



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:05 AM UTC

PDB ID : 1M9Y / pdb_00001m9y
Title : X-ray crystal structure of Cyclophilin A/HIV-1 CA N-terminal domain (1-146)
M-type H87A,G89A Complex.
Authors : Howard, B.R.; Vajdos, F.F.; Li, S.; Sundquist, W.I.; Hill, C.P.
Deposited on : 2002-07-30
Resolution : 1.90 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

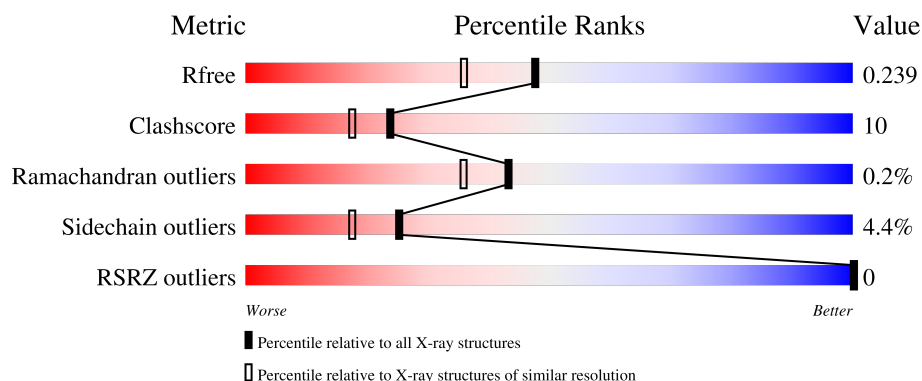
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	165	 88% 11% .
1	B	165	 84% 15% ..
1	E	165	 87% 12% .
1	F	165	 87% 12% ..
2	C	146	 67% 28% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	146	 63% 23% 6% 8%
2	G	146	 79% 18% • •
2	H	146	 55% 29% 7% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10531 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 Cyclophilin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			
1	B	164	Total	C	N	O	S	0	0	0
			1258	797	217	236	8			
1	E	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			
1	F	164	Total	C	N	O	S	0	0	0
			1258	797	217	236	8			

- Molecule 2 is a protein called HIV-1 Capsid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	146	Total	C	N	O	S	0	0	0
			1132	716	198	210	8			
2	D	135	Total	C	N	O	S	0	0	0
			1048	663	183	195	7			
2	G	146	Total	C	N	O	S	0	0	0
			1132	716	198	210	8			
2	H	135	Total	C	N	O	S	0	0	0
			1048	663	183	195	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	87	ALA	HIS	engineered mutation	UNP Q72497
C	89	ALA	GLY	engineered mutation	UNP Q72497
C	120	HIS	ASN	SEE REMARK 999	UNP Q72497
D	87	ALA	HIS	engineered mutation	UNP Q72497
D	89	ALA	GLY	engineered mutation	UNP Q72497
D	120	HIS	ASN	SEE REMARK 999	UNP Q72497
G	87	ALA	HIS	engineered mutation	UNP Q72497
G	89	ALA	GLY	engineered mutation	UNP Q72497

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	120	HIS	ASN	SEE REMARK 999	UNP Q72497
H	87	ALA	HIS	engineered mutation	UNP Q72497
H	89	ALA	GLY	engineered mutation	UNP Q72497
H	120	HIS	ASN	SEE REMARK 999	UNP Q72497

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	171	Total	O	0	0
			171	171		
3	B	177	Total	O	0	0
			177	177		
3	C	178	Total	O	0	0
			178	178		
3	D	61	Total	O	0	0
			61	61		
3	E	201	Total	O	0	0
			201	201		
3	F	89	Total	O	0	0
			89	89		
3	G	135	Total	O	0	0
			135	135		
3	H	111	Total	O	0	0
			111	111		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cyclophilin A

Chain A:  88% 11% .



• Molecule 1: Cyclophilin A

Chain B:  84% 15% ..



• Molecule 1: Cyclophilin A

Chain E:  87% 12% .



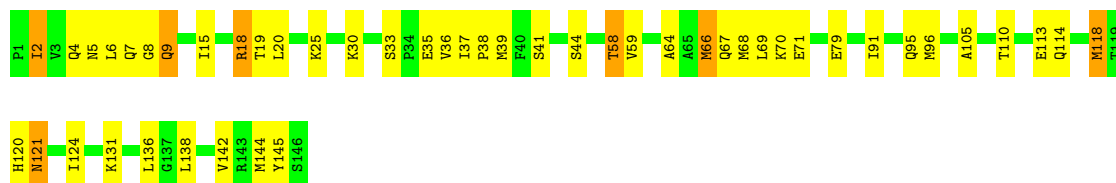
• Molecule 1: Cyclophilin A

Chain F:  87% 12% ..

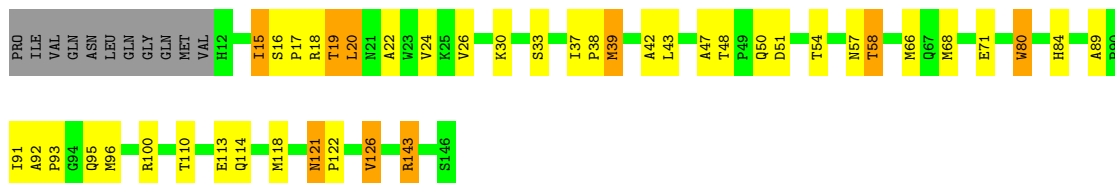


• Molecule 2: HIV-1 Capsid

Chain C:  67% 28% 5%



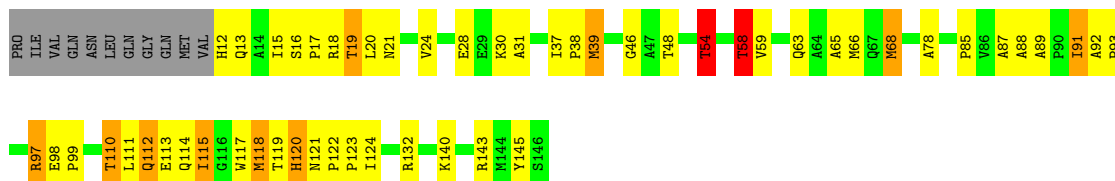
● Molecule 2: HIV-1 Capsid

Chain D:  63% 23% 6% 8%

● Molecule 2: HIV-1 Capsid

Chain G:  79% 18% 3%

● Molecule 2: HIV-1 Capsid

Chain H:  55% 29% 7% 8%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.43Å 111.22Å 67.78Å 89.99° 101.45° 89.75°	Depositor
Resolution (Å)	19.69 – 1.90 19.69 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.69-1.90) 96.3 (19.69-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.162 , 0.234 0.170 , 0.239	Depositor DCC
R_{free} test set	8529 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.319 for -h,k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10531	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.86% 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	0.95	1/1294 (0.1%)	1.63	9/1733 (0.5%)
1	B	1.03	0/1286	1.63	11/1723 (0.6%)
1	E	1.10	2/1294 (0.2%)	1.63	8/1733 (0.5%)
1	F	0.68	0/1286	1.42	2/1723 (0.1%)
2	C	1.07	2/1159 (0.2%)	1.76	14/1577 (0.9%)
2	D	0.80	0/1074	1.58	12/1462 (0.8%)
2	G	0.94	1/1159 (0.1%)	1.64	10/1577 (0.6%)
2	H	1.09	5/1074 (0.5%)	1.68	15/1462 (1.0%)
All	All	0.97	11/9626 (0.1%)	1.62	81/12990 (0.6%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	68	MET	SD-CE	-13.66	1.45	1.79
2	C	66	MET	SD-CE	-9.18	1.56	1.79
2	H	118	MET	SD-CE	-8.43	1.58	1.79
2	H	39	MET	SD-CE	-7.26	1.61	1.79
2	C	118	MET	SD-CE	-6.48	1.63	1.79
1	E	38	ALA	CA-CB	-5.74	1.44	1.53
1	A	38	ALA	CA-CB	-5.65	1.44	1.53
1	E	61	MET	SD-CE	5.40	1.93	1.79
2	H	78	ALA	CA-CB	-5.19	1.44	1.53
2	H	66	MET	SD-CE	5.12	1.92	1.79
2	G	104	ILE	CA-CB	5.01	1.60	1.54

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	145	TYR	CA-C-N	10.22	140.10	121.70
2	C	145	TYR	C-N-CA	10.22	140.10	121.70
2	D	89	ALA	N-CA-C	-9.95	97.37	110.40
1	B	80	GLY	N-CA-C	-9.69	96.61	110.46
1	F	75	GLY	N-CA-C	-8.84	102.39	112.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	89	ALA	N-CA-C	-8.66	99.05	110.40
2	G	58	THR	N-CA-CB	-8.66	96.29	110.40
1	A	120	GLU	N-CA-C	8.63	121.64	111.71
2	H	59	VAL	CB-CA-C	-8.62	101.95	111.35
2	C	124	ILE	N-CA-C	-8.12	98.92	107.60
2	H	98	GLU	N-CA-C	-7.76	100.30	109.93
2	C	58	THR	N-CA-CB	-7.64	97.57	110.41
2	H	115	ILE	N-CA-C	7.64	118.41	110.62
1	B	3	ASN	N-CA-C	7.51	119.18	109.64
2	G	64	ALA	N-CA-C	-7.20	103.47	111.82
1	B	20	VAL	CB-CA-C	-7.17	99.47	110.50
2	D	20	LEU	CB-CA-C	-7.15	99.61	110.90
1	F	124	GLY	N-CA-C	-7.13	105.49	115.32
2	D	126	VAL	N-CA-C	6.79	117.55	110.62
2	H	110	THR	CB-CA-C	-6.78	98.29	110.36
2	D	20	LEU	N-CA-C	6.75	118.43	111.14
2	G	18	ARG	NE-CZ-NH1	-6.54	114.96	121.50
2	G	24	VAL	N-CA-C	6.48	116.64	110.42
2	D	80	TRP	N-CA-C	-6.36	104.28	111.14
2	C	59	VAL	N-CA-C	6.26	117.11	108.84
2	D	39	MET	CB-CA-C	-6.25	100.41	110.79
2	H	59	VAL	N-CA-C	6.23	116.47	108.12
2	G	136	LEU	N-CA-C	-6.22	104.50	111.28
1	E	80	GLY	CA-C-O	6.12	125.92	119.06
2	D	48	THR	N-CA-C	-5.99	102.33	110.36
2	C	69	LEU	N-CA-C	-5.97	104.70	111.14
1	E	70	HIS	N-CA-C	5.96	120.13	112.86
1	B	75	GLY	N-CA-C	-5.94	105.64	112.29
1	A	82	LYS	N-CA-C	-5.91	102.16	110.50
2	C	105	ALA	N-CA-C	5.86	120.04	113.01
2	H	54	THR	OG1-CB-CG2	-5.84	97.62	109.30
2	H	66	MET	CG-SD-CE	-5.84	88.06	100.90
2	C	124	ILE	O-C-N	5.79	126.25	120.92
1	E	132	VAL	N-CA-C	-5.78	102.07	109.30
1	A	61	MET	N-CA-C	5.78	116.92	108.14
1	A	130	GLY	CA-C-O	-5.75	116.02	121.60
2	D	143	ARG	NE-CZ-NH1	-5.74	115.76	121.50
2	C	18	ARG	NE-CZ-NH1	-5.72	115.78	121.50
1	E	164	LEU	CA-C-O	-5.70	114.27	120.36
1	B	48	TYR	N-CA-C	5.68	118.41	111.82
2	D	33	SER	N-CA-C	-5.67	101.88	110.39
2	H	58	THR	N-CA-CB	-5.66	101.50	110.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ILE	N-CA-C	-5.65	106.31	112.80
1	E	61	MET	N-CA-C	5.65	116.72	108.14
2	H	46	GLY	CA-C-O	5.62	125.99	119.13
2	D	39	MET	CG-SD-CE	-5.60	88.59	100.90
2	G	112	GLN	N-CA-C	5.57	117.35	111.28
1	B	129	PHE	CA-C-O	5.52	125.03	118.79
2	H	78	ALA	N-CA-C	5.48	118.01	111.71
2	C	58	THR	CA-CB-OG1	5.44	117.76	109.60
2	H	120	HIS	N-CA-C	5.43	117.96	110.35
1	B	15	GLU	CB-CA-C	-5.41	101.16	108.68
2	G	107	THR	N-CA-C	5.41	117.26	111.36
1	A	70	HIS	N-CA-C	5.39	119.44	112.86
2	C	114	GLN	N-CA-C	-5.38	105.49	111.36
2	C	64	ALA	N-CA-C	-5.38	105.50	111.36
2	G	91	ILE	N-CA-C	5.37	115.93	108.84
2	C	96	MET	CG-SD-CE	5.36	112.69	100.90
1	A	110	SER	N-CA-C	-5.35	106.63	114.39
2	C	136	LEU	N-CA-C	-5.34	105.54	111.36
1	B	82	LYS	N-CA-C	5.32	117.27	109.24
1	E	16	PRO	CA-C-O	5.27	126.87	121.23
2	H	63	GLN	N-CA-C	5.26	117.02	111.28
1	A	139	VAL	N-CA-C	-5.25	105.41	110.72
1	E	74	GLY	N-CA-C	5.24	119.08	112.79
2	G	19	THR	N-CA-C	5.24	116.99	111.28
2	H	88	ALA	CA-C-O	5.18	126.83	120.92
1	A	80	GLY	N-CA-C	-5.17	108.19	115.32
2	D	42	ALA	N-CA-C	5.14	116.57	111.07
2	G	88	ALA	N-CA-C	-5.12	101.61	109.76
1	A	143	GLU	N-CA-CB	5.12	118.89	110.39
1	B	46	PHE	N-CA-C	-5.12	101.28	109.07
2	H	85	PRO	CA-C-O	-5.10	115.44	121.67
2	D	68	MET	CG-SD-CE	-5.06	89.76	100.90
1	B	96	GLY	CA-C-O	-5.06	113.40	119.07
1	E	73	THR	OG1-CB-CG2	-5.00	99.30	109.30

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	1266	0	1237	8	0
1	B	1258	0	1225	10	0
1	E	1266	0	1237	9	0
1	F	1258	0	1225	14	0
2	C	1132	0	1135	52	0
2	D	1048	0	1043	34	0
2	G	1132	0	1135	26	0
2	H	1048	0	1043	47	0
3	A	171	0	0	3	1
3	B	177	0	0	1	0
3	C	178	0	0	8	1
3	D	61	0	0	7	0
3	E	201	0	0	2	1
3	F	89	0	0	3	0
3	G	135	0	0	7	1
3	H	111	0	0	15	0
All	All	10531	0	9280	188	2

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 10.

All (188) 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:68:MET:HE2	3:H:160:HOH:O	1.44	1.16
2:C:30:LYS:NZ	2:C:35:GLU:HG2	1.62	1.13
2:C:6:LEU:HD22	2:C:7:GLN:NE2	1.81	0.95
2:H:115:ILE:O	2:H:119:THR:HG23	1.66	0.94
2:H:91:ILE:HD12	2:H:92:ALA:H	1.39	0.87
2:C:30:LYS:HZ1	2:C:35:GLU:HG2	1.39	0.86
2:C:33:SER:O	2:C:36:VAL:HG12	1.76	0.84
2:C:30:LYS:HZ3	2:C:35:GLU:HG2	1.41	0.81
2:H:91:ILE:HG12	3:H:252:HOH:O	1.81	0.80
2:C:67:GLN:HE22	2:C:70:LYS:NZ	1.80	0.79
2:H:87:ALA:HB3	3:H:225:HOH:O	1.81	0.79
2:C:6:LEU:HD22	2:C:7:GLN:HE21	1.45	0.79
2:D:96:MET:HE3	2:D:96:MET:HA	1.65	0.79
2:C:71:GLU:OE1	3:C:175:HOH:O	2.00	0.78
2:C:30:LYS:HZ1	2:C:35:GLU:CG	1.97	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:71:GLU:OE1	3:G:169:HOH:O	2.03	0.77
2:H:16:SER:HB3	2:H:19:THR:OG1	1.86	0.75
2:H:65:ALA:HA	2:H:68:MET:HE3	1.71	0.73
2:C:39:MET:HE3	2:C:39:MET:HA	1.71	0.73
1:F:6:VAL:HG21	1:F:36:PHE:HE2	1.53	0.73
2:H:112:GLN:H	2:H:112:GLN:CD	1.97	0.72
2:D:71:GLU:OE1	3:D:180:HOH:O	2.07	0.72
2:C:30:LYS:NZ	2:C:35:GLU:CG	2.47	0.69
2:C:66:MET:HA	2:C:66:MET:HE2	1.73	0.69
1:A:44:LYS:NZ	3:A:334:HOH:O	2.17	0.69
2:C:70:LYS:HG3	3:C:200:HOH:O	1.92	0.68
2:C:4:GLN:HE21	2:C:8:GLY:CA	2.06	0.68
2:H:54:THR:HG22	3:H:184:HOH:O	1.94	0.68
2:C:6:LEU:CD2	2:C:7:GLN:NE2	2.57	0.67
2:H:91:ILE:HD13	3:H:196:HOH:O	1.93	0.67
2:D:15:ILE:HD13	2:D:20:LEU:HD11	1.78	0.66
1:E:76:LYS:NZ	3:E:353:HOH:O	2.28	0.66
2:G:144:MET:HG2	3:G:257:HOH:O	1.96	0.66
2:G:68:MET:CE	2:G:144:MET:HE2	2.27	0.65
2:D:39:MET:HE2	3:D:164:HOH:O	1.95	0.65
1:F:30:PRO:HG2	3:F:1093:HOH:O	1.97	0.64
2:D:24:VAL:HG22	2:D:58:THR:HG23	1.80	0.64
2:C:2:ILE:HD13	2:C:118:MET:HE2	1.79	0.64
2:G:65:ALA:HA	2:G:144:MET:HE1	1.80	0.63
2:C:138:LEU:O	2:C:142:VAL:HG13	1.99	0.63
2:G:142:VAL:HG23	2:H:143:ARG:HD3	1.81	0.63
2:H:37:ILE:HB	2:H:38:PRO:HD3	1.81	0.62
2:C:67:GLN:HE22	2:C:70:LYS:HZ1	1.48	0.62
2:C:68:MET:HE1	2:C:144:MET:SD	2.40	0.62
2:H:140:LYS:NZ	3:H:212:HOH:O	2.32	0.61
2:G:142:VAL:CG2	2:H:143:ARG:HD3	2.29	0.61
2:C:19:THR:HG21	3:C:306:HOH:O	2.00	0.61
2:D:22:ALA:O	2:D:26:VAL:HG23	2.00	0.61
2:H:91:ILE:HD12	2:H:92:ALA:N	2.15	0.60
2:C:4:GLN:HE21	2:C:8:GLY:HA2	1.66	0.60
2:G:142:VAL:CG2	2:H:143:ARG:CD	2.80	0.60
2:C:39:MET:HE3	2:C:39:MET:CA	2.27	0.60
2:C:67:GLN:HG2	3:C:180:HOH:O	2.02	0.60
2:C:67:GLN:HE22	2:C:70:LYS:HZ3	1.49	0.59
2:H:24:VAL:CG2	2:H:58:THR:HG23	2.33	0.59
2:C:4:GLN:HE21	2:C:8:GLY:C	2.11	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:138:LEU:O	2:G:142:VAL:HG13	2.02	0.59
2:G:1:PRO:HG2	3:G:258:HOH:O	2.02	0.59
2:D:110:THR:HG23	3:D:195:HOH:O	2.02	0.58
2:H:68:MET:HE1	2:H:145:TYR:HE2	1.67	0.58
2:C:19:THR:CG2	3:C:306:HOH:O	2.52	0.58
2:G:2:ILE:HD12	2:G:12:HIS:HA	1.84	0.58
1:B:31:LYS:NZ	1:B:84:GLU:OE2	2.34	0.58
2:C:15:ILE:HD13	2:C:20:LEU:HD21	1.85	0.58
2:G:128:GLU:CG	3:G:277:HOH:O	2.51	0.58
2:G:24:VAL:HG22	2:G:58:THR:HG23	1.86	0.58
2:H:110:THR:HB	2:H:112:GLN:NE2	2.20	0.57
2:C:95:GLN:OE1	3:C:204:HOH:O	2.17	0.56
1:E:23:GLU:HB2	1:E:133:LYS:HD2	1.88	0.56
2:D:18:ARG:HG3	3:D:189:HOH:O	2.05	0.56
2:H:120:HIS:O	2:H:122:PRO:C	2.49	0.55
2:H:91:ILE:CD1	3:H:196:HOH:O	2.52	0.55
2:D:114:GLN:C	2:D:118:MET:HE3	2.32	0.55
1:F:99:SER:HB3	1:F:113:PHE:CZ	2.41	0.55
2:H:110:THR:O	2:H:114:GLN:HG3	2.06	0.55
2:G:128:GLU:HG3	3:G:277:HOH:O	2.06	0.55
1:B:138:ILE:O	1:B:142:MET:HG3	2.06	0.55
2:C:120:HIS:ND1	2:C:121:ASN:N	2.55	0.54
1:F:6:VAL:HG21	1:F:36:PHE:CE2	2.39	0.54
2:H:87:ALA:CB	3:H:225:HOH:O	2.49	0.54
2:D:57:ASN:ND2	3:D:201:HOH:O	2.39	0.54
2:D:24:VAL:CG2	2:D:58:THR:HG23	2.38	0.54
1:F:20:VAL:HG22	1:F:138:ILE:HB	1.89	0.54
2:G:132:ARG:HD2	3:H:208:HOH:O	2.06	0.54
2:C:4:GLN:NE2	2:C:8:GLY:HA2	2.23	0.54
1:E:25:PHE:CZ	1:E:131:LYS:HG2	2.43	0.54
2:G:142:VAL:HG23	2:H:143:ARG:CD	2.38	0.54
2:H:15:ILE:HG12	2:H:20:LEU:HD21	1.89	0.54
1:E:25:PHE:HZ	1:E:131:LYS:HG2	1.73	0.53
2:G:142:VAL:HG21	2:H:143:ARG:HD2	1.90	0.53
1:F:23:GLU:HB2	3:F:956:HOH:O	2.08	0.53
2:H:111:LEU:O	2:H:115:ILE:HD12	2.08	0.53
2:C:2:ILE:HD13	2:C:118:MET:CE	2.38	0.53
1:B:20:VAL:HG22	1:B:138:ILE:HB	1.89	0.53
2:D:92:ALA:HB3	2:D:95:GLN:HG3	1.89	0.53
2:H:112:GLN:CD	2:H:112:GLN:N	2.66	0.53
2:D:19:THR:O	2:D:22:ALA:HB3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LYS:NZ	3:A:321:HOH:O	2.24	0.52
2:D:110:THR:HG23	2:D:113:GLU:OE1	2.08	0.52
1:B:84:GLU:H	1:B:84:GLU:CD	2.17	0.52
2:C:37:ILE:HB	2:C:38:PRO:HD3	1.91	0.51
2:D:114:GLN:O	2:D:118:MET:HE3	2.10	0.51
2:C:6:LEU:CD2	2:C:7:GLN:HE21	2.18	0.51
1:A:84:GLU:HG2	3:A:313:HOH:O	2.10	0.51
2:H:48:THR:HG22	2:H:118:MET:HE1	1.93	0.51
2:C:44:SER:OG	2:C:131:LYS:HE2	2.11	0.51
1:F:5:THR:HG22	1:F:164:LEU:HB2	1.92	0.50
1:B:13:ASP:HA	3:B:290:HOH:O	2.10	0.50
2:C:4:GLN:NE2	2:C:8:GLY:O	2.44	0.50
2:C:5:ASN:ND2	2:C:9:GLN:HG2	2.26	0.50
2:H:99:PRO:HG3	2:H:124:ILE:HG21	1.94	0.49
2:C:66:MET:HE2	2:C:66:MET:CA	2.43	0.49
2:H:12:HIS:CE1	2:H:13:GLN:O	2.66	0.49
1:A:165:GLU:HG2	1:A:165:GLU:OXT	2.11	0.49
2:G:39:MET:HA	2:G:39:MET:HE3	1.94	0.49
2:G:142:VAL:CG2	2:H:143:ARG:HD2	2.42	0.49
2:H:39:MET:HE3	2:H:39:MET:CA	2.42	0.49
2:C:91:ILE:HG23	2:C:91:ILE:O	2.12	0.49
2:G:141:ILE:O	2:G:144:MET:HB2	2.13	0.49
2:H:117:TRP:HB3	2:H:124:ILE:HB	1.94	0.48
2:D:50:GLN:O	2:D:54:THR:HG23	2.13	0.48
2:H:54:THR:CG2	3:H:184:HOH:O	2.59	0.48
2:D:100:ARG:N	2:D:100:ARG:HD2	2.28	0.47
2:D:118:MET:HE2	2:D:126:VAL:HG23	1.95	0.47
2:D:39:MET:O	2:D:43:LEU:HG	2.15	0.47
2:H:97:ARG:NH1	2:H:113:GLU:OE2	2.48	0.47
2:G:68:MET:HE1	2:G:144:MET:HE2	1.96	0.47
2:G:128:GLU:HG2	3:G:277:HOH:O	2.12	0.47
2:H:140:LYS:NZ	3:H:235:HOH:O	2.47	0.47
1:B:31:LYS:HZ3	1:B:84:GLU:CD	2.23	0.47
2:C:68:MET:CE	2:C:144:MET:HE2	2.44	0.46
2:C:68:MET:HE3	2:C:144:MET:CE	2.45	0.46
2:G:70:LYS:HE2	3:G:202:HOH:O	2.16	0.46
2:D:91:ILE:HG13	2:D:95:GLN:HB2	1.97	0.46
2:D:80:TRP:O	2:D:84:HIS:HD2	1.99	0.46
1:A:57:ILE:CD1	2:D:92:ALA:HB2	2.46	0.46
2:G:24:VAL:CG2	2:G:58:THR:HG23	2.44	0.46
2:C:18:ARG:HD2	3:C:298:HOH:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:91:ILE:HD13	3:H:189:HOH:O	2.16	0.46
2:C:68:MET:CE	2:C:144:MET:CE	2.94	0.45
1:A:66:ASP:OD1	1:A:66:ASP:C	2.58	0.45
2:D:118:MET:HE2	2:D:126:VAL:CG2	2.46	0.45
1:B:148:ARG:O	2:C:95:GLN:NE2	2.49	0.45
2:C:142:VAL:CG2	2:D:143:ARG:HD3	2.47	0.45
2:H:65:ALA:HA	2:H:68:MET:CE	2.43	0.45
2:D:37:ILE:HB	2:D:38:PRO:HD3	1.99	0.45
1:F:84:GLU:H	1:F:84:GLU:CD	2.25	0.44
1:F:13:ASP:OD2	1:F:154:LYS:CD	2.65	0.44
1:B:27:ASP:OD1	1:B:27:ASP:N	2.50	0.44
1:F:118:LYS:HB3	1:F:118:LYS:HE2	1.75	0.43
2:D:15:ILE:HD12	2:D:15:ILE:O	2.18	0.43
2:D:47:ALA:HB1	2:D:51:ASP:HB2	2.01	0.43
2:C:110:THR:OG1	2:C:113:GLU:HG3	2.18	0.43
2:H:30:LYS:O	2:H:31:ALA:C	2.62	0.43
2:G:39:MET:HE3	2:G:39:MET:CA	2.48	0.43
2:H:114:GLN:NE2	3:H:185:HOH:O	2.33	0.43
2:C:5:ASN:HD21	2:C:9:GLN:HG2	1.83	0.42
2:C:70:LYS:HE2	3:C:211:HOH:O	2.18	0.42
2:D:24:VAL:CG2	2:D:58:THR:CG2	2.97	0.42
2:D:113:GLU:OE1	3:D:195:HOH:O	2.21	0.42
1:E:84:GLU:HG2	3:E:314:HOH:O	2.18	0.42
2:C:25:LYS:HE2	2:C:25:LYS:HB3	1.81	0.42
1:E:23:GLU:OE1	1:E:131:LYS:NZ	2.52	0.42
2:C:30:LYS:HZ1	2:C:35:GLU:CD	2.26	0.42
1:E:148:ARG:CZ	1:E:148:ARG:HB3	2.48	0.42
1:F:7:PHE:CD1	1:F:7:PHE:C	2.98	0.42
2:H:132:ARG:HG3	3:H:147:HOH:O	2.20	0.42
2:D:16:SER:HA	2:D:17:PRO:HD3	1.95	0.42
2:D:121:ASN:HA	2:D:122:PRO:HA	1.92	0.42
1:A:60:PHE:CD2	2:D:93:PRO:HD3	2.55	0.42
2:D:91:ILE:O	3:D:147:HOH:O	2.22	0.42
1:B:145:PHE:CE1	1:B:154:LYS:HD2	2.54	0.42
2:H:119:THR:OG1	2:H:120:HIS:N	2.52	0.42
2:C:5:ASN:HD21	2:C:9:GLN:CG	2.33	0.42
2:D:80:TRP:CE2	2:D:84:HIS:CD2	3.08	0.42
2:G:142:VAL:HG21	2:H:143:ARG:CD	2.47	0.42
1:E:7:PHE:CD1	1:E:7:PHE:C	2.98	0.42
2:C:44:SER:OG	2:C:131:LYS:CE	2.68	0.41
2:H:120:HIS:O	2:H:123:PRO:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:THR:HA	1:F:121:TRP:CZ3	2.55	0.41
2:H:17:PRO:HD2	3:H:203:HOH:O	2.20	0.41
1:E:60:PHE:CD2	2:H:93:PRO:HD3	2.55	0.41
1:A:7:PHE:CD1	1:A:7:PHE:C	2.98	0.41
1:B:31:LYS:NZ	1:B:84:GLU:CD	2.79	0.41
1:F:13:ASP:OD2	1:F:154:LYS:CE	2.69	0.41
2:C:33:SER:O	2:C:36:VAL:CG1	2.60	0.40
1:F:164:LEU:O	3:F:1102:HOH:O	2.22	0.40
2:G:12:HIS:HB2	2:G:115:ILE:HD13	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:285:HOH:O	3:E:312:HOH:O[1_645]	2.05	0.15
3:A:269:HOH:O	3:G:192:HOH:O[1_655]	2.18	0.02

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	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
1	B	162/165 (98%)	157 (97%)	5 (3%)	0	100	100
1	E	163/165 (99%)	158 (97%)	5 (3%)	0	100	100
1	F	162/165 (98%)	154 (95%)	8 (5%)	0	100	100
2	C	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	D	133/146 (91%)	126 (95%)	5 (4%)	2 (2%)	8	2
2	G	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
2	H	133/146 (91%)	129 (97%)	4 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1204/1244 (97%)	1161 (96%)	41 (3%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	15	ILE
2	D	30	LYS

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	133/133 (100%)	129 (97%)	4 (3%)	36	30
1	B	132/133 (99%)	127 (96%)	5 (4%)	29	21
1	E	133/133 (100%)	129 (97%)	4 (3%)	36	30
1	F	132/133 (99%)	130 (98%)	2 (2%)	57	56
2	C	122/122 (100%)	116 (95%)	6 (5%)	22	14
2	D	112/122 (92%)	108 (96%)	4 (4%)	31	23
2	G	122/122 (100%)	113 (93%)	9 (7%)	13	6
2	H	112/122 (92%)	102 (91%)	10 (9%)	9	4
All	All	998/1020 (98%)	954 (96%)	44 (4%)	25	17

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	76	LYS
1	A	143	GLU
1	A	165	GLU
1	B	2	VAL
1	B	118	LYS
1	B	137	ASN
1	B	143	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	155	LYS
2	C	2	ILE
2	C	9	GLN
2	C	41	SER
2	C	58	THR
2	C	79	GLU
2	C	121	ASN
2	D	19	THR
2	D	58	THR
2	D	66	MET
2	D	121	ASN
1	E	6	VAL
1	E	29	VAL
1	E	148	ARG
1	E	165	GLU
1	F	2	VAL
1	F	5	THR
2	G	2	ILE
2	G	7	GLN
2	G	15	ILE
2	G	39	MET
2	G	58	THR
2	G	96	MET
2	G	131	LYS
2	G	141	ILE
2	G	146	SER
2	H	18	ARG
2	H	19	THR
2	H	21	ASN
2	H	28	GLU
2	H	54	THR
2	H	58	THR
2	H	91	ILE
2	H	97	ARG
2	H	112	GLN
2	H	121	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	137	ASN
2	C	4	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	7	GLN
2	C	67	GLN
2	C	74	ASN
2	C	95	GLN
2	D	13	GLN
2	D	21	ASN
2	D	50	GLN
2	D	74	ASN
2	D	84	HIS
2	D	139	ASN
2	G	7	GLN
2	G	21	ASN
2	G	74	ASN
2	G	121	ASN
2	H	74	ASN
2	H	121	ASN

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](#)

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	165/165 (100%)	-1.37	0 100 100	15, 23, 38, 63	0
1	B	164/165 (99%)	-1.42	0 100 100	13, 21, 36, 53	0
1	E	165/165 (100%)	-1.45	0 100 100	11, 19, 33, 47	0
1	F	164/165 (99%)	-0.96	0 100 100	27, 41, 59, 70	0
2	C	146/146 (100%)	-1.33	0 100 100	14, 23, 44, 51	0
2	D	135/146 (92%)	-1.10	0 100 100	20, 40, 75, 83	0
2	G	146/146 (100%)	-1.23	0 100 100	17, 28, 58, 85	0
2	H	135/146 (92%)	-1.18	0 100 100	17, 32, 61, 72	0
All	All	1220/1244 (98%)	-1.26	0 100 100	11, 27, 56, 85	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.