



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:53 PM UTC

PDB ID : 6AL8 / pdb_00006al8
Title : Crystal structure HpiC1 Y101F/F138S
Authors : Newmister, S.A.; Li, S.; Garcia-Borrás, M.; Sanders, J.N.; Yang, S.; Lowell, A.N.; Yu, F.; Smith, J.L.; Williams, R.M.; Houk, K.N.; Sherman, D.H.
Deposited on : 2017-08-07
Resolution : 1.64 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

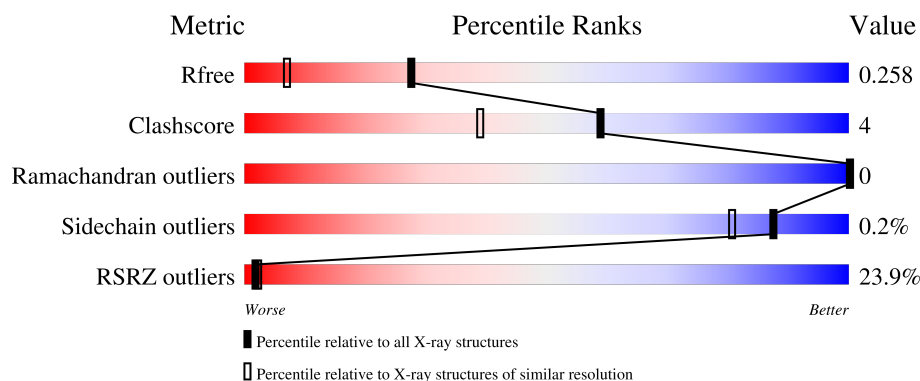
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	225	
1	B	225	
1	D	225	
1	E	225	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6440 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 12-epi-hapalindole C/U synthase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	0	1	0
			1525	975	246	304			
1	B	200	Total	C	N	O	0	0	0
			1536	981	248	307			
1	D	197	Total	C	N	O	0	0	0
			1498	959	241	298			
1	E	175	Total	C	N	O	0	0	0
			1347	862	223	262			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	initiating methionine	UNP A0A076NBW8
A	4	GLY	-	expression tag	UNP A0A076NBW8
A	5	SER	-	expression tag	UNP A0A076NBW8
A	6	SER	-	expression tag	UNP A0A076NBW8
A	7	HIS	-	expression tag	UNP A0A076NBW8
A	8	HIS	-	expression tag	UNP A0A076NBW8
A	9	HIS	-	expression tag	UNP A0A076NBW8
A	10	HIS	-	expression tag	UNP A0A076NBW8
A	11	HIS	-	expression tag	UNP A0A076NBW8
A	12	HIS	-	expression tag	UNP A0A076NBW8
A	13	SER	-	expression tag	UNP A0A076NBW8
A	14	SER	-	expression tag	UNP A0A076NBW8
A	15	GLY	-	expression tag	UNP A0A076NBW8
A	16	LEU	-	expression tag	UNP A0A076NBW8
A	17	VAL	-	expression tag	UNP A0A076NBW8
A	18	PRO	-	expression tag	UNP A0A076NBW8
A	19	ARG	-	expression tag	UNP A0A076NBW8
A	20	GLY	-	expression tag	UNP A0A076NBW8
A	21	SER	-	expression tag	UNP A0A076NBW8
A	22	HIS	-	expression tag	UNP A0A076NBW8
A	23	MET	-	expression tag	UNP A0A076NBW8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ALA	-	expression tag	UNP A0A076NBW8
A	25	SER	-	expression tag	UNP A0A076NBW8
A	101	PHE	TYR	engineered mutation	UNP A0A076NBW8
A	138	SER	PHE	engineered mutation	UNP A0A076NBW8
B	3	MET	-	initiating methionine	UNP A0A076NBW8
B	4	GLY	-	expression tag	UNP A0A076NBW8
B	5	SER	-	expression tag	UNP A0A076NBW8
B	6	SER	-	expression tag	UNP A0A076NBW8
B	7	HIS	-	expression tag	UNP A0A076NBW8
B	8	HIS	-	expression tag	UNP A0A076NBW8
B	9	HIS	-	expression tag	UNP A0A076NBW8
B	10	HIS	-	expression tag	UNP A0A076NBW8
B	11	HIS	-	expression tag	UNP A0A076NBW8
B	12	HIS	-	expression tag	UNP A0A076NBW8
B	13	SER	-	expression tag	UNP A0A076NBW8
B	14	SER	-	expression tag	UNP A0A076NBW8
B	15	GLY	-	expression tag	UNP A0A076NBW8
B	16	LEU	-	expression tag	UNP A0A076NBW8
B	17	VAL	-	expression tag	UNP A0A076NBW8
B	18	PRO	-	expression tag	UNP A0A076NBW8
B	19	ARG	-	expression tag	UNP A0A076NBW8
B	20	GLY	-	expression tag	UNP A0A076NBW8
B	21	SER	-	expression tag	UNP A0A076NBW8
B	22	HIS	-	expression tag	UNP A0A076NBW8
B	23	MET	-	expression tag	UNP A0A076NBW8
B	24	ALA	-	expression tag	UNP A0A076NBW8
B	25	SER	-	expression tag	UNP A0A076NBW8
B	101	PHE	TYR	engineered mutation	UNP A0A076NBW8
B	138	SER	PHE	engineered mutation	UNP A0A076NBW8
D	3	MET	-	initiating methionine	UNP A0A076NBW8
D	4	GLY	-	expression tag	UNP A0A076NBW8
D	5	SER	-	expression tag	UNP A0A076NBW8
D	6	SER	-	expression tag	UNP A0A076NBW8
D	7	HIS	-	expression tag	UNP A0A076NBW8
D	8	HIS	-	expression tag	UNP A0A076NBW8
D	9	HIS	-	expression tag	UNP A0A076NBW8
D	10	HIS	-	expression tag	UNP A0A076NBW8
D	11	HIS	-	expression tag	UNP A0A076NBW8
D	12	HIS	-	expression tag	UNP A0A076NBW8
D	13	SER	-	expression tag	UNP A0A076NBW8
D	14	SER	-	expression tag	UNP A0A076NBW8
D	15	GLY	-	expression tag	UNP A0A076NBW8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	16	LEU	-	expression tag	UNP A0A076NBW8
D	17	VAL	-	expression tag	UNP A0A076NBW8
D	18	PRO	-	expression tag	UNP A0A076NBW8
D	19	ARG	-	expression tag	UNP A0A076NBW8
D	20	GLY	-	expression tag	UNP A0A076NBW8
D	21	SER	-	expression tag	UNP A0A076NBW8
D	22	HIS	-	expression tag	UNP A0A076NBW8
D	23	MET	-	expression tag	UNP A0A076NBW8
D	24	ALA	-	expression tag	UNP A0A076NBW8
D	25	SER	-	expression tag	UNP A0A076NBW8
D	101	PHE	TYR	engineered mutation	UNP A0A076NBW8
D	138	SER	PHE	engineered mutation	UNP A0A076NBW8
E	3	MET	-	initiating methionine	UNP A0A076NBW8
E	4	GLY	-	expression tag	UNP A0A076NBW8
E	5	SER	-	expression tag	UNP A0A076NBW8
E	6	SER	-	expression tag	UNP A0A076NBW8
E	7	HIS	-	expression tag	UNP A0A076NBW8
E	8	HIS	-	expression tag	UNP A0A076NBW8
E	9	HIS	-	expression tag	UNP A0A076NBW8
E	10	HIS	-	expression tag	UNP A0A076NBW8
E	11	HIS	-	expression tag	UNP A0A076NBW8
E	12	HIS	-	expression tag	UNP A0A076NBW8
E	13	SER	-	expression tag	UNP A0A076NBW8
E	14	SER	-	expression tag	UNP A0A076NBW8
E	15	GLY	-	expression tag	UNP A0A076NBW8
E	16	LEU	-	expression tag	UNP A0A076NBW8
E	17	VAL	-	expression tag	UNP A0A076NBW8
E	18	PRO	-	expression tag	UNP A0A076NBW8
E	19	ARG	-	expression tag	UNP A0A076NBW8
E	20	GLY	-	expression tag	UNP A0A076NBW8
E	21	SER	-	expression tag	UNP A0A076NBW8
E	22	HIS	-	expression tag	UNP A0A076NBW8
E	23	MET	-	expression tag	UNP A0A076NBW8
E	24	ALA	-	expression tag	UNP A0A076NBW8
E	25	SER	-	expression tag	UNP A0A076NBW8
E	101	PHE	TYR	engineered mutation	UNP A0A076NBW8
E	138	SER	PHE	engineered mutation	UNP A0A076NBW8

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

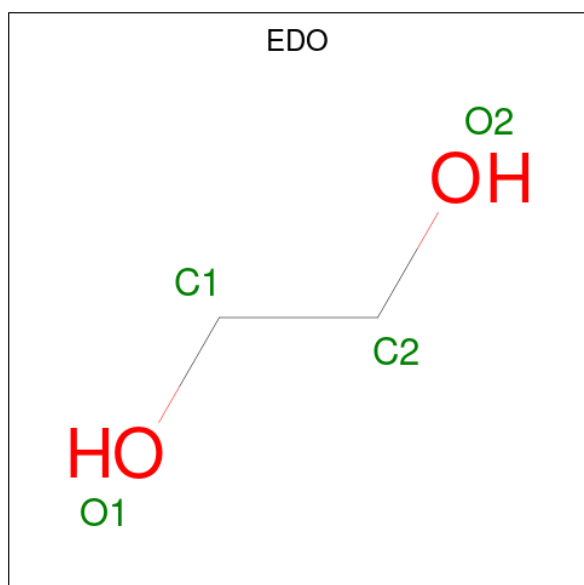
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total 3 Ca 3	0	0
2	B	2	Total 2 Ca 2	0	0
2	D	2	Total 2 Ca 2	0	0
2	E	2	Total 2 Ca 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



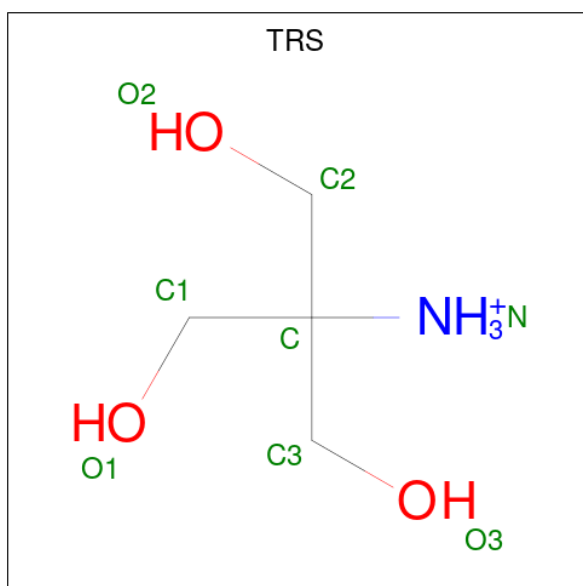
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total 4 C 2 O 2	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	N	O	0	0
			8	4	1	3		

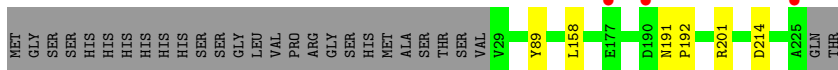
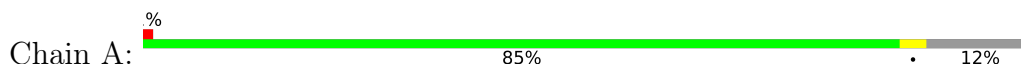
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	228	Total 228	O 228	0	0
6	B	202	Total 202	O 202	0	0
6	D	30	Total 30	O 30	0	0
6	E	49	Total 49	O 49	0	0

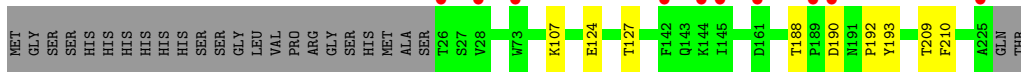
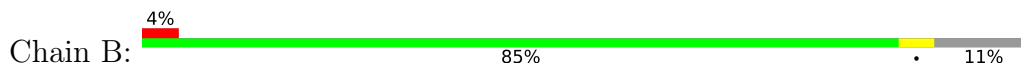
3 Residue-property plots

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.

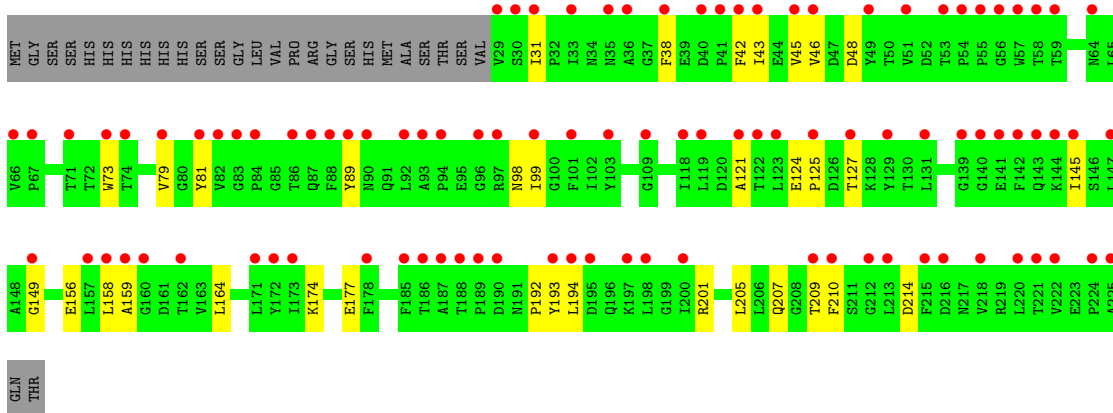
- Molecule 1: 12-epi-hapalindole C/U synthase



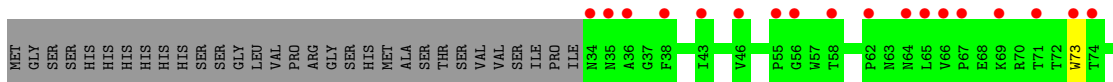
- Molecule 1: 12-epi-hapalindole C/U synthase

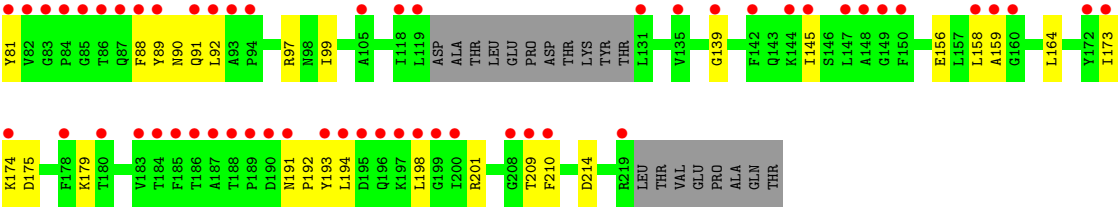


- Molecule 1: 12-epi-hapalindole C/U synthase



- Molecule 1: 12-epi-hapalindole C/U synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.99Å 47.95Å 174.76Å 90.00° 97.05° 90.00°	Depositor
Resolution (Å)	47.50 – 1.64 47.50 – 1.64	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.50-1.64) 97.9 (47.50-1.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.64Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.223 , 0.254 0.229 , 0.258	Depositor DCC
R_{free} test set	6110 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6440	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, EDO, CA, TRS

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	0.35	0/1566	0.57	0/2142
1	B	0.32	0/1574	0.55	0/2155
1	D	0.17	0/1536	0.41	0/2106
1	E	0.23	0/1380	0.46	0/1882
All	All	0.28	0/6056	0.51	0/8285

There are no bond length outliers.

There are no bond angle outliers.

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	1525	0	1468	3	0
1	B	1536	0	1474	6	0
1	D	1498	0	1423	23	0
1	E	1347	0	1289	19	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
3	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	4	0	6	0	0
5	E	8	0	12	0	0
6	A	228	0	0	0	0
6	B	202	0	0	1	0
6	D	30	0	0	0	0
6	E	49	0	0	2	0
All	All	6440	0	5678	51	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 4.

All (51) 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:D:31:ILE:HD11	1:D:121:ALA:HB3	1.43	1.00
1:D:45:VAL:HG13	1:D:48:ASP:HB2	1.64	0.77
1:D:158:LEU:HD11	1:D:201:ARG:HG3	1.67	0.77
1:E:158:LEU:HD11	1:E:201:ARG:HG3	1.82	0.62
1:A:89:TYR:OH	1:A:214:ASP:OD2	2.13	0.60
1:E:210:PHE:HB3	6:E:401:HOH:O	2.03	0.59
1:E:156:GLU:HB2	1:E:201:ARG:HB2	1.84	0.58
1:D:31:ILE:CD1	1:D:121:ALA:HB3	2.28	0.58
1:D:205:LEU:HB3	1:D:207:GLN:HG3	1.86	0.58
1:E:159:ALA:HB2	1:E:164:LEU:HD11	1.86	0.56
1:D:159:ALA:HB2	1:D:164:LEU:HD11	1.86	0.56
1:B:188:THR:OG1	1:B:190:ASP:OD1	2.21	0.56
1:E:174:LYS:HD3	1:E:175:ASP:H	1.71	0.56
1:D:99:ILE:HD13	1:D:214:ASP:HB3	1.87	0.55
1:D:73:TRP:CZ2	1:D:145:ILE:HD13	2.43	0.53
1:E:73:TRP:CZ2	1:E:145:ILE:HD12	2.46	0.51
1:E:90:ASN:ND2	6:E:405:HOH:O	2.43	0.50
1:D:42:PHE:HD1	1:D:43:ILE:N	2.08	0.50
1:E:173:ILE:HG12	1:E:179:LYS:HB2	1.92	0.50
1:E:191:ASN:HB3	1:E:194:LEU:CD2	2.42	0.50
1:A:158:LEU:HD11	1:A:201:ARG:HG3	1.93	0.49
1:D:73:TRP:HZ2	1:D:145:ILE:HD13	1.77	0.49
1:D:46:VAL:HA	1:D:81:TYR:CD2	2.48	0.48
1:E:91:GLN:HG2	1:E:92:LEU:N	2.29	0.47
1:E:209:THR:HA	1:E:210:PHE:C	2.40	0.47
1:B:190:ASP:OD1	6:B:401:HOH:O	2.20	0.47
1:D:38:PHE:HB3	1:D:79:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:ASN:HB3	1:E:194:LEU:HD22	1.97	0.46
1:E:99:ILE:HD13	1:E:214:ASP:HB3	1.98	0.46
1:E:81:TYR:CD1	1:E:97:ARG:HB3	2.51	0.45
1:D:156:GLU:HB2	1:D:201:ARG:HB2	1.98	0.45
1:D:156:GLU:OE1	1:D:201:ARG:NH1	2.47	0.44
1:E:192:PRO:HG2	1:E:193:TYR:CE2	2.52	0.44
1:D:124:GLU:O	1:D:127:THR:HG22	2.17	0.44
1:B:209:THR:HA	1:B:210:PHE:C	2.43	0.44
1:D:89:TYR:OH	1:D:214:ASP:OD2	2.29	0.44
1:D:192:PRO:HG2	1:D:193:TYR:CE2	2.53	0.44
1:D:125:PRO:HB3	1:D:194:LEU:HD11	2.01	0.43
1:D:209:THR:HA	1:D:210:PHE:C	2.44	0.43
1:E:156:GLU:OE1	1:E:201:ARG:HD2	2.18	0.43
1:D:174:LYS:O	1:D:177:GLU:HG2	2.19	0.42
1:B:107:LYS:HE2	1:B:107:LYS:HB2	1.80	0.42
1:E:88:PHE:HA	1:E:139:GLY:O	2.19	0.42
1:D:43:ILE:HG21	1:D:48:ASP:HB3	2.02	0.41
1:D:79:VAL:HG13	1:D:98:ASN:HB3	2.02	0.41
1:B:124:GLU:O	1:B:127:THR:OG1	2.31	0.41
1:D:149:GLY:HA3	1:D:209:THR:O	2.21	0.41
1:E:73:TRP:CH2	1:E:145:ILE:HD12	2.56	0.41
1:E:89:TYR:OH	1:E:214:ASP:OD2	2.34	0.40
1:B:192:PRO:HG2	1:B:193:TYR:CE2	2.56	0.40
1:A:191:ASN:HA	1:A:192:PRO:HD3	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	196/225 (87%)	195 (100%)	1 (0%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	198/225 (88%)	196 (99%)	2 (1%)	0	100	100
1	D	195/225 (87%)	190 (97%)	5 (3%)	0	100	100
1	E	171/225 (76%)	167 (98%)	4 (2%)	0	100	100
All	All	760/900 (84%)	748 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	166/189 (88%)	166 (100%)	0	100	100
1	B	167/189 (88%)	167 (100%)	0	100	100
1	D	160/189 (85%)	160 (100%)	0	100	100
1	E	143/189 (76%)	142 (99%)	1 (1%)	76	62
All	All	636/756 (84%)	635 (100%)	1 (0%)	87	81

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	198	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	170	ASN
1	E	91	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\# Z > 2$
3	EDO	A	304	-	3,3,3	0.31	0	2,2,2	0.13	0
5	TRS	E	304	-	7,7,7	0.22	0	9,9,9	0.44	0
4	DMS	E	303	-	3,3,3	0.60	0	3,3,3	0.29	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
3	EDO	A	304	-	-	1/1/1/1	-
5	TRS	E	304	-	-	2/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	304	TRS	N-C-C1-O1
3	A	304	EDO	O1-C1-C2-O2
5	E	304	TRS	C3-C-C1-O1

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	197/225 (87%)	0.26	3 (1%) 72 77	21, 29, 38, 48	1 (0%)
1	B	200/225 (88%)	0.50	10 (5%) 34 39	22, 31, 42, 49	0
1	D	197/225 (87%)	2.18	98 (49%) 0 0	34, 55, 71, 87	0
1	E	175/225 (77%)	1.87	73 (41%) 0 1	31, 46, 62, 78	0
All	All	769/900 (85%)	1.18	184 (23%) 2 2	21, 39, 65, 87	1 (0%)

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	29	VAL	6.9
1	D	145	ILE	5.3
1	D	142	PHE	5.3
1	E	195	ASP	5.2
1	E	187	ALA	5.0
1	D	225	ALA	4.9
1	E	119	LEU	4.9
1	D	88	PHE	4.9
1	E	194	LEU	4.8
1	D	43	ILE	4.8
1	E	145	ILE	4.8
1	D	224	PRO	4.5
1	E	92	LEU	4.5
1	D	121	ALA	4.5
1	D	194	LEU	4.4
1	D	51	VAL	4.4
1	D	82	VAL	4.3
1	D	89	TYR	4.3
1	D	46	VAL	4.3
1	E	86	THR	4.1
1	D	125	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	81	TYR	4.0
1	D	42	PHE	4.0
1	D	96	GLY	3.9
1	E	188	THR	3.8
1	D	123	LEU	3.8
1	D	198	LEU	3.8
1	E	89	TYR	3.8
1	D	45	VAL	3.7
1	E	73	TRP	3.7
1	E	93	ALA	3.7
1	D	73	TRP	3.7
1	E	118	ILE	3.6
1	E	198	LEU	3.6
1	E	210	PHE	3.6
1	E	105	ALA	3.6
1	D	56	GLY	3.6
1	D	94	PRO	3.5
1	D	31	ILE	3.5
1	D	186	THR	3.5
1	D	36	ALA	3.4
1	E	178	PHE	3.4
1	D	222	VAL	3.4
1	D	59	THR	3.4
1	D	210	PHE	3.4
1	D	129	TYR	3.4
1	E	208	GLY	3.3
1	A	225	ALA	3.3
1	D	53	THR	3.2
1	D	57	TRP	3.2
1	D	49	TYR	3.2
1	E	172	TYR	3.2
1	E	81	TYR	3.1
1	D	99	ILE	3.1
1	D	38	PHE	3.1
1	D	178	PHE	3.1
1	E	185	PHE	3.1
1	E	197	LYS	3.1
1	B	144	LYS	3.1
1	D	101	PHE	3.1
1	B	73	TRP	3.1
1	E	66	VAL	3.1
1	E	83	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	188	THR	3.1
1	E	189	PRO	3.0
1	D	119	LEU	3.0
1	E	74	THR	3.0
1	E	184	THR	3.0
1	E	209	THR	3.0
1	D	118	ILE	3.0
1	D	143	GLN	2.9
1	D	97	ARG	2.9
1	E	174	LYS	2.9
1	D	93	ALA	2.9
1	E	34	ASN	2.9
1	D	158	LEU	2.9
1	E	190	ASP	2.9
1	D	71	THR	2.9
1	D	86	THR	2.9
1	B	225	ALA	2.9
1	D	33	ILE	2.9
1	D	185	PHE	2.8
1	B	190	ASP	2.8
1	E	142	PHE	2.8
1	D	187	ALA	2.8
1	D	66	VAL	2.8
1	D	79	VAL	2.8
1	D	84	PRO	2.8
1	D	90	ASN	2.8
1	E	196	GLN	2.8
1	E	186	THR	2.8
1	B	142	PHE	2.7
1	E	67	PRO	2.7
1	D	122	THR	2.7
1	D	195	ASP	2.7
1	D	221	THR	2.7
1	E	147	LEU	2.7
1	A	190	ASP	2.7
1	E	148	ALA	2.7
1	E	38	PHE	2.6
1	D	64	ASN	2.6
1	D	141	GLU	2.6
1	D	55	PRO	2.6
1	E	88	PHE	2.6
1	E	183	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	159	ALA	2.6
1	D	189	PRO	2.6
1	D	213	LEU	2.6
1	D	220	LEU	2.6
1	E	82	VAL	2.6
1	E	199	GLY	2.5
1	D	193	TYR	2.5
1	D	159	ALA	2.5
1	D	103	TYR	2.5
1	E	84	PRO	2.5
1	B	28	VAL	2.5
1	D	144	LYS	2.5
1	D	215	PHE	2.4
1	D	83	GLY	2.4
1	E	180	THR	2.4
1	D	173	ILE	2.4
1	E	144	LYS	2.4
1	D	30	SER	2.4
1	D	172	TYR	2.4
1	D	197	LYS	2.4
1	D	200	ILE	2.4
1	E	64	ASN	2.3
1	D	54	PRO	2.3
1	D	171	LEU	2.3
1	D	149	GLY	2.3
1	E	219	ARG	2.3
1	D	92	LEU	2.3
1	E	150	PHE	2.3
1	D	218	VAL	2.3
1	E	55	PRO	2.3
1	D	58	THR	2.3
1	D	127	THR	2.3
1	D	147	LEU	2.3
1	E	65	LEU	2.3
1	D	216	ASP	2.3
1	E	135	VAL	2.3
1	E	87	GLN	2.2
1	E	36	ALA	2.2
1	D	109	GLY	2.2
1	E	139	GLY	2.2
1	B	145	ILE	2.2
1	E	58	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	35	ASN	2.2
1	E	131	LEU	2.2
1	E	85	GLY	2.2
1	E	62	PRO	2.2
1	E	94	PRO	2.2
1	D	139	GLY	2.2
1	D	160	GLY	2.2
1	E	56	GLY	2.2
1	E	160	GLY	2.2
1	E	191	ASN	2.2
1	E	193	TYR	2.2
1	D	41	PRO	2.2
1	D	209	THR	2.2
1	A	177	GLU	2.1
1	D	87	GLN	2.1
1	E	149	GLY	2.1
1	B	26	THR	2.1
1	D	74	THR	2.1
1	D	162	THR	2.1
1	E	46	VAL	2.1
1	E	158	LEU	2.1
1	D	140	GLY	2.1
1	E	91	GLN	2.1
1	D	131	LEU	2.1
1	D	157	LEU	2.1
1	D	67	PRO	2.1
1	E	35	ASN	2.0
1	D	190	ASP	2.0
1	E	71	THR	2.0
1	B	189	PRO	2.0
1	D	212	GLY	2.0
1	E	43	ILE	2.0
1	E	173	ILE	2.0
1	E	200	ILE	2.0
1	B	161	ASP	2.0
1	D	40	ASP	2.0
1	E	69	LYS	2.0

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 [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
5	TRS	E	304	8/8	0.77	0.19	46,49,53,58	0
3	EDO	A	304	4/4	0.89	0.27	20,20,20,20	0
2	CA	A	301	1/1	0.89	0.12	65,65,65,65	0
4	DMS	E	303	4/4	0.93	0.15	39,42,46,60	0
2	CA	D	301	1/1	0.94	0.09	49,49,49,49	0
2	CA	E	301	1/1	0.97	0.07	41,41,41,41	0
2	CA	D	302	1/1	0.97	0.06	47,47,47,47	0
2	CA	B	301	1/1	0.98	0.04	28,28,28,28	0
2	CA	A	303	1/1	0.98	0.04	27,27,27,27	0
2	CA	E	302	1/1	0.98	0.07	45,45,45,45	0
2	CA	B	302	1/1	0.99	0.03	26,26,26,26	0
2	CA	A	302	1/1	0.99	0.02	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.