



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:15 PM UTC

PDB ID : 7AVR / pdb_00007avr
Title : The tetrameric structure of haloalkane dehalogenase DpaA from *Paraglaciecola agarilytica* NO2
Authors : Mazur, A.; Kolenko, P.; Prudnikova, T.; Grinkevich, P.; Kuta Smatanova, I.
Deposited on : 2020-11-05
Resolution : 2.00 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

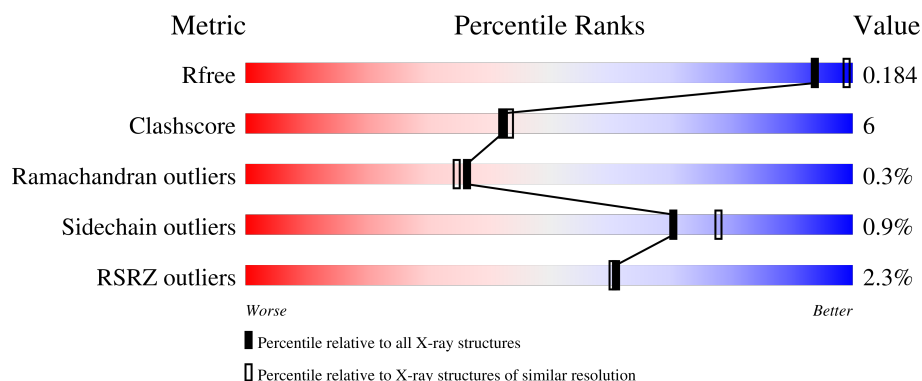
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	307	4% 85% 12% .
1	B	307	% 88% 9% .
1	C	307	2% 84% 11% .
1	D	307	2% 87% 10% .
1	E	307	3% 85% 12% .

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Mol	Chain	Length	Quality of chain
1	F	307	
1	G	307	
1	H	307	

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	CL	F	404	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20821 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 Haloalkane dehalogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	1	0
			2355	1513	380	444	18			
1	B	298	Total	C	N	O	S	0	0	0
			2341	1503	379	441	18			
1	C	299	Total	C	N	O	S	1	1	0
			2354	1511	381	444	18			
1	D	297	Total	C	N	O	S	1	0	0
			2333	1498	378	440	17			
1	E	298	Total	C	N	O	S	0	3	0
			2358	1513	380	447	18			
1	F	298	Total	C	N	O	S	0	1	0
			2348	1508	381	442	17			
1	G	299	Total	C	N	O	S	0	1	0
			2354	1511	381	444	18			
1	H	299	Total	C	N	O	S	0	1	0
			2352	1512	381	441	18			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP K6XNL5
A	2	THR	-	expression tag	UNP K6XNL5
A	302	HIS	-	expression tag	UNP K6XNL5
A	303	HIS	-	expression tag	UNP K6XNL5
A	304	HIS	-	expression tag	UNP K6XNL5
A	305	HIS	-	expression tag	UNP K6XNL5
A	306	HIS	-	expression tag	UNP K6XNL5
A	307	HIS	-	expression tag	UNP K6XNL5
B	1	MET	-	initiating methionine	UNP K6XNL5
B	2	THR	-	expression tag	UNP K6XNL5
B	302	HIS	-	expression tag	UNP K6XNL5
B	303	HIS	-	expression tag	UNP K6XNL5
B	304	HIS	-	expression tag	UNP K6XNL5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	305	HIS	-	expression tag	UNP K6XNL5
B	306	HIS	-	expression tag	UNP K6XNL5
B	307	HIS	-	expression tag	UNP K6XNL5
C	1	MET	-	initiating methionine	UNP K6XNL5
C	2	THR	-	expression tag	UNP K6XNL5
C	302	HIS	-	expression tag	UNP K6XNL5
C	303	HIS	-	expression tag	UNP K6XNL5
C	304	HIS	-	expression tag	UNP K6XNL5
C	305	HIS	-	expression tag	UNP K6XNL5
C	306	HIS	-	expression tag	UNP K6XNL5
C	307	HIS	-	expression tag	UNP K6XNL5
D	1	MET	-	initiating methionine	UNP K6XNL5
D	2	THR	-	expression tag	UNP K6XNL5
D	302	HIS	-	expression tag	UNP K6XNL5
D	303	HIS	-	expression tag	UNP K6XNL5
D	304	HIS	-	expression tag	UNP K6XNL5
D	305	HIS	-	expression tag	UNP K6XNL5
D	306	HIS	-	expression tag	UNP K6XNL5
D	307	HIS	-	expression tag	UNP K6XNL5
E	1	MET	-	initiating methionine	UNP K6XNL5
E	2	THR	-	expression tag	UNP K6XNL5
E	302	HIS	-	expression tag	UNP K6XNL5
E	303	HIS	-	expression tag	UNP K6XNL5
E	304	HIS	-	expression tag	UNP K6XNL5
E	305	HIS	-	expression tag	UNP K6XNL5
E	306	HIS	-	expression tag	UNP K6XNL5
E	307	HIS	-	expression tag	UNP K6XNL5
F	1	MET	-	initiating methionine	UNP K6XNL5
F	2	THR	-	expression tag	UNP K6XNL5
F	302	HIS	-	expression tag	UNP K6XNL5
F	303	HIS	-	expression tag	UNP K6XNL5
F	304	HIS	-	expression tag	UNP K6XNL5
F	305	HIS	-	expression tag	UNP K6XNL5
F	306	HIS	-	expression tag	UNP K6XNL5
F	307	HIS	-	expression tag	UNP K6XNL5
G	1	MET	-	initiating methionine	UNP K6XNL5
G	2	THR	-	expression tag	UNP K6XNL5
G	302	HIS	-	expression tag	UNP K6XNL5
G	303	HIS	-	expression tag	UNP K6XNL5
G	304	HIS	-	expression tag	UNP K6XNL5
G	305	HIS	-	expression tag	UNP K6XNL5
G	306	HIS	-	expression tag	UNP K6XNL5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	307	HIS	-	expression tag	UNP K6XNL5
H	1	MET	-	initiating methionine	UNP K6XNL5
H	2	THR	-	expression tag	UNP K6XNL5
H	302	HIS	-	expression tag	UNP K6XNL5
H	303	HIS	-	expression tag	UNP K6XNL5
H	304	HIS	-	expression tag	UNP K6XNL5
H	305	HIS	-	expression tag	UNP K6XNL5
H	306	HIS	-	expression tag	UNP K6XNL5
H	307	HIS	-	expression tag	UNP K6XNL5

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	3	Total Cl 3 3	0	0
2	D	1	Total Cl 1 1	0	0
2	E	2	Total Cl 2 2	0	0
2	F	6	Total Cl 6 6	0	0
2	G	3	Total Cl 3 3	0	0
2	H	1	Total Cl 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	264	Total O 264 264	0	0
3	B	244	Total O 244 244	0	0
3	C	291	Total O 291 291	0	0
3	D	217	Total O 217 217	0	0
3	E	264	Total O 264 264	0	0

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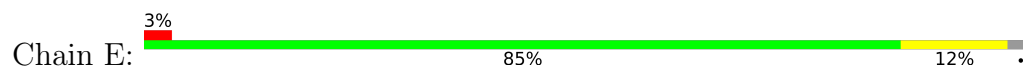
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	298	Total 298	O 298	0	0
3	G	231	Total 231	O 231	0	0
3	H	199	Total 199	O 199	0	0

- Molecule 1: Haloalkane dehalogenase 1

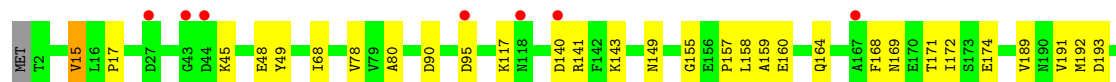
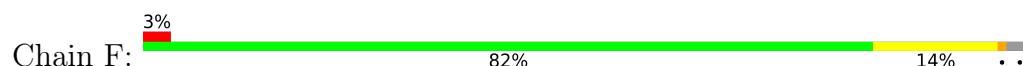




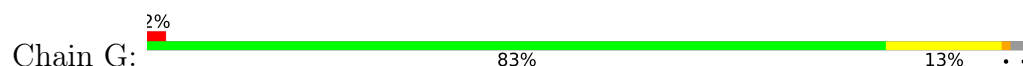
• Molecule 1: Haloalkane dehalogenase 1



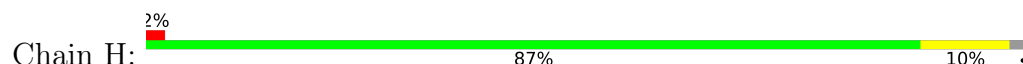
• Molecule 1: Haloalkane dehalogenase 1



• Molecule 1: Haloalkane dehalogenase 1



• Molecule 1: Haloalkane dehalogenase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.39Å 155.51Å 155.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.44 – 2.00 47.44 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.44-2.00) 88.0 (47.44-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.22 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.176 , 0.206 (Not available) , 0.184	Depositor DCC
R_{free} test set	9496 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.105 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20821	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 63.14 % 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 1.0126e-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:
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	1.31	5/2417 (0.2%)	1.14	3/3279 (0.1%)
1	B	1.27	7/2400 (0.3%)	1.16	3/3256 (0.1%)
1	C	1.30	5/2416 (0.2%)	1.14	2/3278 (0.1%)
1	D	1.21	2/2392 (0.1%)	1.11	1/3246 (0.0%)
1	E	1.20	5/2423 (0.2%)	1.12	0/3288
1	F	1.24	1/2407 (0.0%)	1.11	4/3266 (0.1%)
1	G	1.26	4/2416 (0.2%)	1.13	3/3279 (0.1%)
1	H	1.21	4/2414 (0.2%)	1.12	1/3276 (0.0%)
All	All	1.25	33/19285 (0.2%)	1.13	17/26168 (0.1%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	ASP	C-O	-7.56	1.15	1.24
1	H	95	ASP	C-O	-7.22	1.15	1.24
1	A	170[A]	GLU	CA-C	7.13	1.62	1.52
1	A	170[B]	GLU	CA-C	7.13	1.62	1.52
1	C	148	MET	C-O	-6.72	1.14	1.23
1	B	219	THR	CA-C	6.34	1.61	1.52
1	B	33	GLU	C-O	6.31	1.31	1.24
1	C	54	LEU	C-O	-6.22	1.16	1.24
1	G	34	SER	CA-CB	-6.07	1.47	1.54
1	B	26	VAL	C-O	-6.06	1.18	1.24
1	E	95	ASP	C-O	-6.05	1.17	1.24
1	H	280	GLY	C-O	-6.02	1.18	1.24
1	A	280	GLY	C-O	-5.99	1.18	1.24
1	B	220	ASN	CA-C	5.86	1.59	1.52
1	C	11	GLU	C-O	-5.84	1.16	1.24
1	G	56	GLY	N-CA	5.76	1.50	1.45
1	B	95	ASP	C-O	-5.69	1.17	1.24
1	H	138	MET	SD-CE	-5.64	1.65	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	3	ILE	N-CA	5.56	1.52	1.46
1	D	288	VAL	N-CA	5.54	1.53	1.46
1	F	155	GLY	C-O	-5.49	1.16	1.24
1	B	56	GLY	N-CA	5.42	1.50	1.45
1	E	219	THR	CA-C	5.32	1.59	1.52
1	E	278	GLU	N-CA	5.32	1.53	1.46
1	C	53	CYS	C-O	-5.29	1.17	1.24
1	E	54	LEU	C-O	-5.25	1.17	1.24
1	B	199	ALA	N-CA	5.24	1.51	1.46
1	C	168	PHE	C-O	5.17	1.30	1.24
1	A	199	ALA	N-CA	5.14	1.51	1.46
1	E	220	ASN	CA-C	5.09	1.59	1.52
1	D	163	VAL	CA-CB	5.09	1.60	1.54
1	G	26	VAL	C-O	-5.04	1.19	1.24
1	H	199	ALA	N-CA	5.04	1.51	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	268	LYS	N-CA-C	9.03	121.94	111.11
1	H	117	LYS	N-CA-C	8.51	123.53	112.12
1	B	117	LYS	N-CA-C	8.45	123.45	112.12
1	B	119	ILE	N-CA-C	7.48	118.76	108.89
1	G	154	ASN	N-CA-C	-6.38	99.01	109.40
1	A	172	ILE	N-CA-C	5.98	116.97	110.21
1	B	221	ALA	N-CA-C	5.86	119.90	112.87
1	G	154	ASN	CA-C-O	-5.72	114.53	120.70
1	C	139	GLN	CB-CA-C	-5.42	101.80	110.79
1	D	156	GLU	CB-CG-CD	5.36	121.71	112.60
1	G	139	GLN	CB-CA-C	-5.12	102.29	110.79
1	C	184	ASP	N-CA-C	5.10	116.92	111.36
1	F	15	VAL	CA-C-N	5.10	128.25	122.59
1	F	15	VAL	C-N-CA	5.10	128.25	122.59
1	A	170[A]	GLU	N-CA-C	5.07	119.23	113.19
1	A	170[B]	GLU	N-CA-C	5.07	119.23	113.19
1	F	172	ILE	N-CA-C	5.07	115.94	110.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2355	0	2291	33	0
1	B	2341	0	2274	15	0
1	C	2354	0	2289	39	0
1	D	2333	0	2265	24	0
1	E	2358	0	2288	27	0
1	F	2348	0	2281	38	0
1	G	2354	0	2289	45	0
1	H	2352	0	2291	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	3	0	0	1	0
2	D	1	0	0	0	0
2	E	2	0	0	1	0
2	F	6	0	0	2	0
2	G	3	0	0	1	0
2	H	1	0	0	1	0
3	A	264	0	0	17	0
3	B	244	0	0	4	0
3	C	291	0	0	13	0
3	D	217	0	0	4	0
3	E	264	0	0	9	0
3	F	298	0	0	20	0
3	G	231	0	0	9	0
3	H	199	0	0	9	0
All	All	20821	0	18268	233	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 (233) 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:G:156:GLU:HG2	1:G:157:PRO:HD2	1.37	1.03
1:G:182:ALA:HA	1:G:189:VAL:HG21	1.59	0.83
1:E:251:LYS:HZ3	1:G:251:LYS:HD2	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:ALA:HA	1:C:189:VAL:HG21	1.63	0.79
1:G:156:GLU:HG2	1:G:157:PRO:CD	2.11	0.79
1:G:248:ILE:HG22	1:G:250:MET:HE2	1.63	0.79
1:E:251:LYS:NZ	1:G:251:LYS:HD2	1.98	0.79
1:D:15:VAL:HG12	1:D:192:MET:HE1	1.63	0.78
1:H:261:MET:CE	3:H:674:HOH:O	2.30	0.78
1:F:15:VAL:HG12	1:F:192:MET:HE1	1.68	0.75
1:G:8:THR:N	2:G:403:CL:CL	2.56	0.74
1:H:55:HIS:HB2	1:H:59:THR:HG23	1.69	0.74
1:E:121:LEU:HD21	1:E:123:CYS:SG	2.28	0.74
1:C:192:MET:HE1	1:C:195:LEU:HD23	1.68	0.73
1:D:146:ILE:HD11	1:D:298:PHE:CZ	2.24	0.72
1:C:261:MET:HE3	1:C:275:LYS:NZ	2.04	0.72
1:G:248:ILE:CG2	1:G:250:MET:HE2	2.18	0.72
1:D:160:GLU:O	1:D:164:GLN:HG2	1.90	0.71
1:G:145:LEU:HG	1:G:147:VAL:HG23	1.71	0.71
1:E:112:GLU:HG3	3:E:529:HOH:O	1.90	0.70
1:E:118:ASN:HB2	3:E:505:HOH:O	1.91	0.70
1:A:134:ILE:CG2	1:A:138:MET:HE2	2.21	0.70
1:C:192:MET:SD	3:C:695:HOH:O	2.50	0.70
1:G:261:MET:HE3	1:G:275:LYS:NZ	2.07	0.69
1:A:300:MET:SD	3:A:704:HOH:O	2.50	0.69
1:D:95:ASP:OD1	1:D:208:VAL:HG13	1.92	0.68
1:G:145:LEU:HD11	1:G:147:VAL:HG22	1.75	0.68
1:A:118:ASN:ND2	3:A:510:HOH:O	2.27	0.67
1:G:262:GLN:NE2	3:G:503:HOH:O	2.24	0.67
1:C:8:THR:N	2:C:403:CL:CL	2.65	0.66
1:D:95:ASP:HB3	1:D:212:ARG:HD3	1.77	0.66
1:B:42:GLU:HA	3:B:606:HOH:O	1.95	0.66
1:B:145:LEU:HD11	1:B:147:VAL:CG1	2.27	0.65
1:F:210:VAL:HG12	3:F:578:HOH:O	1.96	0.65
1:G:262:GLN:NE2	3:G:506:HOH:O	2.30	0.65
1:B:16:LEU:CD1	1:B:88:ARG:HH21	2.11	0.64
1:G:261:MET:HE1	1:G:273:PRO:HG2	1.80	0.64
1:C:192:MET:HG2	3:C:686:HOH:O	1.99	0.63
1:A:158:LEU:HD23	3:A:628:HOH:O	1.97	0.63
1:E:47:SER:HA	2:E:402:CL:CL	2.36	0.62
1:H:170:GLU:HG2	3:H:603:HOH:O	1.99	0.62
1:A:134:ILE:HG23	1:A:138:MET:HE2	1.82	0.62
1:G:262:GLN:HG3	1:G:263:LEU:N	2.13	0.62
1:E:274:MET:HE3	1:E:293:GLN:OE1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164[A]:GLN:HG2	3:C:618:HOH:O	2.00	0.62
1:F:275:LYS:NZ	3:F:510:HOH:O	2.33	0.61
1:F:95:ASP:HB3	1:F:212:ARG:HD3	1.83	0.61
1:G:250:MET:HE3	1:G:275:LYS:HB3	1.83	0.60
1:B:145:LEU:CG	1:B:147:VAL:HG13	2.31	0.60
1:A:144:LYS:HD2	3:A:704:HOH:O	2.01	0.60
1:G:145:LEU:HG	1:G:147:VAL:CG2	2.31	0.59
1:C:136:MET:O	1:C:139:GLN:NE2	2.27	0.59
1:E:121:LEU:C	1:E:121:LEU:HD23	2.27	0.59
1:B:145:LEU:HD11	1:B:147:VAL:HG13	1.84	0.59
1:C:33:GLU:HB3	3:C:506:HOH:O	2.02	0.59
1:C:248:ILE:CD1	1:C:261:MET:HE2	2.32	0.59
1:G:261:MET:HE3	1:G:275:LYS:HZ1	1.67	0.59
1:A:144:LYS:NZ	1:A:243:GLU:OE2	2.24	0.58
1:D:146:ILE:HD11	1:D:298:PHE:CE2	2.38	0.58
1:F:215:GLN:NE2	3:F:513:HOH:O	2.35	0.58
1:C:182:ALA:HA	1:C:189:VAL:CG2	2.33	0.58
1:C:261:MET:HE1	1:C:273:PRO:HG2	1.85	0.58
1:F:143:LYS:NZ	3:F:508:HOH:O	2.33	0.58
1:H:160:GLU:HA	1:H:163:VAL:HG22	1.84	0.58
1:G:182:ALA:HA	1:G:189:VAL:CG2	2.31	0.58
1:C:192:MET:CE	1:C:195:LEU:HD23	2.32	0.57
1:C:2:THR:HG22	1:C:2:THR:O	2.05	0.57
1:E:121:LEU:CD2	1:E:123:CYS:SG	2.92	0.57
1:F:17:PRO:HD2	1:F:192:MET:HE2	1.87	0.56
1:B:145:LEU:CD1	1:B:147:VAL:HG13	2.35	0.56
1:B:145:LEU:HG	1:B:147:VAL:HG13	1.88	0.56
1:E:121:LEU:HD22	1:E:145:LEU:CD1	2.36	0.56
1:F:245:PHE:HE1	3:F:711:HOH:O	1.87	0.56
1:A:211:LYS:CE	3:A:687:HOH:O	2.54	0.55
1:C:7:ARG:NH1	3:C:502:HOH:O	2.24	0.55
1:G:45:LYS:HG2	3:G:515:HOH:O	2.06	0.55
1:C:192:MET:HE1	1:C:195:LEU:CD2	2.34	0.54
1:A:211:LYS:HE3	3:A:687:HOH:O	2.06	0.54
1:E:12:ARG:HD3	3:E:547:HOH:O	2.08	0.53
1:C:144:LYS:HE3	1:C:243:GLU:OE1	2.07	0.53
1:G:248:ILE:CD1	1:G:261:MET:HE2	2.39	0.53
1:F:204:LYS:HD2	1:F:207:LYS:HB2	1.90	0.53
1:G:160:GLU:O	1:G:164:GLN:HG2	2.09	0.53
1:F:158:LEU:N	2:F:404:CL:CL	2.70	0.52
1:F:191:VAL:HG21	1:G:180:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:189:VAL:HG13	1:H:193:ASP:HB2	1.90	0.52
1:C:148:MET:O	1:C:149:ASN:C	2.53	0.52
1:D:17:PRO:HD2	1:D:192:MET:HE2	1.91	0.52
1:F:189:VAL:HG13	1:F:193:ASP:HB2	1.91	0.52
1:G:145:LEU:CG	1:G:147:VAL:CG2	2.88	0.52
1:A:167:ALA:O	1:A:171:THR:HG23	2.09	0.52
1:G:145:LEU:HD21	1:G:147:VAL:HG21	1.91	0.52
1:A:195:LEU:HD12	3:B:552:HOH:O	2.10	0.51
1:A:189:VAL:HG13	1:A:193:ASP:HB2	1.93	0.51
1:F:169:ASN:O	1:F:211[A]:LYS:HE2	2.11	0.51
1:F:117:LYS:HB2	3:F:610:HOH:O	2.09	0.51
1:D:189:VAL:HG13	1:D:193:ASP:HB2	1.93	0.51
1:A:117:LYS:HD2	3:A:686:HOH:O	2.10	0.51
1:C:17:PRO:HG2	3:C:686:HOH:O	2.10	0.51
1:G:145:LEU:HD21	1:G:147:VAL:CG2	2.41	0.51
1:D:146:ILE:HD12	1:D:245:PHE:HB3	1.93	0.50
1:B:189:VAL:HG13	1:B:193:ASP:HB2	1.93	0.50
1:C:261:MET:HE3	1:C:275:LYS:HZ1	1.74	0.50
1:C:192:MET:HB2	3:C:695:HOH:O	2.12	0.50
1:E:189:VAL:HG13	1:E:193:ASP:HB2	1.93	0.50
1:G:136:MET:C	1:G:139:GLN:OE1	2.55	0.50
1:C:15:VAL:HG12	1:C:192:MET:CE	2.43	0.49
1:G:136:MET:O	1:G:139:GLN:OE1	2.29	0.49
1:F:143:LYS:HE3	3:F:633:HOH:O	2.11	0.49
1:F:95:ASP:OD1	1:F:208:VAL:HG13	2.13	0.49
1:D:145:LEU:O	1:D:146:ILE:HD13	2.13	0.49
1:C:154:ASN:OD1	1:C:156:GLU:HG2	2.13	0.48
1:E:252:ASP:O	3:E:501:HOH:O	2.20	0.48
1:F:168:PHE:CE1	1:G:192:MET:HE1	2.48	0.48
1:H:68:ILE:HG12	1:H:78:VAL:HG11	1.96	0.48
1:F:160:GLU:O	1:F:164:GLN:HG3	2.13	0.48
1:E:261:MET:HE3	1:E:264:LYS:CE	2.44	0.48
1:H:26:VAL:HG23	1:H:39:TYR:CE1	2.49	0.48
1:F:45:LYS:HD2	3:F:669:HOH:O	2.14	0.48
1:G:154:ASN:O	1:G:154:ASN:OD1	2.32	0.47
1:A:272:GLU:CD	1:D:160:GLU:OE1	2.57	0.47
1:E:9:PRO:HG3	3:E:657:HOH:O	2.13	0.47
1:C:10:GLU:HG2	3:C:515:HOH:O	2.14	0.47
1:A:160:GLU:OE2	1:A:164:GLN:HG3	2.14	0.47
1:D:143:LYS:HE3	3:D:632:HOH:O	2.13	0.47
1:F:263:LEU:HB2	3:F:588:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:295:LEU:O	3:F:501:HOH:O	2.20	0.47
1:G:73:ASP:OD1	3:G:501:HOH:O	2.20	0.47
1:B:16:LEU:HD12	1:B:88:ARG:HH21	1.80	0.47
1:C:54:LEU:HA	3:C:606:HOH:O	2.13	0.47
1:E:109:GLN:O	1:E:112:GLU:HG2	2.15	0.47
1:H:160:GLU:O	1:H:164:GLN:HG2	2.15	0.47
1:C:160:GLU:O	1:C:164[B]:GLN:HG2	2.14	0.47
1:F:140:ASP:HA	3:F:583:HOH:O	2.15	0.47
1:G:22[A]:GLN:NE2	3:G:524:HOH:O	2.47	0.47
1:A:144:LYS:CE	3:A:704:HOH:O	2.63	0.47
1:B:68:ILE:HG12	1:B:78:VAL:HG11	1.97	0.46
1:F:160:GLU:OE2	1:F:164:GLN:HG3	2.16	0.46
1:E:68:ILE:HG12	1:E:78:VAL:HG11	1.97	0.46
1:E:20:PRO:HA	3:E:584:HOH:O	2.15	0.46
1:E:46:ASP:O	3:E:502:HOH:O	2.21	0.46
1:H:166:MET:HB3	3:H:553:HOH:O	2.15	0.46
1:G:145:LEU:CD1	1:G:147:VAL:HG22	2.44	0.46
1:D:161:ALA:O	3:D:501:HOH:O	2.20	0.46
1:G:261:MET:CE	1:G:273:PRO:HG2	2.44	0.46
1:D:146:ILE:CD1	1:D:298:PHE:CZ	2.97	0.46
1:D:204:LYS:HD2	1:D:207:LYS:HB2	1.98	0.46
1:G:250:MET:HE3	1:G:275:LYS:CB	2.46	0.46
1:B:47:SER:HA	3:B:579:HOH:O	2.16	0.46
1:C:261:MET:HE3	1:C:275:LYS:HZ3	1.80	0.46
1:E:191:VAL:HG21	1:H:180:LEU:HD12	1.98	0.46
1:H:59:THR:OG1	1:H:63:LEU:HB2	2.16	0.46
1:C:15:VAL:HG12	1:C:192:MET:HE1	1.98	0.46
1:A:170[A]:GLU:HG2	3:A:565:HOH:O	2.16	0.45
1:G:248:ILE:CG2	1:G:250:MET:CE	2.90	0.45
1:A:68:ILE:HG12	1:A:78:VAL:HG11	1.98	0.45
1:F:191:VAL:HG23	3:F:710:HOH:O	2.15	0.45
1:H:159:ALA:HB1	3:H:520:HOH:O	2.15	0.45
1:C:4:LYS:NZ	1:C:94:GLU:OE2	2.45	0.45
1:C:68:ILE:HG12	1:C:78:VAL:HG11	1.98	0.45
1:A:160:GLU:O	1:A:164:GLN:HG3	2.16	0.45
1:A:170[A]:GLU:CG	3:A:565:HOH:O	2.64	0.45
1:E:12:ARG:HD3	3:E:605:HOH:O	2.16	0.45
1:A:105:ASN:ND2	3:A:533:HOH:O	2.48	0.45
1:A:148:MET:SD	1:A:284:GLN:HG3	2.57	0.45
1:F:48:GLU:HG2	1:F:49:TYR:CE2	2.52	0.45
1:A:230:LEU:HD21	3:A:513:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ILE:HG12	1:D:78:VAL:HG11	1.98	0.45
1:F:171:THR:HG21	3:F:736:HOH:O	2.16	0.45
1:H:26:VAL:HG23	1:H:39:TYR:HE1	1.81	0.45
1:C:297:SER:HB2	3:C:698:HOH:O	2.16	0.45
1:G:68:ILE:HG12	1:G:78:VAL:HG11	1.99	0.44
1:C:144:LYS:CE	1:C:243:GLU:OE1	2.65	0.44
1:A:144:LYS:NZ	3:A:505:HOH:O	2.25	0.44
1:C:261:MET:CE	1:C:273:PRO:HG2	2.47	0.44
1:F:222:ASP:OD2	3:F:502:HOH:O	2.21	0.44
1:E:262:GLN:HB3	3:E:509:HOH:O	2.17	0.44
1:F:68:ILE:HG12	1:F:78:VAL:HG11	1.98	0.44
1:F:117:LYS:HD2	1:F:141:ARG:HG2	2.00	0.44
1:F:174:GLU:CB	1:F:204:LYS:HD3	2.48	0.44
1:H:32:TYR:OH	1:H:105:ASN:HB3	2.17	0.44
1:B:139:GLN:HG2	1:B:239:GLU:OE2	2.18	0.44
1:F:90:ASP:OD1	3:F:503:HOH:O	2.21	0.44
1:G:272:GLU:HG3	3:G:577:HOH:O	2.18	0.44
1:H:222:ASP:HB2	3:H:510:HOH:O	2.17	0.44
1:D:145:LEU:C	1:D:146:ILE:HD13	2.43	0.44
1:H:55:HIS:HB2	1:H:59:THR:CG2	2.44	0.44
1:C:34:SER:HB2	3:C:503:HOH:O	2.18	0.43
1:E:156[B]:GLU:HA	1:E:156[B]:GLU:OE1	2.17	0.43
1:H:268:LYS:HA	3:H:506:HOH:O	2.17	0.43
1:A:26:VAL:HG23	1:A:39:TYR:CE1	2.53	0.43
1:C:156:GLU:HG3	3:C:591:HOH:O	2.16	0.43
1:H:265:THR:HG22	3:H:646:HOH:O	2.18	0.43
1:E:139:GLN:HG2	1:E:239:GLU:OE2	2.19	0.43
1:F:159:ALA:HB2	3:F:612:HOH:O	2.19	0.43
1:A:69:PRO:HA	3:A:502:HOH:O	2.18	0.43
1:F:140:ASP:HB3	3:F:530:HOH:O	2.19	0.43
1:F:80:ALA:N	3:F:532:HOH:O	2.51	0.43
1:A:32:TYR:OH	1:A:105:ASN:HB3	2.19	0.42
1:C:44:ASP:OD1	1:C:47:SER:OG	2.37	0.42
1:A:15:VAL:HA	3:A:534:HOH:O	2.19	0.42
1:G:240:TRP:O	1:G:268:LYS:HE2	2.19	0.42
1:A:277:GLU:OE1	1:D:253:ALA:HB2	2.19	0.42
1:A:251:LYS:NZ	1:D:278:GLU:OE2	2.52	0.42
1:G:159:ALA:CB	3:G:698:HOH:O	2.67	0.42
1:A:272:GLU:OE1	1:D:160:GLU:OE1	2.38	0.42
1:F:215:GLN:CD	3:F:513:HOH:O	2.60	0.42
1:B:16:LEU:CD1	1:B:88:ARG:NH2	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:GLU:HG2	2:H:401:CL:CL	2.57	0.41
1:B:72:THR:O	3:B:501:HOH:O	2.21	0.41
1:E:26:VAL:HG13	1:E:39:TYR:HE1	1.85	0.41
1:G:167:ALA:O	1:G:171:THR:HG23	2.20	0.41
1:B:148:MET:O	1:B:149:ASN:C	2.63	0.41
1:C:98:TYR:HB3	1:C:216:MET:CE	2.51	0.41
1:E:22:GLN:H	1:E:22:GLN:HG2	1.76	0.41
1:G:157:PRO:HB3	3:G:685:HOH:O	2.20	0.41
1:H:160:GLU:HB2	3:H:539:HOH:O	2.19	0.41
1:D:17:PRO:CD	1:D:192:MET:HE2	2.51	0.41
1:D:158:LEU:O	3:D:502:HOH:O	2.22	0.41
1:E:109:GLN:OE1	1:E:112:GLU:OE1	2.38	0.41
1:F:216:MET:HG2	3:F:653:HOH:O	2.20	0.41
1:H:261:MET:HE3	3:H:674:HOH:O	2.12	0.41
1:D:44:ASP:OD1	1:D:47:SER:OG	2.39	0.40
1:F:157:PRO:HA	2:F:404:CL:CL	2.58	0.40
1:G:292:GLU:OE2	3:G:502:HOH:O	2.21	0.40
1:C:243:GLU:HA	3:C:588:HOH:O	2.20	0.40
1:A:215:GLN:NE2	3:A:543:HOH:O	2.54	0.40
1:D:45:LYS:HG2	3:D:613:HOH:O	2.20	0.40
1:F:49:TYR:HE1	1:F:143:LYS:HD2	1.86	0.40
1:A:77:ARG:NH1	3:A:501:HOH:O	2.23	0.40
1:C:168:PHE:O	1:C:171:THR:HG22	2.22	0.40
1:G:76:HIS:NE2	1:G:300:MET:HE2	2.37	0.40
1:G:154:ASN:O	1:G:154:ASN:CG	2.64	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	298/307 (97%)	284 (95%)	13 (4%)	1 (0%)	36 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	235/307 (76%)	223 (95%)	12 (5%)	0	100	100
1	C	298/307 (97%)	287 (96%)	10 (3%)	1 (0%)	36	35
1	D	295/307 (96%)	284 (96%)	10 (3%)	1 (0%)	36	35
1	E	299/307 (97%)	288 (96%)	10 (3%)	1 (0%)	36	35
1	F	297/307 (97%)	285 (96%)	11 (4%)	1 (0%)	36	35
1	G	298/307 (97%)	286 (96%)	11 (4%)	1 (0%)	36	35
1	H	298/307 (97%)	284 (95%)	13 (4%)	1 (0%)	36	35
All	All	2318/2456 (94%)	2221 (96%)	90 (4%)	7 (0%)	36	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	149	ASN
1	A	149	ASN
1	D	149	ASN
1	E	149	ASN
1	G	149	ASN
1	H	149	ASN
1	C	149	ASN

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	250/257 (97%)	249 (100%)	1 (0%)	84	89
1	B	248/257 (96%)	246 (99%)	2 (1%)	73	80
1	C	250/257 (97%)	247 (99%)	3 (1%)	63	70
1	D	247/257 (96%)	246 (100%)	1 (0%)	84	89
1	E	251/257 (98%)	248 (99%)	3 (1%)	63	70
1	F	248/257 (96%)	245 (99%)	3 (1%)	63	70
1	G	250/257 (97%)	246 (98%)	4 (2%)	55	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	249/257 (97%)	246 (99%)	3 (1%)	63	70
All	All	1993/2056 (97%)	1973 (99%)	20 (1%)	70	75

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	PHE
1	B	36	ARG
1	B	213	PHE
1	C	11	GLU
1	C	34	SER
1	C	213	PHE
1	D	213	PHE
1	E	101	GLU
1	E	213	PHE
1	E	264	LYS
1	F	211[A]	LYS
1	F	211[B]	LYS
1	F	213	PHE
1	G	44	ASP
1	G	160	GLU
1	G	213	PHE
1	G	262	GLN
1	H	22[A]	GLN
1	H	22[B]	GLN
1	H	158	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	B	109	GLN
1	B	118	ASN
1	B	164	GLN
1	B	205	ASN
1	C	113	HIS
1	F	24	ASN
1	F	118	ASN
1	G	24	ASN
1	G	262	GLN
1	H	24	ASN

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Mol	Chain	Res	Type
1	H	76	HIS

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 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	299/307 (97%)	0.17	11 (3%) 45 44	11, 24, 42, 52	3 (1%)
1	B	298/307 (97%)	0.13	2 (0%) 84 84	14, 27, 44, 67	1 (0%)
1	C	299/307 (97%)	0.13	6 (2%) 65 64	12, 26, 41, 51	2 (0%)
1	D	297/307 (96%)	0.08	6 (2%) 65 64	15, 26, 42, 64	1 (0%)
1	E	298/307 (97%)	0.41	9 (3%) 52 51	16, 29, 41, 61	3 (1%)
1	F	298/307 (97%)	0.38	9 (3%) 52 51	10, 27, 42, 66	1 (0%)
1	G	299/307 (97%)	0.14	6 (2%) 65 64	14, 24, 40, 54	2 (0%)
1	H	299/307 (97%)	0.20	7 (2%) 61 60	17, 26, 44, 65	1 (0%)
All	All	2387/2456 (97%)	0.21	56 (2%) 61 60	10, 26, 42, 67	14 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	140	ASP	4.1
1	A	148	MET	3.8
1	A	20	PRO	3.8
1	E	34[A]	SER	3.5
1	A	74	ALA	3.4
1	D	140	ASP	3.4
1	F	44	ASP	3.4
1	A	237	SER	3.2
1	H	3	ILE	3.1
1	G	154	ASN	2.9
1	C	299	THR	2.9
1	G	299	THR	2.9
1	A	170[A]	GLU	2.8
1	B	300	MET	2.8
1	A	138	MET	2.8
1	H	73	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	118	ASN	2.7
1	C	11	GLU	2.6
1	E	3	ILE	2.5
1	C	2	THR	2.5
1	F	167	ALA	2.5
1	E	263	LEU	2.5
1	C	49	TYR	2.5
1	E	32	TYR	2.5
1	E	108	ILE	2.5
1	H	296	ALA	2.4
1	B	88	ARG	2.4
1	C	28	ASP	2.4
1	A	17	PRO	2.4
1	E	220	ASN	2.3
1	F	95	ASP	2.3
1	G	35	LEU	2.3
1	D	44	ASP	2.3
1	E	113	HIS	2.2
1	A	27	ASP	2.2
1	E	115	ASP	2.2
1	H	74	ALA	2.2
1	D	31	GLY	2.2
1	H	60	TRP	2.2
1	D	95	ASP	2.2
1	H	218	PRO	2.1
1	D	170	GLU	2.1
1	D	118	ASN	2.1
1	G	27	ASP	2.1
1	F	118	ASN	2.1
1	F	27	ASP	2.1
1	C	113	HIS	2.1
1	G	150	THR	2.1
1	F	43	GLY	2.1
1	F	298	PHE	2.1
1	E	160	GLU	2.0
1	G	2	THR	2.0
1	H	167	ALA	2.0
1	A	171	THR	2.0
1	F	299	THR	2.0
1	A	49	TYR	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	CL	F	406	1/1	0.92	0.12	50,50,50,50	0
2	CL	F	401	1/1	0.93	0.14	58,58,58,58	0
2	CL	C	403	1/1	0.93	0.11	47,47,47,47	0
2	CL	E	402	1/1	0.95	0.06	53,53,53,53	0
2	CL	G	402	1/1	0.96	0.07	30,30,30,30	0
2	CL	F	404	1/1	0.97	0.06	35,35,35,35	0
2	CL	H	401	1/1	0.97	0.08	21,21,21,21	0
2	CL	C	402	1/1	0.98	0.04	34,34,34,34	0
2	CL	G	403	1/1	0.98	0.05	29,29,29,29	0
2	CL	F	403	1/1	0.98	0.05	42,42,42,42	0
2	CL	E	401	1/1	0.99	0.03	24,24,24,24	0
2	CL	F	405	1/1	0.99	0.07	33,33,33,33	0
2	CL	C	401	1/1	0.99	0.03	21,21,21,21	0
2	CL	G	401	1/1	0.99	0.03	22,22,22,22	0
2	CL	A	401	1/1	0.99	0.03	18,18,18,18	0
2	CL	F	402	1/1	0.99	0.03	19,19,19,19	0
2	CL	B	401	1/1	0.99	0.03	17,17,17,17	0
2	CL	D	401	1/1	1.00	0.08	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.