



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:57 PM UTC

PDB ID : 2PKH / pdb_00002pkh
Title : Structural Genomics, the crystal structure of the C-terminal domain of histidine utilization repressor from *Pseudomonas syringae* pv. tomato str. DC3000
Authors : Tan, K.; Zhou, M.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2007-04-17
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

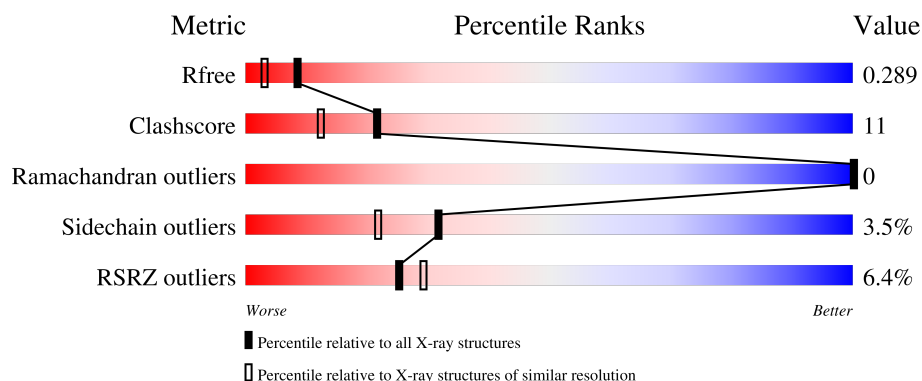
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	148	5% 76% 16% .. 5%
1	B	148	4% 76% 18% ..
1	C	148	7% 76% 18% ..
1	D	148	8% 76% 17% .. 5%
1	E	148	4% 74% 20% ..

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Mol	Chain	Length	Quality of chain
1	F	148	
1	G	148	
1	H	148	

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
2	EDO	B	1026	-	-	X	-
2	EDO	C	1017	-	-	X	-
2	EDO	F	1028	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10115 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 Histidine utilization repressor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	Se	0	0	0
			1127	708	208	206	3	2			
1	B	142	Total	C	N	O	S	Se	0	0	0
			1137	714	211	207	3	2			
1	C	142	Total	C	N	O	S	Se	0	0	0
			1137	714	211	207	3	2			
1	D	141	Total	C	N	O	S	Se	0	0	0
			1127	708	208	206	3	2			
1	E	142	Total	C	N	O	S	Se	0	0	0
			1137	714	211	207	3	2			
1	F	141	Total	C	N	O	S	Se	0	0	0
			1127	708	208	206	3	2			
1	G	141	Total	C	N	O	S	Se	0	0	0
			1127	708	208	206	3	2			
1	H	142	Total	C	N	O	S	Se	0	0	0
			1137	714	211	207	3	2			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	SER	-	cloning artifact	UNP Q87UX0
A	103	ASN	-	cloning artifact	UNP Q87UX0
A	104	ALA	-	cloning artifact	UNP Q87UX0
A	115	MSE	MET	modified residue	UNP Q87UX0
A	132	MSE	MET	modified residue	UNP Q87UX0
B	102	SER	-	cloning artifact	UNP Q87UX0
B	103	ASN	-	cloning artifact	UNP Q87UX0
B	104	ALA	-	cloning artifact	UNP Q87UX0
B	115	MSE	MET	modified residue	UNP Q87UX0
B	132	MSE	MET	modified residue	UNP Q87UX0
C	102	SER	-	cloning artifact	UNP Q87UX0
C	103	ASN	-	cloning artifact	UNP Q87UX0
C	104	ALA	-	cloning artifact	UNP Q87UX0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	115	MSE	MET	modified residue	UNP Q87UX0
C	132	MSE	MET	modified residue	UNP Q87UX0
D	102	SER	-	cloning artifact	UNP Q87UX0
D	103	ASN	-	cloning artifact	UNP Q87UX0
D	104	ALA	-	cloning artifact	UNP Q87UX0
D	115	MSE	MET	modified residue	UNP Q87UX0
D	132	MSE	MET	modified residue	UNP Q87UX0
E	102	SER	-	cloning artifact	UNP Q87UX0
E	103	ASN	-	cloning artifact	UNP Q87UX0
E	104	ALA	-	cloning artifact	UNP Q87UX0
E	115	MSE	MET	modified residue	UNP Q87UX0
E	132	MSE	MET	modified residue	UNP Q87UX0
F	102	SER	-	cloning artifact	UNP Q87UX0
F	103	ASN	-	cloning artifact	UNP Q87UX0
F	104	ALA	-	cloning artifact	UNP Q87UX0
F	115	MSE	MET	modified residue	UNP Q87UX0
F	132	MSE	MET	modified residue	UNP Q87UX0
G	102	SER	-	cloning artifact	UNP Q87UX0
G	103	ASN	-	cloning artifact	UNP Q87UX0
G	104	ALA	-	cloning artifact	UNP Q87UX0
G	115	MSE	MET	modified residue	UNP Q87UX0
G	132	MSE	MET	modified residue	UNP Q87UX0
H	102	SER	-	cloning artifact	UNP Q87UX0
H	103	ASN	-	cloning artifact	UNP Q87UX0
H	104	ALA	-	cloning artifact	UNP Q87UX0
H	115	MSE	MET	modified residue	UNP Q87UX0
H	132	MSE	MET	modified residue	UNP Q87UX0

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	123	Total O 123 123	0	0

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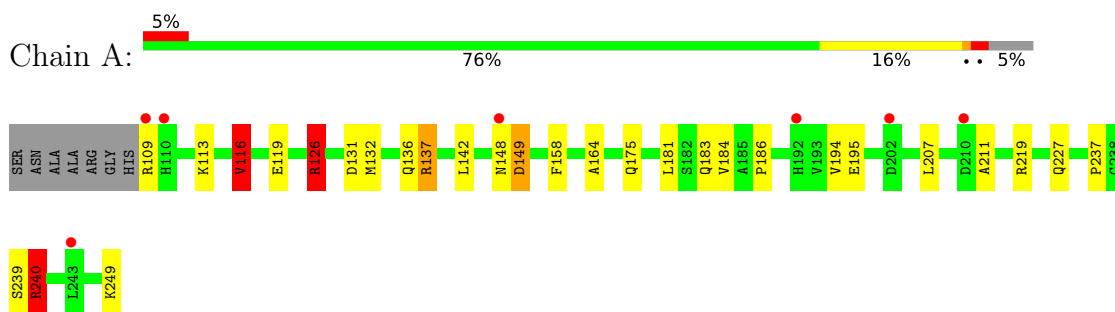
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	116	Total 116	O 116	0	0
3	C	106	Total 106	O 106	0	0
3	D	101	Total 101	O 101	0	0
3	E	121	Total 121	O 121	0	0
3	F	123	Total 123	O 123	0	0
3	G	133	Total 133	O 133	0	0
3	H	108	Total 108	O 108	0	0

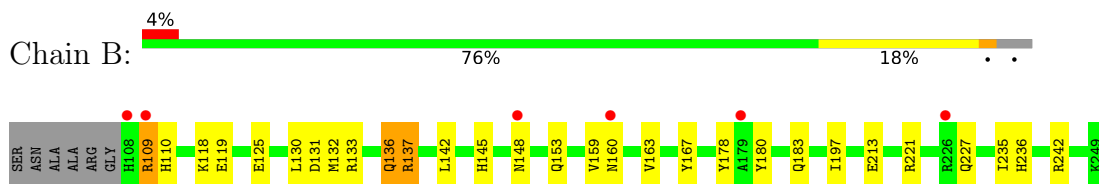
3 Residue-property plots [i](#)

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.

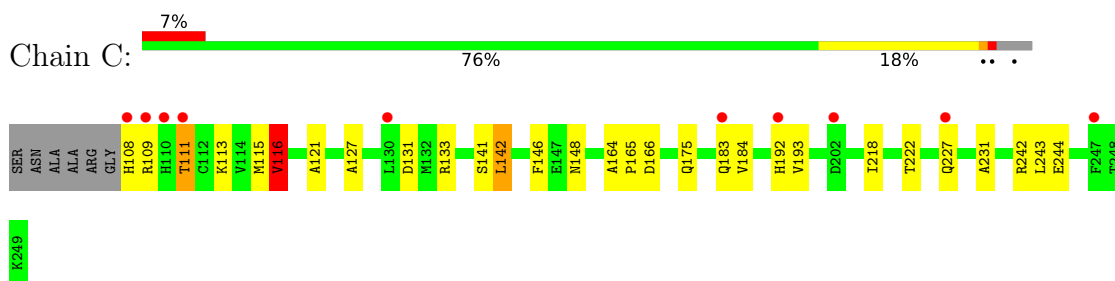
- Molecule 1: Histidine utilization repressor



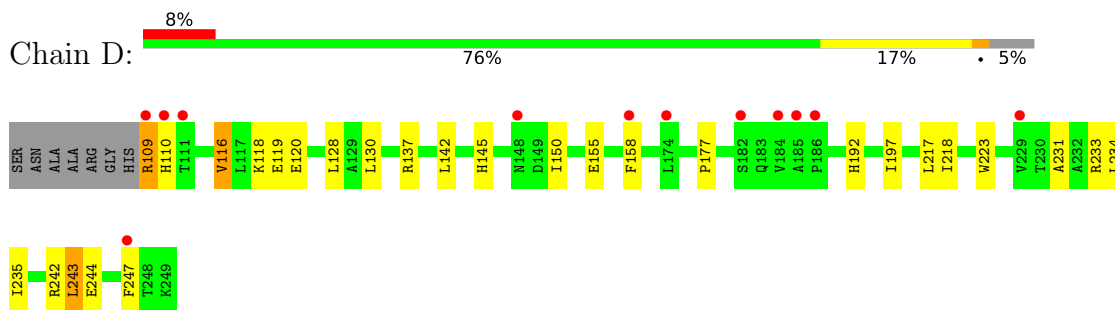
- Molecule 1: Histidine utilization repressor



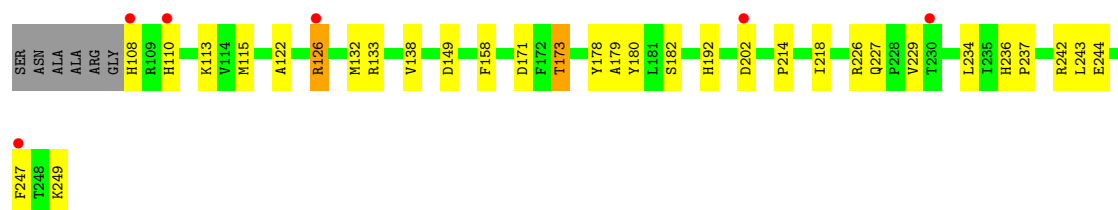
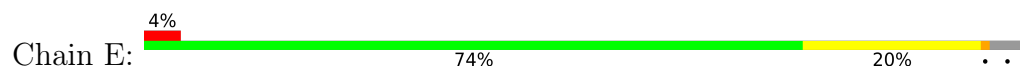
- Molecule 1: Histidine utilization repressor



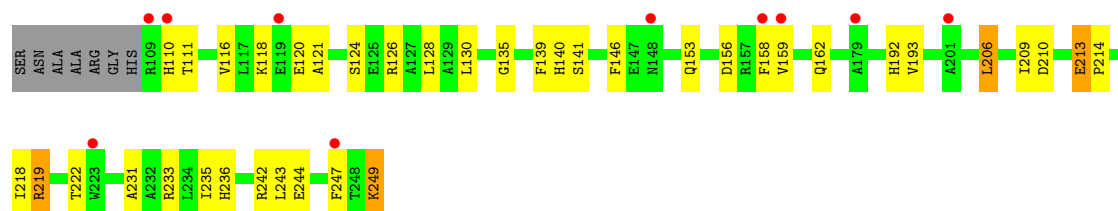
- Molecule 1: Histidine utilization repressor



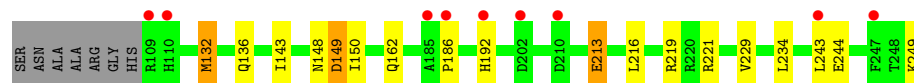
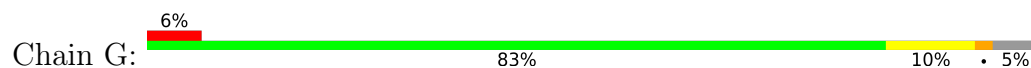
• Molecule 1: Histidine utilization repressor



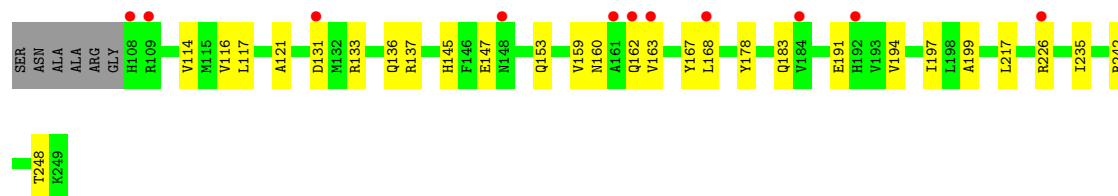
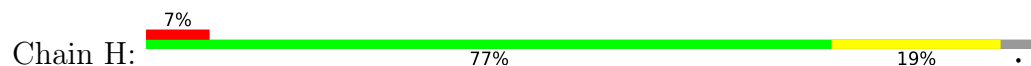
• Molecule 1: Histidine utilization repressor



• Molecule 1: Histidine utilization repressor



• Molecule 1: Histidine utilization repressor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.84Å 100.95Å 130.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.87 – 1.95 39.87 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.87-1.95) 99.3 (39.87-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.277 0.232 , 0.289	Depositor DCC
R_{free} test set	4838 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10115	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 62.56 % 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 1.1050e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.27	4/1147 (0.3%)	1.23	7/1549 (0.5%)
1	B	1.29	0/1158	1.15	0/1564
1	C	1.29	4/1158 (0.3%)	1.17	2/1564 (0.1%)
1	D	1.31	1/1147 (0.1%)	1.16	0/1549
1	E	1.30	2/1158 (0.2%)	1.20	1/1564 (0.1%)
1	F	1.30	0/1147	1.21	6/1549 (0.4%)
1	G	1.34	2/1147 (0.2%)	1.19	3/1549 (0.2%)
1	H	1.42	4/1158 (0.3%)	1.19	0/1564
All	All	1.32	17/9220 (0.2%)	1.19	19/12452 (0.2%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	ALA	CA-CB	8.27	1.62	1.53
1	H	121	ALA	CA-CB	7.40	1.65	1.53
1	H	194	VAL	C-O	7.16	1.31	1.24
1	H	199	ALA	CA-CB	-7.11	1.41	1.53
1	C	127	ALA	CA-CB	-6.74	1.43	1.53
1	A	126	ARG	CD-NE	-6.04	1.37	1.46
1	G	143	ILE	CA-CB	5.96	1.61	1.54
1	G	229	VAL	N-CA	5.83	1.54	1.46
1	E	236	HIS	C-O	-5.63	1.16	1.24
1	D	197	ILE	CA-CB	5.49	1.63	1.54
1	E	180	TYR	C-O	-5.30	1.18	1.24
1	A	194	VAL	CA-CB	5.27	1.60	1.54
1	H	163	VAL	CA-CB	5.20	1.61	1.54
1	A	116	VAL	CA-CB	5.14	1.62	1.54
1	C	116	VAL	CA-CB	5.07	1.62	1.54
1	C	231	ALA	CA-C	5.05	1.58	1.52
1	C	222	THR	C-O	5.00	1.29	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ARG	NE-CZ-NH2	-8.71	111.36	119.20
1	A	240	ARG	NE-CZ-NH1	8.41	129.91	121.50
1	A	240	ARG	NE-CZ-NH2	-7.35	112.58	119.20
1	F	124	SER	N-CA-C	7.35	118.93	111.07
1	G	150	ILE	CB-CA-C	-6.93	102.81	110.78
1	F	121	ALA	N-CA-C	-6.19	101.32	110.48
1	E	229	VAL	N-CA-C	-6.17	106.50	111.81
1	A	149	ASP	CB-CA-C	-6.05	103.84	109.83
1	C	121	ALA	N-CA-C	-6.01	101.58	110.48
1	G	149	ASP	CB-CA-C	-5.89	101.58	110.06
1	A	126	ARG	NE-CZ-NH1	5.79	127.30	121.50
1	A	240	ARG	CD-NE-CZ	5.66	132.32	124.40
1	G	213	GLU	CB-CG-CD	5.62	122.15	112.60
1	A	211	ALA	N-CA-C	5.37	118.63	111.75
1	C	227	GLN	N-CA-C	5.32	116.37	109.72
1	F	206	LEU	CA-CB-CG	5.11	134.17	116.30
1	F	213	GLU	CA-C-N	-5.03	114.77	119.85
1	F	213	GLU	C-N-CA	-5.03	114.77	119.85
1	F	135	GLY	N-CA-C	-5.03	107.82	115.66

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	1127	0	1127	21	0
1	B	1137	0	1134	32	0
1	C	1137	0	1134	32	0
1	D	1127	0	1127	23	0
1	E	1137	0	1134	35	0
1	F	1127	0	1127	39	0
1	G	1127	0	1127	14	0
1	H	1137	0	1134	19	0
2	A	20	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	24	0	36	7	0
2	C	12	0	18	9	0
2	D	12	0	18	2	0
2	E	20	0	30	0	0
2	F	12	0	18	5	0
2	G	8	0	12	2	0
2	H	20	0	30	1	0
3	A	123	0	0	3	0
3	B	116	0	0	3	0
3	C	106	0	0	3	0
3	D	101	0	0	3	0
3	E	121	0	0	1	0
3	F	123	0	0	8	0
3	G	133	0	0	4	0
3	H	108	0	0	6	0
All	All	10115	0	9236	198	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 11.

All (198) 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:113:LYS:HG2	1:C:115:MSE:CE	1.62	1.29
1:C:113:LYS:HG2	1:C:115:MSE:HE1	1.22	1.13
1:E:113:LYS:HG2	1:E:115:MSE:HE1	1.29	1.08
1:E:202:ASP:HB2	3:E:1108:HOH:O	1.55	1.07
1:C:113:LYS:HG2	1:C:115:MSE:HE3	1.44	1.00
1:H:131:ASP:HB3	3:H:1129:HOH:O	1.63	0.99
1:E:113:LYS:HG2	1:E:115:MSE:CE	1.99	0.92
1:E:113:LYS:CG	1:E:115:MSE:HE1	2.00	0.91
1:C:111:THR:HG22	1:C:146:PHE:HB2	1.54	0.88
1:F:111:THR:HG22	3:F:1130:HOH:O	1.79	0.82
1:A:148:ASN:O	1:A:149:ASP:HB2	1.80	0.82
2:B:1026:EDO:H21	3:B:1144:HOH:O	1.79	0.82
2:G:1023:EDO:H11	3:G:1150:HOH:O	1.79	0.80
1:A:119:GLU:OE2	1:A:137:ARG:CD	2.29	0.80
1:E:122:ALA:HB2	1:E:132:MSE:CE	2.11	0.79
1:E:113:LYS:HB3	1:E:115:MSE:HE3	1.65	0.78
1:C:115:MSE:HA	1:C:115:MSE:HE2	1.66	0.77
1:B:197:ILE:HD11	1:B:235:ILE:HD12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:GLU:HB2	2:F:1028:EDO:O1	1.83	0.77
1:A:119:GLU:OE2	1:A:137:ARG:HD3	1.85	0.76
1:H:114:VAL:HG12	3:H:1073:HOH:O	1.85	0.75
1:B:110:HIS:NE2	1:B:145:HIS:HD2	1.85	0.74
1:C:133:ARG:HG2	1:H:242:ARG:HD3	1.70	0.74
1:E:122:ALA:CB	1:E:132:MSE:CE	2.66	0.73
1:B:130:LEU:HB3	1:B:132:MSE:HE3	1.69	0.73
1:C:175:GLN:HE22	1:C:183:GLN:NE2	1.88	0.71
1:E:122:ALA:HB2	1:E:132:MSE:HE1	1.71	0.71
1:C:113:LYS:CG	1:C:115:MSE:CE	2.58	0.71
1:C:113:LYS:CG	1:C:115:MSE:HE1	2.12	0.71
1:G:221:ARG:HD2	3:G:1090:HOH:O	1.91	0.70
1:A:237:PRO:HB2	1:A:240:ARG:HG3	1.73	0.70
1:B:242:ARG:HD3	1:E:133:ARG:HG2	1.72	0.70
1:C:113:LYS:CG	1:C:115:MSE:HE3	2.21	0.69
1:E:244:GLU:HG2	1:F:193:VAL:HG22	1.75	0.69
1:H:133:ARG:NH2	1:H:136:GLN:NE2	2.42	0.68
1:G:148:ASN:O	1:G:149:ASP:HB2	1.93	0.68
1:B:133:ARG:NH2	1:B:136:GLN:OE1	2.28	0.67
1:B:109:ARG:CG	1:B:109:ARG:HH11	2.08	0.65
1:E:126:ARG:HD3	1:E:158:PHE:CD1	2.31	0.65
1:C:184:VAL:HG11	2:C:1017:EDO:H11	1.79	0.65
1:B:132:MSE:HE1	1:B:160:ASN:HD22	1.61	0.65
1:F:153:GLN:HE21	1:F:236:HIS:CE1	2.15	0.65
1:F:111:THR:CG2	1:F:146:PHE:HB2	2.27	0.64
1:H:116:VAL:C	3:H:1073:HOH:O	2.39	0.64
1:A:119:GLU:OE2	1:A:137:ARG:HD2	1.96	0.64
1:F:219:ARG:HD3	3:F:1091:HOH:O	1.97	0.64
1:C:116:VAL:HG13	1:C:142:LEU:HB3	1.80	0.64
1:D:116:VAL:HG13	1:D:142:LEU:HB3	1.79	0.64
1:G:132:MSE:HE2	1:G:136:GLN:HB3	1.80	0.63
1:F:158:PHE:CZ	1:F:231:ALA:HB3	2.33	0.63
1:A:186:PRO:HG3	1:D:110:HIS:HB2	1.80	0.62
1:E:113:LYS:CG	1:E:115:MSE:CE	2.69	0.62
1:B:137:ARG:HG3	1:B:137:ARG:HH21	1.64	0.62
1:B:153:GLN:HE21	1:B:236:HIS:CE1	2.17	0.61
1:A:113:LYS:HD3	3:A:1147:HOH:O	2.00	0.61
1:D:242:ARG:NE	1:D:244:GLU:OE2	2.34	0.61
1:D:109:ARG:HH11	1:D:109:ARG:HB3	1.65	0.61
1:B:160:ASN:OD1	1:B:163:VAL:HG23	2.02	0.60
1:D:158:PHE:CZ	1:D:231:ALA:HB3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LYS:HE2	1:B:178:TYR:OH	2.02	0.60
1:F:111:THR:HG23	1:F:146:PHE:HB2	1.83	0.59
1:C:184:VAL:HG22	2:C:1017:EDO:H22	1.85	0.59
1:A:219:ARG:HH11	1:A:219:ARG:HG2	1.68	0.59
1:D:150:ILE:CD1	1:G:162:GLN:NE2	2.65	0.59
1:C:242:ARG:HD2	1:C:244:GLU:OE2	2.03	0.58
1:F:110:HIS:HB2	1:G:186:PRO:HG3	1.84	0.58
1:D:116:VAL:HG13	1:D:142:LEU:CB	2.33	0.58
1:B:119:GLU:OE2	1:B:137:ARG:NH2	2.35	0.58
1:E:122:ALA:HB2	1:E:132:MSE:HE3	1.86	0.58
1:F:120:GLU:OE2	1:F:126:ARG:NH2	2.33	0.58
1:A:116:VAL:HG13	1:A:142:LEU:HB3	1.86	0.57
1:A:132:MSE:HE2	1:A:136:GLN:HB3	1.87	0.57
2:D:1013:EDO:H22	3:D:1084:HOH:O	2.05	0.57
1:A:240:ARG:HD3	3:A:1136:HOH:O	2.06	0.56
1:B:180:TYR:O	1:B:183:GLN:HB2	2.04	0.56
1:G:216:LEU:HD21	1:G:243:LEU:HG	1.88	0.56
1:F:233:ARG:HG2	1:F:235:ILE:HD11	1.88	0.55
1:H:197:ILE:HD11	1:H:235:ILE:HD12	1.88	0.55
1:B:110:HIS:NE2	1:B:145:HIS:CD2	2.71	0.55
1:E:122:ALA:CB	1:E:132:MSE:HE1	2.35	0.54
1:C:165:PRO:HD2	2:C:1017:EDO:H12	1.90	0.54
1:B:132:MSE:HB2	1:B:136:GLN:HE21	1.72	0.54
1:A:175:GLN:OE1	1:A:183:GLN:NE2	2.41	0.53
1:A:126:ARG:HD3	1:A:158:PHE:CD1	2.43	0.53
1:E:179:ALA:O	1:E:182:SER:HB2	2.08	0.53
1:B:109:ARG:NH1	1:B:109:ARG:HG3	2.24	0.53
1:B:142:LEU:C	1:B:142:LEU:HD23	2.33	0.53
1:C:164:ALA:HA	2:C:1017:EDO:H12	1.91	0.53
1:H:197:ILE:HD13	1:H:217:LEU:HD22	1.91	0.53
1:C:108:HIS:N	3:C:1094:HOH:O	2.42	0.53
1:D:118:LYS:HE3	1:D:120:GLU:OE1	2.09	0.52
1:C:218:ILE:HD11	1:C:243:LEU:HD21	1.91	0.52
1:C:192:HIS:CD2	1:D:247:PHE:HE1	2.28	0.52
1:B:109:ARG:HD3	1:B:148:ASN:OD1	2.08	0.52
1:E:178:TYR:OH	1:F:249:LYS:HE2	2.10	0.52
1:E:113:LYS:CB	1:E:115:MSE:HE3	2.36	0.52
1:H:117:LEU:HG	1:H:168:LEU:HD22	1.92	0.52
1:C:111:THR:HB	3:C:1057:HOH:O	2.09	0.51
1:E:132:MSE:HE1	1:E:138:VAL:CG1	2.41	0.51
1:E:247:PHE:CE2	1:F:192:HIS:HD2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:ARG:HG2	3:F:1091:HOH:O	2.10	0.51
1:B:153:GLN:HE21	1:B:236:HIS:HE1	1.57	0.51
1:F:162:GLN:HG2	3:F:1030:HOH:O	2.11	0.51
1:B:109:ARG:CG	1:B:109:ARG:NH1	2.71	0.51
1:E:122:ALA:HB1	1:E:132:MSE:CE	2.41	0.51
1:B:213:GLU:OE1	2:B:1026:EDO:H11	2.11	0.50
1:C:115:MSE:HE2	1:C:115:MSE:CA	2.39	0.50
1:F:219:ARG:CD	3:F:1091:HOH:O	2.57	0.50
1:D:130:LEU:HD11	1:D:158:PHE:CD1	2.47	0.50
1:H:145:HIS:CD2	1:H:153:GLN:HE21	2.29	0.50
1:E:108:HIS:HB2	1:E:110:HIS:NE2	2.27	0.50
1:F:153:GLN:HE21	1:F:236:HIS:HE1	1.58	0.50
1:F:210:ASP:H	2:F:1028:EDO:C1	2.25	0.50
1:E:108:HIS:HB2	1:E:110:HIS:CD2	2.47	0.49
1:C:175:GLN:HE22	1:C:183:GLN:HE22	1.58	0.49
1:H:133:ARG:NH2	1:H:136:GLN:HE21	2.11	0.49
1:D:110:HIS:CE1	1:D:145:HIS:ND1	2.81	0.49
1:F:118:LYS:HZ2	1:F:120:GLU:CD	2.19	0.49
1:B:109:ARG:HH11	1:B:109:ARG:HG3	1.74	0.49
1:E:242:ARG:HD2	1:E:244:GLU:OE2	2.13	0.49
1:C:109:ARG:NH1	1:C:148:ASN:HD22	2.11	0.48
1:B:213:GLU:OE1	2:B:1026:EDO:C1	2.62	0.48
1:F:139:PHE:HB2	1:F:159:VAL:HG12	1.96	0.48
1:H:160:ASN:OD1	1:H:162:GLN:N	2.47	0.48
1:A:131:ASP:OD1	1:F:242:ARG:NH2	2.46	0.47
1:E:113:LYS:CD	1:E:115:MSE:HE1	2.43	0.47
1:F:110:HIS:CB	1:G:186:PRO:HG3	2.44	0.47
1:C:116:VAL:O	1:C:141:SER:HA	2.13	0.47
1:G:192:HIS:CG	3:G:1082:HOH:O	2.67	0.47
1:H:160:ASN:OD1	1:H:160:ASN:C	2.57	0.47
1:H:162:GLN:NE2	3:H:1089:HOH:O	2.42	0.47
1:B:131:ASP:O	2:B:1029:EDO:H21	2.15	0.46
1:H:137:ARG:HD3	3:H:1085:HOH:O	2.15	0.46
2:C:1002:EDO:H21	1:D:223:TRP:CE2	2.51	0.46
1:E:132:MSE:HE1	1:E:138:VAL:HG13	1.97	0.46
2:D:1003:EDO:H12	3:D:1053:HOH:O	2.14	0.46
1:E:247:PHE:HE2	1:F:192:HIS:HD2	1.63	0.46
1:E:249:LYS:HE3	1:F:222:THR:HG23	1.98	0.46
1:A:207:LEU:O	1:A:240:ARG:NH2	2.49	0.45
1:B:227:GLN:HG3	2:B:1029:EDO:H12	1.98	0.45
1:F:111:THR:CG2	3:F:1130:HOH:O	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:HA	1:A:184:VAL:HG22	1.98	0.45
1:B:137:ARG:HH21	1:B:137:ARG:CG	2.28	0.45
1:E:115:MSE:HA	1:E:115:MSE:HE2	1.99	0.45
1:C:164:ALA:HA	2:C:1017:EDO:C1	2.47	0.45
1:C:193:VAL:HG22	1:D:244:GLU:HG2	1.98	0.45
1:E:113:LYS:HB3	1:E:115:MSE:CE	2.43	0.45
1:F:111:THR:HG22	1:F:146:PHE:HB2	1.99	0.45
1:H:117:LEU:HB2	3:H:1073:HOH:O	2.16	0.45
3:D:1062:HOH:O	1:G:136:GLN:HG2	2.16	0.45
1:C:184:VAL:CG2	2:C:1017:EDO:H22	2.46	0.45
1:C:192:HIS:HD2	1:D:247:PHE:HE1	1.62	0.44
1:F:120:GLU:OE2	1:F:126:ARG:NH1	2.49	0.44
1:A:195:GLU:OE2	1:B:242:ARG:NH1	2.39	0.44
1:D:217:LEU:HD11	1:D:233:ARG:HG3	1.98	0.44
1:E:113:LYS:CB	1:E:115:MSE:CE	2.96	0.44
1:F:116:VAL:O	1:F:141:SER:HA	2.18	0.44
1:G:132:MSE:CE	1:G:136:GLN:HB3	2.45	0.44
1:G:244:GLU:OE1	2:G:1018:EDO:H12	2.18	0.43
1:C:113:LYS:CB	1:C:115:MSE:HE3	2.49	0.43
1:D:192:HIS:CD2	1:D:192:HIS:C	2.97	0.43
1:D:218:ILE:HD11	1:D:243:LEU:HD11	2.00	0.43
1:E:171:ASP:OD1	1:E:173:THR:HB	2.18	0.43
2:B:1026:EDO:C2	3:B:1144:HOH:O	2.53	0.43
1:D:119:GLU:CD	1:D:137:ARG:HD3	2.44	0.43
1:F:219:ARG:HG2	1:F:219:ARG:H	1.75	0.43
1:C:131:ASP:OD2	1:E:226:ARG:NH1	2.45	0.42
2:F:1028:EDO:H21	3:F:1149:HOH:O	2.19	0.42
1:G:249:LYS:HE3	1:H:178:TYR:OH	2.20	0.42
3:C:1085:HOH:O	1:D:242:ARG:NH1	2.43	0.42
1:D:150:ILE:CD1	1:G:162:GLN:HE21	2.31	0.42
1:H:191:GLU:OE2	2:H:1019:EDO:C2	2.67	0.42
1:E:218:ILE:HD11	1:E:243:LEU:HD21	2.02	0.42
1:F:244:GLU:HB2	1:H:248:THR:HG23	2.02	0.42
1:B:130:LEU:CB	1:B:132:MSE:HE3	2.45	0.42
1:A:109:ARG:HG2	1:A:109:ARG:O	2.19	0.42
1:F:130:LEU:HG	1:F:158:PHE:HE2	1.85	0.42
1:F:219:ARG:CG	3:F:1091:HOH:O	2.67	0.42
1:D:155:GLU:HG3	1:D:234:LEU:HD21	2.01	0.41
1:G:219:ARG:HD2	3:G:1074:HOH:O	2.20	0.41
1:B:118:LYS:NZ	3:B:1143:HOH:O	2.53	0.41
1:A:113:LYS:CD	3:A:1147:HOH:O	2.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LYS:NZ	2:B:1016:EDO:H22	2.35	0.41
1:A:239:SER:C	1:A:240:ARG:HG2	2.45	0.41
1:D:110:HIS:HE1	1:D:145:HIS:ND1	2.18	0.41
1:E:192:HIS:CD2	1:F:247:PHE:HE2	2.38	0.41
1:B:183:GLN:HE21	1:B:183:GLN:HB3	1.67	0.41
1:C:184:VAL:HG11	2:C:1017:EDO:C1	2.49	0.41
1:F:140:HIS:NE2	1:F:156:ASP:OD1	2.54	0.41
1:H:159:VAL:HG21	1:H:167:TYR:CE1	2.55	0.41
1:E:214:PRO:HB3	1:F:214:PRO:HB3	2.03	0.40
1:F:193:VAL:HB	1:F:219:ARG:HG3	2.01	0.40
1:F:218:ILE:HD11	1:F:243:LEU:HD21	2.03	0.40
1:D:235:ILE:HD12	1:D:235:ILE:N	2.37	0.40
1:F:209:ILE:HA	2:F:1028:EDO:H11	2.03	0.40
1:F:210:ASP:H	2:F:1028:EDO:H12	1.85	0.40
1:B:159:VAL:HG21	1:B:167:TYR:CE1	2.56	0.40
1:C:166:ASP:N	2:C:1017:EDO:O1	2.46	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	139/148 (94%)	137 (99%)	2 (1%)	0	100	100
1	B	140/148 (95%)	139 (99%)	1 (1%)	0	100	100
1	C	140/148 (95%)	139 (99%)	1 (1%)	0	100	100
1	D	139/148 (94%)	137 (99%)	2 (1%)	0	100	100
1	E	140/148 (95%)	138 (99%)	2 (1%)	0	100	100
1	F	139/148 (94%)	137 (99%)	2 (1%)	0	100	100
1	G	139/148 (94%)	138 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	140/148 (95%)	139 (99%)	1 (1%)	0	100	100
All	All	1116/1184 (94%)	1104 (99%)	12 (1%)	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	120/122 (98%)	115 (96%)	5 (4%)	26	16
1	B	121/122 (99%)	116 (96%)	5 (4%)	27	17
1	C	121/122 (99%)	118 (98%)	3 (2%)	42	34
1	D	120/122 (98%)	115 (96%)	5 (4%)	26	16
1	E	121/122 (99%)	115 (95%)	6 (5%)	22	11
1	F	120/122 (98%)	116 (97%)	4 (3%)	33	24
1	G	120/122 (98%)	117 (98%)	3 (2%)	42	34
1	H	121/122 (99%)	118 (98%)	3 (2%)	42	34
All	All	964/976 (99%)	930 (96%)	34 (4%)	32	22

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	VAL
1	A	126	ARG
1	A	137	ARG
1	A	227	GLN
1	A	240	ARG
1	B	109	ARG
1	B	125	GLU
1	B	136	GLN
1	B	137	ARG
1	B	221	ARG

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Mol	Chain	Res	Type
1	C	111	THR
1	C	116	VAL
1	C	142	LEU
1	D	109	ARG
1	D	116	VAL
1	D	128	LEU
1	D	177	PRO
1	D	243	LEU
1	E	126	ARG
1	E	149	ASP
1	E	173	THR
1	E	227	GLN
1	E	234	LEU
1	E	237	PRO
1	F	128	LEU
1	F	206	LEU
1	F	219	ARG
1	F	249	LYS
1	G	132	MSE
1	G	213	GLU
1	G	234	LEU
1	H	147	GLU
1	H	183	GLN
1	H	226	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	183	GLN
1	B	108	HIS
1	B	145	HIS
1	B	170	GLN
1	B	175	GLN
1	B	183	GLN
1	B	236	HIS
1	C	136	GLN
1	C	148	ASN
1	C	175	GLN
1	C	183	GLN
1	C	192	HIS
1	C	241	HIS

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Mol	Chain	Res	Type
1	D	110	HIS
1	D	148	ASN
1	D	175	GLN
1	D	183	GLN
1	E	175	GLN
1	E	183	GLN
1	E	192	HIS
1	E	227	GLN
1	E	241	HIS
1	F	110	HIS
1	F	153	GLN
1	F	162	GLN
1	F	175	GLN
1	F	183	GLN
1	F	192	HIS
1	F	236	HIS
1	F	241	HIS
1	G	162	GLN
1	G	183	GLN
1	G	236	HIS
1	G	241	HIS
1	H	153	GLN
1	H	170	GLN
1	H	192	HIS

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 ⓘ

32 ligands are modelled in this entry.

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	$\# Z > 2$
2	EDO	A	1024	-	3,3,3	0.49	0	2,2,2	0.15	0
2	EDO	B	1021	-	3,3,3	0.68	0	2,2,2	0.09	0
2	EDO	E	1027	-	3,3,3	0.57	0	2,2,2	0.85	0
2	EDO	B	1032	-	3,3,3	0.58	0	2,2,2	0.21	0
2	EDO	H	1031	-	3,3,3	0.39	0	2,2,2	0.49	0
2	EDO	D	1006	-	3,3,3	0.53	0	2,2,2	0.37	0
2	EDO	C	1017	-	3,3,3	0.46	0	2,2,2	0.46	0
2	EDO	G	1018	-	3,3,3	0.50	0	2,2,2	0.68	0
2	EDO	B	1029	-	3,3,3	1.15	0	2,2,2	1.11	0
2	EDO	H	1008	-	3,3,3	0.42	0	2,2,2	0.44	0
2	EDO	A	1014	-	3,3,3	0.53	0	2,2,2	0.41	0
2	EDO	A	1001	-	3,3,3	0.51	0	2,2,2	0.29	0
2	EDO	F	1007	-	3,3,3	0.36	0	2,2,2	0.64	0
2	EDO	A	1004	-	3,3,3	0.43	0	2,2,2	0.68	0
2	EDO	D	1013	-	3,3,3	0.65	0	2,2,2	0.58	0
2	EDO	B	1016	-	3,3,3	0.75	0	2,2,2	0.08	0
2	EDO	F	1015	-	3,3,3	0.48	0	2,2,2	0.28	0
2	EDO	E	1011	-	3,3,3	0.47	0	2,2,2	0.33	0
2	EDO	A	1009	-	3,3,3	0.62	0	2,2,2	0.28	0
2	EDO	H	1019	-	3,3,3	0.77	0	2,2,2	0.44	0
2	EDO	G	1023	-	3,3,3	0.39	0	2,2,2	0.53	0
2	EDO	E	1005	-	3,3,3	0.70	0	2,2,2	0.47	0
2	EDO	E	1020	-	3,3,3	0.42	0	2,2,2	0.50	0
2	EDO	B	1010	-	3,3,3	0.53	0	2,2,2	0.60	0
2	EDO	B	1026	-	3,3,3	0.81	0	2,2,2	0.24	0
2	EDO	D	1003	-	3,3,3	0.60	0	2,2,2	0.20	0
2	EDO	E	1030	-	3,3,3	0.38	0	2,2,2	0.59	0
2	EDO	H	1022	-	3,3,3	0.47	0	2,2,2	0.25	0
2	EDO	C	1012	-	3,3,3	0.40	0	2,2,2	0.38	0
2	EDO	F	1028	-	3,3,3	0.52	0	2,2,2	0.81	0
2	EDO	H	1025	-	3,3,3	0.57	0	2,2,2	0.06	0
2	EDO	C	1002	-	3,3,3	0.37	0	2,2,2	0.37	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
2	EDO	A	1024	-	-	1/1/1/1	-
2	EDO	B	1021	-	-	1/1/1/1	-
2	EDO	E	1027	-	-	1/1/1/1	-
2	EDO	B	1032	-	-	1/1/1/1	-
2	EDO	H	1031	-	-	0/1/1/1	-
2	EDO	D	1006	-	-	1/1/1/1	-
2	EDO	C	1017	-	-	1/1/1/1	-
2	EDO	G	1018	-	-	0/1/1/1	-
2	EDO	B	1029	-	-	1/1/1/1	-
2	EDO	H	1008	-	-	1/1/1/1	-
2	EDO	A	1014	-	-	1/1/1/1	-
2	EDO	A	1001	-	-	1/1/1/1	-
2	EDO	F	1007	-	-	0/1/1/1	-
2	EDO	A	1004	-	-	1/1/1/1	-
2	EDO	D	1013	-	-	0/1/1/1	-
2	EDO	B	1016	-	-	0/1/1/1	-
2	EDO	F	1015	-	-	1/1/1/1	-
2	EDO	E	1011	-	-	0/1/1/1	-
2	EDO	A	1009	-	-	1/1/1/1	-
2	EDO	H	1019	-	-	0/1/1/1	-
2	EDO	G	1023	-	-	0/1/1/1	-
2	EDO	E	1005	-	-	1/1/1/1	-
2	EDO	E	1020	-	-	0/1/1/1	-
2	EDO	B	1010	-	-	0/1/1/1	-
2	EDO	B	1026	-	-	0/1/1/1	-
2	EDO	D	1003	-	-	0/1/1/1	-
2	EDO	E	1030	-	-	0/1/1/1	-
2	EDO	H	1022	-	-	1/1/1/1	-
2	EDO	C	1012	-	-	1/1/1/1	-
2	EDO	F	1028	-	-	1/1/1/1	-
2	EDO	H	1025	-	-	1/1/1/1	-
2	EDO	C	1002	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1027	EDO	O1-C1-C2-O2
2	A	1001	EDO	O1-C1-C2-O2
2	A	1009	EDO	O1-C1-C2-O2
2	B	1021	EDO	O1-C1-C2-O2
2	B	1029	EDO	O1-C1-C2-O2
2	F	1028	EDO	O1-C1-C2-O2
2	H	1008	EDO	O1-C1-C2-O2
2	A	1004	EDO	O1-C1-C2-O2
2	C	1012	EDO	O1-C1-C2-O2
2	C	1017	EDO	O1-C1-C2-O2
2	E	1005	EDO	O1-C1-C2-O2
2	F	1015	EDO	O1-C1-C2-O2
2	A	1024	EDO	O1-C1-C2-O2
2	B	1032	EDO	O1-C1-C2-O2
2	D	1006	EDO	O1-C1-C2-O2
2	H	1025	EDO	O1-C1-C2-O2
2	A	1014	EDO	O1-C1-C2-O2
2	H	1022	EDO	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1017	EDO	8	0
2	G	1018	EDO	1	0
2	B	1029	EDO	2	0
2	D	1013	EDO	1	0
2	B	1016	EDO	1	0
2	H	1019	EDO	1	0
2	G	1023	EDO	1	0
2	B	1026	EDO	4	0
2	D	1003	EDO	1	0
2	F	1028	EDO	5	0
2	C	1002	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	139/148 (93%)	0.51	7 (5%) 34 40	19, 26, 35, 47	0
1	B	140/148 (94%)	0.69	6 (4%) 40 46	17, 25, 35, 48	0
1	C	140/148 (94%)	0.75	10 (7%) 22 25	20, 27, 38, 60	0
1	D	139/148 (93%)	0.80	12 (8%) 16 19	21, 28, 39, 54	0
1	E	140/148 (94%)	0.75	6 (4%) 40 46	21, 27, 37, 64	0
1	F	139/148 (93%)	0.77	10 (7%) 21 25	22, 28, 38, 55	0
1	G	139/148 (93%)	0.56	9 (6%) 25 28	20, 25, 35, 53	0
1	H	140/148 (94%)	0.78	11 (7%) 18 21	18, 26, 36, 49	0
All	All	1116/1184 (94%)	0.70	71 (6%) 25 29	17, 26, 37, 64	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	110	HIS	4.6
1	F	110	HIS	4.4
1	H	108	HIS	4.1
1	A	210	ASP	4.0
1	F	247	PHE	3.9
1	C	110	HIS	3.9
1	D	229	VAL	3.8
1	B	108	HIS	3.7
1	G	109	ARG	3.5
1	C	247	PHE	3.5
1	G	210	ASP	3.4
1	E	110	HIS	3.3
1	B	148	ASN	3.3
1	H	161	ALA	3.3
1	A	109	ARG	3.2
1	D	247	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	111	THR	3.1
1	G	110	HIS	3.1
1	H	184	VAL	3.1
1	E	108	HIS	3.1
1	H	131	ASP	3.0
1	B	226	ARG	3.0
1	A	110	HIS	2.9
1	D	174	LEU	2.9
1	E	202	ASP	2.9
1	E	247	PHE	2.9
1	G	247	PHE	2.9
1	F	158	PHE	2.8
1	C	108	HIS	2.8
1	H	162	GLN	2.7
1	D	184	VAL	2.7
1	D	185	ALA	2.7
1	D	109	ARG	2.5
1	D	148	ASN	2.5
1	D	111	THR	2.5
1	F	223	TRP	2.5
1	F	201	ALA	2.5
1	C	109	ARG	2.4
1	F	179	ALA	2.4
1	E	230	THR	2.4
1	G	185	ALA	2.4
1	C	183	GLN	2.4
1	H	192	HIS	2.4
1	F	159	VAL	2.4
1	H	168	LEU	2.3
1	F	148	ASN	2.3
1	G	186	PRO	2.3
1	G	243	LEU	2.3
1	B	179	ALA	2.3
1	F	119	GLU	2.3
1	B	109	ARG	2.2
1	D	182	SER	2.2
1	A	148	ASN	2.2
1	C	227	GLN	2.2
1	A	192	HIS	2.2
1	D	158	PHE	2.2
1	C	192	HIS	2.2
1	H	163	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	130	LEU	2.2
1	B	160	ASN	2.1
1	A	202	ASP	2.1
1	G	202	ASP	2.1
1	D	186	PRO	2.1
1	C	202	ASP	2.1
1	H	109	ARG	2.1
1	A	243	LEU	2.1
1	E	126	ARG	2.1
1	G	192	HIS	2.0
1	F	109	ARG	2.0
1	H	226	ARG	2.0
1	H	148	ASN	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($\text{\AA}^2$)	Q<0.9
2	EDO	B	1029	4/4	0.63	0.20	30,33,34,44	0
2	EDO	D	1003	4/4	0.70	0.20	57,57,58,59	0
2	EDO	D	1013	4/4	0.71	0.16	29,30,30,34	0
2	EDO	F	1028	4/4	0.71	0.17	25,28,34,42	0
2	EDO	E	1011	4/4	0.74	0.28	55,57,57,59	0
2	EDO	A	1004	4/4	0.74	0.17	43,44,44,45	0
2	EDO	G	1023	4/4	0.75	0.18	54,56,57,58	0
2	EDO	B	1010	4/4	0.76	0.17	44,45,46,46	0
2	EDO	F	1007	4/4	0.76	0.23	49,50,50,51	0
2	EDO	D	1006	4/4	0.76	0.16	49,51,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	1009	4/4	0.76	0.17	38,38,42,43	0
2	EDO	H	1025	4/4	0.76	0.20	36,37,39,42	0
2	EDO	B	1021	4/4	0.77	0.17	43,45,47,48	0
2	EDO	B	1032	4/4	0.78	0.24	49,53,54,55	0
2	EDO	E	1030	4/4	0.79	0.18	56,57,57,58	0
2	EDO	B	1026	4/4	0.80	0.15	37,38,41,45	0
2	EDO	H	1019	4/4	0.81	0.16	37,40,42,45	0
2	EDO	E	1027	4/4	0.81	0.16	36,37,38,41	0
2	EDO	H	1031	4/4	0.81	0.18	45,49,49,52	0
2	EDO	H	1008	4/4	0.82	0.13	46,46,47,47	0
2	EDO	E	1005	4/4	0.82	0.16	43,43,46,48	0
2	EDO	C	1002	4/4	0.83	0.16	44,46,47,48	0
2	EDO	A	1001	4/4	0.84	0.11	47,49,51,51	0
2	EDO	B	1016	4/4	0.86	0.13	26,36,37,43	0
2	EDO	H	1022	4/4	0.86	0.14	54,55,55,56	0
2	EDO	F	1015	4/4	0.89	0.13	50,51,52,53	0
2	EDO	A	1014	4/4	0.89	0.12	43,44,45,46	0
2	EDO	A	1024	4/4	0.90	0.12	45,46,48,49	0
2	EDO	C	1012	4/4	0.90	0.14	44,45,45,46	0
2	EDO	G	1018	4/4	0.90	0.11	35,39,39,40	0
2	EDO	E	1020	4/4	0.91	0.09	48,48,49,49	0
2	EDO	C	1017	4/4	0.93	0.12	30,31,36,37	0

6.5 Other polymers ⓘ

There are no such residues in this entry.