



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:22 AM UTC

PDB ID : 2PT7 / pdb_00002pt7
Title : Crystal structure of Cag VirB11 (HP0525) and an inhibitory protein (HP1451)
Authors : Hare, S.; Fischer, W.; Williams, R.; Terradot, L.; Bayliss, R.; Haas, R.; Waksman, G.
Deposited on : 2007-05-08
Resolution : 2.40 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

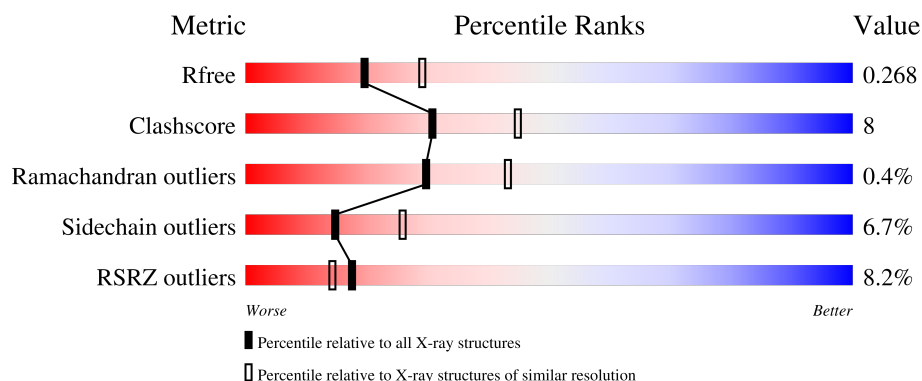
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	330	5% 81% 15% ..
1	B	330	5% 76% 15% • 7%
1	C	330	7% 78% 12% • 7%
1	D	330	4% 80% 16% ..
1	E	330	10% 78% 13% • 7%

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Mol	Chain	Length	Quality of chain
1	F	330	8% 77% 12% • 7%
2	G	152	16% 68% 23% 5% 5%
2	H	152	14% 64% 26% 5% • 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17894 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 Cag-alfa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2565	1625	440	486	14			
1	B	308	Total	C	N	O	S	0	0	0
			2454	1554	422	464	14			
1	C	307	Total	C	N	O	S	0	0	0
			2441	1545	419	463	14			
1	D	323	Total	C	N	O	S	0	0	0
			2568	1627	441	486	14			
1	E	308	Total	C	N	O	S	0	0	0
			2454	1554	422	464	14			
1	F	307	Total	C	N	O	S	0	0	0
			2445	1548	420	463	14			

- Molecule 2 is a protein called Hypothetical protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	145	Total	C	N	O	S	0	0	0
			1140	743	183	212	2			
2	H	145	Total	C	N	O	S	0	0	0
			1140	744	185	208	3			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	124	Total	O	0	0
			124	124		
3	B	107	Total	O	0	0
			107	107		
3	C	109	Total	O	0	0
			109	109		
3	D	137	Total	O	0	0
			137	137		

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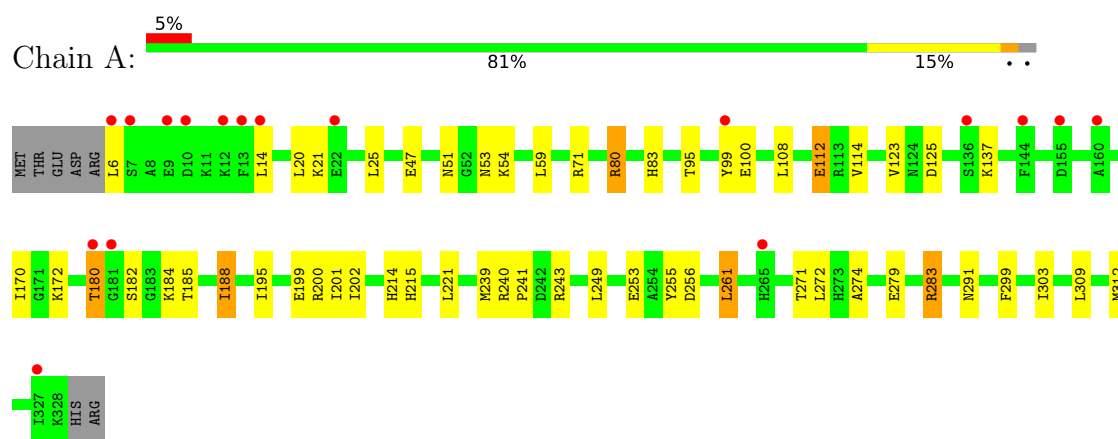
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	77	Total 77	O 77	0	0
3	F	82	Total 82	O 82	0	0
3	G	26	Total 26	O 26	0	0
3	H	25	Total 25	O 25	0	0

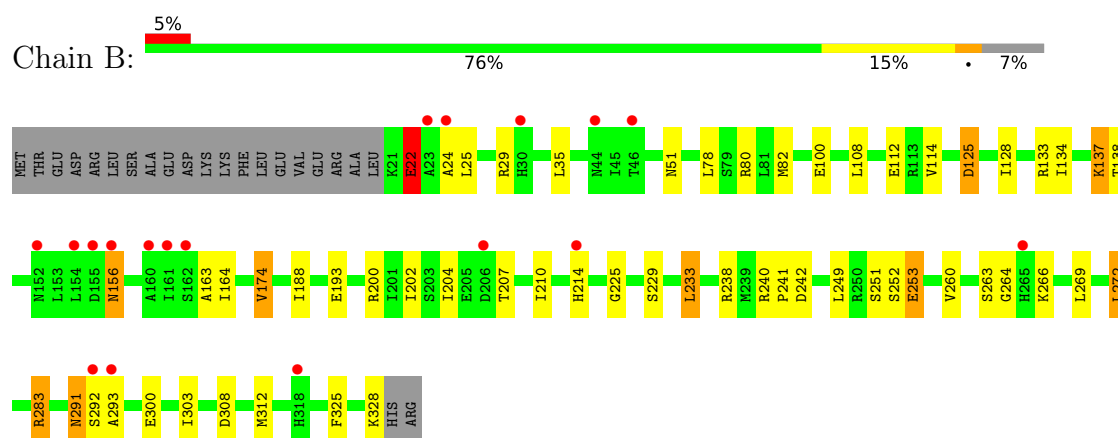
3 Residue-property plots [i](#)

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.

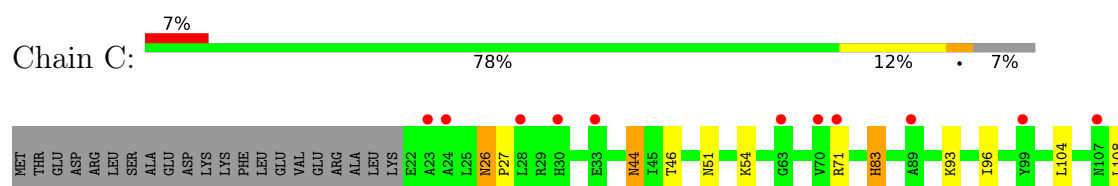
• Molecule 1: Cag-alfa

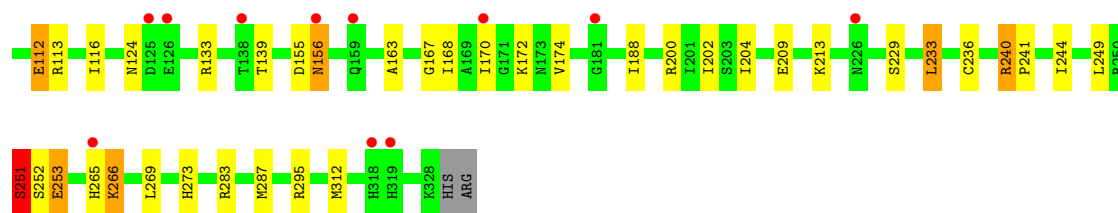


• Molecule 1: Cag-alfa

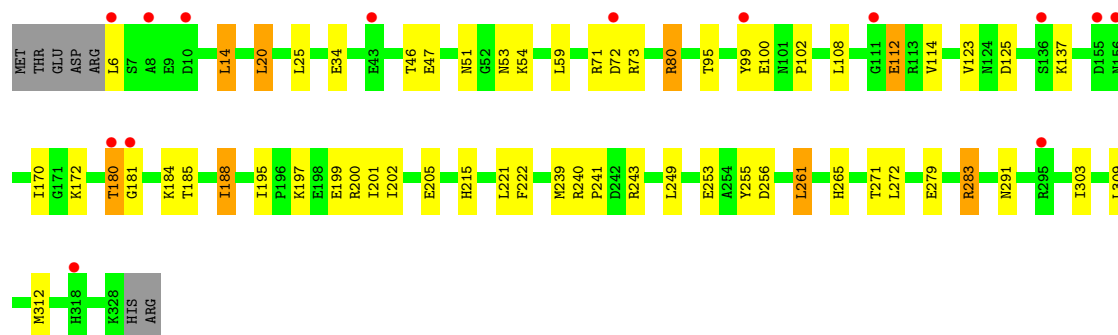
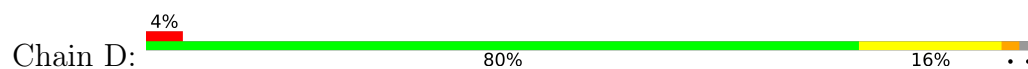


• Molecule 1: Cag-alfa

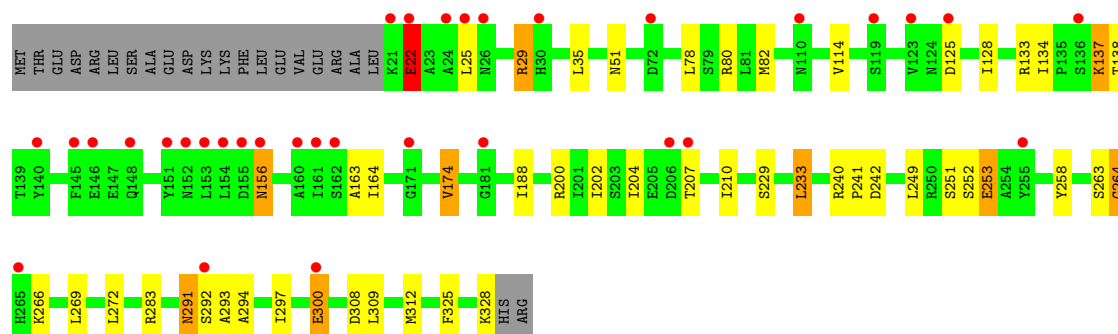
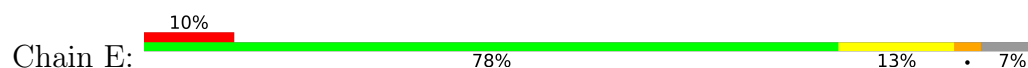




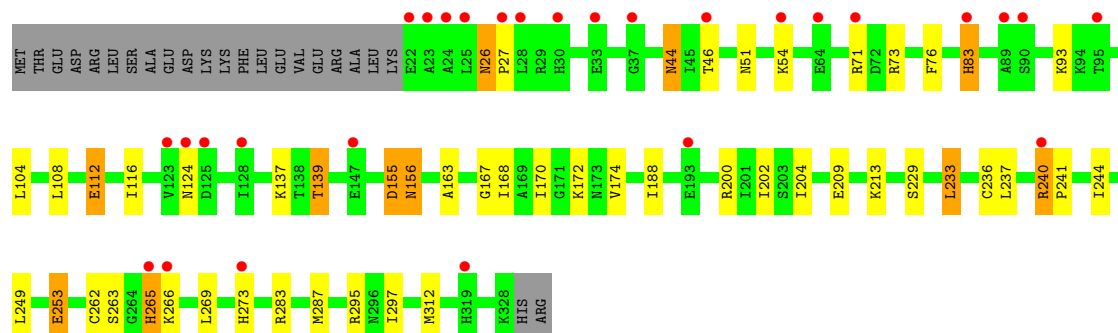
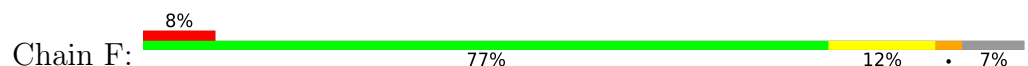
• Molecule 1: Cag-alfa



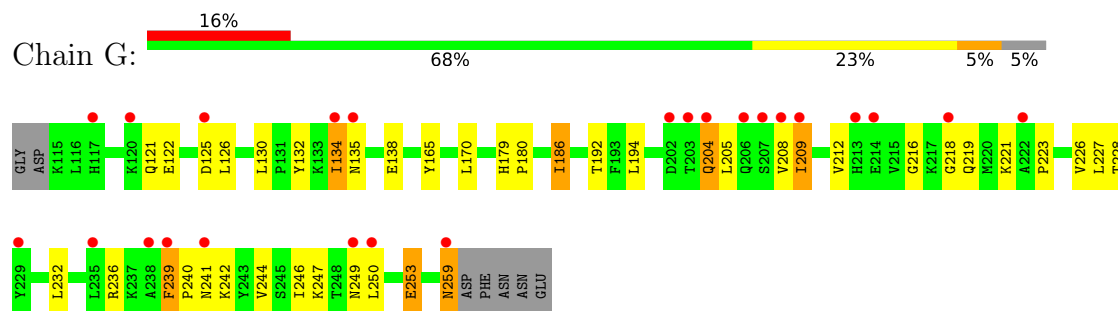
• Molecule 1: Cag-alfa



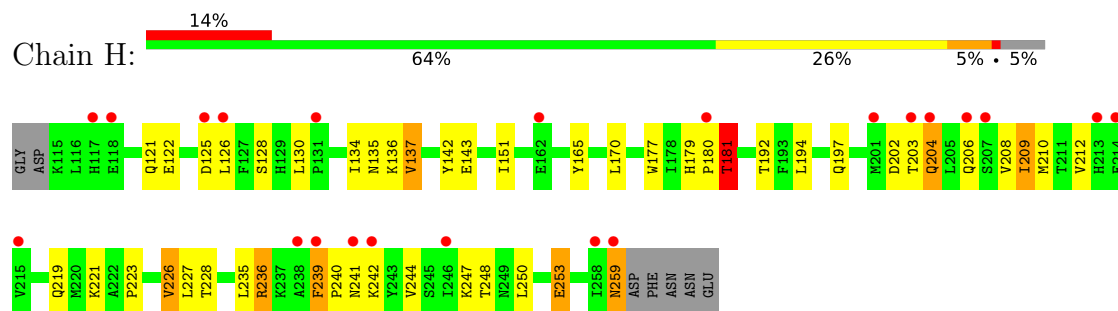
• Molecule 1: Cag-alfa



• Molecule 2: Hypothetical protein



• Molecule 2: Hypothetical protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.85Å 86.90Å 104.13Å 111.04° 95.98° 104.94°	Depositor
Resolution (Å)	40.00 – 2.40 40.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.3 (40.00-2.40) 96.2 (40.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.230 , 0.270 0.229 , 0.268	Depositor DCC
R_{free} test set	5056 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.0	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	0.90	EDS
Total number of atoms	17894	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.43% 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

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	0.57	2/2614 (0.1%)	0.86	4/3522 (0.1%)
1	B	0.65	2/2502 (0.1%)	0.84	2/3370 (0.1%)
1	C	0.62	4/2489 (0.2%)	0.84	2/3355 (0.1%)
1	D	0.58	3/2617 (0.1%)	0.87	4/3525 (0.1%)
1	E	0.80	5/2502 (0.2%)	0.85	2/3370 (0.1%)
1	F	0.65	4/2493 (0.2%)	0.83	1/3359 (0.0%)
2	G	0.76	1/1163 (0.1%)	0.92	3/1579 (0.2%)
2	H	0.85	5/1164 (0.4%)	1.00	5/1580 (0.3%)
All	All	0.67	26/17544 (0.1%)	0.86	23/23660 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	1
2	G	0	1
2	H	0	1
All	All	0	4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	22	GLU	CD-OE2	27.67	1.77	1.25
1	B	22	GLU	CD-OE2	16.38	1.56	1.25
1	F	265	HIS	CE1-NE2	12.71	1.45	1.32
2	G	259	ASN	C-O	9.61	1.42	1.23
1	C	265	HIS	CE1-NE2	9.52	1.42	1.32
1	C	266	LYS	CE-NZ	8.60	1.75	1.49
1	B	22	GLU	CD-OE1	8.45	1.41	1.25
2	H	128	SER	CB-OG	8.00	1.58	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	265	HIS	CG-ND1	7.80	1.46	1.38
2	H	259	ASN	C-O	-7.71	1.08	1.23
1	E	22	GLU	CD-OE1	7.67	1.40	1.25
1	F	265	HIS	CG-CD2	7.18	1.43	1.35
2	H	209	ILE	CG1-CD1	7.12	1.79	1.51
1	E	29	ARG	CZ-NH1	6.44	1.41	1.32
1	F	263	SER	N-CA	6.44	1.54	1.46
2	H	137	VAL	CA-CB	6.37	1.60	1.53
1	C	265	HIS	CG-CD2	5.78	1.42	1.35
1	A	14	LEU	CG-CD2	-5.47	1.34	1.52
1	C	265	HIS	CG-ND1	5.44	1.44	1.38
1	A	20	LEU	CG-CD1	-5.39	1.34	1.52
1	D	20	LEU	CG-CD2	-5.31	1.35	1.52
1	D	14	LEU	CG-CD1	-5.27	1.35	1.52
1	D	20	LEU	CG-CD1	-5.23	1.35	1.52
1	E	22	GLU	CG-CD	5.23	1.65	1.52
1	E	22	GLU	CB-CG	5.08	1.67	1.52
2	H	236	ARG	CZ-NH1	5.05	1.39	1.32

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	22	GLU	CB-CG-CD	-8.46	98.22	112.60
1	A	20	LEU	CD1-CG-CD2	-7.55	94.19	110.80
1	D	14	LEU	CD1-CG-CD2	-7.46	94.38	110.80
1	A	14	LEU	CD1-CG-CD2	-7.10	95.18	110.80
1	D	188	ILE	CB-CA-C	-7.03	102.65	112.14
1	D	20	LEU	CD1-CG-CD2	-6.89	95.64	110.80
1	A	188	ILE	CB-CA-C	-6.52	103.62	111.97
2	H	209	ILE	CB-CG1-CD1	-6.20	100.78	113.80
2	H	181	THR	N-CA-C	6.10	119.19	111.69
1	C	124	ASN	N-CA-C	6.06	116.08	108.45
1	F	124	ASN	N-CA-C	5.92	115.91	108.45
1	A	123	VAL	N-CA-C	5.88	116.61	110.62
1	D	123	VAL	N-CA-C	5.86	116.59	110.62
1	C	266	LYS	CB-CA-C	-5.76	100.35	109.80
1	B	22	GLU	CG-CD-OE1	5.53	131.11	118.40
2	H	137	VAL	CB-CA-C	5.37	116.65	111.23
1	E	22	GLU	CA-CB-CG	-5.29	103.53	114.10
1	B	22	GLU	CG-CD-OE2	-5.21	106.41	118.40
2	H	130	LEU	CA-C-N	5.20	126.01	119.98
2	H	130	LEU	C-N-CA	5.20	126.01	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	130	LEU	CA-C-N	5.13	126.25	119.84
2	G	130	LEU	C-N-CA	5.13	126.25	119.84
2	G	186	ILE	N-CA-C	5.07	117.12	108.86

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	22	GLU	Sidechain
1	E	22	GLU	Sidechain
2	G	239	PHE	Peptide
2	H	239	PHE	Peptide

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	2565	0	2538	46	0
1	B	2454	0	2435	46	0
1	C	2441	0	2411	46	0
1	D	2568	0	2547	42	0
1	E	2454	0	2435	41	0
1	F	2445	0	2422	46	0
2	G	1140	0	1131	32	0
2	H	1140	0	1135	31	0
3	A	124	0	0	4	0
3	B	107	0	0	4	0
3	C	109	0	0	2	0
3	D	137	0	0	2	0
3	E	77	0	0	4	0
3	F	82	0	0	2	0
3	G	26	0	0	1	0
3	H	25	0	0	3	0
All	All	17894	0	17054	285	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 8.

All (285) 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)
2:H:209:ILE:CD1	2:H:209:ILE:CG1	1.79	1.58
1:C:266:LYS:CE	1:C:266:LYS:NZ	1.75	1.47
1:E:22:GLU:CD	1:E:22:GLU:OE2	1.77	1.27
1:A:201:ILE:HD11	1:A:215:HIS:ND1	1.81	0.95
1:E:300:GLU:OE1	3:E:391:HOH:O	1.86	0.93
1:D:201:ILE:HD11	1:D:215:HIS:ND1	1.85	0.91
1:D:200:ARG:HH12	1:E:51:ASN:HD21	1.14	0.90
1:A:200:ARG:HH12	1:B:51:ASN:HD21	1.21	0.86
1:F:237:LEU:HD22	1:F:265:HIS:HE1	1.38	0.85
1:E:308:ASP:O	1:E:328:LYS:NZ	2.08	0.85
2:G:236:ARG:O	2:G:240:PRO:HD3	1.77	0.85
1:B:100:GLU:HG3	3:G:290:HOH:O	1.77	0.83
2:H:236:ARG:O	2:H:240:PRO:HD3	1.78	0.83
1:D:188:ILE:HD11	1:D:271:THR:CG2	2.10	0.81
1:C:240:ARG:NH1	1:D:59:LEU:HD23	1.95	0.81
1:C:156:ASN:HD22	1:C:156:ASN:H	1.28	0.81
1:A:188:ILE:HD11	1:A:271:THR:CG2	2.11	0.80
1:B:25:LEU:HG	1:B:29:ARG:HE	1.47	0.80
2:G:209:ILE:HA	2:G:212:VAL:HG22	1.65	0.79
1:B:308:ASP:O	1:B:328:LYS:NZ	2.15	0.79
2:H:209:ILE:CD1	2:H:209:ILE:CB	2.60	0.78
1:A:201:ILE:HD11	1:A:215:HIS:CE1	2.19	0.78
1:C:266:LYS:NZ	1:C:266:LYS:CD	2.48	0.77
1:E:25:LEU:HG	1:E:29:ARG:HE	1.47	0.77
1:E:82:MET:HE1	3:E:376:HOH:O	1.85	0.76
1:F:156:ASN:HD22	1:F:156:ASN:H	1.30	0.76
1:D:188:ILE:HD11	1:D:271:THR:HG21	1.67	0.75
2:G:212:VAL:HG21	2:G:239:PHE:CZ	2.21	0.75
1:D:201:ILE:HD11	1:D:215:HIS:CE1	2.21	0.75
1:A:201:ILE:CD1	1:A:215:HIS:ND1	2.50	0.74
1:E:156:ASN:HD22	1:E:156:ASN:H	1.35	0.74
1:D:201:ILE:CD1	1:D:215:HIS:ND1	2.50	0.74
1:B:156:ASN:H	1:B:156:ASN:HD22	1.36	0.74
1:E:82:MET:CE	3:E:376:HOH:O	2.36	0.74
1:A:59:LEU:HD23	1:F:240:ARG:NH1	2.03	0.73
1:A:188:ILE:HD11	1:A:271:THR:HG21	1.70	0.73
1:F:240:ARG:HG2	1:F:240:ARG:HH11	1.52	0.73
1:B:82:MET:HE1	3:B:332:HOH:O	1.89	0.72
1:D:200:ARG:HH12	1:E:51:ASN:ND2	1.88	0.72
1:F:237:LEU:HD22	1:F:265:HIS:CE1	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ARG:HH12	1:D:51:ASN:HD21	1.38	0.71
2:G:212:VAL:CG2	2:G:239:PHE:CZ	2.73	0.71
1:A:214:HIS:C	1:A:215:HIS:HD2	1.99	0.71
1:B:200:ARG:HH12	1:C:51:ASN:HD21	1.39	0.70
1:E:200:ARG:HH12	1:F:51:ASN:HD21	1.37	0.69
1:A:51:ASN:HD21	1:F:200:ARG:HH12	1.40	0.69
1:C:240:ARG:HG2	1:C:240:ARG:HH11	1.56	0.69
1:D:197:LYS:HA	1:D:215:HIS:CD2	2.28	0.68
2:H:239:PHE:N	2:H:240:PRO:HD2	2.09	0.67
1:A:214:HIS:O	1:A:215:HIS:HD2	1.78	0.66
1:F:240:ARG:NH1	1:F:240:ARG:HG2	2.10	0.66
2:H:177:TRP:O	2:H:181:THR:HG23	1.97	0.65
1:E:174:VAL:HB	1:E:312:MET:HG3	1.78	0.65
1:F:202:ILE:HD12	1:F:241:PRO:HB3	1.77	0.65
2:H:121:GLN:O	2:H:125:ASP:HB2	1.97	0.65
2:G:209:ILE:HA	2:G:212:VAL:CG2	2.26	0.64
2:G:121:GLN:O	2:G:125:ASP:HB2	1.97	0.64
1:A:188:ILE:HD11	1:A:271:THR:HG23	1.79	0.64
2:H:236:ARG:HG3	2:H:244:VAL:HB	1.80	0.63
1:E:200:ARG:HH12	1:F:51:ASN:ND2	1.96	0.62
1:E:291:ASN:HD22	1:E:293:ALA:H	1.47	0.62
1:D:188:ILE:HD11	1:D:271:THR:HG23	1.80	0.62
1:C:229:SER:HB3	1:C:253:GLU:HG2	1.81	0.62
1:E:82:MET:HE2	1:E:128:ILE:HD11	1.81	0.61
1:E:263:SER:O	1:E:264:GLY:C	2.42	0.61
1:B:174:VAL:HB	1:B:312:MET:HG3	1.82	0.61
1:A:214:HIS:C	1:A:215:HIS:CD2	2.79	0.61
1:F:204:ILE:HD13	1:F:233:LEU:HD13	1.83	0.61
1:B:291:ASN:HD22	1:B:293:ALA:H	1.49	0.61
1:F:240:ARG:HH11	1:F:240:ARG:CG	2.13	0.61
1:B:82:MET:CE	3:B:332:HOH:O	2.48	0.60
1:C:202:ILE:HD12	1:C:241:PRO:HB3	1.81	0.60
1:D:195:ILE:HB	1:D:215:HIS:HE1	1.66	0.60
1:F:229:SER:HB3	1:F:253:GLU:HG2	1.81	0.60
2:G:209:ILE:HB	2:G:239:PHE:CE2	2.37	0.60
1:D:200:ARG:NH1	1:E:51:ASN:HD21	1.93	0.60
1:F:163:ALA:C	1:F:312:MET:HE1	2.27	0.59
2:G:239:PHE:N	2:G:240:PRO:HD2	2.18	0.59
1:C:240:ARG:NH1	1:C:240:ARG:HG2	2.15	0.59
2:G:205:LEU:O	2:G:209:ILE:CG2	2.51	0.59
1:D:199:GLU:OE2	1:D:243:ARG:NE	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LEU:HD21	1:B:29:ARG:HH21	1.67	0.58
2:H:202:ASP:O	2:H:206:GLN:HG2	2.03	0.58
2:G:236:ARG:HG3	2:G:244:VAL:HB	1.86	0.58
2:H:223:PRO:HB2	2:H:227:LEU:HB3	1.86	0.58
1:C:240:ARG:HH11	1:C:240:ARG:CG	2.17	0.58
1:A:180:THR:CG2	1:F:240:ARG:HE	2.16	0.57
1:B:263:SER:O	1:B:264:GLY:C	2.48	0.57
1:A:200:ARG:HH12	1:B:51:ASN:ND2	1.98	0.57
2:G:205:LEU:O	2:G:209:ILE:HG22	2.05	0.57
1:C:204:ILE:HD13	1:C:233:LEU:HD13	1.87	0.57
1:D:197:LYS:HA	1:D:215:HIS:HD2	1.68	0.57
1:B:25:LEU:CD2	1:B:29:ARG:HH21	2.18	0.57
1:F:237:LEU:CD2	1:F:265:HIS:HE1	2.13	0.57
2:G:223:PRO:HB2	2:G:227:LEU:HB3	1.87	0.57
1:C:295:ARG:HH21	1:F:295:ARG:HH21	1.50	0.56
1:C:163:ALA:C	1:C:312:MET:HE1	2.30	0.56
1:E:25:LEU:HD21	1:E:29:ARG:HH21	1.69	0.56
2:H:235:LEU:O	2:H:239:PHE:HB2	2.06	0.56
1:B:202:ILE:HD12	1:B:241:PRO:HB3	1.89	0.55
1:D:185:THR:HA	1:D:188:ILE:HD12	1.88	0.55
1:B:82:MET:HE2	1:B:128:ILE:HD11	1.89	0.54
1:E:252:SER:HB2	2:H:250:LEU:HD21	1.88	0.54
1:B:200:ARG:HH12	1:C:51:ASN:ND2	2.04	0.54
1:C:240:ARG:HE	1:D:180:THR:CG2	2.21	0.54
1:B:204:ILE:HD13	1:B:233:LEU:HD13	1.90	0.54
1:B:252:SER:HB2	2:G:250:LEU:HD21	1.90	0.53
2:G:232:LEU:HB3	2:G:236:ARG:HH11	1.73	0.53
1:A:199:GLU:OE2	1:A:243:ARG:NE	2.40	0.53
2:H:192:THR:O	2:H:192:THR:HG22	2.09	0.53
2:H:204:GLN:O	2:H:208:VAL:HG23	2.09	0.53
1:A:185:THR:HA	1:A:188:ILE:HD12	1.90	0.53
1:B:174:VAL:HG13	1:B:269:LEU:HD13	1.89	0.53
1:E:204:ILE:HD13	1:E:233:LEU:HD13	1.89	0.53
1:A:255:TYR:HB3	1:A:291:ASN:HD22	1.73	0.53
1:B:240:ARG:NH2	1:C:46:THR:OG1	2.33	0.53
1:C:163:ALA:HB1	1:C:312:MET:CE	2.39	0.53
2:H:239:PHE:N	2:H:240:PRO:CD	2.71	0.53
1:A:182:SER:HA	3:A:449:HOH:O	2.08	0.53
1:A:214:HIS:O	1:A:215:HIS:CD2	2.62	0.52
2:G:236:ARG:NE	2:H:241:ASN:HD21	2.07	0.52
1:C:113:ARG:NH2	3:C:428:HOH:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:GLY:HA3	1:C:273:HIS:ND1	2.25	0.52
1:B:80:ARG:HE	1:B:80:ARG:HA	1.75	0.52
2:H:223:PRO:HD2	2:H:228:THR:HA	1.91	0.52
2:H:253:GLU:HG2	3:H:283:HOH:O	2.09	0.52
1:C:44:ASN:N	1:C:44:ASN:HD22	2.09	0.51
1:F:163:ALA:HB1	1:F:312:MET:CE	2.41	0.51
1:A:80:ARG:HH12	1:A:83:HIS:CD2	2.29	0.51
1:A:184:LYS:O	1:A:188:ILE:HG13	2.11	0.51
1:C:163:ALA:HB1	1:C:312:MET:HE1	1.92	0.51
1:B:238:ARG:HD2	3:B:428:HOH:O	2.08	0.51
2:G:212:VAL:HG23	2:G:239:PHE:CZ	2.44	0.51
1:F:73:ARG:O	3:F:406:HOH:O	2.19	0.51
1:C:139:THR:CG2	1:C:213:LYS:HD2	2.41	0.51
1:C:200:ARG:HH12	1:D:51:ASN:ND2	2.08	0.50
1:C:104:LEU:HD23	1:C:116:ILE:HD12	1.93	0.50
1:E:202:ILE:HD12	1:E:241:PRO:HB3	1.92	0.50
1:D:184:LYS:O	1:D:188:ILE:HG13	2.11	0.50
1:D:202:ILE:HD12	1:D:241:PRO:HB3	1.94	0.50
1:F:44:ASN:N	1:F:44:ASN:HD22	2.09	0.50
1:A:108:LEU:HB2	1:A:112:GLU:HG2	1.94	0.50
1:A:99:TYR:OH	1:F:93:LYS:HD2	2.10	0.50
1:A:261:LEU:HB3	1:A:309:LEU:HD13	1.94	0.50
1:F:237:LEU:CD2	1:F:265:HIS:CE1	2.92	0.49
1:A:100:GLU:OE1	3:A:381:HOH:O	2.20	0.49
1:D:255:TYR:HB3	1:D:291:ASN:HD22	1.77	0.49
1:A:202:ILE:HD12	1:A:241:PRO:HB3	1.95	0.49
1:C:236:CYS:SG	1:C:244:ILE:HG12	2.52	0.49
1:A:180:THR:HG22	1:F:240:ARG:HE	1.78	0.49
1:F:236:CYS:SG	1:F:244:ILE:HG12	2.53	0.49
2:G:221:LYS:HE2	2:G:253:GLU:HG3	1.95	0.49
1:A:279:GLU:O	1:A:283:ARG:HB2	2.12	0.48
1:D:279:GLU:O	1:D:283:ARG:HB2	2.13	0.48
1:F:83:HIS:ND1	1:F:83:HIS:C	2.71	0.48
1:F:104:LEU:HD23	1:F:116:ILE:HD12	1.96	0.48
2:G:209:ILE:CA	2:G:212:VAL:HG22	2.41	0.48
1:C:240:ARG:HH11	1:D:59:LEU:HD23	1.73	0.48
2:G:240:PRO:HA	2:G:241:ASN:HA	1.54	0.48
2:H:242:LYS:NZ	3:H:273:HOH:O	2.47	0.48
1:C:93:LYS:HD2	1:D:99:TYR:OH	2.14	0.48
2:G:192:THR:HG22	2:G:192:THR:O	2.14	0.48
1:C:266:LYS:NZ	1:C:266:LYS:HD3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:LEU:HB2	1:D:112:GLU:HG2	1.96	0.48
1:E:80:ARG:HE	1:E:80:ARG:HA	1.78	0.48
1:F:167:GLY:HA2	1:F:172:LYS:HD2	1.96	0.48
1:A:195:ILE:CG2	1:A:215:HIS:HE1	2.28	0.47
1:B:264:GLY:HA3	1:C:273:HIS:HD1	1.78	0.47
1:B:291:ASN:HD22	1:B:292:SER:N	2.12	0.47
2:H:142:TYR:CD2	2:H:143:GLU:HG3	2.48	0.47
1:C:139:THR:HG22	1:C:213:LYS:HD2	1.96	0.47
1:D:221:LEU:HD21	1:D:239:MET:HE1	1.95	0.47
2:G:241:ASN:HD21	2:H:236:ARG:HD3	1.79	0.47
1:E:174:VAL:HG13	1:E:269:LEU:HD13	1.95	0.47
1:B:240:ARG:HH22	1:C:46:THR:HG1	1.58	0.47
1:D:34:GLU:OE2	1:D:80:ARG:HD3	2.14	0.47
2:G:209:ILE:HB	2:G:239:PHE:HE2	1.79	0.47
1:C:240:ARG:HE	1:D:180:THR:HG22	1.80	0.47
1:E:291:ASN:ND2	1:E:293:ALA:H	2.11	0.47
1:D:261:LEU:HB3	1:D:309:LEU:HD13	1.96	0.47
2:H:239:PHE:H	2:H:240:PRO:HD2	1.79	0.47
2:H:239:PHE:O	2:H:242:LYS:N	2.48	0.47
1:C:283:ARG:O	1:C:287:MET:HG3	2.14	0.46
2:G:216:GLY:HA2	2:G:242:LYS:NZ	2.30	0.46
1:C:83:HIS:ND1	1:C:83:HIS:C	2.72	0.46
1:D:54:LYS:HD2	1:D:71:ARG:HA	1.96	0.46
1:D:73:ARG:HD3	3:D:380:HOH:O	2.15	0.46
1:B:225:GLY:O	2:G:249:ASN:ND2	2.49	0.46
1:F:108:LEU:HD12	1:F:112:GLU:CG	2.46	0.46
1:A:283:ARG:NH1	3:A:437:HOH:O	2.17	0.46
1:C:240:ARG:NH1	1:D:47:GLU:HB2	2.31	0.46
1:E:264:GLY:HA3	1:F:273:HIS:ND1	2.31	0.46
1:A:54:LYS:HD2	1:A:71:ARG:HA	1.97	0.46
1:F:139:THR:CG2	1:F:213:LYS:HD2	2.46	0.46
1:C:167:GLY:HA2	1:C:172:LYS:HD2	1.98	0.45
1:E:82:MET:HE3	3:E:376:HOH:O	2.09	0.45
1:F:26:ASN:H	1:F:27:PRO:CD	2.28	0.45
1:F:163:ALA:HB1	1:F:312:MET:HE1	1.99	0.45
1:A:47:GLU:HB2	1:F:240:ARG:NH1	2.31	0.45
1:A:51:ASN:ND2	1:F:200:ARG:HH12	2.12	0.45
1:C:26:ASN:H	1:C:27:PRO:CD	2.29	0.45
1:D:240:ARG:HH21	1:E:133:ARG:HD3	1.81	0.45
1:E:291:ASN:HD22	1:E:292:SER:N	2.14	0.45
1:F:283:ARG:O	1:F:287:MET:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:221:LYS:HE2	2:H:253:GLU:HG3	1.99	0.45
1:B:24:ALA:HA	3:B:386:HOH:O	2.16	0.45
1:E:133:ARG:NH1	1:E:134:ILE:O	2.50	0.45
2:G:223:PRO:HD2	2:G:228:THR:HA	1.97	0.45
1:A:80:ARG:HH11	1:A:80:ARG:HA	1.81	0.45
1:B:137:LYS:H	1:B:137:LYS:HG2	1.56	0.45
2:H:210:MET:O	2:H:210:MET:HG2	2.17	0.44
1:B:291:ASN:ND2	1:B:293:ALA:H	2.12	0.44
2:G:204:GLN:O	2:G:208:VAL:HG23	2.17	0.44
1:A:240:ARG:HH21	1:B:133:ARG:HD3	1.82	0.44
1:B:163:ALA:HB1	1:B:312:MET:HE1	1.98	0.44
2:G:239:PHE:H	2:G:240:PRO:HD2	1.82	0.44
1:B:156:ASN:HD22	1:B:156:ASN:N	2.11	0.44
1:B:242:ASP:O	1:B:266:LYS:HB3	2.17	0.44
1:D:205:GLU:O	1:D:222:PHE:HA	2.17	0.44
1:A:200:ARG:NH1	1:B:51:ASN:HD21	2.02	0.44
1:A:221:LEU:HD21	1:A:239:MET:HE1	1.99	0.44
1:D:195:ILE:HB	1:D:215:HIS:CE1	2.49	0.44
1:F:139:THR:HG22	1:F:213:LYS:HD2	2.00	0.44
1:B:133:ARG:NH1	1:B:134:ILE:O	2.50	0.44
2:G:209:ILE:HB	2:G:239:PHE:CZ	2.53	0.44
1:B:229:SER:HB3	1:B:253:GLU:HG2	2.00	0.43
1:B:164:ILE:HG12	1:B:325:PHE:CZ	2.53	0.43
1:C:108:LEU:HD12	1:C:112:GLU:CG	2.48	0.43
1:C:168:ILE:CD1	1:C:174:VAL:HG21	2.48	0.43
1:E:200:ARG:NH1	1:F:51:ASN:HD21	2.11	0.43
1:E:264:GLY:O	1:F:273:HIS:HE1	2.02	0.43
1:C:96:ILE:HD12	1:C:104:LEU:HB3	2.00	0.43
1:C:251:SER:HB3	1:C:252:SER:H	1.38	0.43
1:D:181:GLY:HA2	3:D:460:HOH:O	2.17	0.43
2:G:212:VAL:HG12	2:G:218:GLY:HA3	2.00	0.43
1:C:240:ARG:HH22	1:D:46:THR:HB	1.83	0.43
1:F:168:ILE:CD1	1:F:174:VAL:HG21	2.48	0.43
1:A:299:PHE:HB2	1:F:297:ILE:HG12	2.00	0.43
1:E:25:LEU:CD2	1:E:29:ARG:HH21	2.30	0.43
1:E:22:GLU:OE2	1:E:25:LEU:HD23	2.19	0.43
1:A:184:LYS:HD2	1:A:271:THR:HB	2.01	0.42
1:A:188:ILE:CD1	1:A:271:THR:HG23	2.47	0.42
2:H:135:ASN:OD1	2:H:136:LYS:N	2.53	0.42
1:B:108:LEU:HB2	1:B:112:GLU:HG2	2.01	0.42
1:F:155:ASP:OD2	1:F:155:ASP:N	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LYS:HD2	1:A:312:MET:HE3	2.02	0.42
1:D:253:GLU:HA	1:D:256:ASP:OD2	2.19	0.42
1:E:163:ALA:HB1	1:E:312:MET:HE1	2.02	0.42
1:E:242:ASP:O	1:E:266:LYS:HB3	2.18	0.42
1:A:253:GLU:HA	1:A:256:ASP:OD2	2.19	0.42
1:D:172:LYS:HD2	1:D:312:MET:HE3	2.02	0.42
1:E:137:LYS:H	1:E:137:LYS:HG2	1.56	0.42
2:H:197:GLN:HB3	2:H:227:LEU:HD21	2.02	0.42
1:A:80:ARG:HA	1:A:80:ARG:HD2	1.89	0.42
1:D:188:ILE:CD1	1:D:271:THR:HG23	2.47	0.42
1:B:272:LEU:HD11	1:B:283:ARG:HG2	2.02	0.41
1:D:184:LYS:HD2	1:D:271:THR:HB	2.02	0.41
1:E:272:LEU:HD11	1:E:283:ARG:HG2	2.02	0.41
1:B:22:GLU:OE2	1:B:25:LEU:HD23	2.20	0.41
1:E:240:ARG:NH2	1:F:46:THR:OG1	2.39	0.41
1:A:274:ALA:HA	1:F:262:CYS:O	2.19	0.41
1:E:294:ALA:HA	1:E:297:ILE:HD12	2.01	0.41
1:F:54:LYS:HD2	1:F:71:ARG:HA	2.01	0.41
1:A:180:THR:HG23	3:A:436:HOH:O	2.21	0.41
2:G:216:GLY:O	2:G:242:LYS:NZ	2.48	0.41
2:H:179:HIS:HB3	2:H:180:PRO:HD3	2.01	0.41
1:B:193:GLU:HG2	1:B:214:HIS:NE2	2.36	0.41
1:C:188:ILE:CG1	1:C:269:LEU:HD23	2.50	0.41
1:D:100:GLU:C	1:D:102:PRO:HD3	2.45	0.41
1:E:229:SER:HB3	1:E:253:GLU:HG2	2.02	0.41
2:G:132:TYR:HB3	2:G:134:ILE:HD13	2.02	0.41
1:E:258:TYR:CE1	1:E:309:LEU:HD12	2.55	0.41
1:C:133:ARG:NE	3:C:392:HOH:O	2.31	0.41
1:E:164:ILE:HG12	1:E:325:PHE:CZ	2.56	0.41
2:H:136:LYS:O	2:H:151:ILE:HA	2.20	0.41
2:H:208:VAL:O	2:H:212:VAL:HG23	2.21	0.41
2:H:223:PRO:HB2	2:H:227:LEU:CB	2.51	0.41
2:H:226:VAL:HG22	3:H:288:HOH:O	2.21	0.41
1:B:164:ILE:HG12	1:B:325:PHE:HZ	1.86	0.40
1:B:233:LEU:HD12	1:B:260:VAL:HG21	2.03	0.40
2:G:179:HIS:HB3	2:G:180:PRO:HD3	2.02	0.40
1:A:21:LYS:NZ	1:B:125:ASP:OD2	2.54	0.40
1:F:188:ILE:CG1	1:F:269:LEU:HD23	2.51	0.40
1:C:54:LYS:HD2	1:C:71:ARG:HA	2.03	0.40
1:F:76:PHE:HB2	3:F:406:HOH:O	2.22	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	321/330 (97%)	312 (97%)	9 (3%)	0	100	100
1	B	306/330 (93%)	296 (97%)	8 (3%)	2 (1%)	18	28
1	C	305/330 (92%)	296 (97%)	7 (2%)	2 (1%)	18	28
1	D	321/330 (97%)	312 (97%)	9 (3%)	0	100	100
1	E	306/330 (93%)	295 (96%)	8 (3%)	3 (1%)	12	20
1	F	305/330 (92%)	296 (97%)	8 (3%)	1 (0%)	36	50
2	G	143/152 (94%)	133 (93%)	10 (7%)	0	100	100
2	H	143/152 (94%)	135 (94%)	8 (6%)	0	100	100
All	All	2150/2284 (94%)	2075 (96%)	67 (3%)	8 (0%)	30	43

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	125	ASP
1	B	125	ASP
1	C	26	ASN
1	F	26	ASN
1	B	251	SER
1	C	251	SER
1	E	251	SER
1	E	264	GLY

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	283/293 (97%)	267 (94%)	16 (6%)	18	33
1	B	273/293 (93%)	255 (93%)	18 (7%)	15	26
1	C	271/293 (92%)	259 (96%)	12 (4%)	25	43
1	D	284/293 (97%)	264 (93%)	20 (7%)	14	24
1	E	273/293 (93%)	258 (94%)	15 (6%)	19	34
1	F	272/293 (93%)	258 (95%)	14 (5%)	21	37
2	G	121/138 (88%)	104 (86%)	17 (14%)	3	4
2	H	121/138 (88%)	105 (87%)	16 (13%)	4	5
All	All	1898/2034 (93%)	1770 (93%)	128 (7%)	15	26

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	25	LEU
1	A	53	ASN
1	A	80	ARG
1	A	95	THR
1	A	112	GLU
1	A	114	VAL
1	A	125	ASP
1	A	137	LYS
1	A	170	ILE
1	A	180	THR
1	A	249	LEU
1	A	261	LEU
1	A	272	LEU
1	A	283	ARG
1	A	303	ILE
1	B	35	LEU
1	B	78	LEU
1	B	114	VAL
1	B	137	LYS
1	B	138	THR
1	B	156	ASN
1	B	174	VAL
1	B	188	ILE
1	B	207	THR
1	B	210	ILE
1	B	233	LEU

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Mol	Chain	Res	Type
1	B	249	LEU
1	B	253	GLU
1	B	272	LEU
1	B	283	ARG
1	B	291	ASN
1	B	300	GLU
1	B	303	ILE
1	C	44	ASN
1	C	83	HIS
1	C	112	GLU
1	C	155	ASP
1	C	156	ASN
1	C	170	ILE
1	C	209	GLU
1	C	233	LEU
1	C	240	ARG
1	C	249	LEU
1	C	251	SER
1	C	253	GLU
1	D	6	LEU
1	D	14	LEU
1	D	20	LEU
1	D	25	LEU
1	D	53	ASN
1	D	72	ASP
1	D	80	ARG
1	D	95	THR
1	D	112	GLU
1	D	114	VAL
1	D	125	ASP
1	D	137	LYS
1	D	170	ILE
1	D	180	THR
1	D	249	LEU
1	D	261	LEU
1	D	265	HIS
1	D	272	LEU
1	D	283	ARG
1	D	303	ILE
1	E	35	LEU
1	E	78	LEU
1	E	114	VAL

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Mol	Chain	Res	Type
1	E	137	LYS
1	E	138	THR
1	E	156	ASN
1	E	174	VAL
1	E	188	ILE
1	E	207	THR
1	E	210	ILE
1	E	233	LEU
1	E	249	LEU
1	E	253	GLU
1	E	291	ASN
1	E	300	GLU
1	F	44	ASN
1	F	83	HIS
1	F	112	GLU
1	F	137	LYS
1	F	139	THR
1	F	155	ASP
1	F	156	ASN
1	F	170	ILE
1	F	209	GLU
1	F	233	LEU
1	F	240	ARG
1	F	249	LEU
1	F	253	GLU
1	F	266	LYS
2	G	122	GLU
2	G	126	LEU
2	G	134	ILE
2	G	135	ASN
2	G	138	GLU
2	G	165	TYR
2	G	170	LEU
2	G	186	ILE
2	G	194	LEU
2	G	204	GLN
2	G	209	ILE
2	G	219	GLN
2	G	226	VAL
2	G	246	ILE
2	G	247	LYS
2	G	253	GLU

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Mol	Chain	Res	Type
2	G	259	ASN
2	H	122	GLU
2	H	126	LEU
2	H	134	ILE
2	H	137	VAL
2	H	165	TYR
2	H	170	LEU
2	H	181	THR
2	H	194	LEU
2	H	203	THR
2	H	204	GLN
2	H	219	GLN
2	H	226	VAL
2	H	247	LYS
2	H	248	THR
2	H	253	GLU
2	H	259	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	53	ASN
1	A	66	GLN
1	A	156	ASN
1	A	159	GLN
1	A	215	HIS
1	A	265	HIS
1	A	273	HIS
1	A	286	ASN
1	B	51	ASN
1	B	83	HIS
1	B	156	ASN
1	B	226	ASN
1	B	265	HIS
1	B	291	ASN
1	C	44	ASN
1	C	51	ASN
1	C	66	GLN
1	C	83	HIS
1	C	156	ASN
1	C	159	GLN

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Mol	Chain	Res	Type
1	C	286	ASN
1	D	51	ASN
1	D	53	ASN
1	D	66	GLN
1	D	156	ASN
1	D	159	GLN
1	D	265	HIS
1	D	273	HIS
1	D	286	ASN
1	D	319	HIS
1	E	51	ASN
1	E	156	ASN
1	E	265	HIS
1	E	291	ASN
1	E	318	HIS
1	E	321	GLN
1	F	44	ASN
1	F	51	ASN
1	F	66	GLN
1	F	156	ASN
1	F	159	GLN
1	F	265	HIS
1	F	273	HIS
1	F	286	ASN
2	G	117	HIS
2	G	196	ASN
2	G	219	GLN
2	G	241	ASN
2	H	196	ASN
2	H	204	GLN
2	H	241	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	323/330 (97%)	0.57	17 (5%)	32 28	21, 31, 46, 56	0
1	B	308/330 (93%)	0.67	18 (5%)	29 25	22, 33, 54, 68	0
1	C	307/330 (93%)	0.63	22 (7%)	21 18	20, 32, 56, 69	0
1	D	323/330 (97%)	0.49	14 (4%)	40 36	21, 31, 46, 56	0
1	E	308/330 (93%)	0.91	33 (10%)	11 8	22, 33, 54, 68	0
1	F	307/330 (93%)	0.69	28 (9%)	15 12	20, 32, 56, 69	0
2	G	145/152 (95%)	1.25	24 (16%)	4 3	25, 38, 43, 46	0
2	H	145/152 (95%)	1.27	22 (15%)	5 4	25, 38, 43, 46	0
All	All	2166/2284 (94%)	0.74	178 (8%)	17 14	20, 33, 52, 69	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	214	GLU	6.0
1	A	144	PHE	5.1
1	A	99	TYR	4.9
2	G	213	HIS	4.2
1	C	24	ALA	4.1
1	E	155	ASP	4.0
2	H	207	SER	4.0
1	A	180	THR	4.0
1	D	136	SER	4.0
1	F	24	ALA	3.8
1	C	28	LEU	3.7
2	H	239	PHE	3.6
1	A	181	GLY	3.5
1	B	206	ASP	3.4
1	E	207	THR	3.4
1	B	162	SER	3.4

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Mol	Chain	Res	Type	RSRZ
2	G	214	GLU	3.4
1	B	24	ALA	3.4
1	B	318	HIS	3.4
1	A	7	SER	3.2
1	E	206	ASP	3.2
1	E	181	GLY	3.2
1	C	71	ARG	3.2
1	B	44	ASN	3.2
1	F	319	HIS	3.2
2	G	204	GLN	3.2
2	H	126	LEU	3.1
1	D	156	ASN	3.1
2	G	239	PHE	3.1
1	A	14	LEU	3.1
1	F	90	SER	3.1
1	D	181	GLY	3.1
1	A	9	GLU	3.0
1	E	22	GLU	3.0
1	B	265	HIS	3.0
1	E	21	LYS	3.0
2	G	207	SER	3.0
2	G	241	ASN	3.0
1	C	181	GLY	3.0
1	E	148	GLN	3.0
1	C	318	HIS	3.0
1	C	125	ASP	3.0
2	H	213	HIS	2.9
1	D	72	ASP	2.9
2	H	259	ASN	2.9
1	F	30	HIS	2.9
1	B	160	ALA	2.9
1	F	128	ILE	2.9
1	C	156	ASN	2.8
1	C	30	HIS	2.8
1	F	125	ASP	2.8
1	B	293	ALA	2.8
1	D	99	TYR	2.8
1	B	292	SER	2.8
1	D	6	LEU	2.8
1	F	23	ALA	2.8
1	D	155	ASP	2.8
1	E	153	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	152	ASN	2.7
2	G	135	ASN	2.7
1	E	25	LEU	2.7
1	C	63	GLY	2.7
2	H	242	LYS	2.7
1	E	154	LEU	2.7
2	H	203	THR	2.7
1	B	214	HIS	2.7
2	H	206	GLN	2.6
1	F	37	GLY	2.6
2	H	180	PRO	2.6
1	C	23	ALA	2.6
2	G	203	THR	2.6
2	H	238	ALA	2.6
1	F	25	LEU	2.6
1	F	266	LYS	2.6
1	A	13	PHE	2.6
1	E	140	TYR	2.6
1	F	33	GLU	2.5
1	F	273	HIS	2.5
1	D	180	THR	2.5
1	D	111	GLY	2.5
1	E	161	ILE	2.5
1	C	265	HIS	2.5
1	C	319	HIS	2.5
1	A	160	ALA	2.5
1	E	136	SER	2.5
2	G	202	ASP	2.5
2	G	209	ILE	2.5
1	E	145	PHE	2.5
1	D	8	ALA	2.5
1	B	46	THR	2.5
2	G	134	ILE	2.4
1	B	154	LEU	2.4
1	C	159	GLN	2.4
1	F	83	HIS	2.4
1	E	156	ASN	2.4
1	F	123	VAL	2.4
1	B	23	ALA	2.4
1	B	30	HIS	2.4
1	F	46	THR	2.4
1	D	43	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	54	LYS	2.4
1	A	6	LEU	2.4
2	G	208	VAL	2.4
2	G	250	LEU	2.3
2	H	246	ILE	2.3
2	H	258	ILE	2.3
1	F	64	GLU	2.3
1	E	162	SER	2.3
2	G	229	TYR	2.3
2	H	215	VAL	2.3
1	F	22	GLU	2.3
1	B	156	ASN	2.3
1	E	24	ALA	2.3
2	G	218	GLY	2.3
2	H	204	GLN	2.3
1	E	125	ASP	2.3
1	C	89	ALA	2.3
2	G	238	ALA	2.3
1	A	265	HIS	2.3
1	E	30	HIS	2.3
1	F	265	HIS	2.3
1	A	12	LYS	2.3
2	G	120	LYS	2.3
1	E	146	GLU	2.3
2	H	131	PRO	2.3
1	C	107	ASN	2.2
1	E	119	SER	2.2
1	B	155	ASP	2.2
2	G	125	ASP	2.2
1	F	147	GLU	2.2
2	H	162	GLU	2.2
1	B	152	ASN	2.2
1	E	123	VAL	2.2
1	C	226	ASN	2.2
2	G	259	ASN	2.2
1	F	193	GLU	2.2
1	D	295	ARG	2.2
1	F	28	LEU	2.1
1	C	126	GLU	2.1
1	A	136	SER	2.1
1	D	10	ASP	2.1
1	E	292	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	206	GLN	2.1
1	F	95	THR	2.1
1	A	327	ILE	2.1
1	E	151	TYR	2.1
1	F	71	ARG	2.1
2	H	117	HIS	2.1
1	E	160	ALA	2.1
2	G	249	ASN	2.1
1	C	138	THR	2.1
1	A	22	GLU	2.1
1	E	255	TYR	2.1
1	E	265	HIS	2.1
2	G	222	ALA	2.1
1	E	171	GLY	2.1
1	A	155	ASP	2.1
1	E	72	ASP	2.1
2	H	201	MET	2.1
1	D	318	HIS	2.1
2	G	117	HIS	2.1
1	C	70	VAL	2.0
1	F	89	ALA	2.0
1	F	124	ASN	2.0
1	C	33	GLU	2.0
2	H	118	GLU	2.0
1	B	161	ILE	2.0
1	C	99	TYR	2.0
1	F	27	PRO	2.0
1	F	240	ARG	2.0
1	E	300	GLU	2.0
2	G	235	LEU	2.0
1	E	26	ASN	2.0
1	E	110	ASN	2.0
2	H	241	ASN	2.0
1	C	170	ILE	2.0
1	A	10	ASP	2.0
2	H	125	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.