



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2021 – 01:12 pm GMT

PDB ID : 7B0D  
Title : Sugar transaminase from *Archaeoglobus veneficus*  
Authors : James, P.; Littlechild, J.A.; De Rose, S.A.; Isupov, M.N.  
Deposited on : 2020-11-19  
Resolution : 1.27 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.

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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 : 1.8.4 (270009), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

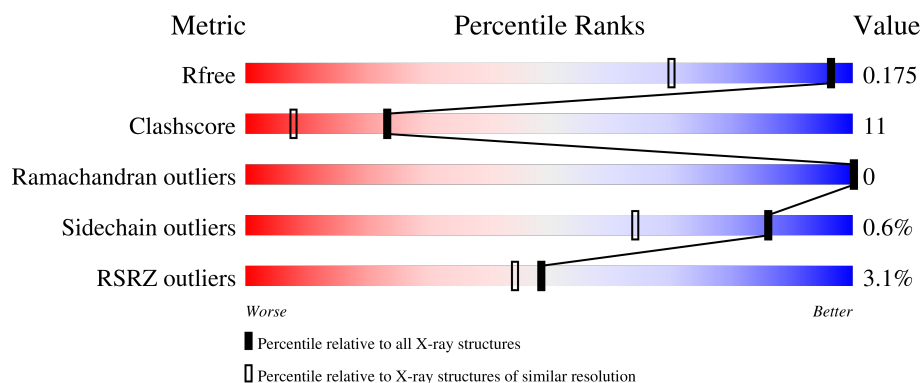
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


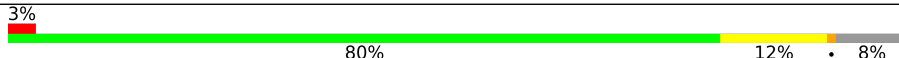
The reported resolution of this entry is 1.27 Å.

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))
$R_{free}$	130704	1850 (1.30-1.26)
Clashscore	141614	1926 (1.30-1.26)
Ramachandran outliers	138981	1860 (1.30-1.26)
Sidechain outliers	138945	1859 (1.30-1.26)
RSRZ outliers	127900	1807 (1.30-1.26)

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	399	
1	B	399	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	401	-	-	X	-
6	TRS	B	2108	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15160 atoms, of which 7341 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 Glutamine--scyllo-inositol transaminase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	368	Total	C	H	N	O	P	S	90	83	0
			7158	2301	3641	556	644	1	15			
1	B	368	Total	C	H	N	O	P	S	87	78	0
			7032	2256	3584	548	626	1	17			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP F2KQE6
A	-26	ALA	-	expression tag	UNP F2KQE6
A	-25	GLY	-	expression tag	UNP F2KQE6
A	-24	SER	-	expression tag	UNP F2KQE6
A	-23	HIS	-	expression tag	UNP F2KQE6
A	-22	HIS	-	expression tag	UNP F2KQE6
A	-21	HIS	-	expression tag	UNP F2KQE6
A	-20	HIS	-	expression tag	UNP F2KQE6
A	-19	HIS	-	expression tag	UNP F2KQE6
A	-18	HIS	-	expression tag	UNP F2KQE6
A	-17	GLY	-	expression tag	UNP F2KQE6
A	-16	MET	-	expression tag	UNP F2KQE6
A	-15	ALA	-	expression tag	UNP F2KQE6
A	-14	SER	-	expression tag	UNP F2KQE6
A	-13	MET	-	expression tag	UNP F2KQE6
A	-12	THR	-	expression tag	UNP F2KQE6
A	-11	GLY	-	expression tag	UNP F2KQE6
A	-10	GLY	-	expression tag	UNP F2KQE6
A	-9	GLN	-	expression tag	UNP F2KQE6
A	-8	GLN	-	expression tag	UNP F2KQE6
A	-7	MET	-	expression tag	UNP F2KQE6
A	-6	GLY	-	expression tag	UNP F2KQE6
A	-5	ARG	-	expression tag	UNP F2KQE6
A	-4	SER	-	expression tag	UNP F2KQE6
A	-3	GLY	-	expression tag	UNP F2KQE6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ASP	-	expression tag	UNP F2KQE6
A	-1	ASP	-	expression tag	UNP F2KQE6
A	0	ASP	-	expression tag	UNP F2KQE6
B	-27	MET	-	initiating methionine	UNP F2KQE6
B	-26	ALA	-	expression tag	UNP F2KQE6
B	-25	GLY	-	expression tag	UNP F2KQE6
B	-24	SER	-	expression tag	UNP F2KQE6
B	-23	HIS	-	expression tag	UNP F2KQE6
B	-22	HIS	-	expression tag	UNP F2KQE6
B	-21	HIS	-	expression tag	UNP F2KQE6
B	-20	HIS	-	expression tag	UNP F2KQE6
B	-19	HIS	-	expression tag	UNP F2KQE6
B	-18	HIS	-	expression tag	UNP F2KQE6
B	-17	GLY	-	expression tag	UNP F2KQE6
B	-16	MET	-	expression tag	UNP F2KQE6
B	-15	ALA	-	expression tag	UNP F2KQE6
B	-14	SER	-	expression tag	UNP F2KQE6
B	-13	MET	-	expression tag	UNP F2KQE6
B	-12	THR	-	expression tag	UNP F2KQE6
B	-11	GLY	-	expression tag	UNP F2KQE6
B	-10	GLY	-	expression tag	UNP F2KQE6
B	-9	GLN	-	expression tag	UNP F2KQE6
B	-8	GLN	-	expression tag	UNP F2KQE6
B	-7	MET	-	expression tag	UNP F2KQE6
B	-6	GLY	-	expression tag	UNP F2KQE6
B	-5	ARG	-	expression tag	UNP F2KQE6
B	-4	SER	-	expression tag	UNP F2KQE6
B	-3	GLY	-	expression tag	UNP F2KQE6
B	-2	ASP	-	expression tag	UNP F2KQE6
B	-1	ASP	-	expression tag	UNP F2KQE6
B	0	ASP	-	expression tag	UNP F2KQE6

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

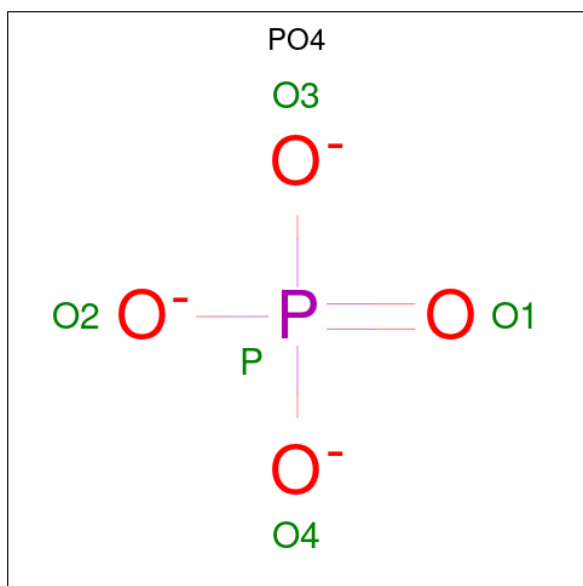


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	1	0
			10	2	6	2		
2	A	1	Total	C	H	O	1	0
			10	2	6	2		
2	A	1	Total	C	H	O	1	0
			10	2	6	2		
2	A	1	Total	C	H	O	1	0
			10	2	6	2		
2	A	1	Total	C	H	O	1	0
			10	2	6	2		
2	A	1	Total	C	H	O	1	0
			10	2	6	2		
2	B	1	Total	C	H	O	1	0
			10	2	6	2		
2	B	1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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		

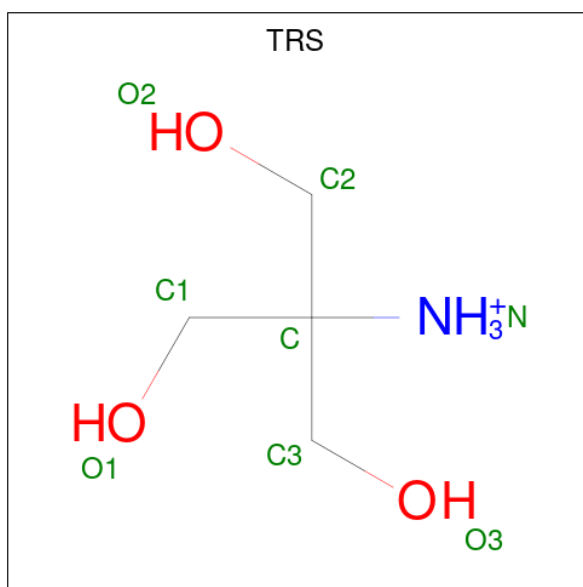
- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



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

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	2	0
			20	4	12	1	3		

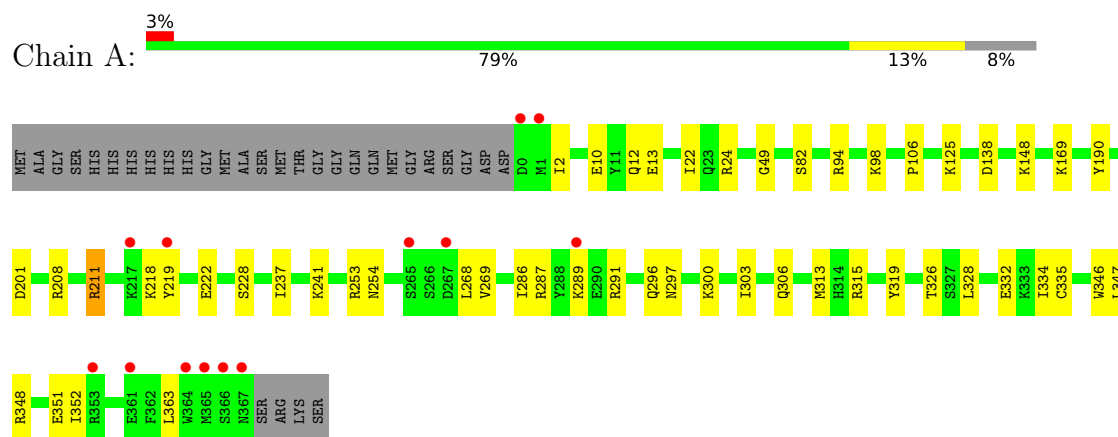
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	392	Total	O	0	0
			392	392		
7	B	333	Total	O	0	0
			333	333		

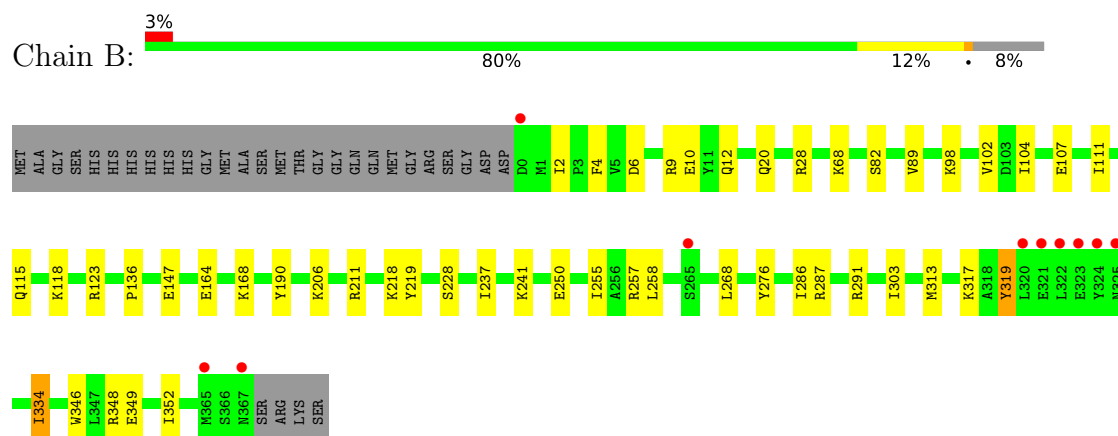
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamine--scyllo-inositol transaminase



- Molecule 1: Glutamine--scyllo-inositol transaminase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.23Å 105.95Å 111.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 1.27 49.24 – 1.27	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.29-1.27) 97.6 (49.24-1.27)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 1.27Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.152 , 0.175 0.152 , 0.175	Depositor DCC
$R_{free}$ test set	10625 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	15160	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, TRS, CA, LLP, PO4, 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	0.72	0/3798	0.85	5/5105 (0.1%)
1	B	0.71	0/3719	0.81	3/5002 (0.1%)
All	All	0.71	0/7517	0.83	8/10107 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	211	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	94	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	319	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	A	208	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	319[A]	TYR	CB-CG-CD1	5.17	124.10	121.00
1	B	319[B]	TYR	CB-CG-CD1	5.17	124.10	121.00
1	B	276	TYR	CB-CG-CD1	5.01	124.00	121.00

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	3517	3641	3705	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3448	3584	3646	99	0
2	A	32	48	47	4	0
2	B	24	36	36	2	0
3	A	1	0	0	0	0
4	A	30	0	0	2	0
4	B	20	0	0	1	0
5	B	14	20	20	4	0
6	B	8	12	12	24	0
7	A	392	0	0	22	0
7	B	333	0	0	17	0
All	All	7819	7341	7466	164	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 11.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250[B]:GLU:HG2	6:B:2108:TRS:C2	1.39	1.52
1:A:315[B]:ARG:CZ	7:A:504:HOH:O	1.68	1.33
1:B:250[B]:GLU:CG	6:B:2108:TRS:H21	1.61	1.30
1:B:250[A]:GLU:CG	6:B:2108:TRS:H21	1.65	1.26
1:A:222[B]:GLU:OE1	1:B:317[B]:LYS:NZ	1.71	1.23
1:A:254[B]:ASN:OD1	7:A:503:HOH:O	1.53	1.20
1:B:250[A]:GLU:HG3	6:B:2108:TRS:C2	1.72	1.18
1:A:222[B]:GLU:CG	1:B:317[B]:LYS:HE3	1.75	1.17
1:B:255[B]:ILE:HD12	1:B:352[B]:ILE:HD11	1.28	1.16
1:A:222[B]:GLU:HG2	1:B:317[B]:LYS:CE	1.78	1.13
1:A:315[B]:ARG:NH1	7:A:504:HOH:O	1.58	1.12
1:A:222[B]:GLU:HG2	1:B:317[B]:LYS:HE3	1.16	1.10
1:A:13[A]:GLU:HG3	1:A:346[A]:TRP:HE1	1.11	1.10
1:A:222[B]:GLU:CD	1:B:317[B]:LYS:NZ	2.05	1.09
1:A:335[B]:CYS:SG	7:A:667:HOH:O	2.09	1.06
1:A:12[B]:GLN:OE1	7:A:505:HOH:O	1.72	1.05
1:B:250[B]:GLU:HG2	6:B:2108:TRS:O2	1.58	1.02
1:A:222[B]:GLU:CG	1:B:317[B]:LYS:CE	2.35	1.01
1:B:6[B]:ASP:OD2	1:B:9[B]:ARG:HD2	1.59	0.99
1:B:250[A]:GLU:HG3	6:B:2108:TRS:H21	1.01	0.99
1:B:190[A]:TYR:CD2	1:B:237[A]:ILE:HD13	1.98	0.98
1:B:250[B]:GLU:CG	6:B:2108:TRS:C2	2.31	0.98
1:B:6[B]:ASP:OD2	1:B:9[B]:ARG:CD	2.11	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10[A]:GLU:HG3	1:B:346[A]:TRP:CZ3	1.99	0.97
1:A:222[B]:GLU:CG	1:B:317[B]:LYS:NZ	2.27	0.97
1:A:24[B]:ARG:HG2	1:A:24[B]:ARG:HH11	1.27	0.96
1:B:250[A]:GLU:CB	6:B:2108:TRS:H21	1.96	0.95
1:B:190[A]:TYR:HD2	1:B:237[A]:ILE:HD13	1.30	0.93
1:A:348[B]:ARG:N	1:A:351[B]:GLU:OE2	2.01	0.93
1:A:346[A]:TRP:HZ3	7:A:527:HOH:O	1.51	0.93
1:B:250[B]:GLU:HG2	6:B:2108:TRS:H21	0.92	0.91
1:A:222[B]:GLU:CD	1:B:317[B]:LYS:HZ1	1.69	0.90
1:A:332[B]:GLU:OE2	7:A:506:HOH:O	1.87	0.90
1:A:13[A]:GLU:HG3	1:A:346[A]:TRP:NE1	1.87	0.88
1:B:10[B]:GLU:OE2	7:B:2203:HOH:O	1.91	0.88
1:A:268:LEU:HD23	1:A:286[B]:ILE:HD12	1.56	0.85
1:A:222[B]:GLU:CD	1:B:317[B]:LYS:HZ2	1.72	0.85
1:A:296:GLN:HE21	1:A:300[A]:LYS:HE3	1.40	0.85
1:A:24[B]:ARG:HH11	1:A:24[B]:ARG:CG	1.90	0.84
1:B:268:LEU:HD23	1:B:286[B]:ILE:HD12	1.59	0.83
1:A:315[B]:ARG:NH2	7:A:504:HOH:O	1.90	0.81
1:B:6[B]:ASP:OD2	1:B:9[B]:ARG:CG	2.31	0.79
1:B:287[A]:ARG:NH1	7:B:2207:HOH:O	2.15	0.79
1:B:268:LEU:HD23	1:B:286[B]:ILE:CD1	2.13	0.78
1:A:222[B]:GLU:HG3	1:B:317[B]:LYS:HE3	1.65	0.77
1:B:6[B]:ASP:OD2	1:B:9[B]:ARG:HG3	1.86	0.76
1:A:2:ILE:HD12	1:A:303[B]:ILE:HD12	1.69	0.75
1:A:348[B]:ARG:NH2	1:A:348[B]:ARG:HB3	2.02	0.75
1:B:250[A]:GLU:HG3	6:B:2108:TRS:C	2.17	0.74
1:B:190[A]:TYR:HD2	1:B:237[A]:ILE:CD1	1.99	0.74
1:B:107[A]:GLU:HG2	5:B:2104:PEG:H11	1.70	0.74
4:A:412:PO4:O1	7:A:507:HOH:O	2.06	0.74
1:B:250[B]:GLU:CB	6:B:2108:TRS:H21	1.98	0.74
1:A:22:ILE:HG13	1:A:237[B]:ILE:HD11	1.70	0.73
1:B:257[A]:ARG:HH12	6:B:2108:TRS:C3	2.01	0.73
1:B:10[B]:GLU:OE2	1:B:241[B]:LYS:NZ	2.22	0.73
1:A:13[A]:GLU:CG	1:A:346[A]:TRP:HE1	1.97	0.72
4:A:410:PO4:O4	7:A:508:HOH:O	2.06	0.71
1:B:255[B]:ILE:HD12	1:B:352[B]:ILE:CD1	2.16	0.71
1:B:257[A]:ARG:HH12	6:B:2108:TRS:H32	1.55	0.71
1:B:250[B]:GLU:CG	6:B:2108:TRS:O2	2.36	0.70
1:B:107[A]:GLU:CG	5:B:2104:PEG:H11	2.22	0.70
1:B:268:LEU:CD2	1:B:286[B]:ILE:HD12	2.23	0.69
1:B:10[A]:GLU:HG3	1:B:346[A]:TRP:CH2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:VAL:HG12	1:B:319[B]:TYR:OH	1.94	0.68
4:B:2111:PO4:O2	7:B:2205:HOH:O	2.10	0.68
1:A:348[B]:ARG:HB3	1:A:348[B]:ARG:CZ	2.23	0.67
1:A:222[B]:GLU:HG3	1:B:317[B]:LYS:CE	2.20	0.67
1:B:12[B]:GLN:CD	7:B:2206:HOH:O	2.31	0.67
1:A:296:GLN:HE21	1:A:300[A]:LYS:CE	2.08	0.67
1:B:12[B]:GLN:OE1	7:B:2206:HOH:O	2.12	0.66
1:A:10:GLU:HG3	1:A:346[A]:TRP:CH2	2.31	0.66
1:A:2:ILE:HD12	1:A:303[B]:ILE:CD1	2.27	0.64
1:A:222[B]:GLU:CG	1:B:317[B]:LYS:HZ1	2.06	0.63
1:B:12[B]:GLN:NE2	7:B:2206:HOH:O	2.31	0.63
1:B:89:VAL:HG12	1:B:319[B]:TYR:CZ	2.34	0.63
1:B:190[A]:TYR:CD2	1:B:237[A]:ILE:CD1	2.77	0.62
1:A:49:GLY:HA3	2:A:401:EDO:H12	1.82	0.62
1:B:68[A]:LYS:HA	2:B:2102:EDO:H11	1.82	0.62
1:B:9[B]:ARG:NH1	1:B:348[B]:ARG:HH12	1.98	0.62
1:A:138[A]:ASP:OD1	7:A:509:HOH:O	2.15	0.61
1:A:347[A]:LEU:HD23	1:A:352:ILE:HD11	1.81	0.61
1:A:169:LYS:H	2:A:401:EDO:H21	1.66	0.61
1:A:326[B]:THR:HG22	1:A:328:LEU:HG	1.84	0.59
1:B:250[B]:GLU:HA	6:B:2108:TRS:C2	2.32	0.59
1:B:4:PHE:O	7:B:2208:HOH:O	2.17	0.58
1:B:82:SER:O	1:B:313[B]:MET:HG2	2.03	0.58
1:B:250[A]:GLU:HA	6:B:2108:TRS:C2	2.33	0.58
1:B:118[A]:LYS:HD3	7:B:2463:HOH:O	2.02	0.58
1:B:68[B]:LYS:HA	2:B:2102:EDO:H11	1.85	0.57
1:B:250[B]:GLU:HA	6:B:2108:TRS:H22	1.87	0.57
1:A:10:GLU:OE1	1:A:241[B]:LYS:NZ	2.35	0.56
1:B:6[B]:ASP:CG	1:B:9[B]:ARG:HG3	2.25	0.56
1:B:250[A]:GLU:HA	6:B:2108:TRS:H22	1.88	0.56
1:A:346[A]:TRP:CZ3	7:A:527:HOH:O	2.38	0.56
1:B:190[B]:TYR:HE1	7:B:2311:HOH:O	1.89	0.56
1:A:125[B]:LYS:HE2	7:A:545:HOH:O	2.06	0.55
1:A:297[B]:ASN:ND2	7:A:522:HOH:O	2.40	0.55
1:B:147[B]:GLU:HG2	7:B:2400:HOH:O	2.06	0.55
1:A:289[B]:LYS:HG2	7:A:763:HOH:O	2.08	0.54
1:A:222[B]:GLU:HG2	1:B:317[B]:LYS:NZ	2.05	0.54
1:B:2:ILE:HD12	1:B:303[B]:ILE:HD12	1.89	0.54
1:A:190[B]:TYR:CD2	1:A:237[B]:ILE:HG13	2.43	0.54
1:B:255[B]:ILE:CD1	1:B:352[B]:ILE:HD11	2.18	0.54
1:A:22:ILE:CG1	1:A:237[B]:ILE:HD11	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201[B]:ASP:OD1	7:A:511:HOH:O	2.18	0.51
1:B:89:VAL:CG1	1:B:319[B]:TYR:CZ	2.94	0.50
1:B:258[A]:LEU:HD21	1:B:349:GLU:HG3	1.94	0.50
1:A:24[B]:ARG:CG	1:A:24[B]:ARG:NH1	2.60	0.50
1:A:348[B]:ARG:HB2	1:A:351[B]:GLU:HG3	1.94	0.50
1:A:296:GLN:NE2	1:A:300[A]:LYS:HE3	2.19	0.49
1:B:107[A]:GLU:HG3	5:B:2104:PEG:H11	1.93	0.49
1:A:24[B]:ARG:HG2	1:A:24[B]:ARG:NH1	2.09	0.49
2:A:401:EDO:H22	7:A:760:HOH:O	2.12	0.49
1:B:2:ILE:HD12	1:B:303[B]:ILE:CD1	2.43	0.49
1:B:10[B]:GLU:OE2	1:B:241[B]:LYS:CE	2.61	0.49
1:A:268:LEU:CD2	1:A:286[B]:ILE:HD12	2.35	0.49
1:B:250[A]:GLU:OE1	6:B:2108:TRS:N	2.44	0.49
1:A:348[B]:ARG:NH2	1:A:348[B]:ARG:CB	2.73	0.48
1:B:10[B]:GLU:OE2	1:B:241[B]:LYS:HE3	2.13	0.48
1:A:268:LEU:HD13	1:A:363:LEU:HD11	1.95	0.48
1:A:218:LYS:HE3	1:A:219[A]:TYR:CZ	2.48	0.48
1:B:250[A]:GLU:HG3	6:B:2108:TRS:N	2.29	0.47
1:B:102[B]:VAL:HG13	1:B:115[B]:GLN:HB2	1.97	0.47
1:B:218:LYS:HE3	1:B:219:TYR:CZ	2.50	0.47
1:A:269:VAL:HB	1:A:287[A]:ARG:HB3	1.97	0.46
1:A:268:LEU:O	7:A:513:HOH:O	2.21	0.46
1:A:348[B]:ARG:HA	1:A:348[B]:ARG:HH21	1.80	0.46
1:B:258[A]:LEU:CD2	1:B:349:GLU:HG3	2.46	0.46
1:A:222[B]:GLU:OE2	7:A:512:HOH:O	2.20	0.45
1:B:9[A]:ARG:NH1	1:B:346[A]:TRP:HD1	2.14	0.45
1:B:250[A]:GLU:HG3	6:B:2108:TRS:O3	2.16	0.45
1:B:9[B]:ARG:CZ	1:B:348[B]:ARG:HH12	2.29	0.45
1:B:268:LEU:HD23	1:B:286[B]:ILE:HD13	1.95	0.45
1:A:347[A]:LEU:CD2	1:A:352:ILE:HD11	2.45	0.44
1:A:169:LYS:H	2:A:401:EDO:C2	2.28	0.44
1:B:206[B]:LYS:HB2	1:B:206[B]:LYS:HE2	1.70	0.43
1:B:168[B]:LYS:HE2	7:B:2308:HOH:O	2.18	0.43
1:B:102[A]:VAL:HG23	1:B:111:ILE:HG13	2.01	0.42
1:A:82:SER:O	1:A:313[B]:MET:HG2	2.20	0.42
1:A:148[B]:LYS:HG3	7:A:644:HOH:O	2.19	0.42
1:A:297[B]:ASN:CG	7:A:522:HOH:O	2.58	0.42
1:A:211:ARG:HB2	1:A:228:SER:O	2.20	0.42
1:B:20[B]:GLN:HG3	7:B:2356:HOH:O	2.20	0.42
1:A:190[B]:TYR:CE2	1:A:237[B]:ILE:HG13	2.55	0.41
1:B:136[B]:PRO:HG2	1:B:164:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250[B]:GLU:CD	7:B:2221:HOH:O	2.57	0.41
1:B:28[B]:ARG:HB3	7:B:2218:HOH:O	2.20	0.41
1:B:123:ARG:HH12	5:B:2107:PEG:H21	1.84	0.41
1:A:98[B]:LYS:HB2	1:A:98[B]:LYS:HE2	1.29	0.41
1:A:106:PRO:O	1:A:287[A]:ARG:NH1	2.54	0.41
1:A:306[A]:GLN:NE2	7:A:507:HOH:O	2.40	0.41
1:B:250[B]:GLU:CA	6:B:2108:TRS:H21	2.47	0.41
1:B:255[B]:ILE:HG23	1:B:352[B]:ILE:HD11	2.02	0.41
1:B:211:ARG:HB2	1:B:228:SER:O	2.20	0.41
1:B:104:ILE:HD11	1:B:334[B]:ILE:HG12	2.02	0.41
1:B:98[B]:LYS:HE2	7:B:2300:HOH:O	2.20	0.41
1:B:258[B]:LEU:HG	7:B:2231:HOH:O	2.21	0.41
1:B:168[B]:LYS:NZ	7:B:2234:HOH:O	2.54	0.40
1:A:348[B]:ARG:HG2	1:A:351[B]:GLU:OE2	2.21	0.40
1:B:257[A]:ARG:NH1	6:B:2108:TRS:H32	2.29	0.40
1:B:250[B]:GLU:HA	6:B:2108:TRS:H21	2.04	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	450/399 (113%)	439 (98%)	11 (2%)	0	100	100
1	B	443/399 (111%)	430 (97%)	13 (3%)	0	100	100
All	All	893/798 (112%)	869 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	405/344 (118%)	403 (100%)	2 (0%)	88	68
1	B	398/344 (116%)	395 (99%)	3 (1%)	81	56
All	All	803/688 (117%)	798 (99%)	5 (1%)	86	64

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	291	ARG
1	A	334	ILE
1	B	291	ARG
1	B	334[A]	ILE
1	B	334[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	296	GLN
1	B	295	GLN
1	B	325	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 1 is monoatomic - leaving 27 for Mogul analysis.

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.

## 5.7 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	367/399 (91%)	-0.23	13 (3%) 44 39	11, 17, 37, 90	0
1	B	367/399 (91%)	-0.28	10 (2%) 54 49	11, 17, 37, 109	0
All	All	734/798 (91%)	-0.25	23 (3%) 49 44	11, 17, 37, 109	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	364[A]	TRP	10.2
1	A	365[A]	MET	7.2
1	A	366	SER	5.8
1	B	324	TYR	5.7
1	A	367	ASN	5.5
1	B	367	ASN	4.3
1	B	325	ASN	4.0
1	B	321	GLU	4.0
1	B	265	SER	3.9
1	B	323	GLU	3.2
1	B	365[A]	MET	3.1
1	A	353	ARG	2.9
1	A	265	SER	2.8
1	B	0	ASP	2.6
1	A	361[A]	GLU	2.6
1	B	320	LEU	2.6
1	A	1[A]	MET	2.5
1	A	217[A]	LYS	2.3
1	A	0	ASP	2.3
1	B	322	LEU	2.2
1	A	267	ASP	2.2
1	A	219[A]	TYR	2.0
1	A	289[A]	LYS	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	LLP	A	185	24/25	0.98	0.07	12,18,25,35	1
1	LLP	B	185	24/25	0.99	0.06	12,17,24,33	1

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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
5	PEG	B	2104	7/7	0.64	0.21	37,46,54,54	17
2	EDO	A	406	4/4	0.77	0.10	46,47,55,58	10
2	EDO	A	407	4/4	0.78	0.08	30,37,40,43	1
4	PO4	B	2111	5/5	0.80	0.19	19,23,29,34	5
6	TRS	B	2108	8/8	0.81	0.30	25,31,48,52	20
2	EDO	B	2103	4/4	0.82	0.15	31,47,61,61	1
2	EDO	A	408	4/4	0.82	0.14	29,32,39,43	10
4	PO4	A	415	5/5	0.83	0.12	24,25,28,42	5
2	EDO	A	404	4/4	0.85	0.18	37,40,50,51	10
2	EDO	B	2102	4/4	0.86	0.12	21,29,32,36	10
2	EDO	B	2109	4/4	0.86	0.16	46,55,58,58	1
2	EDO	B	2105	4/4	0.87	0.10	36,49,53,54	10
5	PEG	B	2107	7/7	0.88	0.19	36,51,57,61	1
2	EDO	A	405	4/4	0.88	0.09	31,34,50,50	1
4	PO4	B	2113	5/5	0.89	0.12	16,30,42,45	5
2	EDO	B	2106	4/4	0.92	0.12	26,30,61,62	1
2	EDO	B	2101	4/4	0.92	0.05	35,38,45,49	10
4	PO4	A	412	5/5	0.92	0.10	24,30,34,35	5
4	PO4	B	2110	5/5	0.93	0.08	24,29,37,39	5
2	EDO	A	402	4/4	0.94	0.17	24,29,35,36	10

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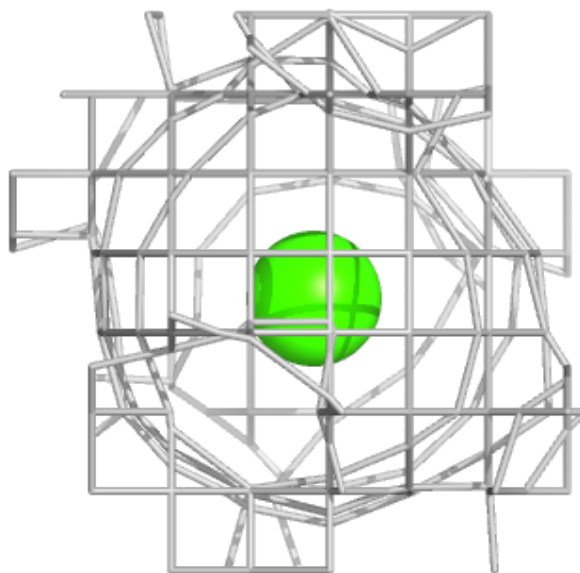
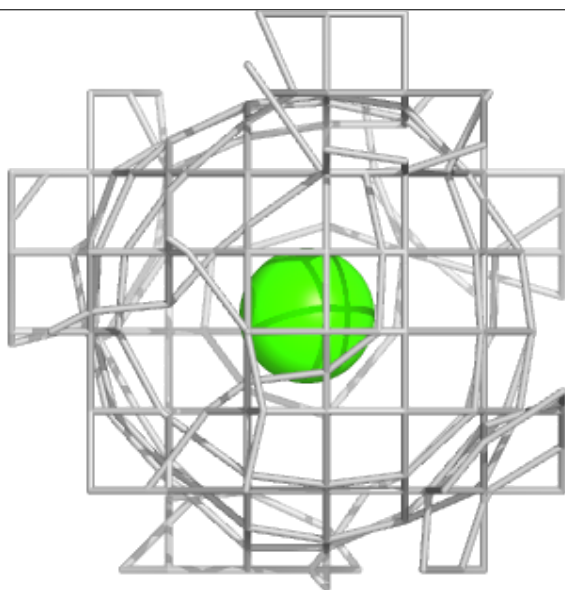
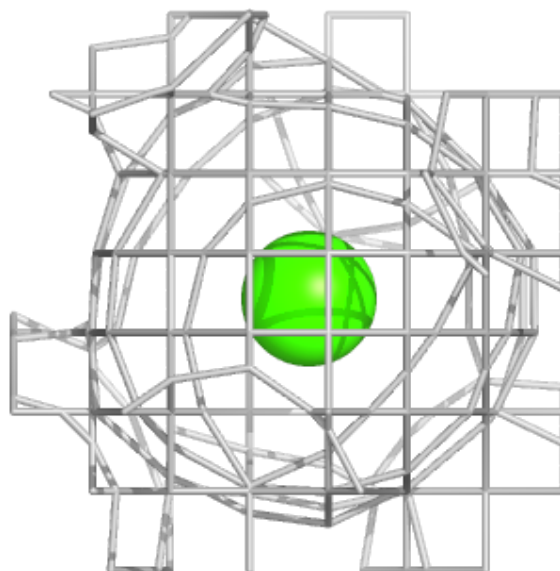
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PO4	A	411	5/5	0.94	0.12	26,27,32,38	5
2	EDO	A	403	4/4	0.95	0.17	24,31,33,34	10
2	EDO	A	401	4/4	0.96	0.16	20,28,52,53	10
4	PO4	B	2112	5/5	0.96	0.17	25,28,32,58	5
4	PO4	A	414	5/5	0.96	0.09	32,35,43,43	5
4	PO4	A	410	5/5	0.97	0.12	23,26,30,45	5
4	PO4	A	413	5/5	0.98	0.08	23,30,39,41	5
3	CA	A	409	1/1	1.00	0.06	14,14,14,14	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around CA A 409:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.