



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:03 AM UTC

PDB ID : 6PD1 / pdb_00006pd1
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

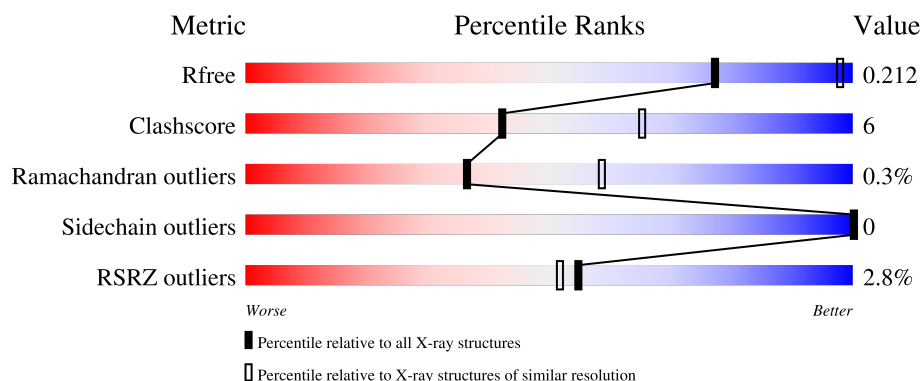
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

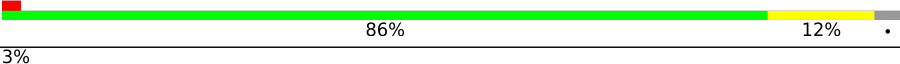
The reported resolution of this entry is 2.72 Å.

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}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (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% 82% 16% ..
1	B	624	 2% 86% 12% .
1	C	624	 3% 84% 14% .
1	D	624	 3% 83% 14% ..

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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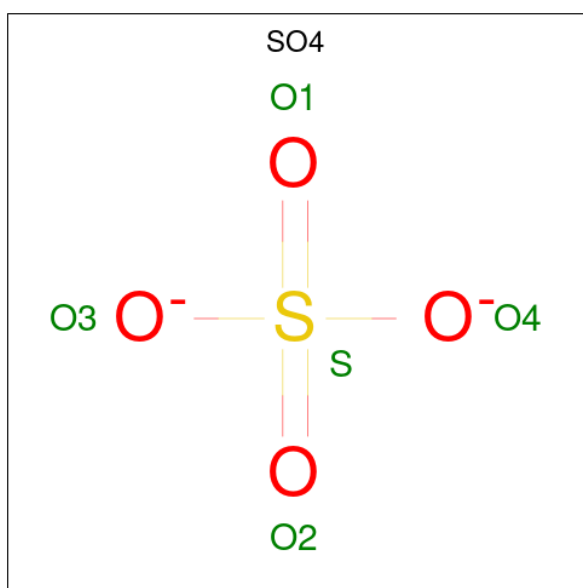
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Chain	Residue	Modelled	Actual	Comment	Reference
C	622	HIS	-	expression tag	UNP Q73MU2
C	623	HIS	-	expression tag	UNP Q73MU2
C	624	HIS	-	expression tag	UNP Q73MU2
D	617	LEU	-	expression tag	UNP Q73MU2
D	618	GLU	-	expression tag	UNP Q73MU2
D	619	HIS	-	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 (CCD ID: MG) (formula: Mg).

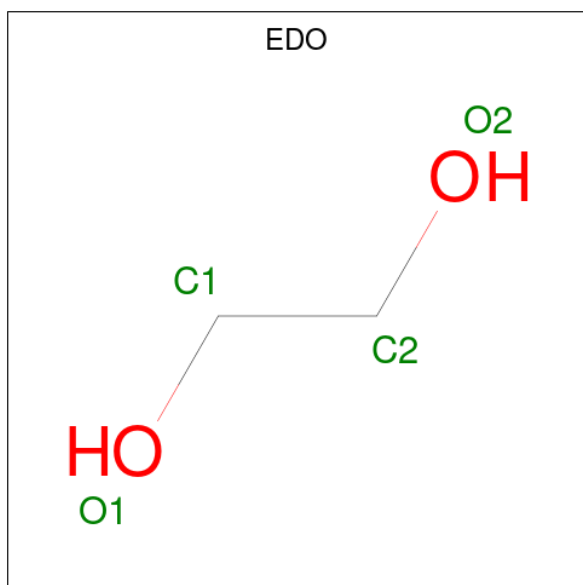
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: 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	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 (CCD ID: EDO) (formula: C₂H₆O₂).



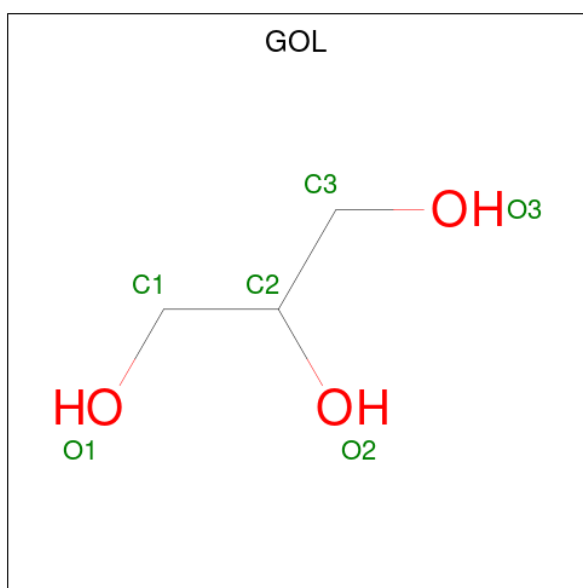
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0

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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 (CCD ID: 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 (CCD ID: NI) (formula: Ni).

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

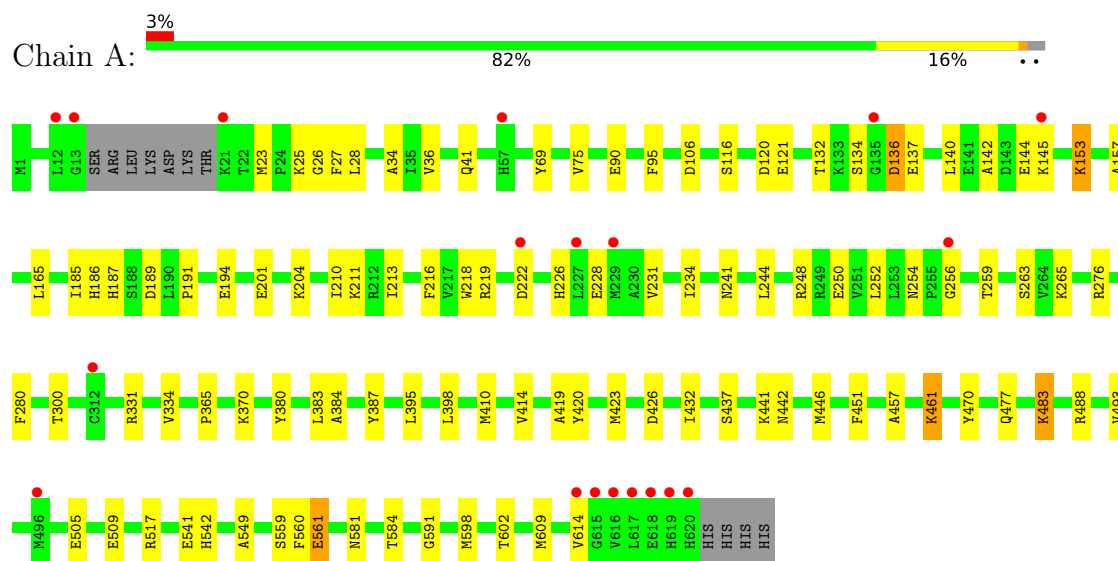
- Molecule 7 is water.

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

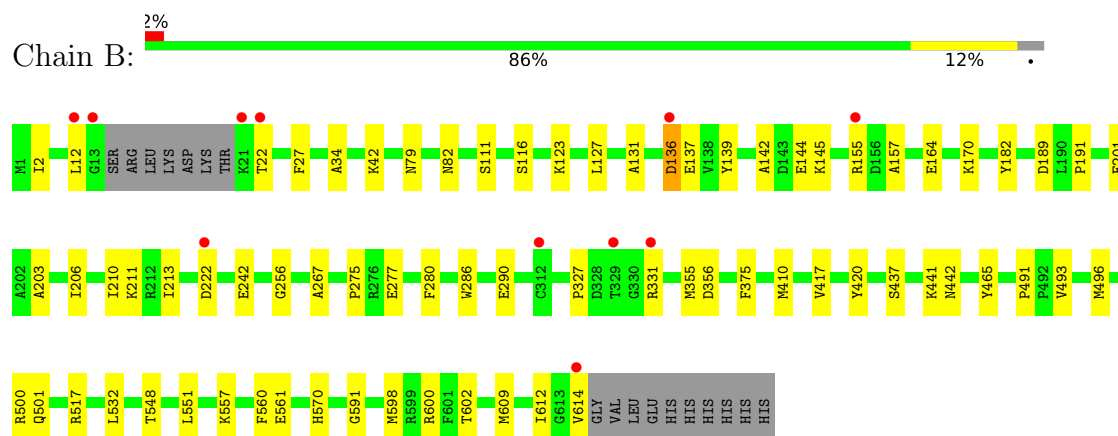
3 Residue-property plots

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

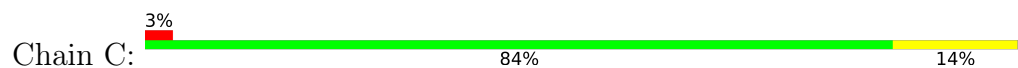
- Molecule 1: Nucleotidyl transferase/aminotransferase, class V



- Molecule 1: Nucleotidyl transferase/aminotransferase, class V



- 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 (Not available) , 0.212	Depositor DCC
R_{free} test set	4104 reflections (4.97%)	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, MG, NI, 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	0.24	1/4912 (0.0%)	0.57	10/6639 (0.2%)
1	B	0.20	0/4862	0.47	4/6571 (0.1%)
1	C	0.23	0/4957	0.53	6/6699 (0.1%)
1	D	0.28	0/4890	0.63	16/6609 (0.2%)
All	All	0.24	1/19621 (0.0%)	0.55	36/26518 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	483	LYS	CE-NZ	6.11	1.67	1.49

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	229	MET	CA-CB-CG	-10.64	92.81	114.10
1	A	461	LYS	CA-CB-CG	-8.25	97.60	114.10
1	D	194	GLU	CA-CB-CG	7.96	130.02	114.10
1	B	561	GLU	N-CA-CB	-7.81	98.69	110.01
1	D	574	ILE	N-CA-CB	7.42	123.47	111.23
1	D	229	MET	CB-CG-SD	7.38	134.85	112.70
1	C	144	GLU	CA-CB-CG	7.12	128.34	114.10
1	A	461	LYS	CB-CG-CD	7.05	127.52	111.30
1	D	145	LYS	CA-CB-CG	-6.70	100.70	114.10
1	B	560	PHE	CA-C-N	6.61	129.03	120.44
1	B	560	PHE	C-N-CA	6.61	129.03	120.44
1	A	541	GLU	CA-CB-CG	6.45	126.99	114.10
1	D	145	LYS	CD-CE-NZ	-6.43	91.33	111.90
1	D	231	VAL	CA-C-N	-6.32	109.90	121.52
1	D	231	VAL	C-N-CA	-6.32	109.90	121.52
1	D	136	ASP	N-CA-CB	-6.31	99.83	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	599	ARG	CD-NE-CZ	5.97	132.76	124.40
1	A	561	GLU	CB-CG-CD	-5.90	102.56	112.60
1	B	561	GLU	CB-CG-CD	-5.82	102.71	112.60
1	C	136	ASP	CA-C-N	-5.64	114.25	122.65
1	C	136	ASP	C-N-CA	-5.64	114.25	122.65
1	A	370	LYS	CA-CB-CG	5.56	125.22	114.10
1	A	145	LYS	CA-CB-CG	5.44	124.97	114.10
1	D	224	GLU	CA-CB-CG	-5.40	103.30	114.10
1	A	153	LYS	CA-CB-CG	5.32	124.73	114.10
1	A	560	PHE	CA-C-N	5.28	127.31	120.44
1	A	560	PHE	C-N-CA	5.28	127.31	120.44
1	C	136	ASP	CB-CA-C	-5.28	102.33	111.30
1	C	144	GLU	N-CA-CB	5.28	118.35	110.22
1	D	144	GLU	CA-C-N	-5.27	114.72	122.83
1	D	144	GLU	C-N-CA	-5.27	114.72	122.83
1	D	541	GLU	CB-CG-CD	-5.16	103.82	112.60
1	D	574	ILE	CB-CA-C	-5.08	102.96	111.29
1	D	121	GLU	N-CA-CB	-5.08	102.40	110.22
1	D	231	VAL	N-CA-C	5.07	115.79	110.62
1	A	483	LYS	CD-CE-NZ	-5.02	95.83	111.90

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	4817	0	4839	64	0
1	B	4769	0	4795	47	0
1	C	4858	0	4866	69	0
1	D	4797	0	4825	70	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	243	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 (243) 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:HE2	1:D:183:ALA:HB2	1.45	0.98
1:D:86:MET:HG3	1:D:193:MET:HE3	1.51	0.92
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:D:491:PRO:HB2	1:D:496:MET:HE1	1.57	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:C:509:GLU:O	1:C:510:THR:OG1	2.03	0.77
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:517:ARG:NH2	1:D:591:GLY:O	2.20	0.74
1:B:491:PRO:HB2	1:B:496:MET:HE1	1.70	0.73
1:D:194:GLU:HG2	1:D:196:GLU:HB2	1.72	0.72
1:D:227:LEU:HD12	1:D:228:GLU:CD	2.14	0.71
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:D:194:GLU:CD	1:D:197:HIS:HB2	2.17	0.69
1:C:313:SER:OG	3:C:1103:SO4:O3	2.10	0.69
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: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:D:86:MET:HE2	1:D:183:ALA:CB	2.24	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: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:D:86:MET:HG3	1:D:193:MET:CE	2.24	0.63
1:A:121:GLU:CD	1:A:121:GLU:H	2.07	0.62
1:C:383:LEU:HB2	1:C:410:MET:HE2	1.81	0.62
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:193:MET:HE3	1:C:198:ALA:HB2	1.85	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: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:B:375:PHE:CG	1:B:410:MET:HE1	2.39	0.57
1:C:120:ASP:OD2	1:C:211:LYS:NZ	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:LEU:HD21	1:C:151:LEU:HD12	1.86	0.57
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:144:GLU:CD	1:A:144:GLU:H	2.13	0.56
1:A:25:LYS:HD3	1:A:106:ASP:HB3	1.87	0.56
1:C:86:MET:HG3	1:C:193:MET:HE3	1.88	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
1:D:388:HIS:HD1	1:D:418:SER:HG	1.54	0.55
1:B:42:LYS:HD3	1:B:111:SER:HB3	1.88	0.55
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: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:C:21:LYS:C	1:C:23:MET:H	2.16	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:419:ALA:HB1	1:C:423:MET:HE3	1.91	0.52
1:A:380:TYR:HB2	1:A:410:MET:HE3	1.90	0.52
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:599:ARG:C	1:C:602:THR:HG22	2.34	0.52
1:B:155:ARG:HH21	1:B:155:ARG:C	2.18	0.52
1:D:332:LEU:O	1:D:355:MET:HA	2.09	0.52
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:265:LYS:HA	1:A:446:MET:HE2	1.92	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:446:MET:HE3	1:C:494:GLN:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:90:GLU:CD	1:A:187:HIS:HE2	2.20	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:B:42:LYS:NZ	1:B:242:GLU:OE2	2.30	0.49
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:292:LYS:HA	1:C:453:ILE:HD13	1.94	0.48
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:CG	1:C:226:HIS:H	2.22	0.48
1:C:223:ASN:HD21	1:C:226:HIS:H	1.62	0.48
1:D:256:GLY:HA2	1:D:257:PRO:C	2.38	0.48
1:C:136:ASP:CG	1:C:136:ASP:O	2.56	0.47
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:C:509:GLU:C	1:C:510:THR:HG1	2.19	0.47
1:B:280:PHE:CE1	1:B:493:VAL:HG13	2.49	0.47
1:C:86:MET:HE2	1:C:183:ALA:HB2	1.97	0.47
1:B:116:SER:OG	1:B:211:LYS:HE2	2.13	0.47
1:B:256:GLY:HA2	1:B:441:LYS:HZ2	1.79	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:D:224:GLU:O	1:D:225:ASP:C	2.57	0.47
1:C:599:ARG:HA	1:C:602:THR:CG2	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:23:MET:HE3	1:A:28:LEU:HD23	1.98	0.45
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:D:224:GLU:OE2	1:D:227:LEU:HB3	2.16	0.45
1:D:383:LEU:HB2	1:D:410:MET:HE2	1.97	0.45
1:A:241:ASN:HA	1:A:244:LEU:HD12	1.98	0.45
1:B:27:PHE:HA	1:B:34:ALA:HB1	1.97	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:C:379:LYS:NZ	7:C:1204:HOH:O	2.49	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:D:427:LEU:HD21	1:D:435:MET:HE3	1.99	0.44
1:D:142:ALA:HB2	1:D:210:ILE:HD12	1.99	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: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:A:120:ASP:OD2	1:A:211:LYS:NZ	2.43	0.43
1:C:528:ALA:HB2	1:C:602:THR:OG1	2.18	0.43
1:D:193:MET:HE3	1:D:198:ALA:HB2	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:123:LYS:HB2	1:B:123:LYS:HE3	1.79	0.42
1:A:383:LEU:HB2	1:A:410:MET:HE2	2.01	0.42
1:A:419:ALA:HB1	1:A:423:MET:HE3	2.01	0.42
1:B:355:MET:HE3	1:B:355:MET:HB2	1.81	0.42
1:A:194:GLU:CD	1:A:194:GLU:H	2.27	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:B:189:ASP:C	1:B:191:PRO:HD3	2.45	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:A:263:SER:OG	1:A:505:GLU:OE2	2.32	0.41
1:B:280:PHE:HZ	1:B:496:MET:HE3	1.85	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: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:A:189:ASP:C	1:A:191:PRO:HD3	2.46	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:D:496:MET:HE3	1:D:496:MET:HB2	1.76	0.41
1:C:212:ARG:NH1	1:C:214:GLU:OE1	2.53	0.41
1:C:229:MET:HB2	1:C:229:MET:HE2	1.59	0.41
1:C:463:LYS:HB2	1:C:475:TYR:CZ	2.56	0.41
1:D:90:GLU:CD	1:D:187:HIS:HE2	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:395:LEU:HD13	1:A:423:MET:HE1	2.03	0.41
1:A:509:GLU:OE2	1:A:517:ARG:NH1	2.48	0.41
1:C:355:MET:HE3	1:C:355:MET:HB2	1.86	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: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:B:491:PRO:HB2	1:B:496:MET:CE	2.44	0.40
1:C:380:TYR:HB2	1:C:410:MET:HE3	2.03	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

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	609/624 (98%)	585 (96%)	22 (4%)	2 (0%)	36	59
1	B	603/624 (97%)	581 (96%)	20 (3%)	2 (0%)	36	59
1	C	613/624 (98%)	589 (96%)	23 (4%)	1 (0%)	43	66
1	D	607/624 (97%)	578 (95%)	27 (4%)	2 (0%)	36	59
All	All	2432/2496 (97%)	2333 (96%)	92 (4%)	7 (0%)	36	59

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 ⓘ

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%)	522 (100%)	0	100	100
1	B	517/533 (97%)	517 (100%)	0	100	100
1	C	526/533 (99%)	526 (100%)	0	100	100
1	D	520/533 (98%)	520 (100%)	0	100	100
All	All	2085/2132 (98%)	2085 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	146	ASN
1	A	444	GLN
1	A	581	ASN
1	A	619	HIS
1	A	620	HIS
1	C	57	HIS
1	C	64	ASN
1	C	82	ASN
1	C	226	HIS
1	C	285	GLN
1	C	440	ASN

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Mol	Chain	Res	Type
1	C	442	ASN
1	D	197	HIS
1	D	226	HIS
1	D	486	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	704	-	3,3,3	0.42	0	2,2,2	0.40	0
3	SO4	C	1103	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	B	702	-	4,4,4	0.23	0	6,6,6	0.11	0
4	EDO	A	705	-	3,3,3	0.43	0	2,2,2	0.38	0
3	SO4	B	705	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	B	704	-	4,4,4	0.22	0	6,6,6	0.07	0
3	SO4	D	704	-	4,4,4	0.24	0	6,6,6	0.09	0
4	EDO	C	1104	-	3,3,3	0.42	0	2,2,2	0.43	0
4	EDO	D	702	-	3,3,3	0.41	0	2,2,2	0.36	0
3	SO4	A	703	-	4,4,4	0.23	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	C	1101	-	3,3,3	0.70	0	2,2,2	0.80	0
3	SO4	D	703	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	706	-	4,4,4	0.25	0	6,6,6	0.08	0
5	GOL	C	1105	-	5,5,5	0.91	0	5,5,5	1.10	0
3	SO4	C	1107	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	B	706	-	4,4,4	0.22	0	6,6,6	0.05	0
4	EDO	B	703	-	3,3,3	0.42	0	2,2,2	0.38	0
3	SO4	A	702	-	4,4,4	0.23	0	6,6,6	0.12	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	A	704	-	-	1/1/1/1	-
4	EDO	A	705	-	-	1/1/1/1	-
4	EDO	D	702	-	-	0/1/1/1	-
4	EDO	C	1104	-	-	1/1/1/1	-
5	GOL	C	1105	-	-	1/4/4/4	-
4	EDO	B	703	-	-	0/1/1/1	-
4	EDO	C	1101	-	-	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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1104	EDO	1	0
3	D	703	SO4	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%)	0.11	19 (3%) 51 48	32, 49, 71, 108	0
1	B	607/624 (97%)	-0.12	11 (1%) 67 65	31, 44, 61, 98	0
1	C	617/624 (98%)	0.13	19 (3%) 51 48	30, 49, 83, 116	0
1	D	611/624 (97%)	-0.02	20 (3%) 49 45	31, 45, 77, 110	0
All	All	2448/2496 (98%)	0.02	69 (2%) 55 52	30, 47, 75, 116	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	616	VAL	5.8
1	A	615	GLY	5.2
1	B	136	ASP	4.5
1	A	13	GLY	4.5
1	A	256	GLY	4.4
1	A	222	ASP	4.2
1	B	13	GLY	4.1
1	A	12	LEU	4.1
1	C	12	LEU	4.1
1	C	227	LEU	4.0
1	C	21	LYS	4.0
1	D	615	GLY	4.0
1	B	12	LEU	3.8
1	D	12	LEU	3.8
1	C	13	GLY	3.7
1	A	227	LEU	3.7
1	D	194	GLU	3.6
1	A	617	LEU	3.6
1	A	21	LYS	3.6
1	C	229	MET	3.6
1	C	23	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	619	HIS	3.3
1	D	614	VAL	3.3
1	C	22	THR	3.3
1	A	57	HIS	3.3
1	D	13	GLY	3.2
1	A	614	VAL	3.2
1	B	22	THR	3.2
1	B	331	ARG	3.2
1	A	145	LYS	3.2
1	D	616	VAL	3.1
1	D	22	THR	3.1
1	A	620	HIS	3.1
1	C	57	HIS	3.1
1	A	312	CYS	3.0
1	B	21	LYS	3.0
1	C	460	GLU	3.0
1	D	21	LYS	2.9
1	B	312	CYS	2.9
1	C	224	GLU	2.9
1	C	146	ASN	2.8
1	C	136	ASP	2.7
1	C	226	HIS	2.7
1	C	32	GLY	2.6
1	C	81	ALA	2.6
1	C	256	GLY	2.6
1	D	188	SER	2.6
1	D	227	LEU	2.5
1	A	496	MET	2.4
1	C	83	THR	2.4
1	A	229	MET	2.4
1	D	136	ASP	2.3
1	A	135	GLY	2.3
1	B	614	VAL	2.3
1	D	23	MET	2.2
1	C	225	ASP	2.2
1	D	229	MET	2.2
1	D	312	CYS	2.2
1	D	145	LYS	2.2
1	D	1	MET	2.2
1	D	276	ARG	2.1
1	D	79	ASN	2.1
1	D	187	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	222	ASP	2.1
1	C	11	GLY	2.0
1	B	155	ARG	2.0
1	A	618	GLU	2.0
1	D	121	GLU	2.0
1	B	329	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å 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	D	701	1/1	0.68	0.20	74,74,74,74	0
2	MG	C	1102	1/1	0.73	0.25	61,61,61,61	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
3	SO4	C	1107	5/5	0.84	0.23	56,63,77,84	0
3	SO4	D	704	5/5	0.84	0.28	65,73,73,88	0
4	EDO	A	705	4/4	0.84	0.21	50,57,58,63	0
3	SO4	B	706	5/5	0.85	0.25	50,51,64,78	0
3	SO4	A	702	5/5	0.86	0.20	55,56,70,80	0
3	SO4	A	703	5/5	0.87	0.18	58,62,82,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	704	4/4	0.87	0.14	39,39,39,40	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	0.95	0.11	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.