



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 11:30 am BST

PDB ID : 2HX1
Title : Crystal structure of possible sugar phosphatase, HAD superfamily (ZP_00311070.1) from CYTOPHAGA HUTCHINSONII ATCC 33406 at 2.10 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2006-08-02
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

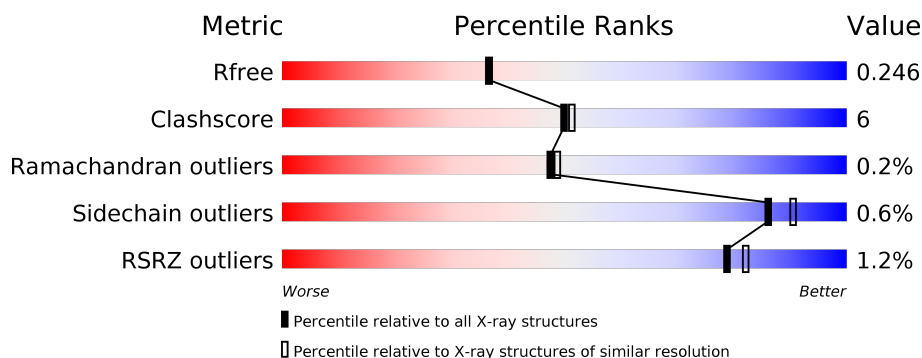
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	284	<div> <div></div> <div>91%</div> <div>8%</div> </div>
1	B	284	<div> <div></div> <div>89%</div> <div>11%</div> </div>
1	C	284	<div> <div></div> <div>83%</div> <div>17%</div> </div>
1	D	284	<div> <div></div> <div>92%</div> <div>8%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	C	306	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10057 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 Predicted sugar phosphatases of the HAD superfamily.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	Se	0	7	0
			2222	1429	359	422	2	10			
1	B	284	Total	C	N	O	S	Se	0	6	0
			2213	1421	355	425	2	10			
1	C	284	Total	C	N	O	S	Se	0	8	0
			2225	1434	352	426	2	11			
1	D	284	Total	C	N	O	S	Se	0	7	0
			2224	1430	357	424	2	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	LEADER SEQUENCE	GB 48856913
A	1	MSE	MET	MODIFIED RESIDUE	GB 48856913
A	84	MSE	MET	MODIFIED RESIDUE	GB 48856913
A	118	MSE	MET	MODIFIED RESIDUE	GB 48856913
A	189	MSE	MET	MODIFIED RESIDUE	GB 48856913
A	208	MSE	MET	MODIFIED RESIDUE	GB 48856913
A	210	MSE	MET	MODIFIED RESIDUE	GB 48856913
A	215	MSE	MET	MODIFIED RESIDUE	GB 48856913
A	220	MSE	MET	MODIFIED RESIDUE	GB 48856913
A	229	MSE	MET	MODIFIED RESIDUE	GB 48856913
B	0	GLY	-	LEADER SEQUENCE	GB 48856913
B	1	MSE	MET	MODIFIED RESIDUE	GB 48856913
B	84	MSE	MET	MODIFIED RESIDUE	GB 48856913
B	118	MSE	MET	MODIFIED RESIDUE	GB 48856913
B	189	MSE	MET	MODIFIED RESIDUE	GB 48856913
B	208	MSE	MET	MODIFIED RESIDUE	GB 48856913
B	210	MSE	MET	MODIFIED RESIDUE	GB 48856913
B	215	MSE	MET	MODIFIED RESIDUE	GB 48856913
B	220	MSE	MET	MODIFIED RESIDUE	GB 48856913
B	229	MSE	MET	MODIFIED RESIDUE	GB 48856913
C	0	GLY	-	LEADER SEQUENCE	GB 48856913

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MSE	MET	MODIFIED RESIDUE	GB 48856913
C	84	MSE	MET	MODIFIED RESIDUE	GB 48856913
C	118	MSE	MET	MODIFIED RESIDUE	GB 48856913
C	189	MSE	MET	MODIFIED RESIDUE	GB 48856913
C	208	MSE	MET	MODIFIED RESIDUE	GB 48856913
C	210	MSE	MET	MODIFIED RESIDUE	GB 48856913
C	215	MSE	MET	MODIFIED RESIDUE	GB 48856913
C	220	MSE	MET	MODIFIED RESIDUE	GB 48856913
C	229	MSE	MET	MODIFIED RESIDUE	GB 48856913
D	0	GLY	-	LEADER SEQUENCE	GB 48856913
D	1	MSE	MET	MODIFIED RESIDUE	GB 48856913
D	84	MSE	MET	MODIFIED RESIDUE	GB 48856913
D	118	MSE	MET	MODIFIED RESIDUE	GB 48856913
D	189	MSE	MET	MODIFIED RESIDUE	GB 48856913
D	208	MSE	MET	MODIFIED RESIDUE	GB 48856913
D	210	MSE	MET	MODIFIED RESIDUE	GB 48856913
D	215	MSE	MET	MODIFIED RESIDUE	GB 48856913
D	220	MSE	MET	MODIFIED RESIDUE	GB 48856913
D	229	MSE	MET	MODIFIED RESIDUE	GB 48856913

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

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

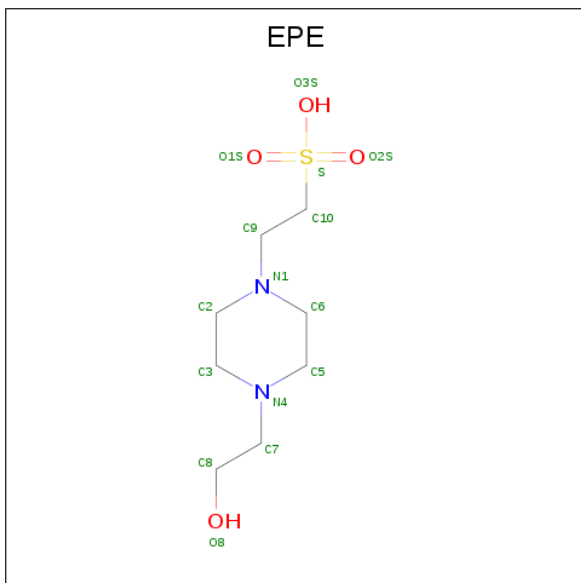
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	5	Total Cl 5 5	0	0
3	A	6	Total Cl 6 6	0	0
3	D	1	Total Cl 1 1	0	0

Continued on next page...

Continued from previous page...

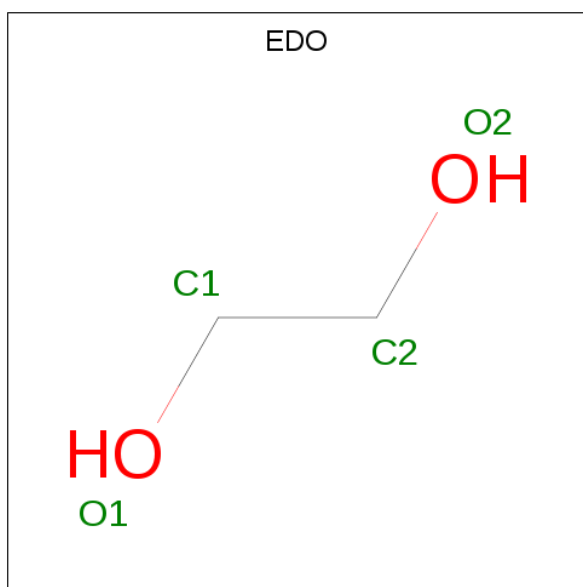
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	3	Total Cl 3 3	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			14	8	2	3	1		
4	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	258	Total	O	0	0
			258	258		
6	B	252	Total	O	0	0
			252	252		
6	C	264	Total	O	0	1
			264	264		
6	D	261	Total	O	0	0
			261	261		

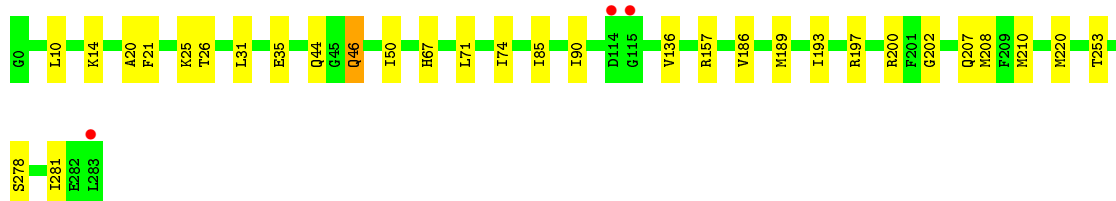
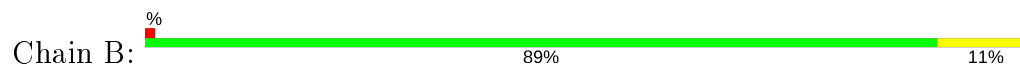
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

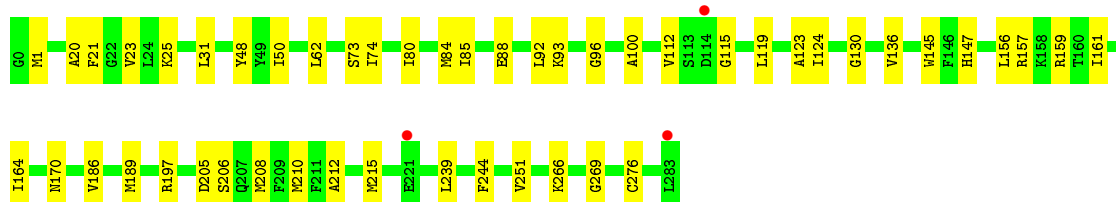
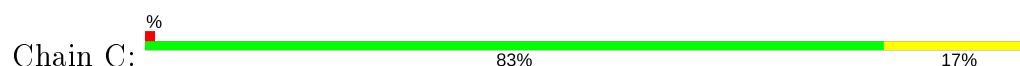
- Molecule 1: Predicted sugar phosphatases of the HAD superfamily



- Molecule 1: Predicted sugar phosphatases of the HAD superfamily



- Molecule 1: Predicted sugar phosphatases of the HAD superfamily



- Molecule 1: Predicted sugar phosphatases of the HAD superfamily



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.62Å 119.46Å 151.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.32 – 2.10 29.33 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.32-2.10) 100.0 (29.33-2.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.179 , 0.234 0.189 , 0.246	Depositor DCC
R_{free} test set	3531 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10057	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.9678e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG, EPE, EDO, CL

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	0.65	0/2273	0.68	0/3059
1	B	0.66	0/2259	0.70	2/3041 (0.1%)
1	C	0.69	0/2277	0.73	1/3064 (0.0%)
1	D	0.72	0/2273	0.71	0/3059
All	All	0.68	0/9082	0.70	3/12223 (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	B	157	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	C	157	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	200	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	2222	0	2254	27	0
1	B	2213	0	2230	23	0
1	C	2225	0	2260	51	0
1	D	2224	0	2256	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6	0	0	1	0
3	B	5	0	0	1	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
4	A	15	0	17	0	0
4	B	14	0	14	0	0
4	C	15	0	18	0	0
4	D	15	0	17	0	0
5	A	12	0	18	1	0
5	B	20	0	30	1	0
5	C	20	0	30	12	0
5	D	8	0	12	2	0
6	A	258	0	0	1	0
6	B	252	0	0	1	0
6	C	264	0	0	5	0
6	D	261	0	0	0	0
All	All	10057	0	9156	106	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 (106) 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:C:84[B]:MSE:HE3	6:C:544:HOH:O	1.68	0.92
1:B:210:MSE:HG2	1:D:210[B]:MSE:HE3	1.57	0.87
1:C:84[B]:MSE:HE2	1:C:85[B]:ILE:HD11	1.59	0.85
1:C:197:ARG:NH2	6:C:331[B]:HOH:O	2.09	0.85
1:C:206[B]:SER:H	5:C:306:EDO:H21	1.41	0.84
1:C:206[A]:SER:H	5:C:306:EDO:H21	1.41	0.84
1:D:210[B]:MSE:HE2	1:D:244:PHE:HE1	1.45	0.79
1:B:26:THR:HG23	1:B:31:LEU:HD11	1.62	0.79
1:C:215:MSE:HG3	6:C:540:HOH:O	1.82	0.79
1:A:210:MSE:HE3	1:C:210[B]:MSE:HG2	1.67	0.75
1:C:84[B]:MSE:HE2	1:C:85[B]:ILE:CD1	2.21	0.71
1:C:21:PHE:CE2	1:C:25:LYS:HE3	2.25	0.71
1:A:210:MSE:HE3	1:C:210[B]:MSE:CG	2.20	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50[B]:ILE:HD11	1:C:74:ILE:HD13	1.75	0.69
1:D:210[B]:MSE:HE2	1:D:244:PHE:CE1	2.27	0.68
1:C:210[B]:MSE:HE2	1:C:244:PHE:CE1	2.30	0.66
1:D:186:VAL:HA	1:D:189:MSE:CE	2.26	0.66
1:B:26:THR:HG23	1:B:31:LEU:CD1	2.25	0.65
1:C:84[B]:MSE:HG2	1:C:85[B]:ILE:HD13	1.77	0.65
1:C:210[B]:MSE:HE2	1:C:244:PHE:HE1	1.63	0.63
1:B:186:VAL:HA	1:B:189:MSE:HE2	1.82	0.62
1:B:14:LYS:HD3	1:B:220:MSE:HE2	1.80	0.62
1:C:186:VAL:HA	1:C:189:MSE:HE2	1.82	0.61
1:A:10:LEU:HD11	1:A:281:ILE:HD11	1.81	0.61
1:D:186:VAL:HA	1:D:189:MSE:HE3	1.82	0.60
1:D:206:SER:O	1:D:210[A]:MSE:HG3	2.01	0.59
1:A:80[A]:ILE:CD1	1:A:212:ALA:HB2	2.32	0.58
1:B:21:PHE:CE2	1:B:25:LYS:HE3	2.39	0.58
1:B:50:ILE:HD11	1:B:74:ILE:HD13	1.88	0.56
1:D:21:PHE:CE2	1:D:25:LYS:HE3	2.41	0.55
1:C:119:LEU:HG	1:C:123:ALA:HB3	1.89	0.54
1:C:100:ALA:HA	1:C:119:LEU:O	2.08	0.53
1:A:80[A]:ILE:HD13	1:A:212:ALA:HB2	1.90	0.53
1:C:206[A]:SER:H	5:C:306:EDO:C2	2.18	0.52
1:C:206[B]:SER:H	5:C:306:EDO:C2	2.18	0.52
1:C:119:LEU:HD23	1:C:124:ILE:HD13	1.92	0.51
1:C:119:LEU:HD23	1:C:124:ILE:CD1	2.40	0.51
1:A:26:THR:HG23	1:A:31:LEU:CD1	2.41	0.50
1:C:156:LEU:HD22	1:C:197:ARG:NH2	2.27	0.50
1:A:186:VAL:HA	1:A:189:MSE:HE2	1.94	0.50
1:A:99:VAL:HG23	1:A:116:ILE:HG21	1.93	0.50
1:A:26:THR:HG23	1:A:31:LEU:HD11	1.93	0.50
1:A:46:GLN:NE2	6:A:458:HOH:O	2.46	0.49
1:B:20:ALA:HB3	3:B:302:CL:CL	2.49	0.49
1:C:159:ARG:HG3	1:C:161:ILE:HG23	1.95	0.48
1:B:90:ILE:HD11	1:B:136:VAL:HG11	1.95	0.48
1:C:145:TRP:HB2	5:D:303:EDO:H21	1.95	0.48
1:C:20:ALA:HB3	5:C:305:EDO:H12	1.96	0.48
1:D:216:LEU:HB3	1:D:222:ILE:HG21	1.96	0.48
1:B:253:THR:HG21	1:B:278:SER:HB2	1.96	0.47
1:D:23:VAL:O	1:D:31[B]:LEU:HD12	2.14	0.47
1:A:207:GLN:HA	1:C:210[A]:MSE:HE1	1.95	0.47
1:B:202:GLY:HA2	1:B:208:MSE:HE2	1.96	0.47
1:A:202:GLY:HA2	1:A:208:MSE:HE2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:GLN:NE2	6:B:486:HOH:O	2.38	0.47
1:C:208:MSE:HB2	6:C:451:HOH:O	2.13	0.47
1:D:3[B]:ILE:HD11	1:D:258:ILE:HD11	1.96	0.47
1:A:210:MSE:CE	1:C:210[B]:MSE:HG2	2.41	0.47
1:C:50[B]:ILE:HD11	1:C:74:ILE:CD1	2.45	0.47
1:C:23:VAL:O	1:C:31:LEU:HD12	2.15	0.47
1:C:84[A]:MSE:HG2	6:C:433:HOH:O	2.16	0.46
1:B:35:GLU:HA	1:B:71:LEU:HD11	1.98	0.46
1:C:96:GLY:HA2	1:C:115:GLY:O	2.16	0.46
1:C:170:ASN:HB3	1:D:193:ILE:HD12	1.97	0.46
1:B:10:LEU:HD11	1:B:281:ILE:HD11	1.98	0.45
1:C:156:LEU:HD22	1:C:197:ARG:CZ	2.46	0.45
1:C:80:ILE:CD1	1:C:212:ALA:HB2	2.47	0.45
5:A:308:EDO:H12	1:C:239:LEU:HD22	1.99	0.45
1:B:10:LEU:O	1:B:46[A]:GLN:NE2	2.50	0.44
1:B:207:GLN:HA	1:D:210[A]:MSE:HE1	2.00	0.44
1:C:251:VAL:HA	1:C:276:CYS:O	2.18	0.44
1:A:10:LEU:N	1:A:11:PRO:CD	2.81	0.44
1:D:225:ARG:CZ	1:D:225:ARG:HA	2.48	0.44
1:A:210:MSE:HG2	1:C:210[B]:MSE:HE3	2.01	0.43
1:D:146:PHE:H	5:D:303:EDO:H22	1.83	0.43
1:A:160:THR:HG23	1:C:266:LYS:HA	2.01	0.43
1:A:210:MSE:HG2	1:C:210[B]:MSE:HG2	1.99	0.43
1:B:25:LYS:NZ	5:B:307:EDO:H12	2.33	0.43
1:C:147:HIS:HA	5:C:307:EDO:C1	2.48	0.43
1:C:88[A]:GLU:HG3	1:C:92:LEU:HD12	2.01	0.43
1:A:242:ASN:HA	1:C:93:LYS:HE2	2.00	0.43
1:A:189:MSE:SE	1:B:193[A]:ILE:HD11	2.69	0.43
1:B:210:MSE:HG2	1:D:210[B]:MSE:CE	2.37	0.42
1:A:227:ILE:HB	1:A:246:LEU:HD22	2.00	0.42
1:A:48:TYR:CD1	1:A:48:TYR:C	2.93	0.42
1:A:26:THR:HA	3:A:305:CL:CL	2.56	0.42
1:C:130:GLY:HA2	5:C:309:EDO:C2	2.49	0.42
1:D:10:LEU:N	1:D:11:PRO:CD	2.83	0.42
1:A:253:THR:HG21	1:A:278:SER:HB2	2.02	0.41
1:A:206:SER:H	5:C:306:EDO:H22	1.85	0.41
1:B:210:MSE:CG	1:D:210[B]:MSE:HE3	2.40	0.41
1:D:186:VAL:HA	1:D:189:MSE:HE2	2.00	0.41
1:B:67:HIS:NE2	1:B:74:ILE:O	2.50	0.41
1:D:31[A]:LEU:HD21	1:D:253:THR:HG21	2.02	0.41
1:B:85:ILE:HD11	1:B:208:MSE:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136[B]:VAL:HG12	1:C:164:ILE:HB	2.01	0.41
1:A:210:MSE:HE3	1:C:210[B]:MSE:HG3	2.00	0.41
1:C:48:TYR:OH	1:C:74:ILE:HA	2.21	0.41
1:C:62:LEU:HD22	5:C:305:EDO:H21	2.03	0.41
1:C:205:ASP:HB3	5:C:306:EDO:O1	2.20	0.41
1:B:21:PHE:CZ	1:B:25:LYS:HE3	2.56	0.40
1:A:10:LEU:CD1	1:A:281:ILE:HD11	2.48	0.40
1:C:147:HIS:HA	5:C:307:EDO:H11	2.01	0.40
1:A:197:ARG:NH1	1:C:269:GLY:HA3	2.36	0.40
1:D:16:ILE:O	1:D:48:TYR:HA	2.21	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	289/284 (102%)	285 (99%)	3 (1%)	1 (0%)	41	41
1	B	288/284 (101%)	283 (98%)	4 (1%)	1 (0%)	41	41
1	C	290/284 (102%)	285 (98%)	5 (2%)	0	100	100
1	D	289/284 (102%)	284 (98%)	5 (2%)	0	100	100
All	All	1156/1136 (102%)	1137 (98%)	17 (2%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	ARG
1	B	197	ARG

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	244/233 (105%)	244 (100%)	0	100	100
1	B	241/233 (103%)	239 (99%)	2 (1%)	81	86
1	C	243/233 (104%)	240 (99%)	3 (1%)	71	77
1	D	242/233 (104%)	240 (99%)	2 (1%)	81	86
All	All	970/932 (104%)	963 (99%)	7 (1%)	86	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	46[A]	GLN
1	B	46[B]	GLN
1	C	1	MSE
1	C	73	SER
1	C	112	VAL
1	D	73	SER
1	D	113	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 38 ligands modelled in this entry, 19 are monoatomic - leaving 19 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
5	EDO	A	308	-	3,3,3	0.46	0	2,2,2	0.32	0
5	EDO	A	310	-	3,3,3	0.66	0	2,2,2	0.27	0
5	EDO	D	304	-	3,3,3	0.51	0	2,2,2	0.33	0
5	EDO	B	309	-	3,3,3	0.42	0	2,2,2	0.51	0
4	EPE	C	304	-	15,15,15	1.05	1 (6%)	18,20,20	1.56	1 (5%)
5	EDO	C	309	-	3,3,3	0.56	0	2,2,2	0.18	0
5	EDO	B	310	-	3,3,3	0.62	0	2,2,2	0.11	0
5	EDO	B	308	-	3,3,3	0.51	0	2,2,2	0.60	0
5	EDO	D	303	-	3,3,3	0.43	0	2,2,2	0.40	0
5	EDO	A	309	-	3,3,3	0.49	0	2,2,2	0.23	0
5	EDO	B	307	-	3,3,3	0.62	0	2,2,2	0.14	0
5	EDO	B	311	-	3,3,3	0.47	0	2,2,2	0.27	0
4	EPE	D	302	-	15,15,15	0.91	1 (6%)	18,20,20	1.78	3 (16%)
5	EDO	C	307	-	3,3,3	0.77	0	2,2,2	0.56	0
4	EPE	A	307	-	15,15,15	0.90	1 (6%)	18,20,20	1.61	3 (16%)
5	EDO	C	306	-	3,3,3	0.61	0	2,2,2	0.44	0
4	EPE	B	306	-	14,14,15	1.09	1 (7%)	17,19,20	1.92	6 (35%)
5	EDO	C	308	-	3,3,3	0.64	0	2,2,2	0.24	0
5	EDO	C	305	-	3,3,3	0.41	0	2,2,2	0.14	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
5	EDO	A	308	-	-	1/1/1/1	-
5	EDO	A	310	-	-	1/1/1/1	-
5	EDO	D	304	-	-	1/1/1/1	-
5	EDO	B	309	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EPE	C	304	-	-	5/9/19/19	0/1/1/1
5	EDO	C	309	-	-	1/1/1/1	-
5	EDO	B	310	-	-	1/1/1/1	-
5	EDO	B	308	-	-	0/1/1/1	-
5	EDO	D	303	-	-	1/1/1/1	-
5	EDO	A	309	-	-	1/1/1/1	-
5	EDO	B	307	-	-	0/1/1/1	-
5	EDO	B	311	-	-	1/1/1/1	-
4	EPE	D	302	-	-	3/9/19/19	0/1/1/1
5	EDO	C	307	-	-	1/1/1/1	-
4	EPE	A	307	-	-	7/9/19/19	0/1/1/1
5	EDO	C	306	-	-	1/1/1/1	-
4	EPE	B	306	-	-	7/8/18/19	0/1/1/1
5	EDO	C	308	-	-	1/1/1/1	-
5	EDO	C	305	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	304	EPE	C10-S	3.67	1.82	1.77
4	B	306	EPE	C10-S	3.62	1.82	1.77
4	A	307	EPE	C10-S	3.03	1.81	1.77
4	D	302	EPE	C10-S	2.88	1.81	1.77

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	302	EPE	C6-C5-N4	5.16	121.24	110.64
4	C	304	EPE	O3S-S-C10	4.99	113.84	105.77
4	A	307	EPE	O3S-S-C10	4.41	112.90	105.77
4	B	306	EPE	O3S-S-C10	4.11	112.42	105.77
4	B	306	EPE	C6-N1-C2	3.26	116.17	108.83
4	B	306	EPE	C2-C3-N4	2.81	116.40	110.64
4	B	306	EPE	C3-C2-N1	2.63	116.03	110.64
4	A	307	EPE	C6-C5-N4	2.49	115.74	110.64
4	B	306	EPE	C6-C5-N4	2.44	115.65	110.64
4	D	302	EPE	C6-N1-C2	2.43	114.30	108.83
4	D	302	EPE	C5-N4-C3	2.22	113.83	108.83
4	A	307	EPE	C6-N1-C2	2.22	113.82	108.83
4	B	306	EPE	O2S-S-C10	2.07	109.41	106.92

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	304	EPE	S-C10-C9-N1
4	C	304	EPE	C9-C10-S-O2S
4	C	304	EPE	C9-C10-S-O3S
4	B	306	EPE	C10-C9-N1-C6
4	B	306	EPE	S-C10-C9-N1
4	B	306	EPE	C9-C10-S-O2S
4	A	307	EPE	C10-C9-N1-C2
4	A	307	EPE	N4-C7-C8-O8
4	A	307	EPE	S-C10-C9-N1
4	A	307	EPE	C9-C10-S-O2S
4	A	307	EPE	C9-C10-S-O3S
4	C	304	EPE	N4-C7-C8-O8
4	B	306	EPE	C9-C10-S-O3S
5	B	311	EDO	O1-C1-C2-O2
5	C	307	EDO	O1-C1-C2-O2
5	B	310	EDO	O1-C1-C2-O2
4	D	302	EPE	C8-C7-N4-C3
5	A	308	EDO	O1-C1-C2-O2
4	B	306	EPE	C10-C9-N1-C2
4	A	307	EPE	C10-C9-N1-C6
5	C	309	EDO	O1-C1-C2-O2
4	D	302	EPE	C8-C7-N4-C5
5	B	309	EDO	O1-C1-C2-O2
5	A	309	EDO	O1-C1-C2-O2
5	D	303	EDO	O1-C1-C2-O2
4	C	304	EPE	C9-C10-S-O1S
4	B	306	EPE	C9-C10-S-O1S
4	A	307	EPE	C9-C10-S-O1S
4	D	302	EPE	N4-C7-C8-O8
4	B	306	EPE	C8-C7-N4-C5
5	A	310	EDO	O1-C1-C2-O2
5	C	306	EDO	O1-C1-C2-O2
5	C	308	EDO	O1-C1-C2-O2
5	D	304	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	308	EDO	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	309	EDO	1	0
5	D	303	EDO	2	0
5	B	307	EDO	1	0
5	C	307	EDO	2	0
5	C	306	EDO	7	0
5	C	305	EDO	2	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	275/284 (96%)	-0.33	3 (1%) 80 84	18, 27, 43, 61	0
1	B	275/284 (96%)	-0.26	3 (1%) 80 84	19, 27, 42, 67	0
1	C	275/284 (96%)	-0.40	3 (1%) 80 84	18, 27, 41, 58	0
1	D	275/284 (96%)	-0.28	4 (1%) 73 77	18, 28, 44, 58	0
All	All	1100/1136 (96%)	-0.32	13 (1%) 79 82	18, 27, 43, 67	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114[A]	ASP	4.2
1	D	221	GLU	3.4
1	D	114	ASP	3.3
1	A	115	GLY	3.1
1	C	221	GLU	2.9
1	B	283	LEU	2.8
1	D	113	SER	2.7
1	C	114	ASP	2.5
1	A	113	SER	2.4
1	B	115	GLY	2.4
1	B	114	ASP	2.3
1	C	283	LEU	2.3
1	D	176	LYS	2.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
5	EDO	C	307	4/4	0.69	0.28	39,49,56,56	0
5	EDO	C	309	4/4	0.79	0.22	53,53,55,55	0
3	CL	A	306	1/1	0.80	0.14	68,68,68,68	0
4	EPE	B	306	14/15	0.81	0.23	78,83,85,86	0
5	EDO	B	309	4/4	0.84	0.25	44,51,54,60	0
5	EDO	B	310	4/4	0.84	0.19	48,50,52,52	0
5	EDO	C	308	4/4	0.84	0.14	35,46,47,48	0
5	EDO	A	309	4/4	0.85	0.16	55,56,60,61	0
5	EDO	C	306	4/4	0.89	0.23	25,30,40,44	0
5	EDO	B	311	4/4	0.90	0.18	51,54,54,54	0
5	EDO	A	310	4/4	0.92	0.14	30,36,42,45	0
3	CL	C	303	1/1	0.92	0.08	51,51,51,51	0
5	EDO	D	304	4/4	0.92	0.14	46,49,51,51	0
4	EPE	A	307	15/15	0.93	0.14	56,71,77,78	0
5	EDO	B	307	4/4	0.93	0.14	31,42,45,48	0
3	CL	B	305	1/1	0.93	0.33	71,71,71,71	0
5	EDO	D	303	4/4	0.93	0.10	28,34,38,40	0
5	EDO	A	308	4/4	0.93	0.13	41,43,45,52	0
4	EPE	D	302	15/15	0.93	0.15	33,56,63,66	0
3	CL	A	305	1/1	0.94	0.10	69,69,69,69	0
5	EDO	B	308	4/4	0.94	0.11	28,31,39,39	0
4	EPE	C	304	15/15	0.96	0.12	27,59,67,70	0
2	MG	D	300	1/1	0.97	0.04	18,18,18,18	0
2	MG	B	300	1/1	0.97	0.05	22,22,22,22	0
2	MG	C	300	1/1	0.98	0.06	24,24,24,24	0
5	EDO	C	305	4/4	0.98	0.09	26,34,36,40	0
3	CL	A	302	1/1	0.99	0.08	32,32,32,32	0
3	CL	C	301	1/1	0.99	0.06	34,34,34,34	0
3	CL	B	301	1/1	0.99	0.06	24,24,24,24	0
3	CL	A	304	1/1	0.99	0.05	30,30,30,30	0
3	CL	C	302	1/1	0.99	0.05	35,35,35,35	0
2	MG	A	300	1/1	0.99	0.03	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	A	301	1/1	0.99	0.07	27,27,27,27	0
3	CL	B	302	1/1	0.99	0.04	40,40,40,40	0
3	CL	A	303	1/1	0.99	0.04	27,27,27,27	0
3	CL	B	304	1/1	1.00	0.03	30,30,30,30	0
3	CL	D	301	1/1	1.00	0.06	33,33,33,33	0
3	CL	B	303	1/1	1.00	0.05	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.