



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:58 PM UTC

PDB ID : 1UF3 / pdb_00001uf3
Title : Crystal structure of TT1561 of thermus thermophilus HB8
Authors : Kato-Murayama, M.; Shirouzu, M.; Terada, T.; Murayama, K.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2003-05-23
Resolution : 2.10 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:

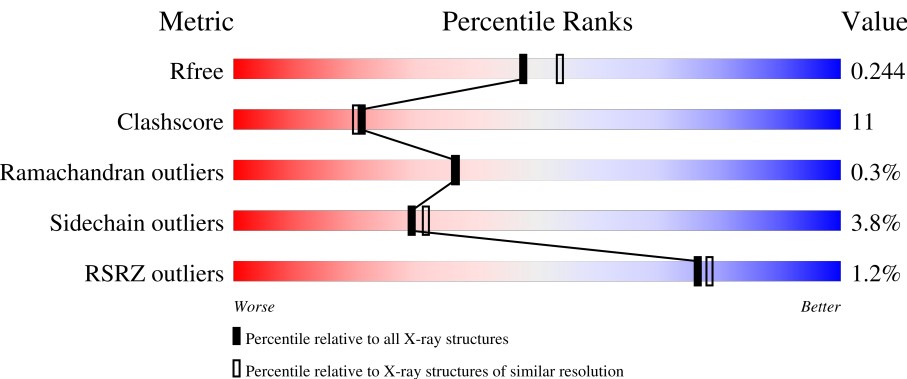
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	228	79%20%.
1	B	228	2% 75%22%..
1	C	228	% 70%25%..
1	D	228	% 71%27%.
1	E	228	2% 71%25%.

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Mol	Chain	Length	Quality of chain
1	F	228	77% 21%
1	G	228	2% 67% 29%
1	H	228	% 72% 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15287 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 hypothetical protein TT1561.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	Se	0	0	0
			1815	1168	314	327	6			
1	B	226	Total	C	N	O	Se	0	0	0
			1796	1157	309	325	5			
1	C	225	Total	C	N	O	Se	0	0	0
			1785	1151	305	324	5			
1	D	228	Total	C	N	O	Se	0	0	0
			1815	1168	314	327	6			
1	E	228	Total	C	N	O	Se	0	0	0
			1815	1168	314	327	6			
1	F	228	Total	C	N	O	Se	0	0	0
			1815	1168	314	327	6			
1	G	228	Total	C	N	O	Se	0	0	0
			1815	1168	314	327	6			
1	H	228	Total	C	N	O	Se	0	0	0
			1815	1168	314	327	6			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	1	Total	Ca	0	0
			1	1		
2	C	2	Total	Ca	0	0
			2	2		
2	D	2	Total	Ca	0	0
			2	2		
2	E	2	Total	Ca	0	0
			2	2		
2	F	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Ca	0	0
			2	2		
2	H	1	Total	Ca	0	0
			1	1		

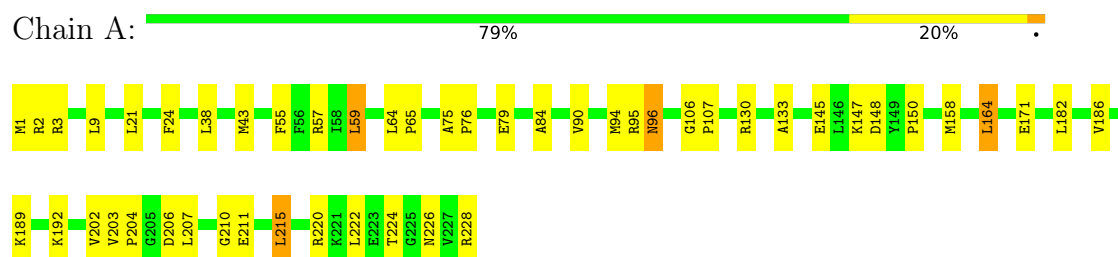
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	124	Total	O	0	0
			124	124		
3	B	89	Total	O	0	0
			89	89		
3	C	83	Total	O	0	0
			83	83		
3	D	84	Total	O	0	0
			84	84		
3	E	82	Total	O	0	0
			82	82		
3	F	140	Total	O	0	0
			140	140		
3	G	102	Total	O	0	0
			102	102		
3	H	98	Total	O	0	0
			98	98		

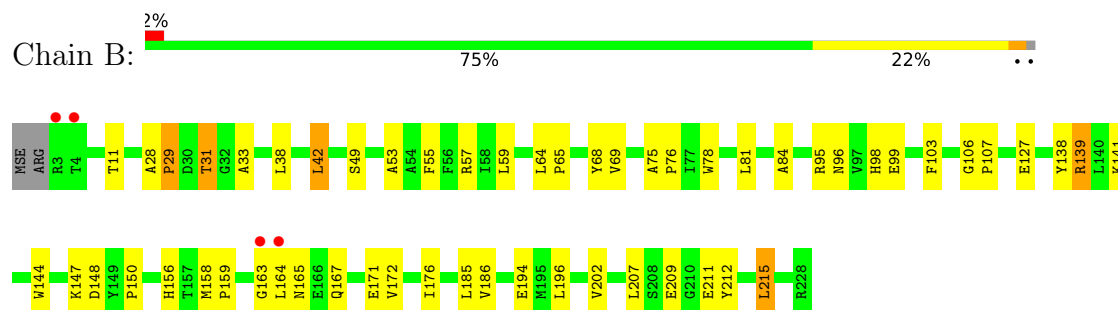
3 Residue-property plots [i](#)

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.

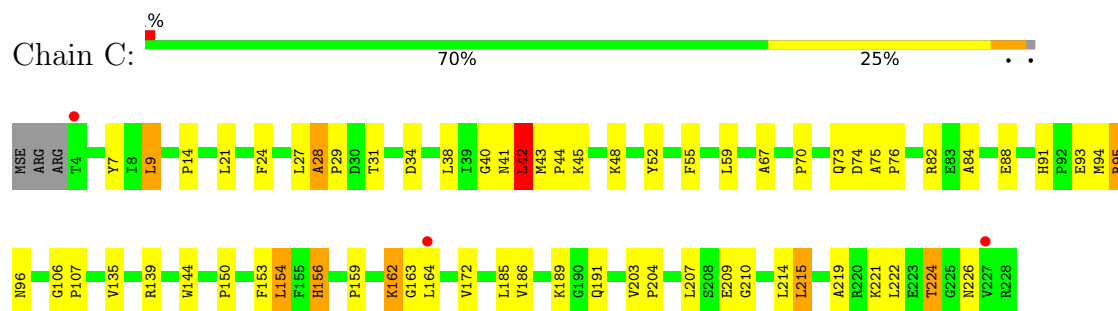
• Molecule 1: hypothetical protein TT1561



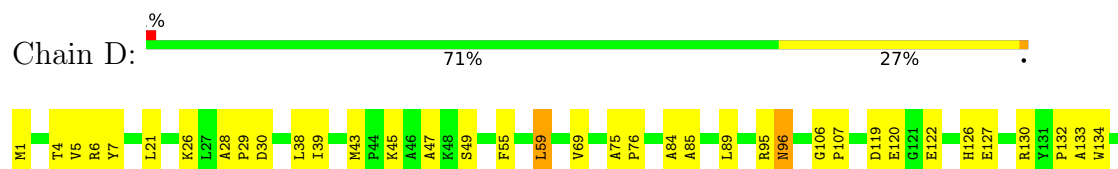
• Molecule 1: hypothetical protein TT1561



• Molecule 1: hypothetical protein TT1561

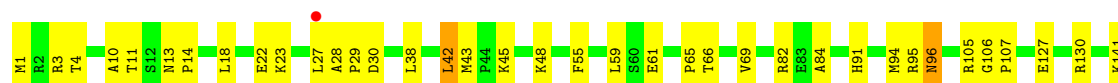
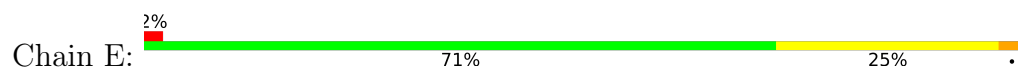


• Molecule 1: hypothetical protein TT1561

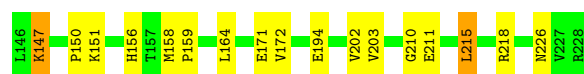
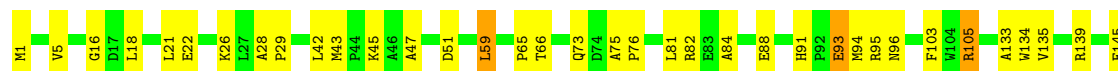
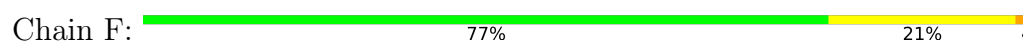




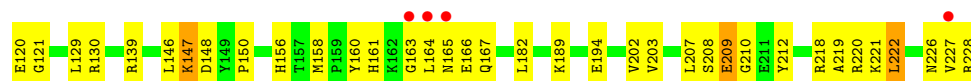
- Molecule 1: hypothetical protein TT1561



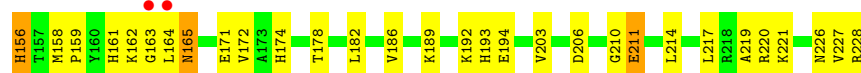
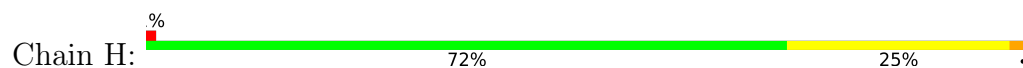
- Molecule 1: hypothetical protein TT1561



- Molecule 1: hypothetical protein TT1561



- Molecule 1: hypothetical protein TT1561



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.38Å 77.34Å 147.80Å 90.00° 127.21° 90.00°	Depositor
Resolution (Å)	29.97 – 2.10 29.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.97-2.10) 98.2 (29.97-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.54 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.245 0.196 , 0.244	Depositor DCC
R_{free} test set	10977 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15287	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.62	0/1861	1.02	9/2520 (0.4%)
1	B	0.52	0/1842	1.03	11/2496 (0.4%)
1	C	0.48	0/1831	0.98	9/2482 (0.4%)
1	D	0.52	0/1861	1.03	11/2520 (0.4%)
1	E	0.52	0/1861	1.03	11/2520 (0.4%)
1	F	0.60	0/1861	1.05	11/2520 (0.4%)
1	G	0.57	0/1861	1.04	17/2520 (0.7%)
1	H	0.58	0/1861	1.04	12/2520 (0.5%)
All	All	0.55	0/14839	1.03	91/20098 (0.5%)

There are no bond length outliers.

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	203	VAL	N-CA-C	-11.50	95.29	107.60
1	H	203	VAL	N-CA-C	-9.97	96.94	107.60
1	D	69	VAL	N-CA-C	-9.19	101.65	109.19
1	D	147	LYS	N-CA-C	8.11	122.65	109.76
1	A	147	LYS	N-CA-C	7.62	122.77	109.96
1	E	156	HIS	N-CA-C	-7.48	103.77	113.12
1	H	147	LYS	N-CA-C	7.26	121.67	109.76
1	E	147	LYS	N-CA-C	7.07	121.35	109.76
1	D	156	HIS	N-CA-C	-7.05	102.65	112.45
1	H	84	ALA	N-CA-C	-7.00	103.58	111.14
1	F	150	PRO	N-CA-C	-6.94	100.34	111.38
1	G	147	LYS	N-CA-C	6.73	118.61	111.28
1	B	49	SER	N-CA-C	6.72	119.17	111.11
1	F	95	ARG	N-CA-C	6.64	119.55	108.13
1	D	150	PRO	N-CA-C	-6.49	101.00	111.19
1	H	211	GLU	N-CA-C	6.47	120.42	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	167	GLN	N-CA-C	-6.43	105.47	113.38
1	E	203	VAL	N-CA-C	-6.33	95.22	108.88
1	D	96	ASN	N-CA-C	-6.29	99.63	109.25
1	C	44	PRO	N-CA-C	-6.12	102.23	111.41
1	C	95	ARG	N-CA-C	6.11	118.00	107.93
1	A	164	LEU	N-CA-C	6.10	119.19	111.69
1	G	156	HIS	N-CA-C	-6.09	103.27	112.04
1	G	202	VAL	N-CA-C	5.95	116.43	108.11
1	E	95	ARG	N-CA-C	5.93	117.71	107.93
1	B	202	VAL	N-CA-C	5.92	116.41	108.11
1	H	42	LEU	N-CA-C	-5.92	104.91	111.36
1	B	78	TRP	N-CA-C	5.85	118.44	111.71
1	B	69	VAL	N-CA-C	-5.84	102.41	109.01
1	B	150	PRO	N-CA-C	-5.78	102.12	111.19
1	E	91	HIS	CA-C-N	5.75	125.43	119.56
1	E	91	HIS	C-N-CA	5.75	125.43	119.56
1	C	150	PRO	N-CA-C	-5.74	102.18	111.14
1	A	148	ASP	N-CA-C	5.73	119.48	111.74
1	D	148	ASP	N-CA-C	5.72	119.32	111.54
1	A	84	ALA	N-CA-C	-5.70	104.98	111.14
1	B	147	LYS	N-CA-C	5.70	119.49	112.54
1	D	95	ARG	N-CA-C	5.70	117.93	108.13
1	F	151	LYS	N-CA-C	5.70	118.84	109.72
1	C	9	LEU	N-CA-C	-5.67	100.74	109.76
1	B	95	ARG	N-CA-C	5.67	117.28	107.93
1	G	150	PRO	N-CA-C	-5.67	102.29	111.19
1	B	211	GLU	N-CA-C	5.67	118.66	110.28
1	A	203	VAL	N-CA-C	-5.65	96.68	108.88
1	F	65	PRO	N-CA-C	-5.63	102.35	111.03
1	H	156	HIS	N-CA-C	-5.61	103.96	112.04
1	F	156	HIS	N-CA-C	-5.59	103.99	112.04
1	F	211	GLU	N-CA-C	5.57	118.72	110.48
1	G	203	VAL	N-CA-C	-5.55	96.88	108.88
1	F	202	VAL	N-CA-C	5.53	115.86	108.11
1	D	208	SER	N-CA-C	-5.53	105.35	111.71
1	H	96	ASN	N-CA-C	-5.51	100.82	109.25
1	A	95	ARG	N-CA-C	5.48	116.97	107.93
1	G	95	ARG	N-CA-C	5.48	117.55	108.13
1	G	65	PRO	N-CA-C	-5.44	102.65	111.03
1	A	96	ASN	N-CA-C	-5.42	100.95	109.25
1	F	147	LYS	N-CA-C	5.42	119.52	113.01
1	C	84	ALA	N-CA-C	-5.42	105.45	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	44	PRO	N-CA-C	-5.42	103.33	111.57
1	C	156	HIS	N-CA-C	-5.42	104.24	112.04
1	A	150	PRO	N-CA-C	-5.41	102.70	111.19
1	C	34	ASP	N-CA-C	-5.37	106.90	113.50
1	A	211	GLU	N-CA-C	5.36	118.42	110.48
1	E	151	LYS	N-CA-C	5.34	118.76	110.17
1	G	78	TRP	N-CA-C	5.32	118.86	112.38
1	D	84	ALA	N-CA-C	-5.28	105.61	111.36
1	H	69	VAL	N-CA-C	-5.24	104.89	109.19
1	H	95	ARG	N-CA-C	5.23	117.13	108.13
1	H	150	PRO	N-CA-C	-5.22	102.39	111.32
1	G	91	HIS	CA-C-N	5.22	125.52	119.47
1	G	91	HIS	C-N-CA	5.22	125.52	119.47
1	G	96	ASN	N-CA-C	-5.22	102.14	109.96
1	G	208	SER	N-CA-C	-5.20	106.03	112.38
1	F	84	ALA	N-CA-C	-5.20	105.52	111.14
1	C	203	VAL	N-CA-C	-5.20	97.66	108.88
1	B	164	LEU	N-CA-C	5.17	119.90	111.37
1	E	65	PRO	N-CA-C	-5.16	103.08	111.03
1	G	146	LEU	CA-C-N	5.16	127.19	120.28
1	G	146	LEU	C-N-CA	5.16	127.19	120.28
1	D	217	LEU	N-CA-C	5.16	116.90	111.28
1	F	145	GLU	N-CA-C	-5.15	106.51	112.89
1	E	10	ALA	N-CA-C	5.12	116.85	109.07
1	H	78	TRP	N-CA-C	5.11	118.61	112.38
1	E	96	ASN	N-CA-C	-5.10	101.44	109.25
1	B	156	HIS	N-CA-C	-5.09	105.37	112.45
1	E	84	ALA	N-CA-C	-5.09	105.63	111.07
1	D	49	SER	N-CA-C	5.05	116.47	111.07
1	B	84	ALA	N-CA-C	-5.03	105.88	111.36
1	G	10	ALA	N-CA-C	5.02	117.02	109.23
1	G	15	MSE	N-CA-C	5.02	118.53	111.90
1	C	42	LEU	N-CA-C	-5.00	105.91	111.36

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	1815	0	1796	32	0
1	B	1796	0	1771	28	0
1	C	1785	0	1758	46	0
1	D	1815	0	1796	38	0
1	E	1815	0	1796	48	0
1	F	1815	0	1796	36	0
1	G	1815	0	1796	59	0
1	H	1815	0	1796	46	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	1	0	0	0	0
3	A	124	0	0	2	0
3	B	89	0	0	3	0
3	C	83	0	0	2	0
3	D	84	0	0	3	0
3	E	82	0	0	4	0
3	F	140	0	0	4	0
3	G	102	0	0	4	0
3	H	98	0	0	1	0
All	All	15287	0	14305	316	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 (316) 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:E:59:LEU:HD22	1:E:94:MSE:HE3	1.45	0.97
1:F:1:MSE:HB2	1:F:105:ARG:HH21	1.32	0.95
1:A:215:LEU:HD22	1:A:222:LEU:HD22	1.51	0.92
1:C:219:ALA:HB1	1:C:221:LYS:HE2	1.48	0.92
1:E:161:HIS:HD2	1:E:196:LEU:HD13	1.35	0.90
1:G:189:LYS:HE3	1:G:209:GLU:HG2	1.56	0.87
1:E:59:LEU:HD21	1:E:66:THR:HG21	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1:MSE:HB2	1:F:105:ARG:NH2	1.92	0.82
1:F:59:LEU:HD13	1:F:94:MSE:HE1	1.66	0.78
1:C:28:ALA:HB3	1:C:29:PRO:HD3	1.67	0.77
1:A:226:ASN:OD1	1:A:228:ARG:HG2	1.85	0.76
1:C:40:GLY:HA2	1:C:42:LEU:HD13	1.65	0.76
1:H:28:ALA:O	1:H:31:THR:HG22	1.83	0.76
1:A:215:LEU:HD22	1:A:222:LEU:CD2	2.15	0.76
1:E:28:ALA:HB3	1:E:29:PRO:HD3	1.66	0.76
1:E:190:GLY:O	1:E:192:LYS:HG3	1.86	0.75
1:E:200:TRP:HB2	1:E:220:ARG:HH11	1.51	0.75
1:G:21:LEU:HD12	1:G:58:ILE:CG2	2.18	0.74
1:A:130:ARG:HD3	3:A:1027:HOH:O	1.87	0.74
1:H:158:MSE:HE3	1:H:164:LEU:HD12	1.70	0.73
1:A:133:ALA:CB	1:A:171:GLU:HG2	2.20	0.72
1:E:18:LEU:O	1:E:22:GLU:HG3	1.90	0.71
1:H:174:HIS:O	1:H:178:THR:HG23	1.91	0.71
1:C:191:GLN:NE2	1:C:224:THR:HG23	2.05	0.71
1:D:4:THR:HG23	1:D:106:GLY:HA2	1.71	0.70
1:E:215:LEU:HD22	1:E:222:LEU:CD2	2.21	0.70
1:B:158:MSE:HG2	1:B:186:VAL:HG21	1.73	0.70
1:G:1:MSE:HG3	1:G:105:ARG:NH1	2.07	0.69
1:C:42:LEU:HD22	1:C:74:ASP:OD2	1.92	0.69
1:H:226:ASN:OD1	1:H:228:ARG:HG2	1.92	0.69
1:H:31:THR:OG1	1:H:214:LEU:HD22	1.93	0.69
1:D:158:MSE:HG2	1:D:165:ASN:HD22	1.58	0.68
1:F:164:LEU:HD12	1:F:194:GLU:HG2	1.73	0.68
1:E:4:THR:HA	1:E:105:ARG:HG3	1.75	0.68
1:A:158:MSE:HE1	1:A:164:LEU:HB3	1.76	0.68
1:B:28:ALA:O	1:B:31:THR:HG22	1.93	0.67
1:F:59:LEU:HD11	1:F:66:THR:HG21	1.76	0.67
1:C:48:LYS:HE2	1:C:48:LYS:HA	1.76	0.67
1:G:182:LEU:HD21	1:G:220:ARG:NH2	2.09	0.67
1:F:164:LEU:CD1	1:F:194:GLU:HG2	2.24	0.67
1:A:90:VAL:HB	1:G:182:LEU:HD23	1.77	0.65
1:G:21:LEU:HD12	1:G:58:ILE:HG22	1.78	0.65
1:C:162:LYS:HB2	1:C:162:LYS:NZ	2.12	0.65
1:H:182:LEU:HD11	1:H:220:ARG:NH1	2.11	0.65
1:E:4:THR:HG23	1:E:106:GLY:HA2	1.79	0.65
1:E:144:TRP:HZ2	1:E:178:THR:HG22	1.62	0.65
1:C:82:ARG:HG2	1:C:82:ARG:HH11	1.63	0.63
1:D:30:ASP:O	1:G:3:ARG:HD3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:158:MSE:HA	1:H:186:VAL:HG11	1.80	0.62
1:F:88:GLU:HG2	1:F:94:MSE:O	1.99	0.62
1:G:158:MSE:HE2	1:G:165:ASN:HD22	1.63	0.62
1:D:28:ALA:HB3	1:D:29:PRO:HD3	1.82	0.62
1:G:163:GLY:C	1:G:164:LEU:HD23	2.24	0.62
1:D:45:LYS:HZ3	1:D:127:GLU:C	2.07	0.62
1:E:23:LYS:HD2	1:E:227:VAL:HG13	1.82	0.61
1:E:161:HIS:CD2	1:E:196:LEU:HD13	2.26	0.61
1:H:161:HIS:ND1	1:H:164:LEU:HD23	2.15	0.61
1:D:1:MSE:HE2	1:F:103:PHE:HB2	1.82	0.61
1:F:43:MSE:HE2	1:F:51:ASP:HB3	1.82	0.61
1:G:88:GLU:HG2	1:G:94:MSE:O	2.01	0.61
1:G:130:ARG:NH1	3:G:946:HOH:O	2.30	0.61
1:A:106:GLY:N	1:A:107:PRO:HA	2.16	0.61
1:C:163:GLY:O	1:C:164:LEU:HD23	2.01	0.61
1:E:59:LEU:O	1:E:59:LEU:HD23	2.00	0.61
1:C:45:LYS:HB2	1:C:73:GLN:HB2	1.82	0.60
1:A:202:VAL:HG13	1:A:222:LEU:HD11	1.83	0.60
1:E:160:TYR:CE1	1:E:166:GLU:HG3	2.36	0.60
1:C:88:GLU:HG2	1:C:94:MSE:O	2.01	0.60
1:B:165:ASN:OD1	1:B:167:GLN:N	2.34	0.60
1:D:106:GLY:N	1:D:107:PRO:HA	2.17	0.59
1:G:27:LEU:HD11	1:G:212:TYR:CE2	2.37	0.59
1:A:38:LEU:HD23	1:A:38:LEU:C	2.27	0.59
1:H:164:LEU:HD23	1:H:164:LEU:H	1.68	0.59
1:G:18:LEU:O	1:G:22:GLU:HG3	2.03	0.59
1:E:209:GLU:HA	1:E:228:ARG:HH21	1.68	0.58
1:F:93:GLU:CD	1:F:93:GLU:H	2.09	0.58
1:D:164:LEU:HG	1:D:194:GLU:HG3	1.86	0.58
1:B:42:LEU:HD13	1:B:55:PHE:CE2	2.38	0.58
1:H:164:LEU:O	1:H:165:ASN:HB2	2.04	0.57
1:E:161:HIS:HE1	1:E:194:GLU:HG2	1.69	0.57
1:A:57:ARG:NH2	1:G:218:ARG:O	2.37	0.57
1:G:219:ALA:HB1	1:G:221:LYS:HE2	1.86	0.56
1:C:219:ALA:O	1:C:221:LYS:HG3	2.05	0.56
1:C:219:ALA:CB	1:C:221:LYS:HE2	2.27	0.56
1:D:38:LEU:C	1:D:38:LEU:HD23	2.30	0.56
1:B:53:ALA:O	1:B:57:ARG:HG3	2.06	0.56
1:B:158:MSE:HG2	1:B:186:VAL:CG2	2.36	0.56
1:F:59:LEU:CD1	1:F:66:THR:HG21	2.36	0.56
1:H:182:LEU:HD12	3:H:915:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:PRO:HB3	1:B:172:VAL:HG12	1.88	0.56
1:D:227:VAL:O	1:D:228:ARG:CB	2.53	0.56
1:C:162:LYS:HB2	1:C:162:LYS:HZ2	1.71	0.55
1:G:160:TYR:CE1	1:G:166:GLU:HA	2.41	0.55
1:E:48:LYS:HD3	3:E:975:HOH:O	2.07	0.55
1:H:18:LEU:O	1:H:22:GLU:HG3	2.06	0.55
1:A:43:MSE:HE3	1:A:55:PHE:HB2	1.89	0.55
1:D:227:VAL:O	1:D:228:ARG:HB3	2.07	0.55
1:H:164:LEU:HD22	1:H:194:GLU:HB2	1.89	0.55
1:G:164:LEU:HD13	1:G:194:GLU:OE2	2.06	0.54
1:C:159:PRO:HB3	1:C:172:VAL:HG12	1.89	0.54
1:E:130:ARG:HD2	3:E:950:HOH:O	2.07	0.54
1:C:210:GLY:O	1:C:226:ASN:HA	2.07	0.54
1:H:31:THR:HG23	1:H:33:ALA:H	1.72	0.54
1:D:159:PRO:HB3	1:D:172:VAL:HG12	1.89	0.54
1:E:162:LYS:HG3	1:E:166:GLU:OE1	2.08	0.54
1:D:45:LYS:NZ	1:D:127:GLU:HA	2.23	0.54
1:B:194:GLU:HG3	3:B:952:HOH:O	2.07	0.53
1:F:75:ALA:HA	1:F:76:PRO:C	2.33	0.53
1:E:161:HIS:CE1	1:E:194:GLU:HG2	2.44	0.53
1:H:210:GLY:O	1:H:226:ASN:HA	2.08	0.53
1:A:59:LEU:HD22	3:A:947:HOH:O	2.08	0.53
1:C:48:LYS:HA	1:C:48:LYS:CE	2.38	0.53
1:D:210:GLY:O	1:D:226:ASN:HA	2.09	0.53
1:G:77:ILE:HG23	1:G:78:TRP:N	2.23	0.53
1:H:106:GLY:N	1:H:107:PRO:HA	2.24	0.53
1:H:228:ARG:O	1:H:228:ARG:HG3	2.09	0.53
1:H:48:LYS:O	1:H:51:ASP:HB2	2.09	0.53
1:F:147:LYS:HG2	3:F:999:HOH:O	2.09	0.53
1:E:59:LEU:HD22	1:E:94:MSE:CE	2.31	0.52
1:G:226:ASN:OD1	1:G:228:ARG:HG3	2.08	0.52
1:D:148:ASP:OD2	1:E:3:ARG:NH1	2.42	0.52
1:G:222:LEU:C	1:G:222:LEU:HD23	2.35	0.52
1:C:189:LYS:HZ3	1:C:209:GLU:CD	2.16	0.52
1:G:212:TYR:CD1	1:G:212:TYR:C	2.87	0.52
1:H:219:ALA:HB1	1:H:221:LYS:HE3	1.92	0.52
1:B:103:PHE:CD1	1:H:1:MSE:HG2	2.45	0.52
1:E:1:MSE:C	1:E:1:MSE:SE	3.03	0.52
1:E:158:MSE:SE	1:E:165:ASN:HD22	2.43	0.52
1:C:91:HIS:HB3	1:C:93:GLU:OE2	2.10	0.51
1:A:220:ARG:HH11	1:A:220:ARG:HG3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:TRP:HZ2	1:D:178:THR:HG22	1.74	0.51
1:C:14:PRO:HD2	1:C:41:ASN:O	2.10	0.51
1:H:220:ARG:HG2	1:H:220:ARG:HH11	1.74	0.51
1:E:30:ASP:HB2	3:E:979:HOH:O	2.10	0.51
1:H:159:PRO:HB3	1:H:172:VAL:HG12	1.92	0.51
1:B:215:LEU:HD23	1:B:215:LEU:N	2.25	0.51
1:E:38:LEU:C	1:E:38:LEU:HD23	2.36	0.51
1:F:91:HIS:HB2	1:F:94:MSE:HG3	1.92	0.51
1:G:210:GLY:HA2	1:G:227:VAL:HG22	1.93	0.51
1:B:103:PHE:CG	1:H:1:MSE:HG2	2.46	0.51
1:D:75:ALA:HA	1:D:76:PRO:C	2.36	0.51
1:C:38:LEU:HD21	1:C:42:LEU:HD12	1.94	0.50
1:E:191:GLN:NE2	1:E:224:THR:HB	2.26	0.50
1:G:222:LEU:HD23	1:G:222:LEU:O	2.10	0.50
1:H:31:THR:OG1	1:H:214:LEU:HD13	2.12	0.50
1:H:158:MSE:HG2	1:H:186:VAL:HG11	1.94	0.50
1:A:133:ALA:HB2	1:A:171:GLU:HG2	1.94	0.50
1:G:226:ASN:OD1	1:G:228:ARG:N	2.45	0.50
1:E:43:MSE:HE3	1:E:55:PHE:HB2	1.93	0.50
1:D:6:ARG:CZ	1:D:7:TYR:OH	2.60	0.50
1:A:76:PRO:HG2	1:A:79:GLU:HG3	1.92	0.50
1:A:182:LEU:HD11	1:A:220:ARG:NH2	2.27	0.50
1:B:144:TRP:HB3	1:G:147:LYS:HD2	1.94	0.50
1:C:9:LEU:HG	1:C:24:PHE:CE1	2.47	0.50
1:C:67:ALA:HA	1:C:95:ARG:O	2.12	0.49
1:C:40:GLY:CA	1:C:42:LEU:HD13	2.40	0.49
1:D:85:ALA:O	1:D:89:LEU:HG	2.12	0.49
1:A:1:MSE:HG2	1:G:103:PHE:CD1	2.46	0.49
1:A:75:ALA:HA	1:A:76:PRO:C	2.37	0.49
1:D:7:TYR:HA	1:D:215:LEU:O	2.13	0.49
1:H:158:MSE:CE	1:H:164:LEU:HD12	2.40	0.49
1:F:16:GLY:HA2	1:F:43:MSE:SE	2.63	0.49
1:A:215:LEU:N	1:A:215:LEU:HD23	2.28	0.49
1:D:133:ALA:CB	1:D:171:GLU:HG2	2.43	0.49
1:F:18:LEU:O	1:F:22:GLU:HG3	2.12	0.48
1:B:98:HIS:O	1:B:99:GLU:HB2	2.13	0.48
1:E:215:LEU:N	1:E:215:LEU:HD23	2.28	0.48
1:B:28:ALA:HB3	1:B:29:PRO:HD3	1.94	0.48
1:C:82:ARG:HH11	1:C:82:ARG:CG	2.26	0.48
1:F:133:ALA:HB2	1:F:171:GLU:HG3	1.96	0.48
1:E:4:THR:HA	1:E:105:ARG:CG	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:GLY:N	1:E:107:PRO:HA	2.28	0.48
1:H:161:HIS:O	1:H:163:GLY:N	2.46	0.48
1:E:82:ARG:HD3	1:F:134:TRP:CE2	2.49	0.48
1:E:226:ASN:OD1	1:E:228:ARG:HG2	2.14	0.48
1:B:138:TYR:CE1	1:B:141:LYS:HE2	2.49	0.47
1:C:7:TYR:HA	1:C:215:LEU:O	2.15	0.47
1:G:59:LEU:HD13	1:G:94:MSE:HE1	1.96	0.47
1:E:59:LEU:HD23	3:E:927:HOH:O	2.15	0.47
1:F:28:ALA:HB3	1:F:29:PRO:HD3	1.96	0.47
1:F:43:MSE:HE3	1:F:47:ALA:HB2	1.97	0.47
1:G:16:GLY:HA2	1:G:43:MSE:CE	2.45	0.47
1:C:144:TRP:HB3	1:F:147:LYS:HE3	1.96	0.47
1:D:164:LEU:HD21	1:D:194:GLU:HG2	1.97	0.47
1:G:21:LEU:CD1	1:G:58:ILE:HG22	2.44	0.47
1:G:71:GLY:O	1:G:129:LEU:HD12	2.15	0.47
1:D:21:LEU:HD22	1:D:55:PHE:CE1	2.50	0.46
1:D:189:LYS:HE3	1:D:209:GLU:HG3	1.98	0.46
1:C:75:ALA:HA	1:C:76:PRO:C	2.40	0.46
1:C:135:VAL:O	1:C:139:ARG:HG2	2.15	0.46
1:E:190:GLY:O	1:E:192:LYS:HE3	2.15	0.46
1:G:23:LYS:O	1:G:27:LEU:HB3	2.15	0.46
1:H:182:LEU:HD11	1:H:220:ARG:HH12	1.81	0.46
1:A:64:LEU:O	1:A:65:PRO:C	2.58	0.46
1:B:99:GLU:HG2	1:B:139:ARG:HG2	1.98	0.46
1:D:180:ASN:ND2	3:D:934:HOH:O	2.48	0.46
1:A:220:ARG:HG3	1:A:220:ARG:NH1	2.31	0.45
1:C:21:LEU:O	1:C:24:PHE:HB3	2.15	0.45
1:C:31:THR:HB	1:C:214:LEU:HD22	1.97	0.45
1:D:132:PRO:HB2	1:D:134:TRP:CD1	2.51	0.45
1:D:138:TYR:O	1:D:141:LYS:HB3	2.16	0.45
1:F:26:LYS:HG2	3:F:1043:HOH:O	2.17	0.45
1:G:14:PRO:HD2	1:G:41:ASN:O	2.16	0.45
1:G:28:ALA:HB3	1:G:29:PRO:HD3	1.98	0.45
1:F:210:GLY:O	1:F:226:ASN:HA	2.16	0.45
1:G:161:HIS:CD2	1:G:164:LEU:HD12	2.51	0.45
1:C:38:LEU:CD2	1:C:42:LEU:HD12	2.46	0.45
1:C:186:VAL:O	1:C:204:PRO:HD2	2.17	0.45
1:D:4:THR:HG22	1:D:5:VAL:N	2.31	0.45
1:E:45:LYS:NZ	1:E:127:GLU:OE1	2.46	0.45
1:E:23:LYS:CD	1:E:227:VAL:HG13	2.44	0.45
1:E:13:ASN:N	1:E:14:PRO:HD3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:ARG:HA	1:E:82:ARG:HD2	1.81	0.45
1:G:1:MSE:HE3	3:G:916:HOH:O	2.17	0.45
1:F:218:ARG:HG3	1:F:218:ARG:HH11	1.82	0.45
1:F:158:MSE:HE2	3:F:1039:HOH:O	2.16	0.44
1:G:52:TYR:OH	1:G:74:ASP:HA	2.18	0.44
1:F:215:LEU:N	1:F:215:LEU:HD23	2.32	0.44
1:G:27:LEU:C	1:G:27:LEU:HD23	2.42	0.44
1:G:139:ARG:NH2	3:G:987:HOH:O	2.50	0.44
1:B:75:ALA:HA	1:B:76:PRO:C	2.43	0.44
1:C:24:PHE:O	1:C:27:LEU:HB2	2.18	0.44
1:F:91:HIS:CB	1:F:94:MSE:HG3	2.48	0.44
1:E:215:LEU:HD22	1:E:222:LEU:HD21	1.95	0.44
1:G:91:HIS:HB2	1:G:94:MSE:HG3	1.99	0.44
1:H:77:ILE:HG23	1:H:78:TRP:N	2.32	0.44
1:H:206:ASP:H	1:H:211:GLU:HB2	1.82	0.44
1:G:38:LEU:C	1:G:38:LEU:HD23	2.43	0.44
1:G:163:GLY:O	1:G:164:LEU:HD23	2.17	0.44
1:A:59:LEU:HD13	1:A:94:MSE:HE3	1.98	0.44
1:E:23:LYS:HD2	1:E:227:VAL:CG1	2.45	0.44
1:H:75:ALA:HA	1:H:76:PRO:C	2.42	0.44
1:C:106:GLY:N	1:C:107:PRO:HA	2.33	0.43
1:F:135:VAL:O	1:F:139:ARG:HG2	2.17	0.43
1:G:57:ARG:NH1	3:G:956:HOH:O	2.51	0.43
1:H:6:ARG:O	1:H:217:LEU:HB2	2.19	0.43
1:H:42:LEU:HD13	1:H:55:PHE:CE2	2.53	0.43
1:H:193:HIS:O	1:H:194:GLU:HG2	2.18	0.43
1:A:158:MSE:HE2	1:A:158:MSE:HB3	1.94	0.43
1:E:23:LYS:O	1:E:27:LEU:HG	2.18	0.43
1:H:72:PRO:HD3	1:H:156:HIS:CD2	2.53	0.43
1:D:226:ASN:C	1:D:228:ARG:H	2.26	0.43
1:D:207:LEU:C	1:D:210:GLY:H	2.26	0.43
1:G:207:LEU:C	1:G:209:GLU:N	2.76	0.43
1:B:11:THR:OG1	1:B:207:LEU:HB2	2.17	0.43
1:C:43:MSE:HE3	1:C:55:PHE:HB2	2.01	0.43
1:A:210:GLY:O	1:A:226:ASN:HA	2.19	0.43
1:G:15:MSE:HE1	1:G:73:GLN:NE2	2.34	0.43
1:A:9:LEU:HG	1:A:24:PHE:CZ	2.54	0.43
1:D:43:MSE:HB3	1:D:47:ALA:CB	2.49	0.43
1:E:206:ASP:OD2	1:E:206:ASP:C	2.62	0.43
1:G:210:GLY:O	1:G:226:ASN:HA	2.18	0.43
1:D:215:LEU:HD12	1:D:215:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:HD22	1:A:55:PHE:CE1	2.54	0.42
1:B:106:GLY:N	1:B:107:PRO:HA	2.34	0.42
1:B:185:LEU:HD21	1:B:215:LEU:HD11	2.00	0.42
1:D:122:GLU:O	1:D:130:ARG:NH1	2.52	0.42
1:G:26:LYS:HD3	1:G:26:LYS:C	2.44	0.42
1:C:27:LEU:O	1:C:28:ALA:C	2.62	0.42
1:C:82:ARG:CG	1:C:82:ARG:NH1	2.83	0.42
1:C:207:LEU:C	1:C:209:GLU:N	2.77	0.42
1:G:40:GLY:HA2	1:G:42:LEU:HD12	2.02	0.42
1:G:82:ARG:HD3	1:H:134:TRP:CE2	2.53	0.42
1:C:185:LEU:HD21	1:C:215:LEU:HD11	2.00	0.42
1:G:164:LEU:HD13	1:G:194:GLU:CD	2.43	0.42
1:G:189:LYS:CE	1:G:209:GLU:HG2	2.37	0.42
1:E:42:LEU:HD13	1:E:55:PHE:CE2	2.54	0.42
1:E:59:LEU:HD23	1:E:59:LEU:C	2.44	0.42
1:B:176:ILE:CG2	1:B:196:LEU:HD22	2.50	0.42
1:G:91:HIS:HB3	1:G:93:GLU:OE2	2.19	0.42
1:B:148:ASP:O	1:H:93:GLU:HB3	2.20	0.42
1:G:120:GLU:HB3	1:G:121:GLY:H	1.70	0.42
1:H:27:LEU:HD11	1:H:227:VAL:HG12	2.02	0.42
1:C:153:PHE:C	1:C:154:LEU:HD23	2.44	0.42
1:D:119:ASP:O	1:D:120:GLU:HG2	2.20	0.42
1:G:119:ASP:O	1:G:120:GLU:HG3	2.20	0.42
1:G:210:GLY:CA	1:G:227:VAL:HG22	2.49	0.42
1:H:189:LYS:O	1:H:192:LYS:NZ	2.52	0.42
1:A:186:VAL:O	1:A:204:PRO:HD2	2.19	0.42
1:H:206:ASP:N	1:H:211:GLU:HB2	2.35	0.41
1:E:11:THR:OG1	1:E:207:LEU:HB2	2.20	0.41
1:F:43:MSE:HE2	1:F:47:ALA:HB1	2.01	0.41
1:F:45:LYS:HA	1:F:73:GLN:O	2.21	0.41
1:C:42:LEU:CD2	1:C:70:PRO:HA	2.51	0.41
1:F:1:MSE:CB	1:F:105:ARG:HH21	2.18	0.41
1:F:133:ALA:CB	1:F:171:GLU:HG3	2.50	0.41
1:G:26:LYS:HD3	1:G:26:LYS:O	2.20	0.41
1:A:3:ARG:NH1	1:H:147:LYS:HB3	2.35	0.41
1:F:158:MSE:HE1	3:F:1036:HOH:O	2.20	0.41
1:H:171:GLU:O	1:H:174:HIS:HB3	2.20	0.41
1:A:145:GLU:HG3	3:B:976:HOH:O	2.20	0.41
1:C:156:HIS:HE1	3:C:967:HOH:O	2.02	0.41
1:D:126:HIS:HD2	3:D:925:HOH:O	2.03	0.41
1:A:2:ARG:HD2	1:G:148:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:PRO:HB3	1:F:172:VAL:HG12	2.02	0.41
1:H:31:THR:HG23	1:H:33:ALA:N	2.36	0.41
1:G:21:LEU:HD12	1:G:58:ILE:HG21	1.97	0.41
1:C:222:LEU:HD12	1:C:222:LEU:C	2.46	0.41
1:H:2:ARG:HH11	1:H:2:ARG:HG2	1.86	0.41
1:C:42:LEU:HD13	1:C:42:LEU:N	2.35	0.41
1:A:189:LYS:HG2	1:A:206:ASP:CB	2.51	0.40
1:B:212:TYR:CD1	1:B:212:TYR:C	2.98	0.40
1:E:141:LYS:NZ	1:F:88:GLU:HB3	2.36	0.40
1:G:78:TRP:CE2	1:H:123:PRO:HB2	2.55	0.40
1:B:31:THR:HG23	1:B:33:ALA:H	1.87	0.40
1:D:4:THR:CG2	1:D:106:GLY:HA2	2.45	0.40
1:G:182:LEU:HD13	1:G:182:LEU:C	2.45	0.40
1:B:38:LEU:O	1:B:68:TYR:HA	2.21	0.40
1:B:139:ARG:HD3	3:B:920:HOH:O	2.21	0.40
1:B:171:GLU:OE1	1:B:171:GLU:HA	2.22	0.40
1:C:52:TYR:HE1	3:C:956:HOH:O	2.04	0.40
1:F:1:MSE:HB2	1:F:105:ARG:CZ	2.50	0.40
1:H:67:ALA:HA	1:H:95:ARG:O	2.21	0.40
1:B:64:LEU:O	1:B:65:PRO:C	2.65	0.40
1:D:39:ILE:HD11	1:D:185:LEU:HB3	2.02	0.40
1:D:59:LEU:HD22	3:D:921:HOH:O	2.22	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	226/228 (99%)	217 (96%)	9 (4%)	0	100	100
1	B	224/228 (98%)	211 (94%)	11 (5%)	2 (1%)	14	10
1	C	223/228 (98%)	210 (94%)	12 (5%)	1 (0%)	30	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	226/228 (99%)	217 (96%)	9 (4%)	0	100	100
1	E	226/228 (99%)	212 (94%)	14 (6%)	0	100	100
1	F	226/228 (99%)	217 (96%)	9 (4%)	0	100	100
1	G	226/228 (99%)	212 (94%)	14 (6%)	0	100	100
1	H	226/228 (99%)	213 (94%)	11 (5%)	2 (1%)	14	10
All	All	1803/1824 (99%)	1709 (95%)	89 (5%)	5 (0%)	36	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	162	LYS
1	H	165	ASN
1	C	28	ALA
1	B	163	GLY
1	B	29	PRO

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	186/180 (103%)	180 (97%)	6 (3%)	34	38
1	B	184/180 (102%)	175 (95%)	9 (5%)	22	22
1	C	183/180 (102%)	176 (96%)	7 (4%)	29	32
1	D	186/180 (103%)	182 (98%)	4 (2%)	45	53
1	E	186/180 (103%)	177 (95%)	9 (5%)	23	23
1	F	186/180 (103%)	176 (95%)	10 (5%)	20	18
1	G	186/180 (103%)	180 (97%)	6 (3%)	34	38
1	H	186/180 (103%)	181 (97%)	5 (3%)	39	45
All	All	1483/1440 (103%)	1427 (96%)	56 (4%)	29	32

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	96	ASN
1	A	192	LYS
1	A	207	LEU
1	A	215	LEU
1	A	224	THR
1	B	31	THR
1	B	42	LEU
1	B	59	LEU
1	B	81	LEU
1	B	96	ASN
1	B	127	GLU
1	B	139	ARG
1	B	209	GLU
1	B	215	LEU
1	C	42	LEU
1	C	59	LEU
1	C	96	ASN
1	C	154	LEU
1	C	162	LYS
1	C	215	LEU
1	C	224	THR
1	D	26	LYS
1	D	59	LEU
1	D	96	ASN
1	D	166	GLU
1	E	42	LEU
1	E	61	GLU
1	E	69	VAL
1	E	96	ASN
1	E	158	MSE
1	E	162	LYS
1	E	209	GLU
1	E	215	LEU
1	E	227	VAL
1	F	5	VAL
1	F	21	LEU
1	F	42	LEU
1	F	59	LEU
1	F	81	LEU
1	F	82	ARG
1	F	93	GLU
1	F	96	ASN

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Mol	Chain	Res	Type
1	F	105	ARG
1	F	215	LEU
1	G	27	LEU
1	G	57	ARG
1	G	59	LEU
1	G	96	ASN
1	G	209	GLU
1	G	222	LEU
1	H	21	LEU
1	H	42	LEU
1	H	59	LEU
1	H	82	ARG
1	H	96	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	91	HIS
1	B	161	HIS
1	B	174	HIS
1	C	156	HIS
1	D	126	HIS
1	D	165	ASN
1	D	174	HIS
1	D	180	ASN
1	E	161	HIS
1	E	170	HIS
1	F	167	GLN
1	G	86	ASN
1	G	161	HIS
1	G	165	ASN
1	G	167	GLN
1	G	180	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 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	222/228 (97%)	-0.24	0 100 100	16, 26, 38, 52	0
1	B	221/228 (96%)	-0.04	4 (1%) 67 70	18, 28, 47, 62	0
1	C	220/228 (96%)	0.23	3 (1%) 73 75	22, 35, 50, 60	0
1	D	222/228 (97%)	0.10	2 (0%) 81 83	18, 31, 44, 65	0
1	E	222/228 (97%)	0.20	5 (2%) 61 64	21, 32, 49, 61	0
1	F	222/228 (97%)	-0.38	0 100 100	15, 23, 37, 54	0
1	G	222/228 (97%)	-0.00	4 (1%) 67 70	17, 30, 45, 64	0
1	H	222/228 (97%)	-0.13	3 (1%) 73 75	16, 27, 43, 59	0
All	All	1773/1824 (97%)	-0.03	21 (1%) 76 78	15, 29, 46, 65	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	GLY	4.2
1	D	228	ARG	4.1
1	B	164	LEU	3.7
1	E	27	LEU	3.5
1	E	163	GLY	3.3
1	H	163	GLY	3.1
1	B	3	ARG	3.0
1	H	164	LEU	3.0
1	E	222	LEU	2.9
1	E	164	LEU	2.8
1	G	163	GLY	2.4
1	G	164	LEU	2.3
1	D	167	GLN	2.3
1	B	4	THR	2.2
1	C	164	LEU	2.2
1	C	227	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	4	THR	2.2
1	G	227	VAL	2.1
1	G	165	ASN	2.0
1	E	227	VAL	2.0
1	H	27	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	909	1/1	0.95	0.05	45,45,45,45	0
2	CA	A	901	1/1	0.96	0.06	29,29,29,29	0
2	CA	E	911	1/1	0.97	0.03	45,45,45,45	0
2	CA	D	904	1/1	0.98	0.03	35,35,35,35	0
2	CA	D	913	1/1	0.98	0.07	30,30,30,30	0
2	CA	E	905	1/1	0.98	0.04	32,32,32,32	0
2	CA	C	910	1/1	0.98	0.03	51,51,51,51	0
2	CA	G	912	1/1	0.98	0.05	45,45,45,45	0
2	CA	B	902	1/1	0.99	0.02	32,32,32,32	0
2	CA	F	906	1/1	0.99	0.02	26,26,26,26	0
2	CA	F	914	1/1	0.99	0.05	31,31,31,31	0
2	CA	G	907	1/1	0.99	0.04	34,34,34,34	0
2	CA	C	903	1/1	0.99	0.02	39,39,39,39	0
2	CA	H	908	1/1	0.99	0.02	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.