



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 09:22 PM EST

PDB ID : 6PD1
Title : PntC-AEPT: fusion protein of phosphonate-specific cytidyltransferase and 2-aminoethylphosphonate (AEP) transaminase from *Treponema denticola*
Authors : Suits, M.D.L.; Whiteside, J.
Deposited on : 2019-06-18
Resolution : 2.72 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

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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

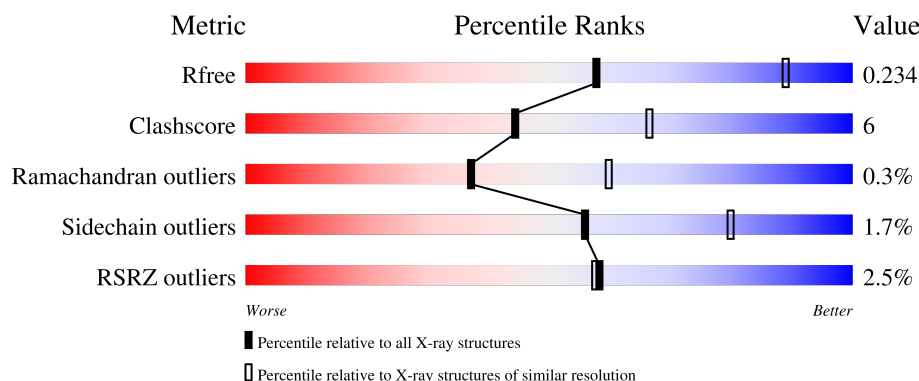
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4050 (2.74-2.70)
Clashscore	180529	4439 (2.74-2.70)
Ramachandran outliers	177936	4374 (2.74-2.70)
Sidechain outliers	177891	4375 (2.74-2.70)
RSRZ outliers	164620	4050 (2.74-2.70)

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 ≥ 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	624	 3% 83% 14% ..
1	B	624	 % 86% 11% .
1	C	624	 3% 84% 13% ..
1	D	624	 3% 82% 15% ..

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	C	1101	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19503 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 Nucleotidyl transferase/aminotransferase, class V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4817	3077	795	910	35			
1	B	607	Total	C	N	O	S	0	0	0
			4769	3047	785	902	35			
1	C	617	Total	C	N	O	S	0	0	0
			4858	3101	807	915	35			
1	D	611	Total	C	N	O	S	0	0	0
			4797	3065	789	908	35			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	617	LEU	-	expression tag	UNP Q73MU2
A	618	GLU	-	expression tag	UNP Q73MU2
A	619	HIS	-	expression tag	UNP Q73MU2
A	620	HIS	-	expression tag	UNP Q73MU2
A	621	HIS	-	expression tag	UNP Q73MU2
A	622	HIS	-	expression tag	UNP Q73MU2
A	623	HIS	-	expression tag	UNP Q73MU2
A	624	HIS	-	expression tag	UNP Q73MU2
B	617	LEU	-	expression tag	UNP Q73MU2
B	618	GLU	-	expression tag	UNP Q73MU2
B	619	HIS	-	expression tag	UNP Q73MU2
B	620	HIS	-	expression tag	UNP Q73MU2
B	621	HIS	-	expression tag	UNP Q73MU2
B	622	HIS	-	expression tag	UNP Q73MU2
B	623	HIS	-	expression tag	UNP Q73MU2
B	624	HIS	-	expression tag	UNP Q73MU2
C	617	LEU	-	expression tag	UNP Q73MU2
C	618	GLU	-	expression tag	UNP Q73MU2
C	619	HIS	-	expression tag	UNP Q73MU2
C	620	HIS	-	expression tag	UNP Q73MU2
C	621	HIS	-	expression tag	UNP Q73MU2

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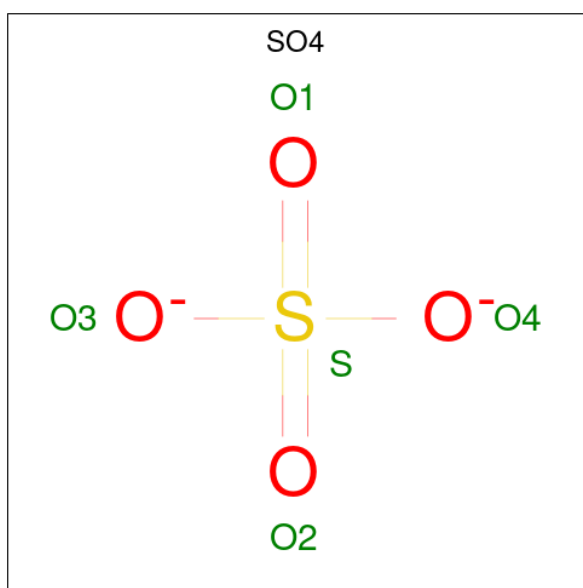
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Chain	Residue	Modelled	Actual	Comment	Reference
C	622	HIS	-	expression tag	UNP Q73MU2
C	623	HIS	-	expression tag	UNP Q73MU2
C	624	HIS	-	expression tag	UNP Q73MU2
D	617	LEU	-	expression tag	UNP Q73MU2
D	618	GLU	-	expression tag	UNP Q73MU2
D	619	HIS	-	expression tag	UNP Q73MU2
D	620	HIS	-	expression tag	UNP Q73MU2
D	621	HIS	-	expression tag	UNP Q73MU2
D	622	HIS	-	expression tag	UNP Q73MU2
D	623	HIS	-	expression tag	UNP Q73MU2
D	624	HIS	-	expression tag	UNP Q73MU2

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

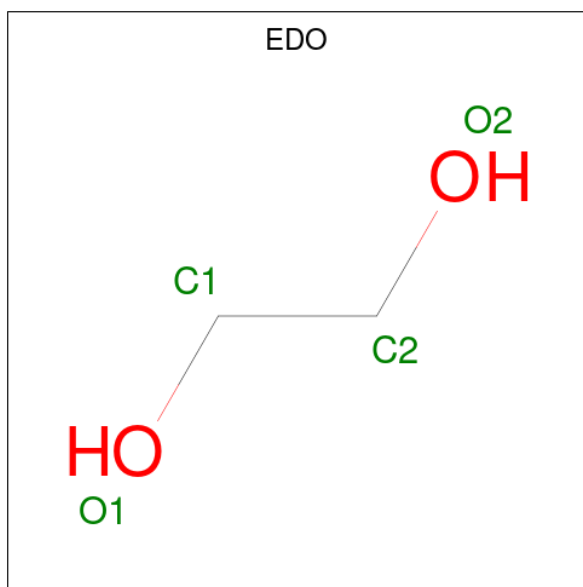
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total 1 Mg 1	0	0
2	B	1	Total 1 Mg 1	0	0
2	C	1	Total 1 Mg 1	0	0
2	D	1	Total 1 Mg 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



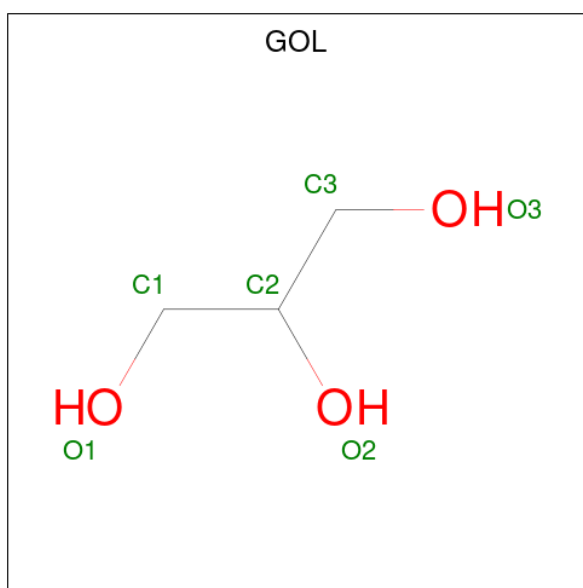
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		

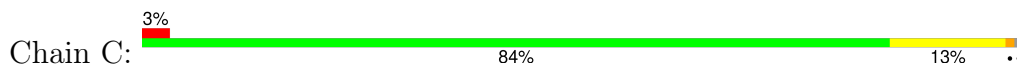
- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

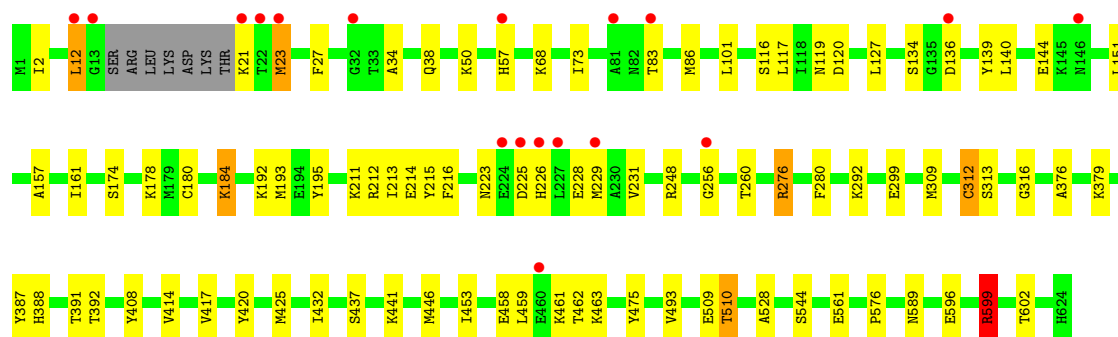
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Ni	0	0
			1	1		

- Molecule 7 is water.

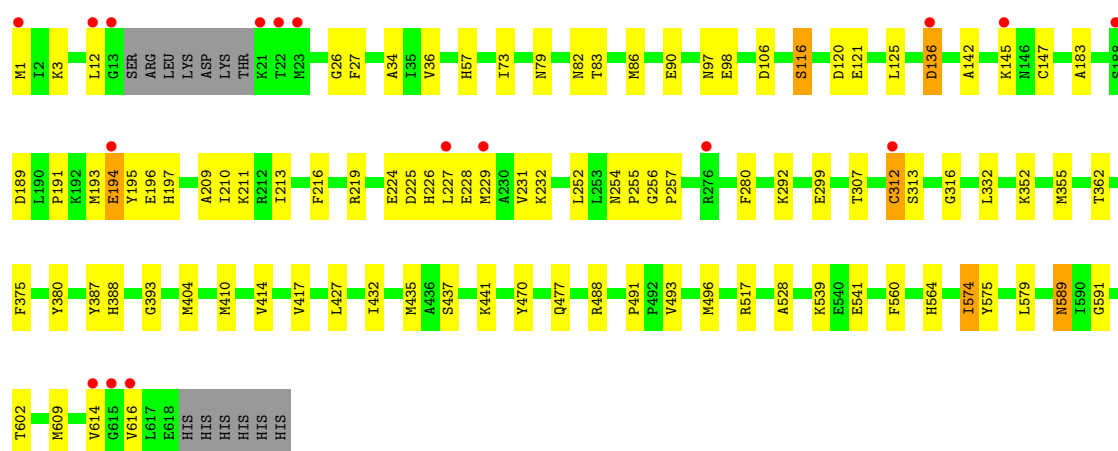
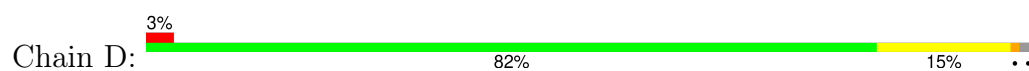
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	49	Total 49	O 49	0	0
7	B	47	Total 47	O 47	0	0
7	C	38	Total 38	O 38	0	0
7	D	38	Total 38	O 38	0	0

- Molecule 1: Nucleotidyl transferase/aminotransferase, class V





- Molecule 1: Nucleotidyl transferase/aminotransferase, class V



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.05Å 129.01Å 135.80Å 90.00° 92.99° 90.00°	Depositor
Resolution (Å)	38.00 – 2.72 38.00 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.00-2.72) 99.8 (38.00-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.199 , 0.233 0.201 , 0.234	Depositor DCC
R_{free} test set	4107 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19503	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: EDO, GOL, NI, MG, SO4

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	0.34	3/4912 (0.1%)	0.58	9/6639 (0.1%)
1	B	0.30	1/4862 (0.0%)	0.50	1/6571 (0.0%)
1	C	0.31	0/4957	0.58	7/6699 (0.1%)
1	D	0.36	2/4890 (0.0%)	0.63	10/6609 (0.2%)
All	All	0.33	6/19621 (0.0%)	0.57	27/26518 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	483	LYS	CE-NZ	7.45	1.67	1.49
1	D	232	LYS	CD-CE	5.85	1.65	1.51
1	A	561	GLU	CB-CG	-5.43	1.41	1.52
1	D	232	LYS	CE-NZ	5.31	1.62	1.49
1	A	541	GLU	CD-OE2	5.15	1.31	1.25
1	B	561	GLU	CB-CG	-5.08	1.42	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	229	MET	CA-CB-CG	-12.05	92.81	113.30
1	C	248	ARG	NE-CZ-NH2	-10.63	114.98	120.30
1	D	145	LYS	CD-CE-NZ	-8.86	91.33	111.70
1	C	599	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	C	599	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	A	12	LEU	CB-CG-CD2	7.57	123.88	111.00
1	D	194	GLU	CA-CB-CG	7.56	130.02	113.40
1	C	248	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	D	229	MET	CB-CG-SD	7.48	134.85	112.40
1	A	461	LYS	CA-CB-CG	-7.18	97.60	113.40
1	A	483	LYS	CD-CE-NZ	-6.90	95.83	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	144	GLU	CA-CB-CG	6.79	128.34	113.40
1	B	561	GLU	N-CA-CB	-6.62	98.69	110.60
1	C	599	ARG	CD-NE-CZ	6.54	132.76	123.60
1	D	574	ILE	CG1-CB-CG2	-6.29	97.57	111.40
1	A	541	GLU	CA-CB-CG	6.18	126.99	113.40
1	D	73	ILE	CG1-CB-CG2	6.14	124.92	111.40
1	A	461	LYS	CB-CG-CD	6.12	127.52	111.60
1	D	136	ASP	N-CA-CB	-5.99	99.83	110.60
1	D	145	LYS	CA-CB-CG	-5.77	100.70	113.40
1	D	574	ILE	N-CA-CB	5.51	123.47	110.80
1	A	370	LYS	CA-CB-CG	5.37	125.22	113.40
1	A	12	LEU	CA-CB-CG	5.26	127.41	115.30
1	A	145	LYS	CA-CB-CG	5.26	124.97	113.40
1	C	510	THR	CA-CB-CG2	-5.15	105.19	112.40
1	A	153	LYS	CA-CB-CG	5.15	124.73	113.40
1	D	231	VAL	CG1-CB-CG2	-5.10	102.74	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	4817	0	4839	56	0
1	B	4769	0	4795	45	0
1	C	4858	0	4866	63	0
1	D	4797	0	4825	72	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	15	0	0	0	0
3	B	20	0	0	0	0
3	C	10	0	0	1	0
3	D	10	0	0	1	0
4	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	6	0	0
4	C	8	0	11	1	0
4	D	4	0	6	0	0
5	C	6	0	8	0	0
6	C	1	0	0	0	0
7	A	49	0	0	0	0
7	B	47	0	0	1	0
7	C	38	0	0	1	0
7	D	38	0	0	0	0
All	All	19503	0	19368	230	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 6.

All (230) 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:483:LYS:CE	1:A:483:LYS:NZ	1.67	1.55
1:D:224:GLU:OE2	1:D:228:GLU:OE1	1.64	1.13
1:D:86:MET:HG3	1:D:193:MET:HE3	1.37	1.02
1:C:599:ARG:O	1:C:602:THR:HG22	1.73	0.88
1:C:134:SER:HB2	1:C:226:HIS:HE1	1.40	0.86
1:A:483:LYS:NZ	1:A:483:LYS:CD	2.40	0.84
1:C:223:ASN:ND2	1:C:226:HIS:HD2	1.79	0.80
1:D:12:LEU:HD21	1:D:57:HIS:CG	2.17	0.80
1:C:86:MET:HG2	1:C:195:TYR:HA	1.64	0.80
1:A:228:GLU:HA	1:A:231:VAL:HG12	1.63	0.78
1:A:470:TYR:O	1:A:488:ARG:NH2	2.17	0.78
1:A:517:ARG:NH2	1:A:591:GLY:O	2.17	0.78
1:B:155:ARG:O	1:B:155:ARG:NH2	2.18	0.77
1:C:134:SER:HB2	1:C:226:HIS:CE1	2.20	0.77
1:C:596:GLU:OE1	1:C:599:ARG:NE	2.18	0.76
1:B:517:ARG:NH2	1:B:591:GLY:O	2.19	0.75
1:A:549:ALA:HB1	1:A:584:THR:HG21	1.69	0.74
1:D:517:ARG:NH2	1:D:591:GLY:O	2.20	0.74
1:C:509:GLU:O	1:C:510:THR:OG1	2.03	0.72
1:D:194:GLU:HG2	1:D:196:GLU:HB2	1.72	0.72
1:A:457:ALA:O	1:A:461:LYS:HG3	1.90	0.71
1:D:194:GLU:OE2	1:D:197:HIS:HB2	1.90	0.71
1:C:86:MET:HG3	1:C:193:MET:HE3	1.73	0.70
1:C:313:SER:OG	3:C:1103:SO4:O3	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:SD	1:D:3:LYS:NZ	2.65	0.68
1:B:127:LEU:HD11	1:B:213:ILE:HD12	1.75	0.68
1:D:86:MET:HG2	1:D:195:TYR:HA	1.75	0.68
1:D:227:LEU:HD12	1:D:228:GLU:CD	2.14	0.68
1:D:560:PHE:CE1	1:D:574:ILE:HD12	2.28	0.68
1:C:391:THR:HG23	1:C:392:THR:HG23	1.75	0.67
1:B:331:ARG:CZ	1:B:356:ASP:OD1	2.24	0.65
1:B:267:ALA:HB2	1:B:501:GLN:HG3	1.78	0.65
1:D:194:GLU:CD	1:D:197:HIS:HB2	2.17	0.65
1:A:609:MET:HB3	1:A:614:VAL:HG21	1.80	0.64
1:D:120:ASP:OD2	1:D:211:LYS:NZ	2.30	0.64
1:B:12:LEU:HD23	1:B:12:LEU:H	1.64	0.63
1:C:223:ASN:HD21	1:C:226:HIS:HD2	1.46	0.62
1:D:470:TYR:O	1:D:488:ARG:NH2	2.31	0.61
1:C:223:ASN:ND2	1:C:225:ASP:HB2	2.15	0.61
1:A:559:SER:OG	1:A:561:GLU:HB2	2.01	0.61
1:A:559:SER:OG	1:A:561:GLU:OE1	2.19	0.60
1:A:331:ARG:HG2	1:A:380:TYR:HD1	1.68	0.59
1:B:609:MET:HB3	1:B:614:VAL:HB	1.85	0.59
1:B:137:GLU:HG3	1:B:139:TYR:CZ	2.38	0.59
1:C:509:GLU:C	1:C:510:THR:HG1	1.99	0.59
1:A:219:ARG:HG3	1:A:234:ILE:HG13	1.85	0.58
1:A:116:SER:OG	1:A:211:LYS:HE2	2.03	0.58
1:C:414:VAL:HG21	1:C:432:ILE:HG12	1.85	0.58
1:C:599:ARG:HA	1:C:602:THR:HG22	1.85	0.58
1:D:227:LEU:HD12	1:D:228:GLU:OE1	2.04	0.58
1:D:86:MET:HG3	1:D:193:MET:CE	2.24	0.58
1:D:227:LEU:HD12	1:D:228:GLU:OE2	2.04	0.58
1:D:313:SER:OG	3:D:703:SO4:O2	2.21	0.57
1:B:331:ARG:NH1	1:B:356:ASP:OD1	2.36	0.57
1:C:120:ASP:OD2	1:C:211:LYS:NZ	2.34	0.57
1:C:140:LEU:HD21	1:C:151:LEU:HD12	1.86	0.57
1:D:86:MET:HE2	1:D:183:ALA:HB2	1.86	0.57
1:A:121:GLU:CD	1:A:121:GLU:H	2.07	0.56
1:A:185:ILE:HG13	1:A:186:HIS:CD2	2.40	0.56
1:A:213:ILE:HB	1:A:216:PHE:HB2	1.87	0.56
1:A:609:MET:HB3	1:A:614:VAL:CG2	2.35	0.56
1:A:25:LYS:HD3	1:A:106:ASP:HB3	1.87	0.56
1:A:380:TYR:HB2	1:A:410:MET:HE3	1.86	0.55
1:C:213:ILE:HB	1:C:216:PHE:HB2	1.89	0.55
1:D:194:GLU:CG	1:D:196:GLU:HB2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LYS:HD3	1:B:111:SER:HB3	1.88	0.55
1:B:491:PRO:HB2	1:B:496:MET:HE1	1.90	0.54
1:D:86:MET:CE	1:D:183:ALA:HB2	2.36	0.54
1:A:477:GLN:OE1	1:A:488:ARG:NH1	2.40	0.54
1:C:12:LEU:HD23	1:C:57:HIS:CD2	2.42	0.54
1:D:312:CYS:SG	1:D:316:GLY:HA3	2.47	0.54
1:D:491:PRO:HB2	1:D:496:MET:HE1	1.90	0.54
1:D:26:GLY:O	1:D:36:VAL:HG22	2.07	0.53
1:A:218:TRP:O	1:A:219:ARG:HG2	2.09	0.53
1:C:309:MET:HB2	4:C:1104:EDO:H21	1.89	0.53
1:D:12:LEU:HD21	1:D:57:HIS:CD2	2.43	0.53
1:D:27:PHE:HA	1:D:34:ALA:HB1	1.90	0.53
1:C:312:CYS:SG	1:C:316:GLY:HA3	2.50	0.52
1:D:299:GLU:N	1:D:299:GLU:OE1	2.43	0.52
1:A:581:ASN:HD21	1:B:551:LEU:HD22	1.75	0.52
1:C:420:TYR:HA	1:C:425:MET:HE1	1.91	0.52
1:D:332:LEU:O	1:D:355:MET:HA	2.09	0.52
1:A:144:GLU:CD	1:A:144:GLU:H	2.13	0.51
1:A:250:GLU:O	1:A:259:THR:OG1	2.26	0.51
1:A:276:ARG:HE	1:C:576:PRO:HG3	1.75	0.51
1:B:142:ALA:HB2	1:B:210:ILE:HD12	1.93	0.51
1:D:539:LYS:HB3	1:D:541:GLU:OE1	2.09	0.51
1:B:144:GLU:HG2	1:B:145:LYS:N	2.25	0.51
1:A:248:ARG:HB2	1:C:119:ASN:O	2.11	0.51
1:A:26:GLY:O	1:A:36:VAL:HG22	2.11	0.51
1:A:27:PHE:HA	1:A:34:ALA:HB1	1.93	0.51
1:C:561:GLU:OE2	1:C:561:GLU:N	2.36	0.51
1:D:219:ARG:HD2	1:D:226:HIS:ND1	2.26	0.51
1:C:180:CYS:O	1:C:184:LYS:HD2	2.10	0.50
1:A:222:ASP:OD1	1:A:222:ASP:N	2.29	0.50
1:C:276:ARG:HG2	1:C:276:ARG:O	2.12	0.50
1:D:560:PHE:CE1	1:D:574:ILE:CD1	2.94	0.50
1:D:609:MET:HB3	1:D:614:VAL:HG21	1.92	0.50
1:A:136:ASP:HB2	1:A:153:LYS:HE2	1.94	0.50
1:D:491:PRO:HB2	1:D:496:MET:CE	2.41	0.50
1:D:12:LEU:CD2	1:D:57:HIS:CG	2.92	0.49
1:D:147:CYS:HA	1:D:209:ALA:HA	1.94	0.49
1:D:194:GLU:OE2	1:D:197:HIS:CB	2.60	0.49
1:A:598:MET:O	1:A:602:THR:HG23	2.13	0.48
1:C:21:LYS:C	1:C:23:MET:H	2.16	0.48
1:C:292:LYS:HA	1:C:453:ILE:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:GLU:HG2	1:D:197:HIS:H	1.78	0.48
1:B:417:VAL:HA	1:B:437:SER:HA	1.96	0.48
1:A:276:ARG:O	1:A:276:ARG:HG2	2.14	0.48
1:C:223:ASN:ND2	1:C:226:HIS:H	2.12	0.48
1:C:223:ASN:HD21	1:C:226:HIS:H	1.62	0.48
1:B:388:HIS:CD2	1:B:544:SER:HG	2.31	0.48
1:D:213:ILE:HB	1:D:216:PHE:HB2	1.96	0.47
1:A:280:PHE:CE1	1:A:493:VAL:HG13	2.49	0.47
1:B:491:PRO:HB2	1:B:496:MET:CE	2.44	0.47
1:B:280:PHE:CE1	1:B:493:VAL:HG13	2.49	0.47
1:B:116:SER:OG	1:B:211:LYS:HE2	2.13	0.47
1:B:155:ARG:HH21	1:B:155:ARG:C	2.18	0.47
1:B:277:GLU:OE2	1:D:564:HIS:NE2	2.37	0.47
1:C:2:ILE:HG21	1:C:101:LEU:HG	1.97	0.47
1:C:459:LEU:O	1:C:462:THR:HB	2.14	0.47
1:C:599:ARG:HA	1:C:602:THR:CG2	2.44	0.47
1:D:388:HIS:HE2	1:D:393:GLY:HA2	1.80	0.47
1:C:139:TYR:HB3	1:C:161:ILE:HD12	1.96	0.46
1:C:280:PHE:CE1	1:C:493:VAL:HG13	2.50	0.46
1:B:2:ILE:HD11	1:B:170:LYS:HD2	1.97	0.46
1:D:116:SER:OG	1:D:211:LYS:HE2	2.15	0.46
1:A:201:GLU:HA	1:A:204:LYS:HE3	1.98	0.46
1:D:125:LEU:HD21	1:D:211:LYS:HB2	1.97	0.46
1:B:22:THR:O	1:B:22:THR:HG22	2.16	0.46
1:B:203:ALA:HA	1:B:206:ILE:O	2.15	0.46
1:B:286:TRP:CZ3	1:B:500:ARG:HG3	2.51	0.46
1:D:224:GLU:O	1:D:224:GLU:HG3	2.12	0.46
1:D:417:VAL:HA	1:D:437:SER:HA	1.98	0.46
1:C:223:ASN:HD21	1:C:226:HIS:CD2	2.30	0.46
1:D:477:GLN:OE1	1:D:488:ARG:NH1	2.39	0.46
1:B:79:ASN:OD1	1:B:82:ASN:HB2	2.16	0.46
1:C:256:GLY:HA2	1:C:441:LYS:NZ	2.31	0.46
1:D:83:THR:HA	1:D:191:PRO:O	2.15	0.46
1:B:420:TYR:O	1:B:442:ASN:HB2	2.16	0.46
1:D:560:PHE:HE1	1:D:574:ILE:HD12	1.79	0.46
1:C:27:PHE:HA	1:C:34:ALA:HB1	1.97	0.45
1:A:334:VAL:HG22	1:A:384:ALA:HB3	1.98	0.45
1:A:90:GLU:CD	1:A:187:HIS:HE2	2.20	0.45
1:D:224:GLU:OE2	1:D:227:LEU:HB3	2.16	0.45
1:B:256:GLY:HA2	1:B:441:LYS:HZ2	1.81	0.45
1:A:241:ASN:HA	1:A:244:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:PHE:HA	1:B:34:ALA:HB1	1.97	0.45
1:C:599:ARG:C	1:C:602:THR:HG22	2.34	0.45
1:D:255:PRO:O	1:D:441:LYS:NZ	2.40	0.45
1:C:260:THR:HG21	1:C:446:MET:CE	2.46	0.45
1:C:299:GLU:OE1	1:C:299:GLU:N	2.50	0.45
1:B:57:HIS:CE1	1:B:58:CYS:HG	2.35	0.44
1:B:327:PRO:HD3	1:B:465:TYR:CE2	2.52	0.44
1:D:528:ALA:HB2	1:D:602:THR:HG23	1.99	0.44
1:C:50:LYS:HD2	1:C:73:ILE:HD12	2.00	0.44
1:D:194:GLU:HB2	1:D:196:GLU:OE1	2.17	0.44
1:C:379:LYS:NZ	7:C:1204:HOH:O	2.49	0.44
1:D:142:ALA:HB2	1:D:210:ILE:HD12	1.99	0.44
1:C:388:HIS:CD2	1:C:544:SER:HG	2.36	0.44
1:B:201:GLU:OE1	1:B:204:LYS:NZ	2.47	0.44
1:C:228:GLU:O	1:C:231:VAL:HG12	2.18	0.44
1:A:256:GLY:HA2	1:A:441:LYS:NZ	2.33	0.44
1:A:300:THR:HG21	1:A:426:ASP:OD1	2.17	0.43
1:C:223:ASN:CG	1:C:226:HIS:H	2.22	0.43
1:D:427:LEU:HD21	1:D:435:MET:HE2	2.00	0.43
1:C:223:ASN:OD1	1:C:226:HIS:N	2.49	0.43
1:C:417:VAL:HA	1:C:437:SER:HA	1.99	0.43
1:D:86:MET:O	1:D:90:GLU:HG3	2.19	0.43
1:C:136:ASP:CG	1:C:136:ASP:O	2.56	0.43
1:C:528:ALA:HB2	1:C:602:THR:OG1	2.18	0.43
1:D:414:VAL:HG21	1:D:432:ILE:HG12	2.01	0.43
1:A:331:ARG:HG2	1:A:380:TYR:CD1	2.52	0.43
1:D:280:PHE:CE1	1:D:493:VAL:HG13	2.54	0.43
1:D:496:MET:HB2	1:D:496:MET:HE3	1.58	0.43
1:A:581:ASN:ND2	1:B:551:LEU:HD22	2.33	0.43
1:B:570:HIS:O	1:B:600:ARG:NH2	2.52	0.43
1:B:598:MET:O	1:B:602:THR:HG23	2.18	0.43
1:C:214:GLU:HG2	1:C:215:TYR:CE2	2.53	0.43
1:D:79:ASN:OD1	1:D:82:ASN:HB2	2.18	0.43
1:D:256:GLY:HA2	1:D:257:PRO:C	2.38	0.43
1:D:362:THR:HG21	1:D:579:LEU:CD2	2.49	0.43
1:A:252:LEU:HB3	1:A:254:ASN:OD1	2.19	0.43
1:C:34:ALA:O	1:C:38:GLN:HG3	2.19	0.43
1:C:117:LEU:HD11	1:C:127:LEU:HB2	2.01	0.43
1:D:292:LYS:HB3	1:D:307:THR:OG1	2.19	0.42
1:A:414:VAL:HG21	1:A:432:ILE:HG12	2.00	0.42
1:A:437:SER:HB3	1:A:451:PHE:CE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LYS:HB2	1:B:123:LYS:HE3	1.79	0.42
1:D:224:GLU:O	1:D:225:ASP:C	2.57	0.42
1:C:599:ARG:CA	1:C:602:THR:HG22	2.48	0.42
1:B:222:ASP:OD1	1:B:222:ASP:N	2.52	0.42
1:C:420:TYR:HA	1:C:425:MET:CE	2.50	0.42
1:C:458:GLU:HA	1:C:461:LYS:HE3	2.02	0.42
1:A:420:TYR:O	1:A:442:ASN:HB2	2.20	0.42
1:D:97:ASN:OD1	1:D:98:GLU:HG3	2.19	0.42
1:A:57:HIS:CE1	1:A:58:CYS:HG	2.38	0.42
1:B:136:ASP:OD1	1:B:136:ASP:O	2.38	0.41
1:D:12:LEU:CD2	1:D:57:HIS:CD2	3.03	0.41
1:D:352:LYS:HA	1:D:352:LYS:HD3	1.78	0.41
1:C:83:THR:O	1:C:192:LYS:HE3	2.19	0.41
1:A:142:ALA:HB2	1:A:210:ILE:HD12	2.02	0.41
1:C:596:GLU:OE2	1:C:599:ARG:HD3	2.21	0.41
1:D:528:ALA:CB	1:D:602:THR:HG23	2.50	0.41
1:B:548:THR:HG23	7:B:801:HOH:O	2.21	0.41
1:D:380:TYR:HB2	1:D:410:MET:HE3	2.02	0.41
1:C:226:HIS:HA	1:C:229:MET:HG3	2.02	0.41
1:D:106:ASP:OD1	1:D:106:ASP:N	2.50	0.41
1:D:194:GLU:HG2	1:D:197:HIS:N	2.36	0.41
1:B:275:PRO:HD3	1:D:257:PRO:HG2	2.03	0.41
1:B:182:TYR:CD1	1:B:201:GLU:HG2	2.55	0.41
1:B:532:LEU:HD12	1:B:532:LEU:HA	1.85	0.41
1:C:212:ARG:NH1	1:C:214:GLU:OE1	2.53	0.41
1:C:463:LYS:HB2	1:C:475:TYR:CZ	2.56	0.41
1:D:252:LEU:HB3	1:D:254:ASN:OD1	2.21	0.41
1:D:589:ASN:O	1:D:589:ASN:ND2	2.51	0.41
1:A:41:GLN:NE2	1:A:69:TYR:OH	2.51	0.41
1:A:75:VAL:HG21	1:A:95:PHE:HE2	1.85	0.41
1:A:132:THR:HG22	1:A:137:GLU:HG2	2.03	0.41
1:A:365:PRO:HG3	1:A:542:HIS:CD2	2.56	0.41
1:A:509:GLU:OE2	1:A:517:ARG:NH1	2.48	0.41
1:A:140:LEU:HD21	1:A:165:LEU:HB2	2.03	0.41
1:B:131:ALA:HA	1:B:164:GLU:OE1	2.22	0.40
1:C:376:ALA:HA	1:C:408:TYR:CE2	2.56	0.40
1:A:120:ASP:OD2	1:A:211:LYS:NZ	2.43	0.40
1:B:557:LYS:HB3	1:B:612:ILE:HB	2.04	0.40
1:B:286:TRP:CE2	1:B:290:GLU:HG3	2.57	0.40
1:A:134:SER:HB2	1:A:226:HIS:NE2	2.37	0.40
1:A:387:TYR:CG	1:A:398:LEU:HD22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:PHE:CE2	1:D:404:MET:HE3	2.57	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	609/624 (98%)	585 (96%)	22 (4%)	2 (0%)	37	60
1	B	603/624 (97%)	581 (96%)	20 (3%)	2 (0%)	37	60
1	C	613/624 (98%)	589 (96%)	23 (4%)	1 (0%)	44	67
1	D	607/624 (97%)	578 (95%)	27 (4%)	2 (0%)	37	60
All	All	2432/2496 (97%)	2333 (96%)	92 (4%)	7 (0%)	37	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ALA
1	B	136	ASP
1	D	136	ASP
1	A	136	ASP
1	B	157	ALA
1	C	157	ALA
1	D	616	VAL

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	522/533 (98%)	510 (98%)	12 (2%)	45	73
1	B	517/533 (97%)	513 (99%)	4 (1%)	79	91
1	C	526/533 (99%)	514 (98%)	12 (2%)	45	73
1	D	520/533 (98%)	513 (99%)	7 (1%)	65	84
All	All	2085/2132 (98%)	2050 (98%)	35 (2%)	56	80

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	21	LYS
1	A	57	HIS
1	A	77	ASN
1	A	219	ARG
1	A	228	GLU
1	A	331	ARG
1	A	355	MET
1	A	387	TYR
1	A	483	LYS
1	A	589	ASN
1	A	600	ARG
1	B	155	ARG
1	B	331	ARG
1	B	387	TYR
1	B	589	ASN
1	C	12	LEU
1	C	23	MET
1	C	68	LYS
1	C	116	SER
1	C	174	SER
1	C	178	LYS
1	C	184	LYS
1	C	276	ARG
1	C	312	CYS
1	C	387	TYR
1	C	589	ASN
1	C	599	ARG
1	D	116	SER
1	D	121	GLU

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Mol	Chain	Res	Type
1	D	189	ASP
1	D	312	CYS
1	D	387	TYR
1	D	575	TYR
1	D	589	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	581	ASN
1	A	620	HIS
1	C	57	HIS
1	C	64	ASN
1	C	226	HIS
1	D	197	HIS
1	D	226	HIS
1	D	486	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 5 are monoatomic - leaving 18 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	703	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	A	704	-	3,3,3	0.42	0	2,2,2	0.40	0
4	EDO	A	705	-	3,3,3	0.43	0	2,2,2	0.38	0
3	SO4	A	702	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	B	704	-	4,4,4	0.22	0	6,6,6	0.07	0
3	SO4	C	1103	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	D	704	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	A	706	-	4,4,4	0.25	0	6,6,6	0.08	0
4	EDO	D	702	-	3,3,3	0.41	0	2,2,2	0.36	0
5	GOL	C	1105	-	5,5,5	0.91	0	5,5,5	1.10	0
4	EDO	C	1101	-	3,3,3	0.70	0	2,2,2	0.80	0
3	SO4	B	705	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	A	703	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	B	706	-	4,4,4	0.22	0	6,6,6	0.05	0
3	SO4	B	702	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	D	703	-	4,4,4	0.24	0	6,6,6	0.08	0
4	EDO	C	1104	-	3,3,3	0.42	0	2,2,2	0.43	0
3	SO4	C	1107	-	4,4,4	0.24	0	6,6,6	0.11	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	703	-	-	0/1/1/1	-
4	EDO	A	704	-	-	1/1/1/1	-
4	EDO	A	705	-	-	1/1/1/1	-
4	EDO	D	702	-	-	0/1/1/1	-
5	GOL	C	1105	-	-	1/4/4/4	-
4	EDO	C	1101	-	-	1/1/1/1	-
4	EDO	C	1104	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1101	EDO	O1-C1-C2-O2
5	C	1105	GOL	O1-C1-C2-C3
4	A	705	EDO	O1-C1-C2-O2
4	C	1104	EDO	O1-C1-C2-O2
4	A	704	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1103	SO4	1	0
3	D	703	SO4	1	0
4	C	1104	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, 95th 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 ²)	Q<0.9
1	A	613/624 (98%)	-0.02	18 (2%) 54 53	32, 49, 71, 108	0
1	B	607/624 (97%)	-0.25	8 (1%) 74 75	31, 44, 61, 98	0
1	C	617/624 (98%)	-0.00	18 (2%) 54 53	30, 49, 83, 116	0
1	D	611/624 (97%)	-0.15	17 (2%) 55 54	31, 45, 77, 110	0
All	All	2448/2496 (98%)	-0.11	61 (2%) 58 57	30, 47, 75, 116	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	616	VAL	5.7
1	A	615	GLY	5.1
1	B	136	ASP	4.5
1	A	13	GLY	4.3
1	A	222	ASP	4.2
1	A	256	GLY	4.2
1	B	13	GLY	4.0
1	A	12	LEU	4.0
1	C	12	LEU	4.0
1	C	21	LYS	3.9
1	C	227	LEU	3.9
1	D	615	GLY	3.8
1	B	12	LEU	3.6
1	D	12	LEU	3.6
1	A	227	LEU	3.6
1	C	13	GLY	3.6
1	A	21	LYS	3.6
1	D	194	GLU	3.6
1	A	617	LEU	3.5
1	C	229	MET	3.4
1	C	23	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	619	HIS	3.2
1	D	614	VAL	3.2
1	B	331	ARG	3.2
1	B	22	THR	3.1
1	C	22	THR	3.1
1	A	57	HIS	3.1
1	D	13	GLY	3.1
1	A	614	VAL	3.1
1	A	145	LYS	3.1
1	D	22	THR	3.0
1	C	57	HIS	3.0
1	D	616	VAL	3.0
1	C	460	GLU	3.0
1	A	620	HIS	3.0
1	B	21	LYS	2.9
1	A	312	CYS	2.9
1	D	21	LYS	2.8
1	C	224	GLU	2.8
1	B	312	CYS	2.8
1	C	146	ASN	2.7
1	C	136	ASP	2.6
1	C	226	HIS	2.6
1	C	81	ALA	2.5
1	D	188	SER	2.5
1	C	32	GLY	2.5
1	C	256	GLY	2.5
1	D	227	LEU	2.3
1	A	496	MET	2.3
1	A	229	MET	2.3
1	C	83	THR	2.3
1	D	136	ASP	2.3
1	B	614	VAL	2.2
1	A	135	GLY	2.2
1	C	225	ASP	2.2
1	D	229	MET	2.1
1	D	23	MET	2.1
1	D	312	CYS	2.1
1	D	145	LYS	2.1
1	D	1	MET	2.0
1	D	276	ARG	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 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, 95th 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(\AA^2)	Q<0.9
4	EDO	C	1101	4/4	0.48	0.41	42,54,55,77	0
3	SO4	B	705	5/5	0.63	0.14	61,71,97,109	0
2	MG	C	1102	1/1	0.63	0.27	61,61,61,61	0
2	MG	D	701	1/1	0.66	0.20	74,74,74,74	0
3	SO4	B	702	5/5	0.77	0.25	57,67,80,95	0
3	SO4	D	703	5/5	0.79	0.12	45,57,64,83	0
3	SO4	B	704	5/5	0.81	0.12	49,58,67,81	0
3	SO4	A	706	5/5	0.82	0.12	49,65,69,83	0
3	SO4	C	1103	5/5	0.82	0.13	48,56,62,75	0
5	GOL	C	1105	6/6	0.82	0.18	49,51,58,60	0
4	EDO	B	703	4/4	0.83	0.14	47,48,49,50	0
4	EDO	A	705	4/4	0.84	0.21	50,57,58,63	0
3	SO4	C	1107	5/5	0.84	0.23	56,63,77,84	0
3	SO4	B	706	5/5	0.85	0.25	50,51,64,78	0
3	SO4	D	704	5/5	0.85	0.28	65,73,73,88	0
3	SO4	A	702	5/5	0.86	0.20	55,56,70,80	0
4	EDO	A	704	4/4	0.86	0.14	39,39,39,40	0
3	SO4	A	703	5/5	0.87	0.18	58,62,82,87	0
4	EDO	C	1104	4/4	0.89	0.20	45,46,50,51	0
4	EDO	D	702	4/4	0.91	0.14	40,41,43,43	0
2	MG	B	701	1/1	0.93	0.18	34,34,34,34	0
2	MG	A	701	1/1	0.94	0.12	50,50,50,50	0
6	NI	C	1106	1/1	0.97	0.27	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.