.97	0.15	-	35,58,69,73	1
4	SO4	B	824	5/5	0.86	0.16	-	24,36,50,63	5
4	SO4	C	822	5/5	0.81	0.18	-	22,30,60,60	5
5	EDO	C	828	4/4	0.73	0.17	-	52,68,69,81	0
4	SO4	B	822	5/5	0.91	0.15	-	36,45,57,61	4
4	SO4	B	825	5/5	0.93	0.10	-	36,54,58,69	1
5	EDO	A	829	4/4	0.91	0.11	-	35,39,48,50	0

## 6.5 Other polymers

There are no such residues in this entry.