



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:50 PM GMT

PDB ID : 1M9Y
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

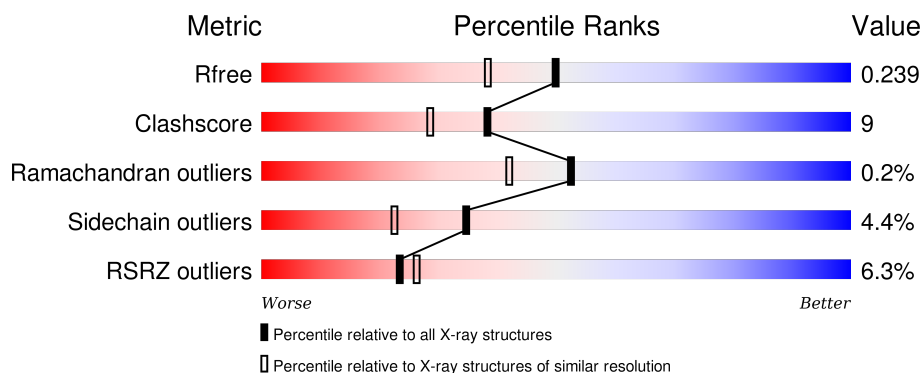
1 Overall quality at a glance ⓘ

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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 91%, yellow 9%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 91% 9% </div> </div>
1	B	165	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 87%, yellow 12%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 87% 12% .. </div> </div>
1	E	165	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 86%, yellow 13%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 86% 13% . </div> </div>
1	F	165	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 26%, green 87%, yellow 12%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 26% 87% 12% . </div> </div>
2	C	146	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 68%, yellow 27%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 68% 27% 5% </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	146	<div><div></div><div>8%</div><div>66%</div><div>22%</div><div>5%</div><div>8%</div></div>
2	G	146	<div><div></div><div>8%</div><div>84%</div><div>15%</div><div>••</div></div>
2	H	146	<div><div></div><div>5%</div><div>62%</div><div>25%</div><div>5%</div><div>•</div><div>8%</div></div>

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	UNP Q72497
C	89	ALA	GLY	ENGINEERED	UNP Q72497
C	120	HIS	ASN	SEE REMARK 999	UNP Q72497
D	87	ALA	HIS	ENGINEERED	UNP Q72497
D	89	ALA	GLY	ENGINEERED	UNP Q72497
D	120	HIS	ASN	SEE REMARK 999	UNP Q72497
G	87	ALA	HIS	ENGINEERED	UNP Q72497
G	89	ALA	GLY	ENGINEERED	UNP Q72497

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

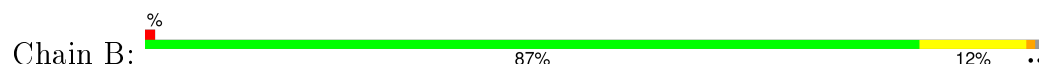
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



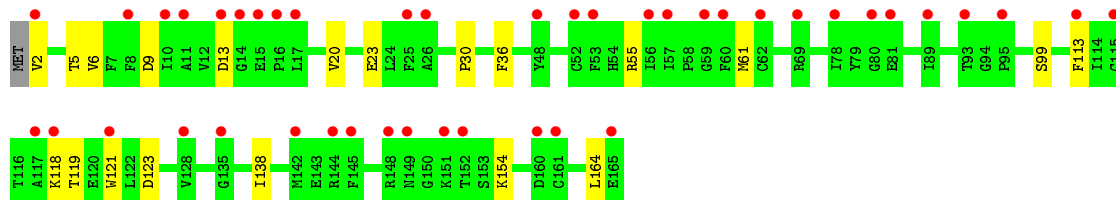
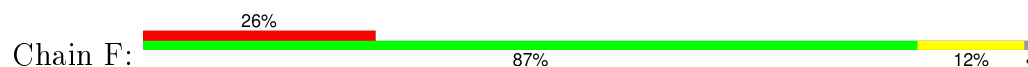
- Molecule 1: Cyclophilin A



- Molecule 1: Cyclophilin A



- Molecule 1: Cyclophilin A

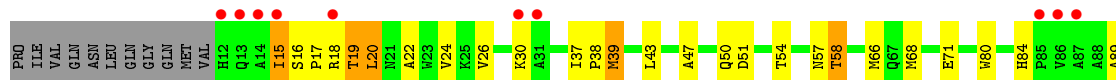


- Molecule 2: HIV-1 Capsid

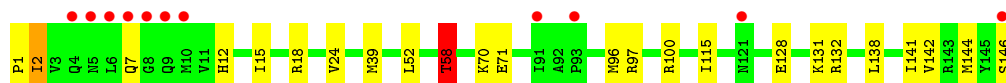
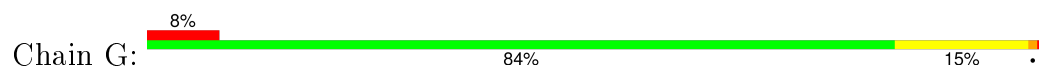




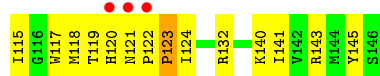
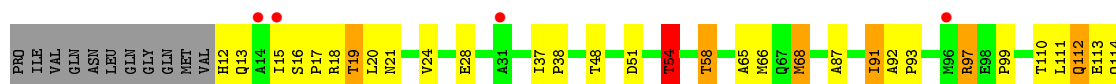
• Molecule 2: HIV-1 Capsid



• Molecule 2: HIV-1 Capsid



• Molecule 2: HIV-1 Capsid



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 19.68 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.69-1.90) 96.2 (19.68-1.90)	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	Depositor
R, R_{free}	0.162 , 0.234 0.170 , 0.239	Depositor DCC
R_{free} test set	8529 reflections (11.22%)	DCC
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.0	EDS
Estimated twinning fraction	0.319 for -h,k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 84527 reflections	Xtriage
F_o, F_c correlation	0.96	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.80	0/1294	1.36	4/1733 (0.2%)
1	B	0.85	0/1286	1.41	7/1723 (0.4%)
1	E	0.92	0/1294	1.44	14/1733 (0.8%)
1	F	0.56	0/1286	1.15	3/1723 (0.2%)
2	C	0.83	0/1159	1.44	12/1577 (0.8%)
2	D	0.62	0/1074	1.28	8/1462 (0.5%)
2	G	0.72	0/1159	1.30	6/1577 (0.4%)
2	H	0.81	1/1074 (0.1%)	1.31	3/1462 (0.2%)
All	All	0.77	1/9626 (0.0%)	1.34	57/12990 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	68	MET	SD-CE	-5.79	1.45	1.77

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	18	ARG	NE-CZ-NH1	-10.68	114.96	120.30
2	D	143	ARG	NE-CZ-NH1	-9.07	115.76	120.30
2	C	18	ARG	NE-CZ-NH1	-9.03	115.78	120.30
1	B	27	ASP	CB-CG-OD2	8.79	126.21	118.30
1	B	37	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	E	13	ASP	CB-CG-OD1	8.04	125.53	118.30
2	C	82	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	B	69	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	B	19	ARG	NE-CZ-NH2	-7.84	116.38	120.30
2	C	96	MET	CG-SD-CE	7.80	112.69	100.20
2	H	66	MET	CG-SD-CE	-7.59	88.06	100.20
2	G	97	ARG	NE-CZ-NH1	-7.44	116.58	120.30
2	G	58	THR	N-CA-CB	-7.38	96.29	110.30
2	C	145	TYR	C-N-CA	7.36	140.10	121.70
2	D	39	MET	CG-SD-CE	-7.26	88.59	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	85	ASP	CB-CG-OD2	7.23	124.81	118.30
1	F	55	ARG	NE-CZ-NH2	-7.04	116.78	120.30
2	C	100	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	E	55	ARG	NE-CZ-NH2	-6.83	116.89	120.30
2	C	58	THR	N-CA-CB	-6.70	97.57	110.30
1	E	155	LYS	CD-CE-NZ	6.65	127.00	111.70
1	B	80	GLY	N-CA-C	-6.60	96.61	113.10
1	E	116	THR	CA-CB-CG2	-6.54	103.24	112.40
2	D	68	MET	CG-SD-CE	-6.52	89.76	100.20
1	B	123	ASP	CB-CG-OD1	6.37	124.03	118.30
2	D	143	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	B	20	VAL	CB-CA-C	-6.28	99.47	111.40
1	E	19	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	E	37	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	E	134	GLU	OE1-CD-OE2	-6.16	115.91	123.30
2	C	81	ASP	CB-CG-OD2	6.13	123.82	118.30
2	D	144	MET	CG-SD-CE	6.07	109.91	100.20
1	A	55	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	27	ASP	CB-CG-OD2	5.96	123.66	118.30
1	E	165	GLU	OE1-CD-OE2	5.96	130.45	123.30
1	F	123	ASP	CB-CG-OD1	5.87	123.58	118.30
2	C	36	VAL	CG1-CB-CG2	-5.66	101.85	110.90
1	E	69	ARG	NE-CZ-NH1	5.59	123.10	120.30
2	D	20	LEU	CB-CA-C	-5.58	99.61	110.20
1	A	85	ASP	CB-CG-OD2	5.49	123.24	118.30
2	G	100	ARG	NE-CZ-NH2	5.44	123.02	120.30
2	C	132	ARG	NE-CZ-NH1	-5.44	117.58	120.30
2	H	54	THR	OG1-CB-CG2	-5.38	97.62	110.00
2	D	103	ASP	CB-CG-OD2	5.33	123.10	118.30
1	E	13	ASP	OD1-CG-OD2	-5.33	113.18	123.30
1	A	69	ARG	NE-CZ-NH1	5.31	122.96	120.30
2	C	103	ASP	CB-CG-OD1	5.31	123.08	118.30
2	C	146	SER	N-CA-CB	5.28	118.42	110.50
1	E	144	ARG	CB-CA-C	-5.26	99.87	110.40
2	C	68	MET	CG-SD-CE	5.21	108.54	100.20
1	E	164	LEU	CB-CG-CD1	-5.14	102.25	111.00
2	H	51	ASP	CB-CG-OD1	5.09	122.88	118.30
2	G	97	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	E	143	GLU	CG-CD-OE1	-5.06	108.19	118.30
1	F	9	ASP	CB-CG-OD2	5.05	122.85	118.30
2	G	52	LEU	CB-CG-CD2	-5.05	102.41	111.00
2	D	89	ALA	N-CA-C	-5.05	97.37	111.00

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	6	0
1	B	1258	0	1225	8	0
1	E	1266	0	1237	8	0
1	F	1258	0	1225	12	0
2	C	1132	0	1135	50	0
2	D	1048	0	1043	29	0
2	G	1132	0	1135	23	0
2	H	1048	0	1043	46	0
3	A	171	0	0	2	1
3	B	177	0	0	1	0
3	C	178	0	0	8	1
3	D	61	0	0	6	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	170	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 9.

All (170) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:G:71:GLU:OE1	3:G:169:HOH:O	2.03	0.77
2:H:68:MET:HE1	3:H:160:HOH:O	1.85	0.75
2:H:16:SER:HB3	2:H:19:THR:OG1	1.86	0.75
1:F:6:VAL:HG21	1:F:36:PHE:HE2	1.53	0.73
2:D:71:GLU:OE1	3:D:180:HOH:O	2.07	0.72
2:C:67:GLN:HE22	2:C:70:LYS:HZ1	1.38	0.72
2:C:30:LYS:NZ	2:C:35:GLU:CG	2.47	0.69
2:H:68:MET:CE	3:H:160:HOH:O	2.38	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:C:39:MET:HA	2:C:39:MET:HE3	1.74	0.68
2:H:54:THR:HG22	3:H:184:HOH:O	1.94	0.68
1:A:118:LYS:NZ	3:A:321:HOH:O	2.24	0.68
2:H:112:GLN:CD	2:H:112:GLN:H	1.97	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
2:G:144:MET:HG2	3:G:257:HOH:O	1.96	0.66
1:F:30:PRO:HG2	3:F:1093:HOH:O	1.97	0.64
2:H:65:ALA:HA	2:H:68:MET:HE2	1.80	0.64
2:D:24:VAL:HG22	2:D:58:THR:HG23	1.80	0.64
2:C:138:LEU:O	2:C:142:VAL:HG13	1.99	0.63
2:C:68:MET:HE1	2:C:144:MET:SD	2.38	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:G:142:VAL:CG2	2:H:143:ARG:HD3	2.29	0.61
2:D:22:ALA:O	2:D:26:VAL:HG23	2.00	0.61
2:C:19:THR:HG21	3:C:306:HOH:O	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:67:GLN:HG2	3:C:180:HOH:O	2.02	0.60
2:H:24:VAL:CG2	2:H:58:THR:HG23	2.33	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110:THR:HG23	3:D:195:HOH:O	2.02	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:C:39:MET:HE3	2:C:39:MET:CA	2.35	0.56
2:D:18:ARG:HG3	3:D:189:HOH:O	2.05	0.56
2:H:91:ILE:CD1	3:H:196:HOH:O	2.52	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
2:H:87:ALA:CB	3:H:225:HOH:O	2.49	0.54
1:F:6:VAL:HG21	1:F:36:PHE:CE2	2.39	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
2:G:132:ARG:HD2	3:H:208:HOH:O	2.06	0.54
1:F:20:VAL:HG22	1:F:138:ILE:HB	1.89	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:C:4:GLN:HE21	2:C:8:GLY:C	2.11	0.53
2:G:142:VAL:HG21	2:H:143:ARG:HD2	1.90	0.53
2:H:111:LEU:O	2:H:115:ILE:HD12	2.08	0.53
1:F:23:GLU:HB2	3:F:956:HOH:O	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:D:19:THR:O	2:D:22:ALA:HB3	2.09	0.53
2:D:110:THR:HG23	2:D:113:GLU:OE1	2.08	0.52
2:C:37:ILE:HB	2:C:38:PRO:HD3	1.91	0.51
2:C:6:LEU:CD2	2:C:7:GLN:HE21	2.18	0.51
2:H:120:HIS:O	2:H:122:PRO:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLU:HG2	3:A:313:HOH:O	2.10	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:H:12:HIS:CE1	2:H:13:GLN:O	2.66	0.49
1:A:165:GLU:OXT	1:A:165:GLU:HG2	2.11	0.49
2:G:142:VAL:CG2	2:H:143:ARG:HD2	2.42	0.49
2:G:141:ILE:O	2:G:144:MET:HB2	2.13	0.49
2:C:91:ILE:HG23	2:C:91:ILE:O	2.12	0.49
2:H:117:TRP:HB3	2:H:124:ILE:HB	1.94	0.48
2:H:112:GLN:CD	2:H:112:GLN:N	2.66	0.48
2:H:65:ALA:HA	2:H:68:MET:CE	2.43	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:C:66:MET:HA	2:C:66:MET:HE2	1.95	0.47
2:D:100:ARG:N	2:D:100:ARG:HD2	2.28	0.47
1:B:84:GLU:H	1:B:84:GLU:CD	2.17	0.47
2:G:39:MET:HE2	2:G:39:MET:HB3	1.84	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:C:67:GLN:HE22	2:C:70:LYS:HZ3	1.59	0.47
2:G:128:GLU:HG2	3:G:277:HOH:O	2.12	0.47
2:G:70:LYS:HE2	3:G:202:HOH:O	2.16	0.46
2:D:96:MET:CE	2:D:96:MET:HA	2.46	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:H:91:ILE:HD13	3:H:189:HOH:O	2.16	0.46
2:C:18:ARG:HD2	3:C:298:HOH:O	2.16	0.46
2:C:68:MET:CE	2:C:144:MET:CE	2.94	0.45
1:E:76:LYS:NZ	3:E:353:HOH:O	2.28	0.45
2:H:68:MET:HE1	2:H:145:TYR:HE2	1.81	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:G:39:MET:HA	2:G:39:MET:HE3	1.99	0.45
2:D:37:ILE:HB	2:D:38:PRO:HD3	1.99	0.45
1:F:13:ASP:OD2	1:F:154:LYS:CD	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:48:THR:HA	2:H:118:MET:HE1	1.99	0.44
1:B:27:ASP:N	1:B:27:ASP:OD1	2.50	0.44
1:F:118:LYS:HE2	1:F:118:LYS:HB3	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:114:GLN:NE2	3:H:185:HOH:O	2.33	0.43
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
2:C:5:ASN:HD21	2:C:9:GLN:HG2	1.83	0.42
2:C:66:MET:CE	2:C:66:MET:HA	2.49	0.42
1:E:84:GLU:HG2	3:E:314:HOH:O	2.18	0.42
1:E:23:GLU:OE1	1:E:131:LYS:NZ	2.52	0.42
2:C:25:LYS:HE2	2:C:25:LYS:HB3	1.81	0.42
1:E:148:ARG:HB3	1:E:148:ARG:CZ	2.48	0.42
2:H:132:ARG:HG3	3:H:147:HOH:O	2.20	0.42
2:D:121:ASN:HA	2:D:122:PRO:HA	1.92	0.42
2:D:16:SER:HA	2:D:17:PRO:HD3	1.95	0.42
2:D:91:ILE:O	3:D:147:HOH:O	2.22	0.42
1:A:60:PHE:CD2	2:D:93:PRO:HD3	2.55	0.42
2:H:119:THR:OG1	2:H:120:HIS:N	2.52	0.42
1:B:145:PHE:CE1	1:B:154:LYS:HD2	2.54	0.42
2:G:142:VAL:HG21	2:H:143:ARG:CD	2.47	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:H:120:HIS:O	2:H:123:PRO:N	2.53	0.41
2:C:44:SER:OG	2:C:131:LYS:CE	2.68	0.41
2:H:17:PRO:HD2	3:H:203:HOH:O	2.20	0.41
1:F:119:THR:HA	1:F:121:TRP:CZ3	2.55	0.41
1:E:60:PHE:CD2	2:H:93:PRO:HD3	2.55	0.41
2:C:68:MET:HE3	2:C:144:MET:CE	2.51	0.41
2:H:140:LYS:NZ	3:H:212:HOH:O	2.32	0.41
1:A:66:ASP:C	1:A:66:ASP:OD1	2.58	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
2:C:68:MET:HE1	2:C:144:MET:CE	2.51	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
2:H:68:MET:HE3	2:H:141:ILE:HG12	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry 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 [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	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%)	13	3
2	G	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
2	H	133/146 (91%)	129 (97%)	4 (3%)	0	100	100
All	All	1204/1244 (97%)	1161 (96%)	41 (3%)	2 (0%)	52	42

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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%)	128 (96%)	5 (4%)	40	28
1	B	132/133 (99%)	126 (96%)	6 (4%)	34	21
1	E	133/133 (100%)	130 (98%)	3 (2%)	58	51
1	F	132/133 (99%)	130 (98%)	2 (2%)	72	69
2	C	122/122 (100%)	116 (95%)	6 (5%)	31	18
2	D	112/122 (92%)	108 (96%)	4 (4%)	42	30
2	G	122/122 (100%)	115 (94%)	7 (6%)	25	13
2	H	112/122 (92%)	101 (90%)	11 (10%)	10	3
All	All	998/1020 (98%)	954 (96%)	44 (4%)	35	22

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

Mol	Chain	Res	Type
1	A	29	VAL
1	A	61	MET
1	A	76	LYS
1	A	131	LYS
1	A	143	GLU
1	B	2	VAL
1	B	61	MET
1	B	118	LYS
1	B	137	ASN
1	B	143	GLU
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	29	VAL
1	E	61	MET
1	E	148	ARG

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Mol	Chain	Res	Type
1	F	2	VAL
1	F	61	MET
2	G	2	ILE
2	G	7	GLN
2	G	15	ILE
2	G	58	THR
2	G	96	MET
2	G	131	LYS
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
2	H	123	PRO

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

Mol	Chain	Res	Type
1	A	137	ASN
1	B	137	ASN
2	C	4	GLN
2	C	7	GLN
2	C	67	GLN
2	C	74	ASN
2	D	13	GLN
2	D	21	ASN
2	D	50	GLN
2	D	74	ASN
2	D	84	HIS
2	G	7	GLN
2	G	21	ASN
2	G	74	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 carbohydrates 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	165/165 (100%)	-0.54	1 (0%) 90 91	15, 23, 38, 63	0
1	B	164/165 (99%)	-0.29	1 (0%) 90 91	13, 21, 36, 53	0
1	E	165/165 (100%)	-0.53	0 100 100	11, 19, 33, 47	0
1	F	164/165 (99%)	1.48	43 (26%) 1 1	27, 41, 59, 70	0
2	C	146/146 (100%)	-0.35	2 (1%) 78 80	14, 23, 44, 51	0
2	D	135/146 (92%)	0.37	12 (8%) 12 13	20, 40, 75, 83	0
2	G	146/146 (100%)	0.20	11 (7%) 17 19	17, 28, 58, 85	0
2	H	135/146 (92%)	0.05	7 (5%) 31 34	17, 32, 61, 72	0
All	All	1220/1244 (98%)	0.04	77 (6%) 23 26	11, 27, 56, 85	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	8	GLY	8.6
2	D	121	ASN	7.9
1	F	148	ARG	5.9
2	G	10	MET	5.6
1	F	60	PHE	5.3
1	F	2	VAL	5.3
2	G	6	LEU	5.1
2	G	4	GLN	4.9
2	C	146	SER	4.9
2	G	5	ASN	4.9
1	F	11	ALA	4.2
2	D	18	ARG	4.2
1	A	165	GLU	4.2
2	G	9	GLN	4.2
1	F	17	LEU	4.2
1	F	165	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	81	GLU	3.9
1	F	144	ARG	3.9
1	F	62	CYS	3.7
1	F	152	THR	3.7
1	F	161	CYS	3.6
1	F	93	THR	3.6
2	D	14	ALA	3.5
2	D	87	ALA	3.5
2	G	146	SER	3.5
2	G	93	PRO	3.5
2	D	13	GLN	3.4
1	F	57	ILE	3.3
2	G	91	ILE	3.3
2	D	31	ALA	3.3
2	D	12	HIS	3.3
1	F	10	ILE	3.3
1	F	56	ILE	3.3
1	F	13	ASP	3.1
1	F	117	ALA	3.0
2	D	112	GLN	3.0
1	F	48	TYR	2.8
1	F	15	GLU	2.8
2	H	31	ALA	2.8
2	G	121	ASN	2.8
1	F	59	GLY	2.8
1	F	160	ASP	2.7
1	F	78	ILE	2.7
2	D	85	PRO	2.7
1	F	80	GLY	2.7
2	D	15	ILE	2.6
2	D	30	LYS	2.6
1	F	142	MET	2.6
2	D	86	VAL	2.6
2	H	121	ASN	2.6
1	F	121	TRP	2.5
1	F	145	PHE	2.5
1	F	89	ILE	2.5
2	H	122	PRO	2.5
2	C	6	LEU	2.5
1	F	135	GLY	2.5
1	F	26	ALA	2.4
1	B	2	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	14	GLY	2.4
1	F	113	PHE	2.4
1	F	149	ASN	2.3
1	F	16	PRO	2.3
1	F	69	ARG	2.3
1	F	52	CYS	2.2
2	H	96	MET	2.2
2	H	120	HIS	2.2
1	F	8	PHE	2.1
2	H	15	ILE	2.1
1	F	25	PHE	2.1
1	F	115	CYS	2.1
1	F	128	VAL	2.1
2	H	14	ALA	2.1
1	F	95	PRO	2.1
1	F	151	LYS	2.0
2	G	7	GLN	2.0
1	F	53	PHE	2.0
1	F	118	LYS	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 carbohydrates 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.