



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:27 AM 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 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/ValidationPDFNotes.html>

---

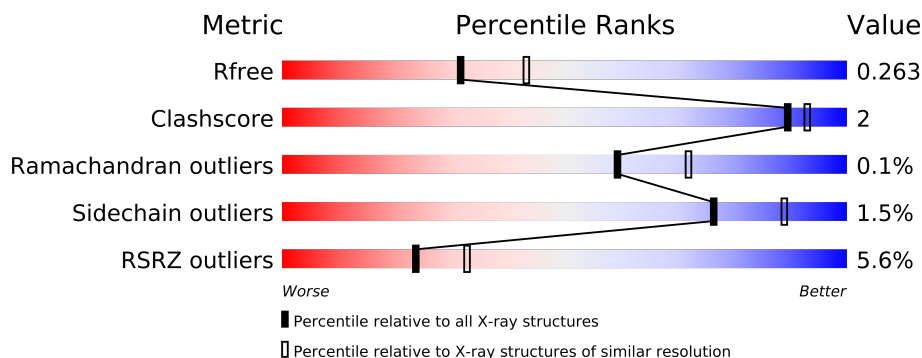
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	822	
1	B	822	
1	C	822	
1	D	822	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NA	A	902	-	X
3	NA	B	902	-	X
3	NA	C	902	-	X
5	EDO	A	827	-	X
5	EDO	C	827	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25742 atoms, of which 0 are hydrogen and 0 are deuterium.

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

*Continued on next page...*

Continued from previous page...

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

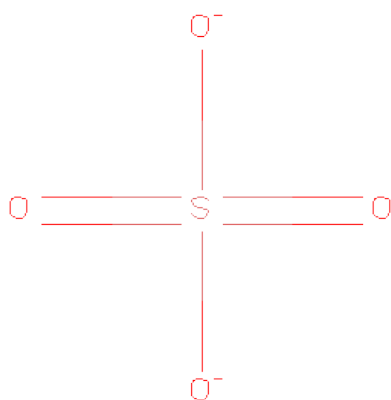
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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).



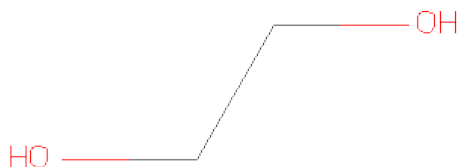
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total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

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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.

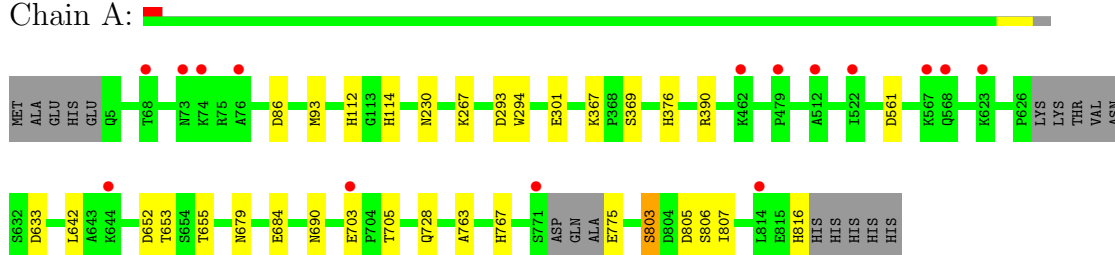
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	262	Total	O	0	0
			262	262		
6	B	283	Total	O	0	0
			283	283		
6	C	177	Total	O	0	0
			177	177		
6	D	106	Total	O	0	0
			106	106		

### 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.

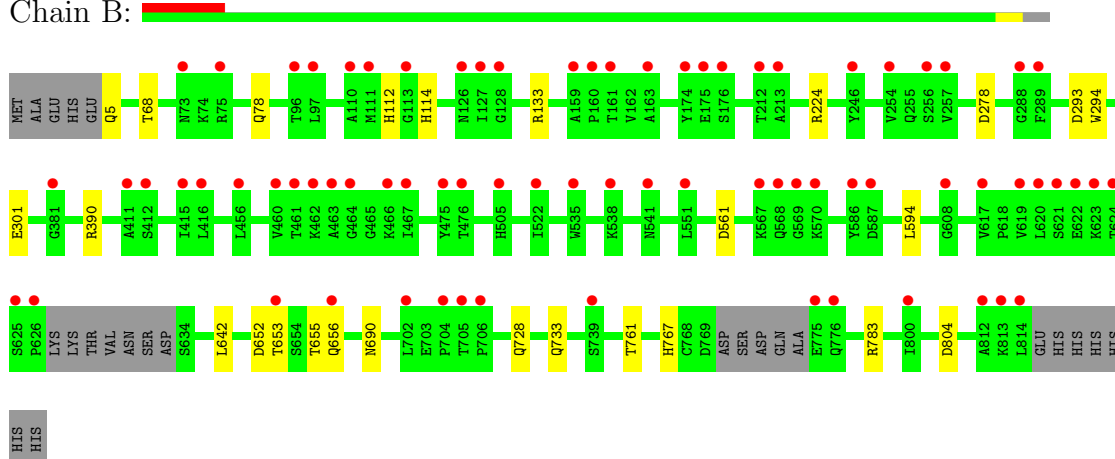
- Molecule 1: Exo-1,3/1,4-beta-glucanase

Chain A:



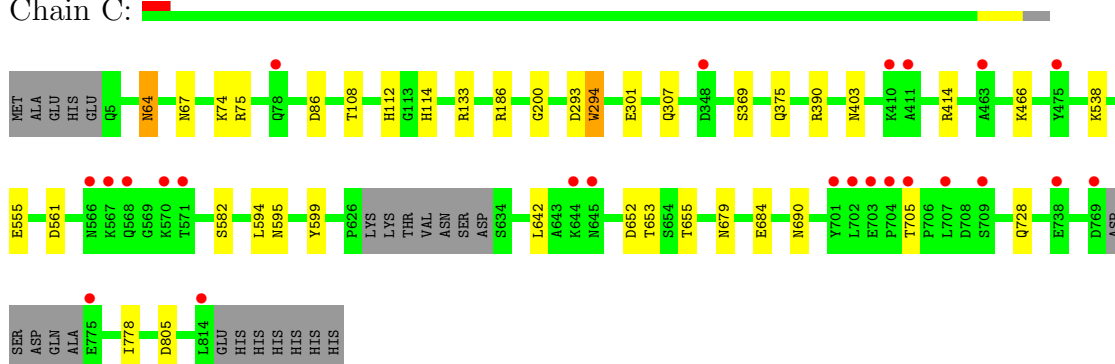
- Molecule 1: Exo-1,3/1,4-beta-glucanase

Chain B:



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

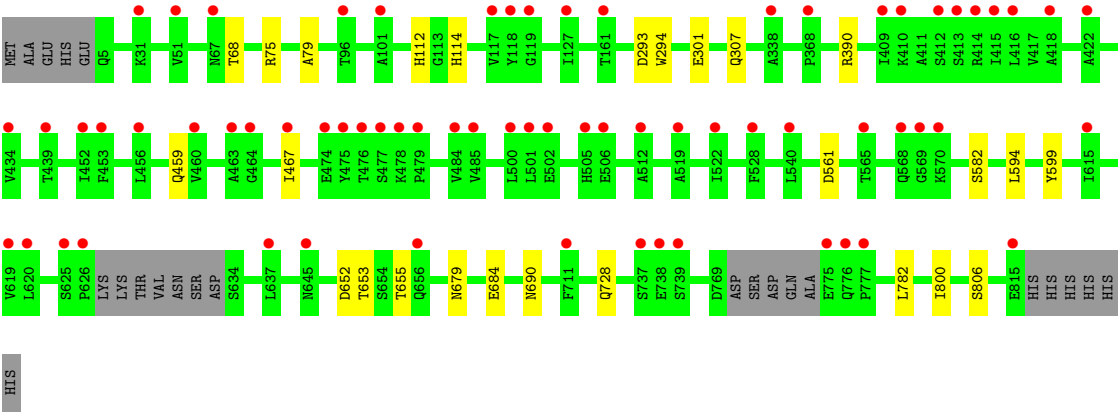
Chain C:





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

Chain D: 



## 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 0.215 , 0.263	Depositor DCC
$R_{free}$ test set	7206 reflections (5.03%)	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 , 29.2	EDS
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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.

## 5 Model quality

### 5.1 Standard geometry

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 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the

Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6228	0	0	15	0
1	B	6181	0	0	12	0
1	C	6181	0	0	20	0
1	D	6190	0	0	9	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	1	0
4	C	25	0	0	2	0
4	D	15	0	0	0	0
5	A	12	0	18	0	0
5	B	8	0	12	0	0
5	C	8	0	12	0	0
5	D	8	0	12	0	0
6	A	262	0	0	3	0
6	B	283	0	0	6	0
6	C	177	0	0	8	0
6	D	106	0	0	1	0
All	All	25742	0	54	54	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (54) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:367:LYS:NZ	1:C:375:GLN:OE1	2.10	0.85
1:B:656:GLN:NE2	6:B:1083:HOH:O	2.24	0.70
1:C:414:ARG:NH2	6:C:991:HOH:O	2.25	0.69
1:A:301:GLU:OE1	1:A:690:ASN:ND2	2.31	0.64
1:A:703:GLU:N	6:A:1021:HOH:O	2.33	0.61
1:B:767:HIS:NE2	6:B:1029:HOH:O	2.31	0.60
1:D:301:GLU:OE1	1:D:690:ASN:ND2	2.36	0.59
1:C:301:GLU:OE1	1:C:690:ASN:ND2	2.37	0.57
1:C:64:ASN:OD1	1:C:108:THR:OG1	2.21	0.57
1:C:466:LYS:NZ	6:C:1006:HOH:O	2.38	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:301:GLU:OE1	1:B:690:ASN:ND2	2.38	0.56
1:A:767:HIS:NE2	1:A:816:HIS:O	2.39	0.56
1:C:186:ARG:NH2	6:C:1000:HOH:O	2.38	0.56
1:C:200:GLY:N	6:C:836:HOH:O	2.40	0.55
1:A:376:HIS:NE2	1:D:79:ALA:O	2.40	0.54
1:B:733:GLN:OE1	1:B:783:ARG:NH1	2.41	0.54
1:D:652:ASP:OD1	1:D:655:THR:OG1	2.29	0.50
1:C:595:ASN:N	6:C:964:HOH:O	2.44	0.50
1:A:652:ASP:OD1	1:A:655:THR:OG1	2.30	0.50
1:B:278:ASP:OD2	6:B:858:HOH:O	2.20	0.50
1:C:293:ASP:OD1	1:C:294:TRP:N	2.45	0.50
1:A:803:SER:O	1:A:806:SER:OG	2.31	0.49
1:C:555:GLU:N	6:C:853:HOH:O	2.46	0.49
1:C:133:ARG:NE	4:C:824:SO4:O4	2.46	0.49
1:D:293:ASP:OD1	1:D:294:TRP:N	2.46	0.48
1:B:652:ASP:OD1	1:B:655:THR:OG1	2.33	0.47
1:C:652:ASP:OD1	1:C:655:THR:OG1	2.33	0.46
1:C:86:ASP:OD2	1:C:369:SER:OG	2.32	0.46
1:B:293:ASP:OD1	1:B:294:TRP:N	2.49	0.46
1:A:230:ASN:ND2	6:A:884:HOH:O	2.49	0.46
1:C:403:ASN:OD1	6:C:1002:HOH:O	2.21	0.45
1:B:390:ARG:NE	1:B:561:ASP:OD2	2.50	0.45
1:C:582:SER:OG	1:C:599:TYR:OH	2.36	0.44
1:C:705:THR:O	1:C:778:ILE:N	2.50	0.44
1:B:133:ARG:NH2	4:B:825:SO4:O1	2.51	0.44
1:A:293:ASP:OD1	1:A:294:TRP:N	2.52	0.43
1:B:5:GLN:N	6:B:1095:HOH:O	2.51	0.43
1:D:582:SER:OG	1:D:599:TYR:OH	2.36	0.43
1:C:390:ARG:NE	1:C:561:ASP:OD2	2.52	0.43
1:A:390:ARG:NE	1:A:561:ASP:OD2	2.51	0.43
1:C:186:ARG:NH1	6:C:856:HOH:O	2.51	0.42
1:D:467:ILE:N	6:D:899:HOH:O	2.53	0.42
1:D:390:ARG:NE	1:D:561:ASP:OD2	2.52	0.42
1:A:679:ASN:OD1	1:A:684:GLU:N	2.53	0.42
1:A:763:ALA:N	1:A:807:ILE:O	2.53	0.42
1:C:538:LYS:NZ	4:C:826:SO4:O1	2.53	0.41
1:B:224:ARG:NH2	6:B:986:HOH:O	2.53	0.41
1:C:679:ASN:OD1	1:C:684:GLU:N	2.53	0.41
1:A:805:ASP:N	6:A:1024:HOH:O	2.53	0.41
1:D:459:GLN:NE2	1:D:561:ASP:OD1	2.54	0.41
1:D:679:ASN:OD1	1:D:684:GLU:N	2.53	0.41
1:B:761:THR:N	6:B:924:HOH:O	2.54	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:86:ASP:OD2	1:A:369:SER:OG	2.40	0.40
1:A:633:ASP:N	1:A:633:ASP:OD1	2.55	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	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%)	50	60
1	D	793/822 (96%)	760 (96%)	33 (4%)	0	100	100
All	All	3175/3288 (97%)	3039 (96%)	134 (4%)	2 (0%)	59	72

All (2) Ramachandran outliers are listed below:

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

### 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	664/680 (98%)	655 (99%)	9 (1%)	78	90
1	B	658/680 (97%)	649 (99%)	9 (1%)	78	90
1	C	658/680 (97%)	647 (98%)	11 (2%)	73	87

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	659/680 (97%)	648 (98%)	11 (2%)	73	87
All	All	2639/2720 (97%)	2599 (98%)	40 (2%)	76	89

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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 chains 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	0.31	0	6,6,6	0.16	0
4	SO4	A	824	-	4,4,4	0.31	0	6,6,6	0.13	0
4	SO4	A	825	-	4,4,4	0.19	0	6,6,6	0.25	0
4	SO4	A	826	-	4,4,4	0.27	0	6,6,6	0.11	0
5	EDO	A	827	-	3,3,3	0.54	0	2,2,2	0.72	0
5	EDO	A	828	-	3,3,3	0.56	0	2,2,2	0.43	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	829	-	3,3,3	0.53	0	2,2,2	0.48	0
4	SO4	B	822	-	4,4,4	0.26	0	6,6,6	0.19	0
4	SO4	B	823	-	4,4,4	0.23	0	6,6,6	0.17	0
4	SO4	B	824	-	4,4,4	0.17	0	6,6,6	0.14	0
4	SO4	B	825	-	4,4,4	0.16	0	6,6,6	0.23	0
4	SO4	B	826	-	4,4,4	0.26	0	6,6,6	0.13	0
5	EDO	B	827	-	3,3,3	0.49	0	2,2,2	0.72	0
5	EDO	B	828	-	3,3,3	0.54	0	2,2,2	0.43	0
4	SO4	C	822	-	4,4,4	0.11	0	6,6,6	0.30	0
4	SO4	C	823	-	4,4,4	0.36	0	6,6,6	0.38	0
4	SO4	C	824	-	4,4,4	0.19	0	6,6,6	0.07	0
4	SO4	C	825	-	4,4,4	0.20	0	6,6,6	0.14	0
4	SO4	C	826	-	4,4,4	0.11	0	6,6,6	0.13	0
5	EDO	C	827	-	3,3,3	0.56	0	2,2,2	0.14	0
5	EDO	C	828	-	3,3,3	0.58	0	2,2,2	0.34	0
4	SO4	D	822	-	4,4,4	0.19	0	6,6,6	0.09	0
4	SO4	D	823	-	4,4,4	0.23	0	6,6,6	0.18	0
4	SO4	D	824	-	4,4,4	0.19	0	6,6,6	0.21	0
5	EDO	D	825	-	3,3,3	0.54	0	2,2,2	0.63	0
5	EDO	D	826	-	3,3,3	0.55	0	2,2,2	0.33	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

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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%)	0.05	15 (1%) 64 73	16, 38, 71, 98	48 (5%)
1	B	798/822 (97%)	0.44	75 (9%) 9 14	20, 43, 74, 90	50 (6%)
1	C	798/822 (97%)	0.14	24 (3%) 48 58	16, 40, 70, 92	40 (5%)
1	D	799/822 (97%)	0.48	68 (8%) 11 17	23, 43, 74, 91	51 (6%)
All	All	3199/3288 (97%)	0.28	182 (5%) 24 32	16, 41, 72, 98	189 (5%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	475	TYR	7.4
1	D	415	ILE	6.4
1	B	814	LEU	6.0
1	B	624	THR	6.0
1	B	626	PRO	5.9
1	C	568	GLN	5.5
1	D	477	SER	5.4
1	B	73	ASN	5.3
1	D	476	THR	5.1
1	D	519	ALA	4.6
1	C	775	GLU	4.5
1	B	620	LEU	4.4
1	B	111	MET	4.3
1	D	619	VAL	4.3
1	C	567	LYS	4.3
1	D	474	GLU	4.3
1	B	461	THR	4.2
1	D	501	LEU	4.2
1	D	464	GLY	4.1
1	B	127	ILE	4.1
1	B	460	VAL	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	625	SER	4.0
1	D	500	LEU	4.0
1	B	625	SER	3.9
1	B	706	PRO	3.9
1	A	567	LYS	3.8
1	A	73	ASN	3.8
1	B	623	LYS	3.8
1	D	512	ALA	3.7
1	D	485	VAL	3.7
1	D	522	ILE	3.7
1	D	506	GLU	3.6
1	D	101	ALA	3.5
1	D	479	PRO	3.5
1	B	415	ILE	3.5
1	A	74	LYS	3.5
1	B	161	THR	3.4
1	B	96	THR	3.4
1	C	738	GLU	3.4
1	B	411	ALA	3.4
1	B	254	VAL	3.3
1	B	570	LYS	3.3
1	B	812	ALA	3.3
1	C	411	ALA	3.3
1	D	739	SER	3.3
1	C	571	THR	3.3
1	C	475	TYR	3.3
1	B	126	ASN	3.3
1	B	412	SER	3.3
1	D	570	LYS	3.3
1	D	776	GLN	3.2
1	B	463	ALA	3.2
1	D	413	SER	3.2
1	A	814	LEU	3.2
1	B	535	TRP	3.2
1	C	704	PRO	3.1
1	D	815	GLU	3.1
1	A	568	GLN	3.1
1	B	619	VAL	3.1
1	B	464	GLY	3.1
1	D	118	TYR	3.1
1	D	565	THR	3.0
1	B	621	SER	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	460	VAL	3.0
1	B	257	VAL	2.9
1	B	213	ALA	2.9
1	D	117	VAL	2.9
1	C	644	LYS	2.9
1	C	814	LEU	2.9
1	D	505	HIS	2.9
1	B	381	GLY	2.9
1	B	569	GLY	2.9
1	A	703	GLU	2.9
1	D	409	ILE	2.8
1	D	645	ASN	2.8
1	B	617	VAL	2.8
1	D	463	ALA	2.8
1	B	110	ALA	2.8
1	A	462	LYS	2.8
1	D	412	SER	2.8
1	C	645	ASN	2.7
1	D	434	VAL	2.7
1	B	505	HIS	2.7
1	A	76	ALA	2.7
1	D	467	ILE	2.7
1	D	711	PHE	2.7
1	B	567	LYS	2.7
1	D	414	ARG	2.7
1	A	522	ILE	2.7
1	B	97	LEU	2.6
1	B	212	THR	2.6
1	D	615	ILE	2.6
1	D	368	PRO	2.6
1	A	644	LYS	2.6
1	D	777	PRO	2.6
1	D	119	GLY	2.6
1	A	771	SER	2.6
1	C	705	THR	2.6
1	B	653	THR	2.6
1	D	96	THR	2.6
1	D	31	LYS	2.6
1	B	704	PRO	2.5
1	B	813	LYS	2.5
1	D	484	VAL	2.5
1	D	67	ASN	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	701	TYR	2.5
1	B	160	PRO	2.5
1	C	463	ALA	2.5
1	D	439	THR	2.5
1	B	462	LYS	2.5
1	B	256	SER	2.5
1	D	528	PHE	2.5
1	B	586	TYR	2.5
1	B	128	GLY	2.5
1	D	478	LYS	2.5
1	B	159	ALA	2.5
1	B	775	GLU	2.4
1	D	51	VAL	2.4
1	D	453	PHE	2.4
1	B	739	SER	2.4
1	D	620	LEU	2.4
1	C	78	GLN	2.4
1	D	568	GLN	2.4
1	D	738	GLU	2.4
1	B	174	TYR	2.3
1	B	475	TYR	2.3
1	D	540	LEU	2.3
1	D	338	ALA	2.3
1	D	410	LYS	2.3
1	B	587	ASP	2.3
1	C	566	ASN	2.3
1	A	68	THR	2.3
1	D	502	GLU	2.3
1	B	541	ASN	2.3
1	D	569	GLY	2.3
1	D	737	SER	2.3
1	C	707	LEU	2.2
1	B	800	ILE	2.2
1	B	568	GLN	2.2
1	C	709	SER	2.2
1	A	512	ALA	2.2
1	B	456	LEU	2.2
1	B	246	TYR	2.2
1	B	467	ILE	2.2
1	D	161	THR	2.2
1	B	466	LYS	2.2
1	D	626	PRO	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	622	GLU	2.2
1	C	410	LYS	2.2
1	C	703	GLU	2.2
1	D	775	GLU	2.2
1	C	702	LEU	2.2
1	A	623	LYS	2.1
1	B	175	GLU	2.1
1	D	452	ILE	2.1
1	A	479	PRO	2.1
1	B	288	GLY	2.1
1	B	289	PHE	2.1
1	D	422	ALA	2.1
1	B	176	SER	2.1
1	B	522	ILE	2.1
1	D	418	ALA	2.1
1	D	656	GLN	2.1
1	B	705	THR	2.1
1	D	416	LEU	2.1
1	B	608	GLY	2.1
1	B	416	LEU	2.1
1	C	570	LYS	2.1
1	B	113	GLY	2.1
1	B	776	GLN	2.1
1	B	476	THR	2.1
1	C	769	ASP	2.1
1	D	127	ILE	2.1
1	B	551	LEU	2.0
1	B	538	LYS	2.0
1	B	75	ARG	2.0
1	B	163	ALA	2.0
1	B	656	GLN	2.0
1	D	456	LEU	2.0
1	C	348	ASP	2.0
1	B	702	LEU	2.0
1	D	637	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	C	827	4/4	0.23	6.15	51,54,59,59	0
3	NA	C	902	1/1	0.23	4.73	24,24,24,24	0
3	NA	B	902	1/1	0.20	2.65	24,24,24,24	0
5	EDO	A	827	4/4	0.17	2.39	31,32,39,58	0
3	NA	A	902	1/1	0.18	2.36	18,18,18,18	0
5	EDO	B	827	4/4	0.21	1.94	51,54,57,58	0
5	EDO	D	825	4/4	0.29	1.89	57,60,65,65	0
4	SO4	A	823	5/5	0.22	1.84	32,50,61,82	0
4	SO4	A	825	5/5	0.19	1.43	19,33,50,52	4
4	SO4	B	823	5/5	0.14	1.34	35,58,69,73	1
4	SO4	A	822	5/5	0.13	1.31	43,67,84,90	0
4	SO4	D	824	5/5	0.19	1.24	40,55,84,90	1
4	SO4	C	822	5/5	0.17	0.82	22,30,60,60	5
4	SO4	C	823	5/5	0.21	0.77	31,34,45,72	0
4	SO4	B	824	5/5	0.14	0.57	24,36,50,63	5
2	CA	C	901	1/1	0.14	0.41	31,31,31,31	0
2	CA	B	901	1/1	0.17	0.38	40,40,40,40	0
4	SO4	A	826	5/5	0.10	0.29	29,34,66,83	1
5	EDO	C	828	4/4	0.16	-0.09	52,68,69,81	0
4	SO4	B	822	5/5	0.14	-0.11	36,45,57,61	4
5	EDO	A	828	4/4	0.11	-0.44	44,60,63,64	0
4	SO4	C	824	5/5	0.10	-0.85	61,65,79,81	1
3	NA	D	902	1/1	0.12	-0.91	27,27,27,27	0
5	EDO	A	829	4/4	0.10	-0.92	35,39,48,50	0
2	CA	A	901	1/1	0.12	-0.98	30,30,30,30	0
4	SO4	A	824	5/5	0.13	-1.02	26,31,42,43	5
4	SO4	C	825	5/5	0.11	-1.16	28,28,44,47	5
4	SO4	D	822	5/5	0.12	-1.17	45,52,64,66	1
5	EDO	B	828	4/4	0.10	-1.38	30,42,66,67	0
4	SO4	B	826	5/5	0.08	-1.55	48,61,68,77	1

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	D	826	4/4	0.10	-1.70	46,46,53,56	0
2	CA	D	901	1/1	0.10	-1.73	36,36,36,36	0
4	SO4	C	826	5/5	0.09	-1.87	59,64,81,85	0
4	SO4	D	823	5/5	0.14	-1.94	52,55,65,68	0
4	SO4	B	825	5/5	0.10	-3.77	36,54,58,69	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.