



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:53 AM UTC

PDB ID : 4GGH / pdb_00004ggh
Title : Crystal structure of an enolase family member from vibrio harveyi (efi-target 501692) with homology to mannonate dehydratase, with mg, hepes, and ethylene glycol bound (ordered loops, space group c2221)
Authors : Vetting, M.W.; Toro, R.; Bhosle, R.; Al Obaidi, N.F.; Morisco, L.L.; Wasserman, S.R.; Sojitra, S.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Hillerich, B.; Love, J.; Seidel, R.D.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on : 2012-08-06
Resolution : 1.90 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)

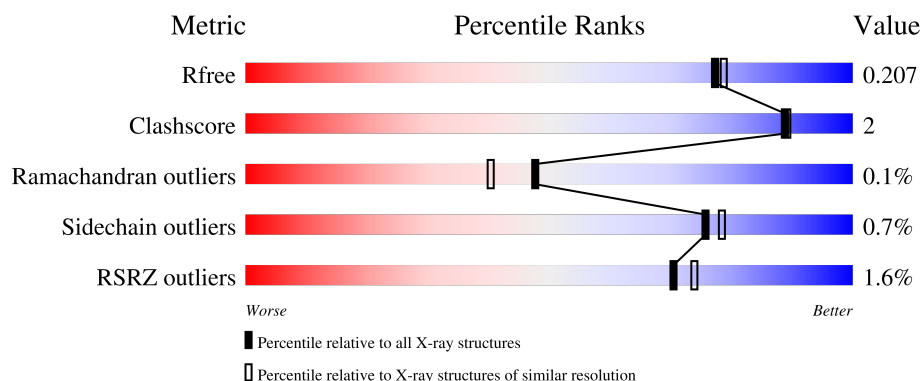
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	422	
1	B	422	
1	C	422	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	422	% 88% 6% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14691 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	1	0
			3199	2029	554	600	16			
1	B	397	Total	C	N	O	S	0	0	0
			3190	2024	553	597	16			
1	C	397	Total	C	N	O	S	0	2	0
			3212	2036	561	599	16			
1	D	397	Total	C	N	O	S	0	2	0
			3208	2034	557	601	16			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP D0X4R4
A	-21	HIS	-	expression tag	UNP D0X4R4
A	-20	HIS	-	expression tag	UNP D0X4R4
A	-19	HIS	-	expression tag	UNP D0X4R4
A	-18	HIS	-	expression tag	UNP D0X4R4
A	-17	HIS	-	expression tag	UNP D0X4R4
A	-16	HIS	-	expression tag	UNP D0X4R4
A	-15	SER	-	expression tag	UNP D0X4R4
A	-14	SER	-	expression tag	UNP D0X4R4
A	-13	GLY	-	expression tag	UNP D0X4R4
A	-12	VAL	-	expression tag	UNP D0X4R4
A	-11	ASP	-	expression tag	UNP D0X4R4
A	-10	LEU	-	expression tag	UNP D0X4R4
A	-9	GLY	-	expression tag	UNP D0X4R4
A	-8	THR	-	expression tag	UNP D0X4R4
A	-7	GLU	-	expression tag	UNP D0X4R4
A	-6	ASN	-	expression tag	UNP D0X4R4
A	-5	LEU	-	expression tag	UNP D0X4R4
A	-4	TYR	-	expression tag	UNP D0X4R4
A	-3	PHE	-	expression tag	UNP D0X4R4
A	-2	GLN	-	expression tag	UNP D0X4R4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP D0X4R4
A	0	MET	-	expression tag	UNP D0X4R4
B	-22	MET	-	initiating methionine	UNP D0X4R4
B	-21	HIS	-	expression tag	UNP D0X4R4
B	-20	HIS	-	expression tag	UNP D0X4R4
B	-19	HIS	-	expression tag	UNP D0X4R4
B	-18	HIS	-	expression tag	UNP D0X4R4
B	-17	HIS	-	expression tag	UNP D0X4R4
B	-16	HIS	-	expression tag	UNP D0X4R4
B	-15	SER	-	expression tag	UNP D0X4R4
B	-14	SER	-	expression tag	UNP D0X4R4
B	-13	GLY	-	expression tag	UNP D0X4R4
B	-12	VAL	-	expression tag	UNP D0X4R4
B	-11	ASP	-	expression tag	UNP D0X4R4
B	-10	LEU	-	expression tag	UNP D0X4R4
B	-9	GLY	-	expression tag	UNP D0X4R4
B	-8	THR	-	expression tag	UNP D0X4R4
B	-7	GLU	-	expression tag	UNP D0X4R4
B	-6	ASN	-	expression tag	UNP D0X4R4
B	-5	LEU	-	expression tag	UNP D0X4R4
B	-4	TYR	-	expression tag	UNP D0X4R4
B	-3	PHE	-	expression tag	UNP D0X4R4
B	-2	GLN	-	expression tag	UNP D0X4R4
B	-1	SER	-	expression tag	UNP D0X4R4
B	0	MET	-	expression tag	UNP D0X4R4
C	-22	MET	-	initiating methionine	UNP D0X4R4
C	-21	HIS	-	expression tag	UNP D0X4R4
C	-20	HIS	-	expression tag	UNP D0X4R4
C	-19	HIS	-	expression tag	UNP D0X4R4
C	-18	HIS	-	expression tag	UNP D0X4R4
C	-17	HIS	-	expression tag	UNP D0X4R4
C	-16	HIS	-	expression tag	UNP D0X4R4
C	-15	SER	-	expression tag	UNP D0X4R4
C	-14	SER	-	expression tag	UNP D0X4R4
C	-13	GLY	-	expression tag	UNP D0X4R4
C	-12	VAL	-	expression tag	UNP D0X4R4
C	-11	ASP	-	expression tag	UNP D0X4R4
C	-10	LEU	-	expression tag	UNP D0X4R4
C	-9	GLY	-	expression tag	UNP D0X4R4
C	-8	THR	-	expression tag	UNP D0X4R4
C	-7	GLU	-	expression tag	UNP D0X4R4
C	-6	ASN	-	expression tag	UNP D0X4R4

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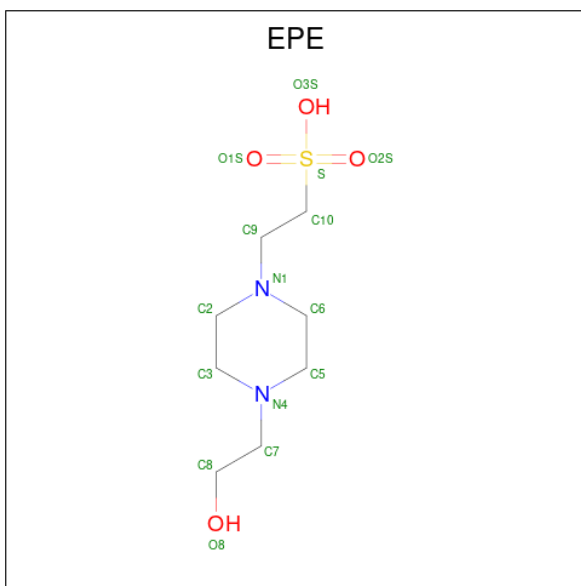
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	LEU	-	expression tag	UNP D0X4R4
C	-4	TYR	-	expression tag	UNP D0X4R4
C	-3	PHE	-	expression tag	UNP D0X4R4
C	-2	GLN	-	expression tag	UNP D0X4R4
C	-1	SER	-	expression tag	UNP D0X4R4
C	0	MET	-	expression tag	UNP D0X4R4
D	-22	MET	-	initiating methionine	UNP D0X4R4
D	-21	HIS	-	expression tag	UNP D0X4R4
D	-20	HIS	-	expression tag	UNP D0X4R4
D	-19	HIS	-	expression tag	UNP D0X4R4
D	-18	HIS	-	expression tag	UNP D0X4R4
D	-17	HIS	-	expression tag	UNP D0X4R4
D	-16	HIS	-	expression tag	UNP D0X4R4
D	-15	SER	-	expression tag	UNP D0X4R4
D	-14	SER	-	expression tag	UNP D0X4R4
D	-13	GLY	-	expression tag	UNP D0X4R4
D	-12	VAL	-	expression tag	UNP D0X4R4
D	-11	ASP	-	expression tag	UNP D0X4R4
D	-10	LEU	-	expression tag	UNP D0X4R4
D	-9	GLY	-	expression tag	UNP D0X4R4
D	-8	THR	-	expression tag	UNP D0X4R4
D	-7	GLU	-	expression tag	UNP D0X4R4
D	-6	ASN	-	expression tag	UNP D0X4R4
D	-5	LEU	-	expression tag	UNP D0X4R4
D	-4	TYR	-	expression tag	UNP D0X4R4
D	-3	PHE	-	expression tag	UNP D0X4R4
D	-2	GLN	-	expression tag	UNP D0X4R4
D	-1	SER	-	expression tag	UNP D0X4R4
D	0	MET	-	expression tag	UNP D0X4R4

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	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

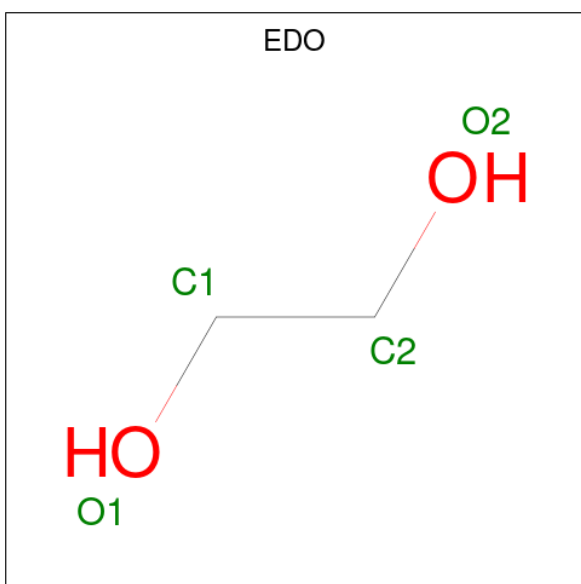
- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD

ID: EPE) (formula: $\text{C}_8\text{H}_{18}\text{N}_2\text{O}_4\text{S}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 2 2	0	1
5	C	3	Total Cl 5 5	0	2

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

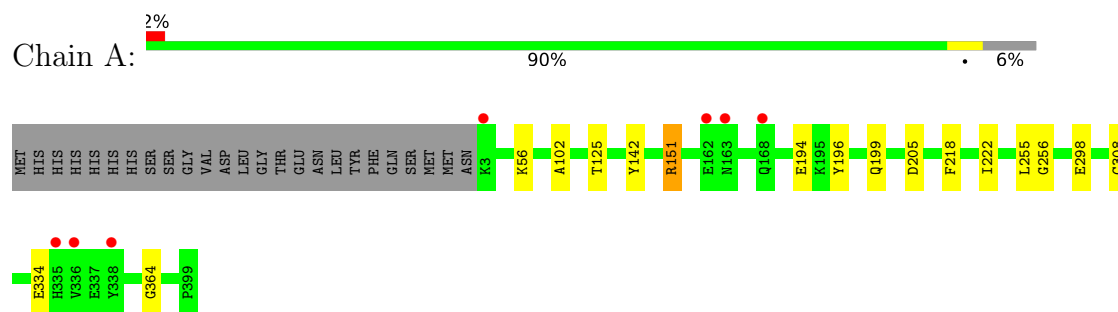
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	427	Total	O	0	10
			438	438		
7	B	406	Total	O	0	5
			411	411		
7	C	430	Total	O	0	10
			440	440		
7	D	431	Total	O	0	18
			449	449		

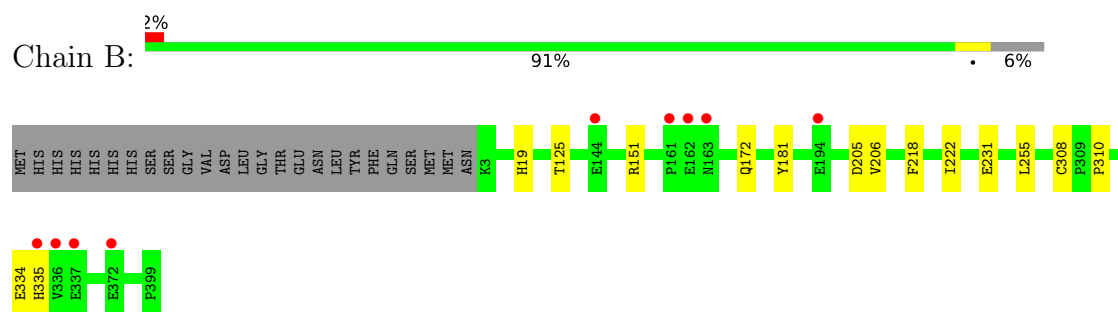
3 Residue-property plots [i](#)

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.

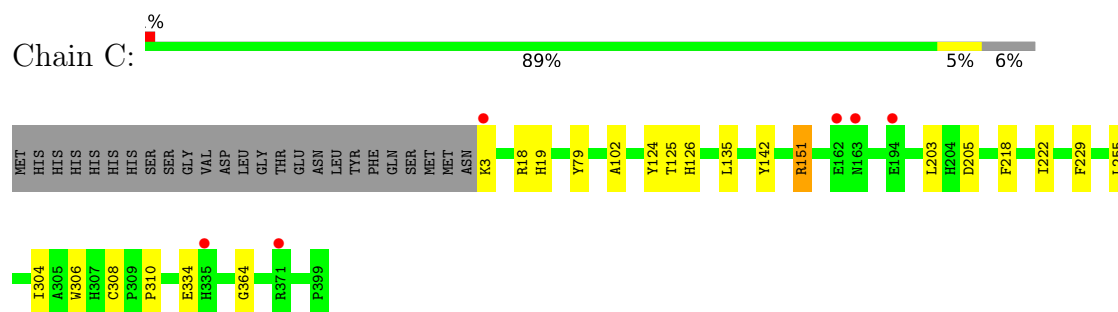
- Molecule 1: Putative uncharacterized protein



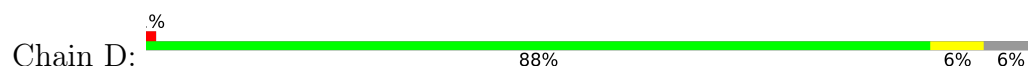
- Molecule 1: Putative uncharacterized protein

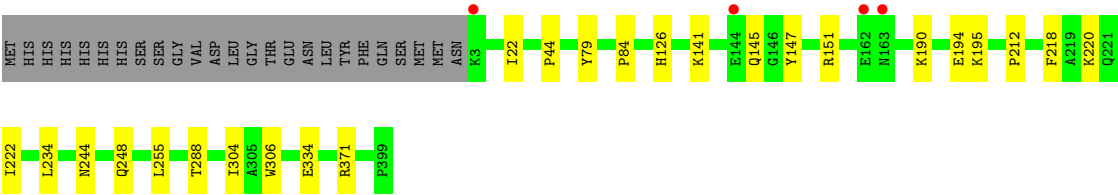


- Molecule 1: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	92.95Å 209.55Å 208.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.62 – 1.90 93.62 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (93.62-1.90) 98.8 (93.62-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.168 , 0.203 0.173 , 0.207	Depositor DCC
R_{free} test set	4762 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14691	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: EPE, GOL, CL, MG, 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	0.43	0/3282	0.76	1/4463 (0.0%)
1	B	0.42	0/3273	0.76	0/4451
1	C	0.45	0/3295	0.75	0/4479
1	D	0.42	0/3291	0.77	2/4475 (0.0%)
All	All	0.43	0/13141	0.76	3/17868 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	288	THR	CA-C-N	-5.77	113.82	119.64
1	D	288	THR	C-N-CA	-5.77	113.82	119.64
1	A	256	GLY	N-CA-C	5.08	122.11	114.95

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	3199	0	3084	10	0
1	B	3190	0	3079	7	0
1	C	3212	0	3103	15	0
1	D	3208	0	3093	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	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	17	0	0
3	B	15	0	17	0	0
3	C	15	0	17	1	0
3	D	15	0	17	2	0
4	A	16	0	24	1	0
4	B	16	0	24	1	0
4	C	16	0	24	0	0
4	D	12	0	18	0	0
5	A	2	0	0	0	0
5	C	5	0	0	2	0
6	C	6	0	8	0	0
6	D	6	0	8	0	0
7	A	438	0	0	4	0
7	B	411	0	0	1	1
7	C	440	0	0	2	0
7	D	449	0	0	2	0
All	All	14691	0	12533	49	1

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 2.

All (49) 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:151:ARG:HG2	1:A:151:ARG:HH21	1.42	0.83
1:C:151[A]:ARG:HG2	1:C:151[A]:ARG:HH21	1.46	0.80
5:C:410:CL:CL	7:C:720:HOH:O	2.35	0.80
1:C:308:CYS:HB2	1:C:334:GLU:HB3	1.70	0.73
1:A:298:GLU:OE2	7:A:832:HOH:O	2.07	0.73
1:D:190:LYS:NZ	1:D:194:GLU:OE2	2.23	0.71
1:C:18:ARG:NH2	3:C:403:EPE:O2S	2.26	0.69
1:B:308:CYS:HB2	1:B:334:GLU:HB3	1.80	0.63
1:D:195:LYS:NZ	7:D:724[B]:HOH:O	2.39	0.56
4:A:407:EDO:H11	7:A:921:HOH:O	2.07	0.55
1:C:151[A]:ARG:HG2	1:C:151[A]:ARG:NH2	2.18	0.53
1:C:126:HIS:HE2	1:C:334:GLU:HG2	1.77	0.50
1:A:196:TYR:O	1:A:199:GLN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:CYS:HB2	1:A:334:GLU:HB3	1.94	0.49
4:B:405:EDO:H11	7:B:802:HOH:O	2.14	0.48
1:C:218:PHE:O	1:C:222:ILE:HG13	2.14	0.48
5:C:408[A]:CL:CL	1:D:84:PRO:HD2	2.51	0.47
1:C:19:HIS:CE1	1:C:310:PRO:HB2	2.50	0.47
1:A:218:PHE:O	1:A:222:ILE:HG13	2.16	0.46
1:B:151:ARG:HD2	1:B:205:ASP:HB2	1.97	0.45
3:D:403:EPE:H81	3:D:403:EPE:H52	1.80	0.44
1:B:181:TYR:OH	1:B:206:VAL:HA	2.18	0.44
1:C:102:ALA:HB3	1:C:364:GLY:HA2	1.98	0.44
1:C:124:TYR:CZ	1:C:334:GLU:HG3	2.53	0.44
1:A:102:ALA:HB3	1:A:364:GLY:HA2	2.00	0.44
1:C:151[B]:ARG:HD2	1:C:205:ASP:HB2	2.00	0.44
1:D:141:LYS:HE3	1:D:145:GLN:OE1	2.18	0.43
3:D:403:EPE:H102	3:D:403:EPE:H62	1.44	0.43
1:D:304:ILE:HG21	1:D:306:TRP:CE2	2.54	0.43
1:C:3:LYS:N	7:C:643:HOH:O	2.51	0.43
1:D:218:PHE:O	1:D:222:ILE:HG13	2.19	0.43
1:D:22:ILE:HD11	1:D:44:PRO:HA	2.00	0.43
1:B:218:PHE:O	1:B:222:ILE:HG13	2.19	0.42
1:C:203:LEU:HD23	1:C:229:PHE:CZ	2.54	0.42
1:D:145:GLN:HE21	1:D:147:TYR:HE2	1.66	0.42
1:A:151:ARG:HD2	1:A:205:ASP:HB2	2.02	0.42
1:B:205:ASP:HA	1:B:231:GLU:HB3	2.00	0.42
1:C:125:THR:HG21	1:C:142:TYR:CG	2.55	0.42
1:B:125:THR:HA	1:B:335:HIS:HB3	2.03	0.41
1:C:135:LEU:HD23	1:C:135:LEU:HA	1.94	0.41
1:D:220:LYS:HE2	7:D:925:HOH:O	2.21	0.41
1:A:56:LYS:NZ	7:A:828:HOH:O	2.51	0.41
1:D:126:HIS:HE1	1:D:334:GLU:HG3	1.85	0.41
1:C:304:ILE:HG21	1:C:306:TRP:CE2	2.56	0.41
1:A:125:THR:HG21	1:A:142:TYR:CD1	2.56	0.40
1:B:19:HIS:CE1	1:B:310:PRO:HB2	2.56	0.40
1:D:212:PRO:HA	1:D:234:LEU:HD21	2.04	0.40
1:A:194:GLU:HG3	7:A:644:HOH:O	2.21	0.40
1:D:244:ASN:O	1:D:248:GLN:HG2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:830:HOH:O	7:B:830:HOH:O[3_454]	2.19	0.01

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	396/422 (94%)	387 (98%)	9 (2%)	0	100	100
1	B	395/422 (94%)	384 (97%)	11 (3%)	0	100	100
1	C	397/422 (94%)	388 (98%)	8 (2%)	1 (0%)	36	29
1	D	397/422 (94%)	388 (98%)	8 (2%)	1 (0%)	36	29
All	All	1585/1688 (94%)	1547 (98%)	36 (2%)	2 (0%)	48	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	79	TYR
1	C	79	TYR

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	345/367 (94%)	343 (99%)	2 (1%)	78	81
1	B	344/367 (94%)	342 (99%)	2 (1%)	78	81
1	C	346/367 (94%)	343 (99%)	3 (1%)	70	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	346/367 (94%)	343 (99%)	3 (1%)	70	73
All	All	1381/1468 (94%)	1371 (99%)	10 (1%)	76	78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	ARG
1	A	255	LEU
1	B	172	GLN
1	B	255	LEU
1	C	151[A]	ARG
1	C	151[B]	ARG
1	C	255	LEU
1	D	151	ARG
1	D	255	LEU
1	D	371	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	226	ASN
1	A	238	GLN
1	B	87	ASN
1	B	88	ASN
1	B	145	GLN
1	B	226	ASN
1	B	238	GLN
1	B	343	GLN
1	C	88	ASN
1	C	122	GLN
1	C	238	GLN
1	D	88	ASN
1	D	238	GLN

5.3.3 RNA ⓘ

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 33 ligands modelled in this entry, 12 are monoatomic - leaving 21 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	C	404	-	3,3,3	0.49	0	2,2,2	0.45	0
3	EPE	B	402	-	15,15,15	0.92	1 (6%)	19,20,20	1.86	6 (31%)
3	EPE	C	403	-	15,15,15	0.91	1 (6%)	19,20,20	1.82	7 (36%)
4	EDO	B	403	-	3,3,3	0.47	0	2,2,2	0.46	0
4	EDO	C	406	-	3,3,3	0.42	0	2,2,2	0.35	0
4	EDO	A	407	-	3,3,3	0.44	0	2,2,2	0.37	0
4	EDO	A	404	-	3,3,3	0.47	0	2,2,2	0.45	0
6	GOL	C	402	-	5,5,5	0.33	0	5,5,5	0.21	0
4	EDO	D	406	-	3,3,3	0.41	0	2,2,2	0.68	0
6	GOL	D	402	-	5,5,5	0.46	0	5,5,5	0.36	0
4	EDO	C	407	-	3,3,3	0.40	0	2,2,2	0.40	0
4	EDO	D	405	-	3,3,3	0.48	0	2,2,2	0.32	0
4	EDO	D	404	-	3,3,3	0.47	0	2,2,2	0.50	0
4	EDO	A	405	-	3,3,3	0.48	0	2,2,2	0.34	0
3	EPE	A	403	-	15,15,15	0.89	1 (6%)	19,20,20	1.78	5 (26%)
4	EDO	B	404	-	3,3,3	0.43	0	2,2,2	0.51	0
4	EDO	B	406	-	3,3,3	0.49	0	2,2,2	0.34	0
3	EPE	D	403	-	15,15,15	0.80	1 (6%)	19,20,20	1.67	6 (31%)
4	EDO	C	405	-	3,3,3	0.45	0	2,2,2	0.41	0
4	EDO	B	405	-	3,3,3	0.45	0	2,2,2	0.25	0
4	EDO	A	406	-	3,3,3	0.43	0	2,2,2	0.60	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	C	404	-	-	0/1/1/1	-
3	EPE	B	402	-	-	3/9/19/19	0/1/1/1
3	EPE	C	403	-	-	3/9/19/19	0/1/1/1
4	EDO	B	403	-	-	0/1/1/1	-
4	EDO	C	406	-	-	0/1/1/1	-
4	EDO	A	407	-	-	0/1/1/1	-
4	EDO	A	404	-	-	0/1/1/1	-
6	GOL	C	402	-	-	0/4/4/4	-
4	EDO	D	406	-	-	0/1/1/1	-
6	GOL	D	402	-	-	0/4/4/4	-
4	EDO	C	407	-	-	0/1/1/1	-
4	EDO	D	405	-	-	0/1/1/1	-
4	EDO	D	404	-	-	0/1/1/1	-
4	EDO	A	405	-	-	0/1/1/1	-
3	EPE	A	403	-	-	4/9/19/19	0/1/1/1
4	EDO	B	404	-	-	0/1/1/1	-
4	EDO	B	406	-	-	1/1/1/1	-
3	EPE	D	403	-	-	5/9/19/19	0/1/1/1
4	EDO	C	405	-	-	0/1/1/1	-
4	EDO	B	405	-	-	0/1/1/1	-
4	EDO	A	406	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	EPE	C10-S	3.21	1.82	1.77
3	B	402	EPE	C10-S	3.16	1.82	1.77
3	A	403	EPE	C10-S	3.10	1.81	1.77
3	D	403	EPE	C10-S	2.73	1.81	1.77

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	EPE	C5-N4-C3	4.35	118.22	108.84
3	D	403	EPE	C5-N4-C3	4.30	118.09	108.84
3	A	403	EPE	C5-N4-C3	4.29	118.08	108.84
3	C	403	EPE	C5-N4-C3	4.11	117.69	108.84
3	A	403	EPE	O1S-S-C10	3.09	111.39	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	EPE	C7-N4-C3	2.95	119.10	111.24
3	B	402	EPE	C7-N4-C3	2.92	119.03	111.24
3	A	403	EPE	C7-N4-C3	2.84	118.81	111.24
3	A	403	EPE	C7-N4-C5	2.80	118.71	111.24
3	D	403	EPE	C7-N4-C3	2.74	118.53	111.24
3	C	403	EPE	C7-N4-C5	2.65	118.31	111.24
3	B	402	EPE	C7-N4-C5	2.64	118.28	111.24
3	B	402	EPE	O2S-S-C10	2.64	110.72	106.73
3	B	402	EPE	C6-N1-C2	2.53	114.30	108.84
3	C	403	EPE	O3S-S-C10	2.36	110.63	106.00
3	C	403	EPE	O1S-S-C10	2.29	110.18	106.73
3	D	403	EPE	C7-N4-C5	2.25	117.23	111.24
3	D	403	EPE	O3S-S-C10	2.19	110.30	106.00
3	D	403	EPE	O1S-S-C10	2.15	109.98	106.73
3	B	402	EPE	O1S-S-C10	2.13	109.94	106.73
3	C	403	EPE	C6-N1-C2	2.12	113.42	108.84
3	C	403	EPE	O2S-S-C10	2.12	109.93	106.73
3	A	403	EPE	O3S-S-C10	2.11	110.13	106.00
3	D	403	EPE	O2S-S-O1S	-2.00	107.31	113.82

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	EPE	C10-C9-N1-C2
3	A	403	EPE	C8-C7-N4-C3
3	A	403	EPE	S-C10-C9-N1
3	B	402	EPE	C10-C9-N1-C2
3	B	402	EPE	C8-C7-N4-C3
3	C	403	EPE	C10-C9-N1-C2
3	C	403	EPE	C8-C7-N4-C3
3	D	403	EPE	C10-C9-N1-C6
3	D	403	EPE	C9-C10-S-O1S
3	D	403	EPE	C9-C10-S-O3S
3	D	403	EPE	C8-C7-N4-C5
3	B	402	EPE	C10-C9-N1-C6
3	D	403	EPE	C9-C10-S-O2S
3	C	403	EPE	C10-C9-N1-C6
4	B	406	EDO	O1-C1-C2-O2
3	A	403	EPE	N4-C7-C8-O8

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	EPE	1	0
4	A	407	EDO	1	0
3	D	403	EPE	2	0
4	B	405	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	397/422 (94%)	-0.17	7 (1%) 67 71	9, 15, 33, 58	1 (0%)
1	B	397/422 (94%)	-0.12	9 (2%) 61 65	8, 15, 34, 60	0
1	C	397/422 (94%)	-0.21	6 (1%) 72 75	8, 14, 31, 69	2 (0%)
1	D	397/422 (94%)	-0.19	4 (1%) 79 82	8, 14, 30, 55	2 (0%)
All	All	1588/1688 (94%)	-0.17	26 (1%) 70 74	8, 14, 32, 69	5 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	335	HIS	3.6
1	B	162	GLU	3.0
1	A	336	VAL	2.9
1	B	163	ASN	2.8
1	B	144	GLU	2.8
1	B	336	VAL	2.7
1	B	335	HIS	2.5
1	C	3	LYS	2.5
1	C	163	ASN	2.5
1	A	163	ASN	2.4
1	A	162	GLU	2.4
1	A	3	LYS	2.4
1	D	144	GLU	2.4
1	C	162	GLU	2.4
1	A	168	GLN	2.4
1	B	337	GLU	2.3
1	D	162	GLU	2.3
1	D	3	LYS	2.3
1	B	194	GLU	2.2
1	C	371	ARG	2.2
1	B	161	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	338	TYR	2.1
1	B	372	GLU	2.1
1	A	335	HIS	2.1
1	D	163	ASN	2.1
1	C	194	GLU	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	B	406	4/4	0.73	0.24	42,42,47,52	0
3	EPE	D	403	15/15	0.81	0.19	37,40,51,51	15
3	EPE	A	403	15/15	0.85	0.16	28,37,44,50	15
3	EPE	B	402	15/15	0.86	0.16	34,38,43,46	15
3	EPE	C	403	15/15	0.86	0.15	19,28,36,40	15
4	EDO	C	404	4/4	0.86	0.14	18,20,22,29	0
4	EDO	A	405	4/4	0.87	0.14	25,27,32,35	0
4	EDO	C	407	4/4	0.87	0.14	31,35,36,36	0
4	EDO	D	404	4/4	0.87	0.14	22,26,26,29	0
4	EDO	A	404	4/4	0.88	0.12	19,22,22,26	0
4	EDO	B	403	4/4	0.89	0.12	20,22,25,33	0
4	EDO	B	405	4/4	0.89	0.11	19,20,23,24	0
4	EDO	A	407	4/4	0.89	0.11	16,18,20,27	0
4	EDO	D	405	4/4	0.89	0.10	26,27,29,32	0
4	EDO	C	406	4/4	0.91	0.14	20,26,36,39	0
4	EDO	A	406	4/4	0.91	0.11	21,21,27,35	0
5	CL	A	408[A]	1/1	0.91	0.08	17,17,17,17	1
5	CL	A	408[B]	1/1	0.91	0.08	29,29,29,29	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	404	4/4	0.92	0.11	19,19,21,24	0
5	CL	C	410	1/1	0.92	0.15	49,49,49,49	0
4	EDO	D	406	4/4	0.93	0.10	18,20,21,28	0
2	MG	A	401	1/1	0.94	0.15	8,8,8,8	0
5	CL	C	408[A]	1/1	0.94	0.11	12,12,12,12	1
5	CL	C	408[B]	1/1	0.94	0.11	7,7,7,7	1
4	EDO	C	405	4/4	0.94	0.09	12,18,21,21	0
6	GOL	D	402	6/6	0.94	0.12	18,23,31,31	0
5	CL	C	409[B]	1/1	0.95	0.07	25,25,25,25	1
2	MG	C	401	1/1	0.95	0.05	11,11,11,11	0
6	GOL	C	402	6/6	0.95	0.09	16,19,23,26	0
5	CL	C	409[A]	1/1	0.95	0.07	18,18,18,18	1
2	MG	A	402	1/1	0.96	0.08	13,13,13,13	0
2	MG	D	401	1/1	0.97	0.06	13,13,13,13	0
2	MG	B	401	1/1	0.99	0.03	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.