Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:50 PM GMT

PDB ID	:	1M9X
Title	:	X-ray crystal structure of Cyclophilin A/HIV-1 CA N-terminal domain (1-146) M-type H87A,A88M,G89A Complex.
Authors	:	Howard, B.R.; Vajdos, F.F.; Li, S.; Sundquist, W.I.; Hill, C.P.
Deposited on	:	2002-07-30
Resolution	:	1.70 Å(reported)

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

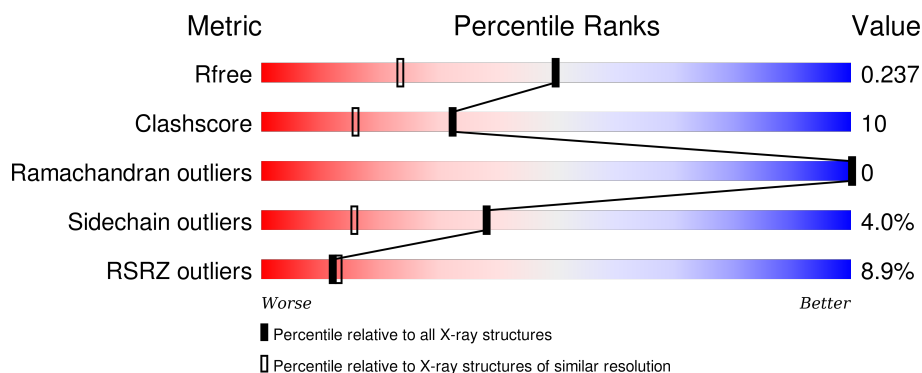|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 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	Percentile Ranks	Value
Rfree		0.237
Clashscore		10
Ramachandran outliers		0
Sidechain outliers		4.0%
RSRZ outliers		8.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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 <=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	% 85% 12% •
1	B	165	86% 12% ••
1	E	165	% 92% 7% •
1	F	165	33% 84% 14% ••
2	C	146	3% 75% 22% •

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Mol	Chain	Length	Quality of chain
2	D	146	11% · 70% · 19% · · 8%
2	G	146	12% · 75% · 23% ·
2	H	146	8% · 64% · 24% · · 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10972 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 1266	C 802	N 218	O 237	S 9	0	0	0
1	B	164	Total 1258	C 797	N 217	O 236	S 8	0	0	0
1	E	165	Total 1266	C 802	N 218	O 237	S 9	0	0	0
1	F	164	Total 1258	C 797	N 217	O 236	S 8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	146	Total 1163	C 737	N 202	O 214	S 10	0	4	0
2	D	135	Total 1051	C 665	N 183	O 195	S 8	0	0	0
2	G	146	Total 1163	C 737	N 202	O 214	S 10	0	4	0
2	H	135	Total 1051	C 665	N 183	O 195	S 8	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	87	ALA	HIS	ENGINEERED	UNP Q72497
C	88	MET	ALA	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	88	MET	ALA	ENGINEERED	UNP Q72497
D	89	ALA	GLY	ENGINEERED	UNP Q72497
D	120	HIS	ASN	SEE REMARK 999	UNP Q72497

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Chain	Residue	Modelled	Actual	Comment	Reference
G	87	ALA	HIS	ENGINEERED	UNP Q72497
G	88	MET	ALA	ENGINEERED	UNP Q72497
G	89	ALA	GLY	ENGINEERED	UNP Q72497
G	120	HIS	ASN	SEE REMARK 999	UNP Q72497
H	87	ALA	HIS	ENGINEERED	UNP Q72497
H	88	MET	ALA	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	256	Total 256	O 256	0	0
3	B	226	Total 226	O 226	0	0
3	C	189	Total 189	O 189	0	0
3	D	122	Total 122	O 122	0	0
3	E	254	Total 254	O 254	0	0
3	F	138	Total 138	O 138	0	0
3	G	163	Total 163	O 163	0	0
3	H	148	Total 148	O 148	0	0

3 Residue-property plots ⓘ

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.
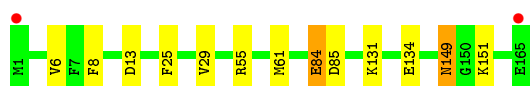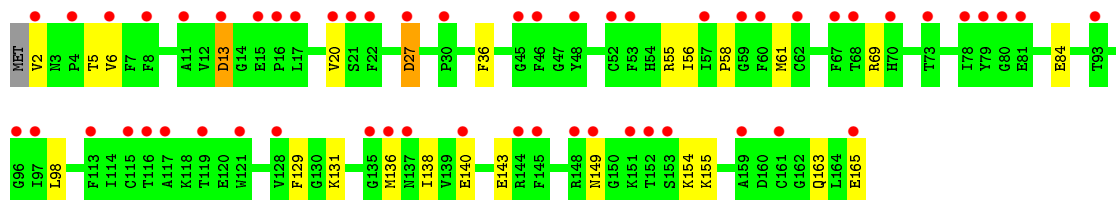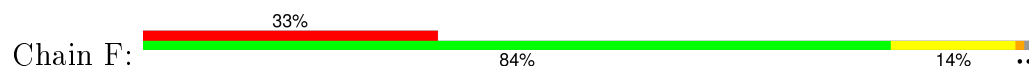
- Molecule 1: Cyclophilin A
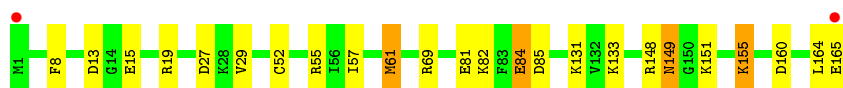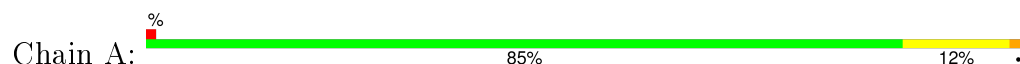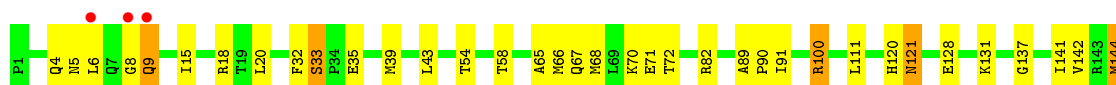

- Molecule 1: Cyclophilin A
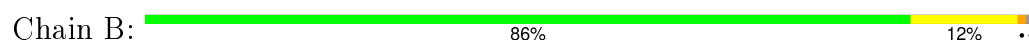
- Molecule 1: Cyclophilin A

- Molecule 1: Cyclophilin A

- Molecule 2: HIV-1 Capsid

Y145 S146

• **Molecule 2: HIV-1 Capsid**

Chain D:

• **Molecule 2: HIV-1 Capsid**

Chain G:

• **Molecule 2: HIV-1 Capsid**

Chain H:
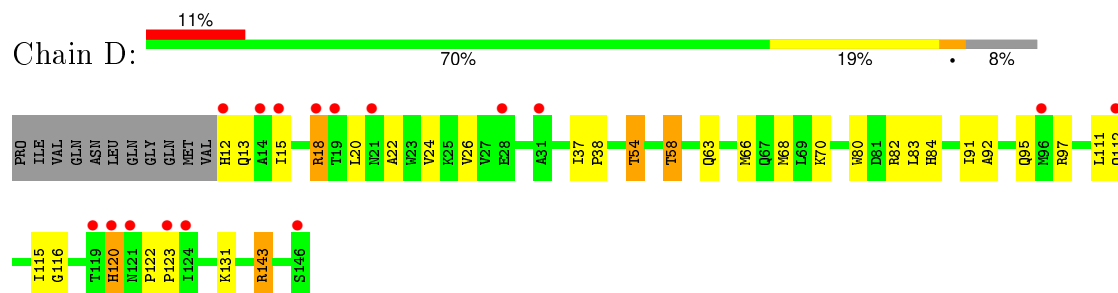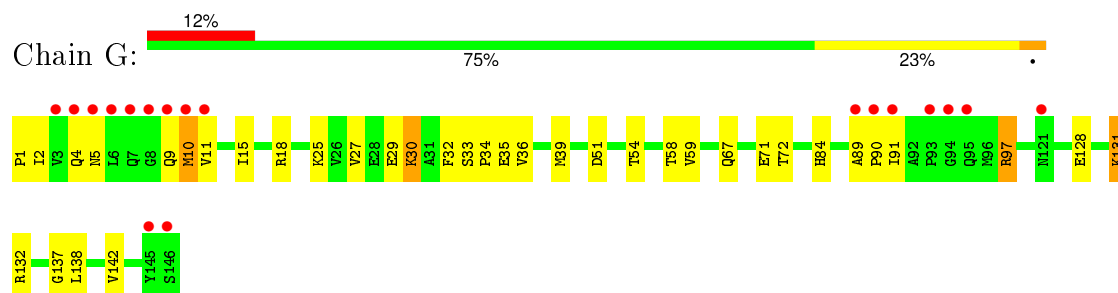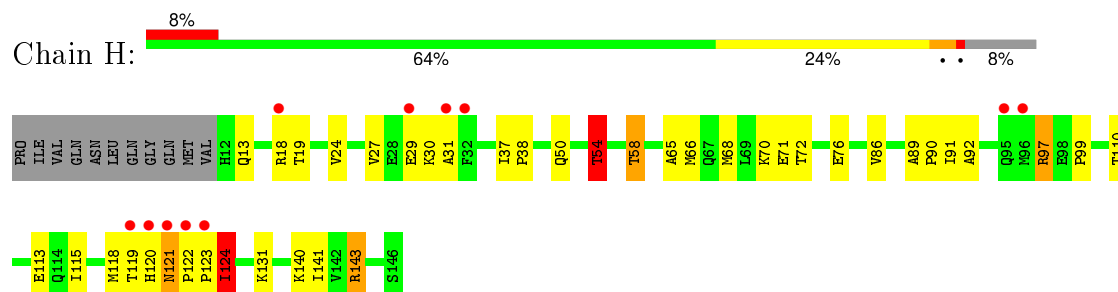
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	38.47Å 111.12Å 67.91Å 89.98° 101.60° 89.90°	Depositor
Resolution (Å)	19.69 – 1.70 19.69 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.1 (19.69-1.70) 96.6 (19.69-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.165 , 0.230 0.175 , 0.237	Depositor DCC
R_{free} test set	11826 reflections (11.18%)	DCC
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 33.4	EDS
Estimated twinning fraction	0.379 for -h,k,-l	Xtriage
L-test for twinning [2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 117637 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10972	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.89	0/1294	1.36	13/1733 (0.8%)
1	B	0.90	0/1286	1.33	7/1723 (0.4%)
1	E	0.95	0/1294	1.36	10/1733 (0.6%)
1	F	0.67	0/1286	1.17	4/1723 (0.2%)
2	C	0.86	1/1191 (0.1%)	1.36	10/1620 (0.6%)
2	D	0.78	0/1077	1.24	5/1465 (0.3%)
2	G	0.82	0/1191	1.19	3/1620 (0.2%)
2	H	0.82	0/1077	1.28	7/1465 (0.5%)
All	All	0.84	1/9696 (0.0%)	1.29	59/13082 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	66	MET	SD-CE	-6.13	1.43	1.77

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	100	ARG	NE-CZ-NH1	15.43	128.01	120.30
2	C	100	ARG	NE-CZ-NH2	-13.61	113.50	120.30
2	D	143	ARG	NE-CZ-NH1	-11.58	114.51	120.30
1	E	55	ARG	NE-CZ-NH2	-11.31	114.64	120.30
1	A	27	ASP	CB-CG-OD2	9.57	126.92	118.30
1	E	85	ASP	CB-CG-OD2	9.32	126.69	118.30
2	G	97	ARG	NE-CZ-NH1	-9.22	115.69	120.30
1	F	27	ASP	CB-CG-OD2	8.33	125.80	118.30
1	E	8	PHE	CB-CG-CD1	8.26	126.58	120.80
2	H	143	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	B	8	PHE	CB-CG-CD2	-8.02	115.19	120.80
1	A	55	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	19	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	84	GLU	CG-CD-OE1	6.83	131.95	118.30
2	H	18	ARG	NE-CZ-NH2	6.82	123.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	100	ARG	CD-NE-CZ	6.77	133.07	123.60
1	A	85	ASP	CB-CG-OD2	6.65	124.28	118.30
2	C	18	ARG	NE-CZ-NH1	-6.64	116.98	120.30
2	H	54	THR	OG1-CB-CG2	-6.62	94.77	110.00
2	C	82	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	F	69	ARG	NE-CZ-NH1	6.51	123.56	120.30
2	C	100	ARG	CG-CD-NE	-6.49	98.17	111.80
1	A	8	PHE	CB-CG-CD1	6.45	125.31	120.80
2	G	97	ARG	NE-CZ-NH2	6.38	123.49	120.30
2	C	82	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	55	ARG	NE-CZ-NH1	6.20	123.40	120.30
2	C	144	MET	CA-CB-CG	6.08	123.63	113.30
1	A	155	LYS	CD-CE-NZ	6.03	125.56	111.70
1	B	160	ASP	CB-CG-OD1	6.02	123.71	118.30
1	A	69	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	8	PHE	CB-CG-CD1	5.99	124.99	120.80
1	A	84	GLU	OE1-CD-OE2	-5.90	116.22	123.30
2	D	18	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	B	69	ARG	NE-CZ-NH2	-5.85	117.37	120.30
2	H	66	MET	CG-SD-CE	-5.69	91.10	100.20
1	E	84	GLU	OE1-CD-OE2	-5.68	116.48	123.30
1	E	6	VAL	CA-CB-CG2	-5.68	102.38	110.90
1	E	8	PHE	CB-CG-CD2	-5.65	116.84	120.80
1	A	61	MET	CA-CB-CG	5.64	122.88	113.30
1	E	13	ASP	CB-CG-OD1	5.62	123.35	118.30
2	H	124	ILE	N-CA-C	-5.62	95.84	111.00
2	G	18	ARG	NE-CZ-NH1	-5.59	117.51	120.30
2	D	143	ARG	CD-NE-CZ	-5.50	115.90	123.60
1	E	84	GLU	CG-CD-OE1	5.42	129.14	118.30
2	C	111	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	B	27	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	82	LYS	CD-CE-NZ	5.29	123.85	111.70
1	F	55	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	F	13	ASP	CB-CG-OD2	5.23	123.00	118.30
1	E	55	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	E	134	GLU	OE1-CD-OE2	-5.17	117.09	123.30
1	B	69	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	D	68	MET	CG-SD-CE	-5.14	91.98	100.20
2	D	54	THR	OG1-CB-CG2	-5.12	98.22	110.00
2	H	97	ARG	NE-CZ-NH2	5.09	122.84	120.30
2	C	43	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	A	27	ASP	OD1-CG-OD2	-5.02	113.77	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	118	MET	CG-SD-CE	5.01	108.22	100.20
1	A	160	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	13	0
1	B	1258	0	1225	14	0
1	E	1266	0	1237	5	0
1	F	1258	0	1225	16	0
2	C	1163	0	1170	41	0
2	D	1051	0	1047	24	0
2	G	1163	0	1170	46	0
2	H	1051	0	1047	43	0
3	A	256	0	0	4	0
3	B	226	0	0	2	0
3	C	189	0	0	17	0
3	D	122	0	0	11	0
3	E	254	0	0	0	1
3	F	138	0	0	2	0
3	G	163	0	0	20	0
3	H	148	0	0	17	1
All	All	10972	0	9358	197	1

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 (197) 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:89[B]:ALA:CB	3:C:147:HOH:O	1.66	1.32
2:G:89[B]:ALA:N	3:G:147:HOH:O	1.72	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:89[B]:ALA:CB	3:C:148:HOH:O	1.89	1.17
2:C:89[B]:ALA:HB2	3:C:148:HOH:O	1.46	1.11
2:C:89[B]:ALA:N	3:C:148:HOH:O	1.85	1.06
2:D:91:ILE:HD12	3:D:147:HOH:O	1.62	0.99
2:C:4:GLN:HE21	2:C:8:GLY:HA2	1.29	0.98
2:G:89[B]:ALA:CB	3:G:147:HOH:O	2.12	0.96
2:C:5:ASN:HD21	2:C:9:GLN:HE21	1.14	0.93
2:H:115:ILE:O	2:H:119:THR:HG23	1.67	0.92
1:A:52:CYS:SG	3:A:329:HOH:O	2.32	0.86
2:D:54:THR:HG22	3:D:194:HOH:O	1.75	0.86
2:H:86:VAL:HG23	3:H:286:HOH:O	1.75	0.85
2:H:65:ALA:HA	2:H:68:MET:CE	2.07	0.84
2:G:89[B]:ALA:HB2	3:G:147:HOH:O	1.74	0.83
1:B:149:ASN:HD22	1:B:149:ASN:H	1.27	0.82
2:C:100:ARG:HD3	3:C:201:HOH:O	1.80	0.81
2:H:54:THR:HG22	3:H:179:HOH:O	1.80	0.81
2:C:70:LYS:HG3	3:C:209:HOH:O	1.79	0.81
2:C:89[B]:ALA:HB1	3:C:147:HOH:O	1.53	0.80
1:F:13:ASP:OD2	1:F:154:LYS:HG2	1.83	0.79
2:C:89[B]:ALA:HB2	3:C:147:HOH:O	1.52	0.77
2:D:15:ILE:HD12	2:D:20:LEU:HD21	1.67	0.77
1:F:20:VAL:HG22	1:F:138:ILE:HB	1.66	0.75
1:F:5:THR:N	1:F:165:GLU:OXT	2.17	0.74
2:C:67:GLN:HG3	3:C:309:HOH:O	1.88	0.74
2:H:65:ALA:HA	2:H:68:MET:HE3	1.70	0.73
1:A:81:GLU:OE2	3:A:304:HOH:O	2.06	0.73
2:G:30:LYS:HE2	3:G:278:HOH:O	1.87	0.73
2:G:132:ARG:HD3	3:G:204:HOH:O	1.88	0.73
2:C:6:LEU:HD12	2:C:6:LEU:H	1.52	0.73
2:G:128:GLU:OE2	2:G:131:LYS:NZ	2.20	0.72
2:D:97:ARG:HD3	3:D:242:HOH:O	1.89	0.72
2:H:91:ILE:HD12	3:H:226:HOH:O	1.91	0.71
2:C:128:GLU:HG2	3:C:205:HOH:O	1.89	0.70
2:H:120:HIS:O	2:H:122:PRO:C	2.30	0.70
2:C:15:ILE:HD13	2:C:20:LEU:HD21	1.73	0.70
1:B:56:ILE:CD1	1:B:156:ILE:HD12	2.23	0.69
2:G:5:ASN:OD1	2:G:9:GLN:HG2	1.93	0.69
1:B:147:SER:OG	1:B:149:ASN:ND2	2.25	0.68
2:G:131:LYS:CD	3:G:293:HOH:O	2.41	0.68
2:D:37:ILE:HB	2:D:38:PRO:HD3	1.76	0.67
2:H:68:MET:HE1	2:H:141:ILE:HG12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:5:ASN:HD21	2:C:9:GLN:NE2	1.91	0.66
2:H:65:ALA:HA	2:H:68:MET:HE2	1.76	0.66
2:D:24:VAL:HG22	2:D:58:THR:HG23	1.76	0.66
2:D:66:MET:CE	3:D:202:HOH:O	2.44	0.66
1:F:149:ASN:HB2	3:F:223:HOH:O	1.96	0.65
2:D:63:GLN:NE2	3:D:228:HOH:O	2.26	0.65
2:C:5:ASN:OD1	2:C:9:GLN:HG2	1.97	0.64
2:H:68:MET:CE	2:H:141:ILE:HG12	2.28	0.64
1:B:20:VAL:CG2	1:B:138:ILE:HB	2.27	0.64
2:H:76:GLU:OE1	3:H:235:HOH:O	2.15	0.63
2:H:37:ILE:HB	2:H:38:PRO:HD3	1.80	0.63
2:G:89[B]:ALA:HB1	2:G:90[B]:PRO:HA	1.81	0.62
2:D:111:LEU:O	2:D:115:ILE:HD12	1.99	0.62
2:H:99:PRO:HG3	2:H:124:ILE:HG21	1.80	0.62
2:C:4:GLN:NE2	2:C:8:GLY:HA2	2.10	0.61
2:G:128:GLU:HG3	3:G:282:HOH:O	1.99	0.61
1:B:56:ILE:HD12	1:B:156:ILE:HD12	1.83	0.60
2:C:91[B]:ILE:HD13	3:C:207:HOH:O	2.00	0.60
2:G:30:LYS:CE	3:G:278:HOH:O	2.46	0.59
2:G:128:GLU:CG	3:G:282:HOH:O	2.50	0.59
2:D:22:ALA:O	2:D:26:VAL:HG23	2.02	0.59
2:C:89[B]:ALA:CA	3:C:148:HOH:O	2.23	0.59
1:B:149:ASN:H	1:B:149:ASN:ND2	1.98	0.58
2:D:15:ILE:HD12	2:D:20:LEU:CD2	2.33	0.58
2:G:39:MET:HA	2:G:39:MET:HE3	1.85	0.58
2:H:97:ARG:NH1	3:H:264:HOH:O	2.36	0.58
2:H:120:HIS:O	2:H:123:PRO:N	2.37	0.58
2:H:124:ILE:HD11	3:H:269:HOH:O	2.03	0.58
2:G:131:LYS:HD2	3:G:293:HOH:O	2.02	0.57
2:G:142:VAL:CG2	2:H:143:ARG:HD3	2.34	0.57
2:H:30:LYS:O	2:H:31:ALA:HB3	2.03	0.57
2:H:50:GLN:NE2	3:H:211:HOH:O	2.36	0.57
2:C:89[B]:ALA:HB1	2:C:90[B]:PRO:HA	1.86	0.57
2:D:91:ILE:HD13	3:D:217:HOH:O	2.05	0.56
2:H:91:ILE:HD12	2:H:92:ALA:H	1.71	0.55
2:D:15:ILE:CD1	2:D:20:LEU:HD21	2.34	0.55
2:G:32:PHE:O	2:G:142:VAL:HG12	2.06	0.55
1:B:20:VAL:HG22	1:B:138:ILE:HB	1.89	0.55
2:G:142:VAL:HG23	2:H:143:ARG:HD3	1.88	0.54
2:H:24:VAL:HG22	2:H:58:THR:HG23	1.89	0.54
2:G:138:LEU:O	2:G:142:VAL:HG13	2.08	0.53

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:ILE:HG21	1:F:143:GLU:HA	1.89	0.53
1:F:163:GLN:NE2	1:F:165:GLU:O	2.38	0.53
2:H:140:LYS:CE	3:H:280:HOH:O	2.57	0.53
2:C:145:TYR:O	3:C:280:HOH:O	2.19	0.52
2:H:19:THR:HG23	3:H:271:HOH:O	2.09	0.52
2:H:110:THR:OG1	2:H:113:GLU:HG3	2.08	0.52
1:F:20:VAL:HG22	1:F:138:ILE:CB	2.36	0.52
2:H:97:ARG:NH1	2:H:113:GLU:OE2	2.41	0.52
2:G:15:ILE:HD12	2:G:51:ASP:HB3	1.91	0.51
2:G:132:ARG:HD2	3:H:190:HOH:O	2.10	0.51
2:C:5:ASN:ND2	2:C:9:GLN:HE21	1.95	0.51
1:F:6:VAL:HG21	1:F:36:PHE:HE2	1.75	0.51
2:G:33:SER:HB2	2:G:34:PRO:HD2	1.92	0.51
2:H:91:ILE:CD1	3:H:226:HOH:O	2.52	0.50
2:G:132:ARG:NE	3:G:232:HOH:O	2.39	0.50
1:B:56:ILE:HD11	1:B:156:ILE:HD12	1.92	0.50
1:A:149:ASN:HD22	1:A:149:ASN:C	2.14	0.49
2:G:89[A]:ALA:O	2:G:90[A]:PRO:C	2.48	0.49
2:H:29:GLU:HG3	2:H:30:LYS:HD3	1.93	0.49
1:E:25:PHE:HZ	1:E:131:LYS:HG2	1.77	0.49
2:H:91:ILE:HD13	3:H:197:HOH:O	2.11	0.49
1:A:13:ASP:OD1	1:A:155:LYS:NZ	2.37	0.49
2:G:89[B]:ALA:CA	3:G:147:HOH:O	2.28	0.49
2:C:120:HIS:CG	2:C:121:ASN:H	2.30	0.49
1:A:84:GLU:H	1:A:84:GLU:CD	2.16	0.49
2:C:91[A]:ILE:HG23	2:C:91[A]:ILE:O	2.12	0.49
2:C:32:PHE:O	2:C:142:VAL:HG12	2.12	0.49
2:G:91[A]:ILE:O	2:G:91[A]:ILE:HG23	2.13	0.49
2:C:67:GLN:HG2	3:C:187:HOH:O	2.11	0.49
2:H:91:ILE:CD1	3:H:197:HOH:O	2.59	0.49
2:C:70:LYS:HE3	3:C:236:HOH:O	2.12	0.49
2:H:70:LYS:HE2	3:H:289:HOH:O	2.12	0.49
2:C:131:LYS:HE2	3:C:223:HOH:O	2.13	0.49
1:F:20:VAL:CG2	1:F:138:ILE:HB	2.37	0.49
2:H:124:ILE:N	2:H:124:ILE:CD1	2.76	0.49
2:H:70:LYS:CE	3:H:289:HOH:O	2.61	0.49
1:E:84:GLU:H	1:E:84:GLU:CD	2.16	0.48
1:F:136:MET:O	1:F:140:GLU:HG3	2.14	0.48
2:C:120:HIS:CG	2:C:121:ASN:N	2.80	0.48
2:H:72:THR:OG1	2:H:140:LYS:HE3	2.13	0.48
2:G:5:ASN:OD1	2:G:9:GLN:CG	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:71:GLU:OE1	3:C:165:HOH:O	2.20	0.47
2:D:66:MET:HE1	3:D:202:HOH:O	2.11	0.47
1:E:25:PHE:CZ	1:E:131:LYS:HG2	2.49	0.47
1:A:15:GLU:OE1	3:A:383:HOH:O	2.20	0.47
3:F:201:HOH:O	2:G:90[B]:PRO:HA	2.13	0.47
1:E:149:ASN:ND2	1:E:151:LYS:H	2.13	0.47
1:F:84:GLU:CD	1:F:84:GLU:H	2.18	0.47
2:D:80:TRP:O	2:D:84:HIS:HD2	1.98	0.47
2:D:116:GLY:O	2:D:120:HIS:N	2.48	0.47
2:G:4:GLN:HB3	2:G:10:MET:SD	2.55	0.47
2:G:29:GLU:CD	3:G:300:HOH:O	2.54	0.46
2:G:54:THR:O	2:G:58:THR:HG23	2.15	0.46
2:D:12:HIS:CE1	2:D:111:LEU:HD11	2.51	0.46
2:H:27:VAL:O	3:H:253:HOH:O	2.20	0.46
2:G:27:VAL:HG11	2:G:59:VAL:HG13	1.97	0.46
2:D:91:ILE:HA	3:D:221:HOH:O	2.15	0.46
2:G:33:SER:O	2:G:36:VAL:HG12	2.16	0.46
2:G:30:LYS:HE3	2:G:35:GLU:HB2	1.98	0.46
2:C:68:MET:SD	2:C:141:ILE:HG22	2.56	0.46
2:C:120:HIS:ND1	2:C:121:ASN:N	2.64	0.46
1:F:131:LYS:O	1:F:131:LYS:HG3	2.15	0.46
1:B:145:PHE:HB2	1:B:156:ILE:HD11	1.98	0.46
1:A:81:GLU:HG3	1:A:82:LYS:O	2.15	0.45
2:H:89:ALA:HB1	2:H:90:PRO:HA	1.99	0.45
2:D:95:GLN:HG2	3:D:256:HOH:O	2.16	0.45
2:C:33:SER:OG	2:C:35:GLU:OE1	2.30	0.45
1:A:57:ILE:HD13	2:D:92:ALA:HB2	1.99	0.45
1:E:149:ASN:HD22	1:E:149:ASN:C	2.20	0.45
1:A:165:GLU:CG	1:A:165:GLU:OXT	2.64	0.45
2:C:39:MET:HB3	2:C:39:MET:HE2	1.92	0.45
2:G:131:LYS:HD3	3:G:293:HOH:O	2.13	0.44
1:A:149:ASN:ND2	1:A:151:LYS:H	2.15	0.44
2:C:54:THR:O	2:C:58:THR:HG23	2.18	0.44
1:F:56:ILE:CG2	1:F:143:GLU:HA	2.48	0.44
2:D:82:ARG:NH2	2:D:83:LEU:HD21	2.33	0.44
2:H:30:LYS:O	2:H:31:ALA:CB	2.67	0.43
2:D:66:MET:HE3	3:D:202:HOH:O	2.11	0.43
1:F:58:PRO:HG3	1:F:143:GLU:O	2.18	0.43
2:G:67:GLN:HG2	3:G:187:HOH:O	2.17	0.43
1:B:149:ASN:ND2	3:B:365:HOH:O	2.51	0.43
2:D:70:LYS:NZ	3:D:243:HOH:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:MET:HE3	2:H:68:MET:HB2	1.60	0.43
2:C:5:ASN:CG	2:C:9:GLN:HG2	2.39	0.43
2:C:68:MET:HE3	2:C:144:MET:HE1	2.01	0.43
2:G:71:GLU:OE1	3:G:160:HOH:O	2.20	0.42
1:F:6:VAL:HG21	1:F:36:PHE:CE2	2.54	0.42
2:C:65:ALA:HB1	2:C:141:ILE:HD12	2.01	0.42
2:D:122:PRO:CB	2:D:123:PRO:CD	2.97	0.42
1:A:149:ASN:C	1:A:149:ASN:ND2	2.73	0.42
2:G:30:LYS:HE3	2:G:35:GLU:CB	2.50	0.42
2:G:72:THR:HG21	2:G:137:GLY:HA2	2.02	0.42
1:F:98:LEU:HG	1:F:129:PHE:CZ	2.55	0.42
2:C:6:LEU:CD1	2:C:6:LEU:H	2.24	0.42
2:H:121:ASN:HA	2:H:122:PRO:HA	1.86	0.42
2:G:84:HIS:HE1	3:G:243:HOH:O	2.01	0.42
2:G:142:VAL:HG21	2:H:143:ARG:CD	2.50	0.41
2:H:71:GLU:OE1	3:H:225:HOH:O	2.22	0.41
2:G:5:ASN:HD21	2:G:9:GLN:HG3	1.85	0.41
2:G:30:LYS:CD	3:G:278:HOH:O	2.68	0.41
1:A:164:LEU:O	1:A:165:GLU:HB3	2.20	0.41
2:G:1:PRO:HG2	3:G:265:HOH:O	2.20	0.41
2:G:142:VAL:CG2	2:H:143:ARG:CD	2.98	0.41
2:C:72:THR:HG21	2:C:137:GLY:HA2	2.03	0.41
2:G:39:MET:HB3	2:G:39:MET:HE2	1.88	0.41
2:G:97:ARG:HG3	3:G:295:HOH:O	2.21	0.41
1:B:153:SER:HA	3:B:366:HOH:O	2.20	0.41
1:B:20:VAL:HG22	1:B:135:GLY:O	2.21	0.41
1:B:31:LYS:HG2	1:B:79:TYR:CZ	2.56	0.41
1:A:133:LYS:NZ	3:A:409:HOH:O	2.54	0.41
2:H:68:MET:HE3	2:H:141:ILE:HG12	2.03	0.41
2:C:65:ALA:HA	2:C:144:MET:HE1	2.03	0.40
1:B:98:LEU:HG	1:B:129:PHE:CZ	2.57	0.40

All (1) 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:E:405:HOH:O	3:H:228:HOH:O[1_655]	2.10	0.10

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%)	157 (96%)	6 (4%)	0	100	100
1	B	162/165 (98%)	156 (96%)	6 (4%)	0	100	100
1	E	163/165 (99%)	155 (95%)	8 (5%)	0	100	100
1	F	162/165 (98%)	153 (94%)	9 (6%)	0	100	100
2	C	148/146 (101%)	147 (99%)	1 (1%)	0	100	100
2	D	133/146 (91%)	127 (96%)	6 (4%)	0	100	100
2	G	148/146 (101%)	145 (98%)	3 (2%)	0	100	100
2	H	133/146 (91%)	129 (97%)	4 (3%)	0	100	100
All	All	1212/1244 (97%)	1169 (96%)	43 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	17
1	B	132/133 (99%)	126 (96%)	6 (4%)	34	13
1	E	133/133 (100%)	130 (98%)	3 (2%)	58	37
1	F	132/133 (99%)	128 (97%)	4 (3%)	48	26
2	C	126/123 (102%)	123 (98%)	3 (2%)	57	36
2	D	113/123 (92%)	106 (94%)	7 (6%)	23	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	126/123 (102%)	120 (95%)	6 (5%)	31	12
2	H	113/123 (92%)	107 (95%)	6 (5%)	28	9
All	All	1008/1024 (98%)	968 (96%)	40 (4%)	38	16

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	61	MET
1	A	131	LYS
1	A	148	ARG
1	A	149	ASN
1	B	2	VAL
1	B	29	VAL
1	B	31	LYS
1	B	61	MET
1	B	84	GLU
1	B	149	ASN
2	C	9	GLN
2	C	33	SER
2	C	121	ASN
2	D	13	GLN
2	D	18	ARG
2	D	58	THR
2	D	112	GLN
2	D	120	HIS
2	D	131	LYS
2	D	143	ARG
1	E	29	VAL
1	E	61	MET
1	E	149	ASN
1	F	2	VAL
1	F	27	ASP
1	F	61	MET
1	F	155	LYS
2	G	2	ILE
2	G	10	MET
2	G	11	VAL
2	G	25	LYS
2	G	30	LYS
2	G	131	LYS

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Mol	Chain	Res	Type
2	H	13	GLN
2	H	54	THR
2	H	58	THR
2	H	121	ASN
2	H	124	ILE
2	H	131	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	B	149	ASN
2	C	4	GLN
2	C	9	GLN
2	C	74	ASN
2	D	12	HIS
2	D	21	ASN
2	D	74	ASN
2	D	84	HIS
1	E	149	ASN
1	F	149	ASN
2	G	9	GLN
2	G	50	GLN
2	G	74	ASN
2	G	95	GLN
2	H	21	ASN
2	H	74	ASN
2	H	95	GLN
2	H	112	GLN
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 (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%)	-0.34	2 (1%)	81	85	10, 17, 30, 58	0
1	B	164/165 (99%)	0.17	0	100	100	10, 19, 32, 48	0
1	E	165/165 (100%)	-0.27	2 (1%)	81	85	8, 15, 28, 42	0
1	F	164/165 (99%)	1.76	55 (33%)	0	0	18, 29, 45, 59	0
2	C	146/146 (100%)	0.10	4 (2%)	58	62	10, 21, 43, 57	0
2	D	135/146 (92%)	0.60	16 (11%)	6	7	15, 29, 56, 72	0
2	G	146/146 (100%)	0.61	18 (12%)	5	6	13, 24, 52, 75	0
2	H	135/146 (92%)	0.41	11 (8%)	15	16	14, 26, 49, 66	0
All	All	1220/1244 (98%)	0.37	108 (8%)	12	13	8, 22, 46, 75	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	8	GLY	7.9
1	F	144	ARG	7.7
2	G	6	LEU	7.7
1	F	2	VAL	7.1
2	G	10	MET	6.3
2	G	5	ASN	6.3
2	G	91[A]	ILE	6.1
2	G	89[A]	ALA	5.8
1	A	165	GLU	5.6
2	D	14	ALA	5.5
2	G	9	GLN	5.0
2	C	6	LEU	4.9
1	F	80	GLY	4.8
2	D	121	ASN	4.8
2	G	4	GLN	4.8
2	C	146	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	145	PHE	4.6
2	G	121	ASN	4.5
1	F	148	ARG	4.3
1	F	115	CYS	4.3
1	F	17	LEU	4.3
1	F	57	ILE	4.2
1	F	60	PHE	4.1
2	D	15	ILE	4.1
1	F	165	GLU	4.1
2	D	112	GLN	4.0
1	F	59	GLY	3.9
2	G	7	GLN	3.8
1	F	121	TRP	3.8
1	F	20	VAL	3.7
1	F	62	CYS	3.6
1	F	13	ASP	3.6
2	G	11	VAL	3.5
1	F	149	ASN	3.5
2	D	31	ALA	3.5
1	F	161	CYS	3.5
2	G	93	PRO	3.4
2	H	122	PRO	3.4
1	A	1	MET	3.4
1	F	117	ALA	3.4
1	F	46	PHE	3.3
1	F	152	THR	3.3
2	G	145	TYR	3.3
1	F	52	CYS	3.3
1	F	15	GLU	3.2
1	F	113	PHE	3.2
1	F	159	ALA	3.2
1	F	48	TYR	3.2
1	F	93	THR	3.2
2	G	95	GLN	3.1
2	H	120	HIS	3.1
1	F	67	PHE	3.1
1	F	81	GLU	3.1
1	F	68	THR	3.1
2	H	121	ASN	3.1
2	D	119	THR	3.0
2	G	94	GLY	3.0
2	D	12	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	29	GLU	2.9
2	C	8	GLY	2.9
2	D	96	MET	2.8
2	G	146	SER	2.8
2	H	31	ALA	2.8
2	C	9	GLN	2.8
1	F	6	VAL	2.8
1	F	8	PHE	2.7
1	F	78	ILE	2.6
1	F	53	PHE	2.6
2	D	123	PRO	2.6
1	F	73	THR	2.5
1	F	30	PRO	2.5
1	F	153	SER	2.5
1	E	165	GLU	2.5
1	F	128	VAL	2.5
1	F	45	GLY	2.5
2	D	146	SER	2.5
1	F	22	PHE	2.5
2	D	18	ARG	2.4
2	G	3	VAL	2.4
2	D	120	HIS	2.4
2	H	96	MET	2.4
1	F	11	ALA	2.4
2	H	119	THR	2.3
1	F	151	LYS	2.3
1	E	1	MET	2.3
1	F	97	ILE	2.3
1	F	140	GLU	2.3
1	F	16	PRO	2.3
2	D	21	ASN	2.3
1	F	21	SER	2.3
1	F	96	GLY	2.3
1	F	70	HIS	2.2
2	D	124	ILE	2.2
1	F	79	TYR	2.2
1	F	137	ASN	2.2
1	F	116	THR	2.2
1	F	119	THR	2.2
2	H	95	GLN	2.2
1	F	136	MET	2.1
1	F	27	ASP	2.1

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Full wwPDB X-ray Structure Validation Report

Mol	Chain	Res	Type	RSRZ
1	F	135	GLY	2.1
2	D	28	GLU	2.1
2	D	19	THR	2.1
2	H	18	ARG	2.1
2	H	32	PHE	2.1
2	H	123	PRO	2.1
1	F	4	PRO	2.0
2	G	90[A]	PRO	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.