Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 09:37 AM EDT

PDB ID	:	4EN2
Title	:	HIV-1 Nef in complex with MHC-I cytoplasmic domain and Mu1 adaptin subunit of AP1 adaptor (second domain)
Authors	:	Jia, X.; Xiong, Y.
Deposited on	:	2012-04-12
Resolution	:	2.58 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 (i) 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 (1)) were used in the production of this report:

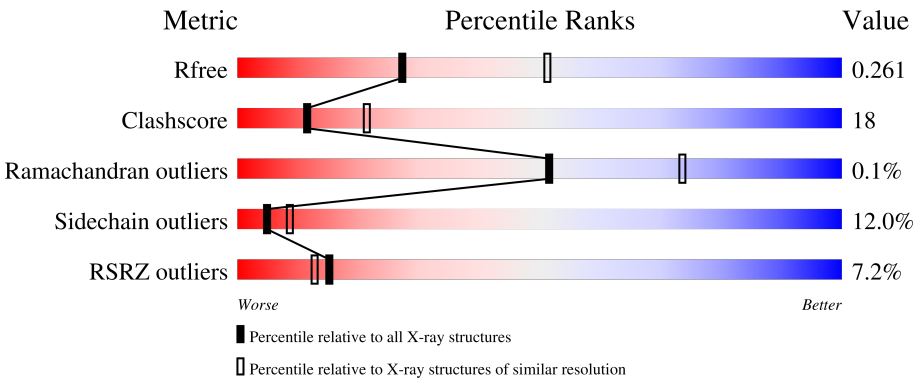
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.58 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}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 <=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	266	7% 66% 22% 8% •
1	M	266	5% 69% 23% • • •
2	B	206	3% 47% 22% • 28%
2	C	206	9% 43% 17% • 35%
3	D	28	7% 14% 29% 57%

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Mol	Chain	Length	Quality of chain
3	E	28	57% 7% 36%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6783 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 AP-1 complex subunit mu-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	M	256	2085	1339	365	375	6	0	0	0
1	A	255	2081	1335	366	374	6	0	1	0

- Molecule 2 is a protein called Protein Nef.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	149	1238	798	218	219	3	0	0	0
2	C	133	1123	733	195	192	3	0	0	0

- Molecule 3 is a protein called MHC-I.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	12	81	46	14	21	0	0	0
3	E	18	121	68	24	29	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	M	18	18	18	0	0
4	B	16	16	16	0	0
4	C	4	4	4	0	0
4	A	13	14	14	0	1

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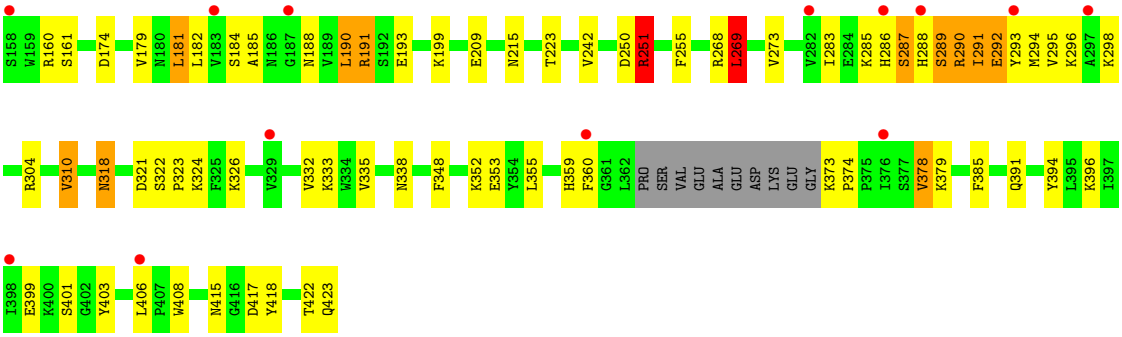
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	1	1	1	0	0
			Total	O		
4	E	1	1	1	0	0

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.

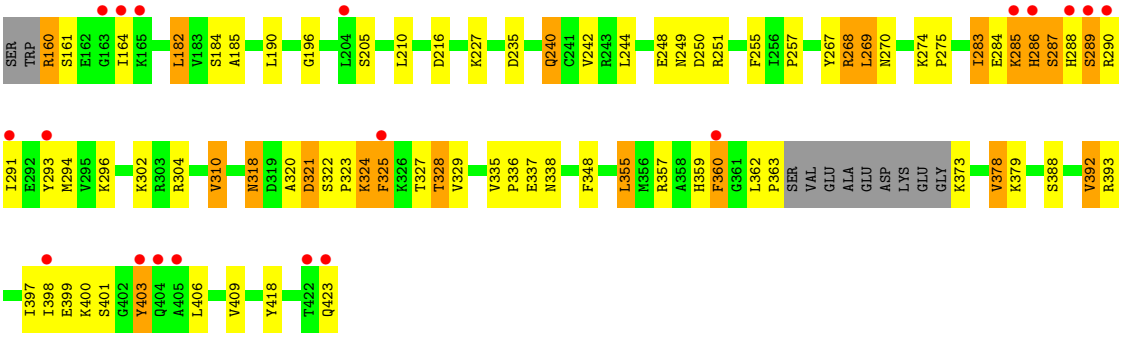
• Molecule 1: AP-1 complex subunit mu-1

Chain M:



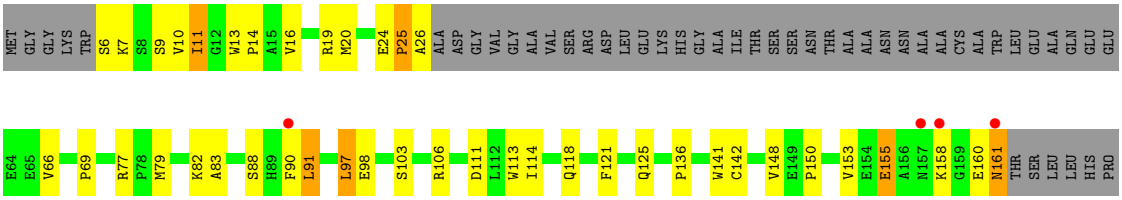
• Molecule 1: AP-1 complex subunit mu-1

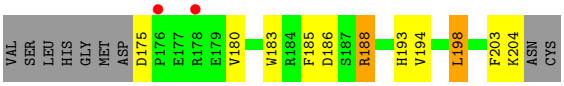
Chain A:



• Molecule 2: Protein Nef

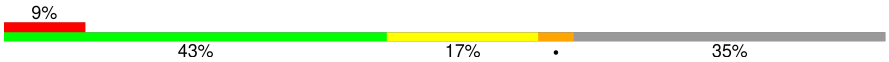
Chain B:

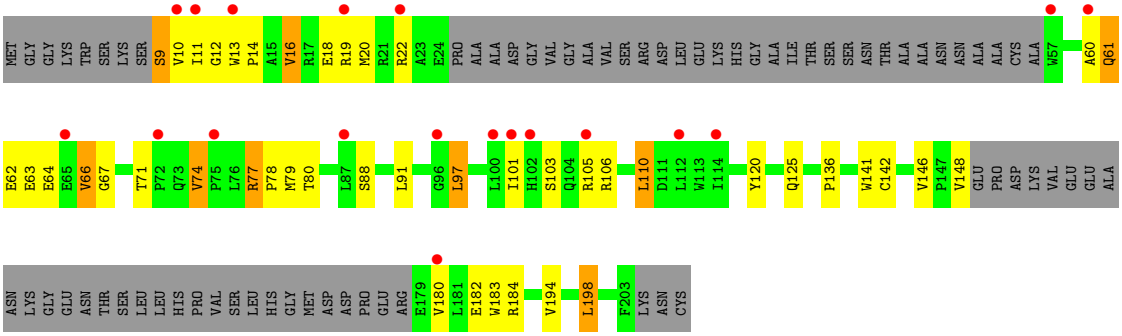




- Molecule 2: Protein Nef

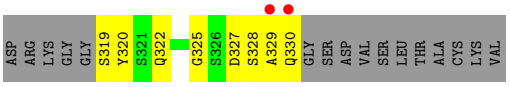
Chain C:





- Molecule 3: MHC-I

Chain D:



- Molecule 3: MHC-I

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.03Å 98.13Å 112.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 2.58 48.88 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.88-2.58) 98.5 (48.88-2.58)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.258 0.211 , 0.261	Depositor DCC
R_{free} test set	1561 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	63.2	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6783	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.76	0/2132	0.89	1/2875 (0.0%)
1	M	0.76	0/2134	0.89	2/2880 (0.1%)
2	B	0.79	0/1279	0.80	0/1736
2	C	0.76	0/1163	0.79	0/1582
3	D	0.78	0/81	0.73	0/108
3	E	0.79	0/121	0.84	0/159
All	All	0.77	0/6910	0.86	3/9340 (0.0%)

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
2	C	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	251	ARG	CG-CD-NE	-6.90	97.31	111.80
1	M	269	LEU	CA-CB-CG	6.33	129.86	115.30
1	A	268	ARG	NE-CZ-NH1	5.46	123.03	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	64	GLU	Peptide

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	2081	0	2115	99	0
1	M	2085	0	2111	58	1
2	B	1238	0	1191	42	1
2	C	1123	0	1075	42	0
3	D	81	0	66	10	0
3	E	121	0	105	1	0
4	A	14	0	0	1	0
4	B	16	0	0	1	0
4	C	4	0	0	1	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	M	18	0	0	1	0
All	All	6783	0	6663	235	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 18.

All (235) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:296:LYS:HG2	1:M:355:LEU:CD2	1.43	1.45
1:M:296:LYS:CG	1:M:355:LEU:HD21	1.63	1.26
1:A:323:PRO:CA	1:A:360:PHE:HB3	1.84	1.08
1:A:320:ALA:HB2	1:A:362:LEU:HD12	1.31	1.04
1:A:205:SER:O	1:A:403:TYR:OH	1.79	1.00
1:A:323:PRO:HA	1:A:360:PHE:HB3	1.44	0.98
1:A:291:ILE:CG2	1:A:360:PHE:CE1	2.47	0.97
1:A:321:ASP:OD2	1:A:322:SER:HB3	1.65	0.96
1:A:323:PRO:CB	1:A:360:PHE:HB3	1.98	0.93
2:B:79:MET:HE2	2:B:83:ALA:HB3	1.51	0.92
1:M:296:LYS:CG	1:M:355:LEU:CD2	2.33	0.87
1:A:323:PRO:HB3	1:A:360:PHE:HB3	1.57	0.87
1:A:291:ILE:HG22	1:A:360:PHE:CE1	2.11	0.84
1:M:286:HIS:CD2	1:M:287:SER:OG	2.32	0.82
1:M:287:SER:O	1:M:290:ARG:HB2	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:PRO:HA	1:A:360:PHE:CB	2.10	0.81
1:M:288:HIS:CD2	1:M:289:SER:H	2.00	0.80
1:M:288:HIS:CG	1:M:289:SER:H	2.02	0.78
2:B:79:MET:CE	2:B:83:ALA:HB3	2.12	0.78
1:M:185:ALA:HB2	1:M:423:GLN:HA	1.64	0.78
1:A:291:ILE:CG2	1:A:360:PHE:HE1	1.95	0.77
1:A:392:VAL:HG11	1:A:409:VAL:HG21	1.65	0.77
1:A:286:HIS:ND1	1:A:286:HIS:N	2.35	0.74
1:M:323:PRO:HB3	1:M:360:PHE:CE1	2.24	0.73
1:A:321:ASP:OD2	1:A:322:SER:CB	2.35	0.73
2:C:13:TRP:N	2:C:14:PRO:HD2	2.04	0.72
1:A:392:VAL:CG1	1:A:409:VAL:HG21	2.20	0.72
2:C:20:MET:O	2:C:106:ARG:HD3	1.91	0.71
1:A:320:ALA:CB	1:A:362:LEU:HD12	2.18	0.70
2:B:193:HIS:ND1	4:B:309:HOH:O	2.24	0.70
1:A:336:PRO:HD2	1:A:337:GLU:OE2	1.93	0.69
1:A:328:THR:HG22	1:A:355:LEU:O	1.92	0.69
1:M:286:HIS:HB2	1:M:292:GLU:HB2	1.75	0.69
2:B:20:MET:O	2:B:106:ARG:HD3	1.94	0.67
1:M:296:LYS:HG2	1:M:355:LEU:HD21	0.70	0.67
1:M:296:LYS:HA	1:M:355:LEU:HD23	1.76	0.67
1:M:290:ARG:HE	1:M:359:HIS:CE1	2.13	0.67
1:A:289:SER:O	1:A:362:LEU:N	2.28	0.66
2:B:103:SER:OG	2:B:106:ARG:HG3	1.96	0.66
2:C:63:GLU:HB3	1:A:335:VAL:HG22	1.79	0.65
1:A:289:SER:O	1:A:362:LEU:O	2.15	0.64
2:C:103:SER:OG	2:C:106:ARG:HG3	1.97	0.64
1:A:160:ARG:HD2	1:A:257:PRO:O	1.98	0.64
1:M:399:GLU:HG2	1:M:403:TYR:CE2	2.33	0.63
1:M:318:ASN:OD1	1:M:318:ASN:N	2.31	0.63
2:B:7:LYS:O	2:B:11:ILE:HG23	1.99	0.63
1:A:321:ASP:OD2	1:A:321:ASP:C	2.37	0.63
1:M:288:HIS:CG	1:M:289:SER:N	2.67	0.63
1:M:373:LYS:HB3	1:M:374:PRO:HD2	1.81	0.62
1:M:385:PHE:CZ	2:C:67:GLY:HA3	2.34	0.62
2:C:71:THR:OG1	2:C:74:VAL:HG13	1.99	0.62
1:A:323:PRO:CA	1:A:360:PHE:CB	2.67	0.62
2:B:150:PRO:O	2:B:153:VAL:HG12	1.99	0.62
1:A:321:ASP:OD2	1:A:322:SER:N	2.32	0.62
2:C:60:ALA:HB3	1:A:323:PRO:HG2	1.80	0.62
1:A:294:MET:HE3	1:A:357:ARG:HD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:394:TYR:CE1	3:D:327:ASP:HB2	2.36	0.61
1:A:185:ALA:HB2	1:A:423:GLN:O	2.01	0.61
1:M:188:ASN:O	1:M:190:LEU:HD13	2.00	0.61
1:M:296:LYS:HG2	1:M:355:LEU:HD23	1.70	0.60
1:A:328:THR:CG2	1:A:355:LEU:H	2.15	0.60
2:B:79:MET:CE	2:B:83:ALA:CB	2.79	0.60
2:C:146:VAL:HG21	2:C:184:ARG:HG3	1.82	0.60
1:M:290:ARG:NH2	1:M:322:SER:O	2.32	0.60
2:C:105:ARG:NH2	1:A:321:ASP:OD2	2.34	0.60
1:A:323:PRO:HA	1:A:360:PHE:CA	2.32	0.60
2:C:146:VAL:CG2	2:C:184:ARG:HG3	2.32	0.60
1:A:362:LEU:HG	1:A:363:PRO:HD2	1.84	0.60
2:B:24:GLU:HG3	2:B:25:PRO:HD2	1.85	0.59
2:C:146:VAL:HG22	2:C:184:ARG:HG2	1.85	0.59
1:A:235:ASP:OD1	1:A:268:ARG:NH1	2.36	0.59
1:A:250:ASP:O	1:A:251:ARG:HB2	2.02	0.59
2:C:80:THR:HA	3:D:328:SER:HB3	1.85	0.59
1:A:289:SER:HA	1:A:362:LEU:O	2.03	0.58
1:A:378:VAL:HG13	1:A:418:TYR:CD2	2.39	0.58
2:B:24:GLU:O	2:B:26:ALA:N	2.36	0.58
1:A:283:ILE:HG22	1:A:293:TYR:CD1	2.39	0.58
3:D:329:ALA:O	3:D:330:GLN:HB2	2.04	0.58
2:C:88:SER:HB3	2:C:142:CYS:HB2	1.86	0.57
2:B:79:MET:HE3	2:B:79:MET:HA	1.87	0.57
1:A:310:VAL:HA	1:A:379:LYS:O	2.04	0.57
1:M:373:LYS:HB3	1:M:374:PRO:CD	2.35	0.57
1:A:328:THR:HG21	1:A:355:LEU:H	1.69	0.56
2:C:194:VAL:HG12	2:C:198:LEU:HD22	1.86	0.56
2:B:79:MET:HE1	2:B:83:ALA:CB	2.35	0.56
2:B:160:GLU:O	2:B:188:ARG:NH2	2.38	0.56
1:A:360:PHE:CD1	1:A:360:PHE:C	2.78	0.56
1:A:291:ILE:HG22	1:A:360:PHE:HE1	1.59	0.56
1:A:290:ARG:NH1	1:A:360:PHE:HA	2.20	0.56
2:B:16:VAL:HG21	2:B:113:TRP:CD2	2.41	0.56
2:B:186:ASP:OD2	2:B:188:ARG:HG2	2.05	0.56
2:B:24:GLU:C	2:B:26:ALA:H	2.09	0.56
2:B:194:VAL:HG12	2:B:198:LEU:HD22	1.87	0.56
2:C:12:GLY:O	2:C:16:VAL:HG12	2.06	0.56
1:M:310:VAL:HA	1:M:379:LYS:O	2.04	0.56
1:A:378:VAL:HG13	1:A:418:TYR:HD2	1.71	0.56
2:C:16:VAL:O	2:C:16:VAL:HG23	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:SER:HB3	2:B:142:CYS:HB2	1.87	0.55
1:A:240:GLN:H	1:A:240:GLN:HE21	1.55	0.55
2:C:146:VAL:HG22	2:C:184:ARG:CG	2.37	0.54
1:M:273:VAL:CG1	2:C:66:VAL:HG13	2.37	0.54
2:B:24:GLU:C	2:B:26:ALA:N	2.61	0.54
2:C:71:THR:OG1	2:C:74:VAL:CG1	2.55	0.54
1:M:273:VAL:HG11	2:C:66:VAL:HG13	1.89	0.54
1:A:360:PHE:C	1:A:360:PHE:HD1	2.10	0.54
1:M:287:SER:O	1:M:290:ARG:N	2.37	0.54
2:B:13:TRP:N	2:B:14:PRO:HD2	2.23	0.53
2:C:79:MET:O	3:D:328:SER:HB2	2.08	0.53
1:M:191:ARG:NH2	1:M:193:GLU:OE1	2.41	0.53
2:B:79:MET:HE1	2:B:83:ALA:HB1	1.90	0.53
1:A:323:PRO:HA	1:A:360:PHE:HA	1.91	0.52
2:C:9:SER:OG	2:C:10:VAL:N	2.39	0.52
2:C:13:TRP:N	2:C:14:PRO:CD	2.71	0.52
2:C:13:TRP:HA	2:C:16:VAL:HG13	1.90	0.52
1:M:223:THR:HB	3:D:330:GLN:OE1	2.10	0.52
2:C:61:GLN:HE21	2:C:61:GLN:HA	1.75	0.52
2:C:10:VAL:HG12	2:C:11:ILE:HD12	1.92	0.51
1:A:362:LEU:CD2	1:A:363:PRO:O	2.59	0.51
1:A:323:PRO:HB3	1:A:360:PHE:CD2	2.45	0.51
2:B:16:VAL:HG21	2:B:113:TRP:CG	2.46	0.51
1:M:283:ILE:CG2	1:M:291:ILE:HD11	2.41	0.51
1:A:321:ASP:CG	1:A:322:SER:N	2.65	0.51
2:C:148:VAL:HG11	2:C:182:GLU:CD	2.31	0.50
2:B:6:SER:O	2:B:10:VAL:HG23	2.12	0.50
2:C:74:VAL:HG22	2:C:74:VAL:O	2.11	0.50
2:B:98:GLU:OE1	2:B:185:PHE:N	2.33	0.50
2:B:121:PHE:CE1	1:A:393:ARG:HA	2.46	0.50
1:M:406:LEU:HD22	3:D:322:GLN:NE2	2.26	0.50
1:A:318:ASN:OD1	1:A:318:ASN:N	2.30	0.50
1:M:378:VAL:HG13	1:M:418:TYR:CD2	2.46	0.50
1:A:294:MET:CE	1:A:357:ARG:HD2	2.41	0.50
1:M:292:GLU:HG3	1:M:293:TYR:N	2.27	0.50
1:A:362:LEU:HD23	1:A:363:PRO:O	2.12	0.50
1:A:399:GLU:HG2	1:A:403:TYR:CE1	2.46	0.49
1:A:335:VAL:HG12	1:A:338:ASN:H	1.78	0.49
2:B:97:LEU:HD22	2:B:183:TRP:CG	2.47	0.49
2:C:146:VAL:CG2	2:C:184:ARG:CG	2.91	0.49
1:A:283:ILE:HD13	1:A:283:ILE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:PRO:HB3	1:A:360:PHE:CB	2.35	0.49
1:A:289:SER:CA	1:A:362:LEU:O	2.61	0.49
1:M:321:ASP:OD2	1:M:322:SER:N	2.45	0.49
1:A:373:LYS:O	1:A:423:GLN:HG2	2.13	0.49
1:M:373:LYS:HD3	4:M:514:HOH:O	2.12	0.49
2:B:160:GLU:HB2	2:B:188:ARG:HH22	1.77	0.49
3:D:329:ALA:O	3:D:330:GLN:CB	2.61	0.49
1:M:287:SER:O	1:M:290:ARG:CB	2.56	0.48
2:B:111:ASP:OD1	2:B:125:GLN:NE2	2.46	0.48
1:A:406:LEU:HD22	3:E:322:GLN:NE2	2.29	0.48
1:A:289:SER:C	1:A:362:LEU:O	2.52	0.48
1:M:291:ILE:HG12	1:M:292:GLU:N	2.27	0.48
1:A:294:MET:HE2	1:A:357:ARG:HD3	1.95	0.48
1:A:325:PHE:C	1:A:325:PHE:CD2	2.87	0.48
1:M:250:ASP:O	1:M:251:ARG:CB	2.60	0.48
1:A:205:SER:C	1:A:403:TYR:OH	2.52	0.48
2:C:12:GLY:O	2:C:16:VAL:CG1	2.62	0.47
1:A:323:PRO:HA	1:A:359:HIS:O	2.14	0.47
1:M:332:VAL:HG12	1:M:333:LYS:N	2.29	0.47
2:C:136:PRO:HB3	2:C:141:TRP:HD1	1.80	0.47
2:C:16:VAL:O	2:C:16:VAL:CG2	2.54	0.47
1:M:290:ARG:NE	1:M:359:HIS:CE1	2.82	0.47
1:A:327:THR:HG22	1:A:328:THR:N	2.29	0.47
1:M:286:HIS:HD2	1:M:287:SER:OG	1.94	0.47
2:C:61:GLN:HE21	2:C:61:GLN:CA	2.27	0.47
1:A:269:LEU:HD13	1:A:388:SER:HB3	1.97	0.47
1:A:362:LEU:HD23	1:A:362:LEU:C	2.35	0.47
1:A:327:THR:HG22	1:A:329:VAL:H	1.80	0.46
1:A:283:ILE:HG22	1:A:293:TYR:CE1	2.51	0.46
1:M:396:LYS:HA	3:D:325:GLY:O	2.15	0.46
1:A:288:HIS:O	1:A:362:LEU:O	2.33	0.46
1:M:422:THR:O	1:M:423:GLN:HB3	2.15	0.46
1:A:323:PRO:HB3	1:A:360:PHE:HD2	1.79	0.46
1:A:337:GLU:CD	1:A:337:GLU:H	2.16	0.46
1:A:362:LEU:HD23	1:A:363:PRO:C	2.35	0.46
1:A:284:GLU:O	1:A:286:HIS:HE1	1.98	0.46
1:A:296:LYS:HG3	1:A:355:LEU:CD1	2.46	0.46
1:A:324:LYS:N	1:A:359:HIS:O	2.42	0.46
2:B:136:PRO:HB3	2:B:141:TRP:HD1	1.80	0.45
1:A:294:MET:CE	1:A:357:ARG:CD	2.94	0.45
1:M:179:VAL:O	1:M:415:ASN:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:ILE:O	2:B:118:GLN:HB2	2.16	0.45
1:A:291:ILE:HG21	1:A:360:PHE:HE1	1.75	0.45
1:M:335:VAL:HG12	1:M:338:ASN:H	1.80	0.45
1:M:181:LEU:HD22	1:M:182:LEU:N	2.32	0.45
2:B:203:PHE:O	2:B:204:LYS:C	2.56	0.45
2:C:9:SER:O	2:C:12:GLY:N	2.49	0.45
1:A:291:ILE:HG21	1:A:360:PHE:CE1	2.42	0.45
1:M:290:ARG:NE	1:M:359:HIS:ND1	2.44	0.44
1:M:378:VAL:HG13	1:M:418:TYR:HD2	1.81	0.44
1:A:360:PHE:HD1	1:A:360:PHE:O	2.01	0.44
2:B:69:PRO:HG2	1:A:304[B]:ARG:CZ	2.47	0.44
1:A:327:THR:HG23	1:A:355:LEU:O	2.18	0.44
1:M:286:HIS:CD2	1:M:286:HIS:C	2.90	0.44
2:C:74:VAL:O	2:C:74:VAL:CG2	2.65	0.44
1:M:215:ASN:HB3	1:M:391:GLN:HE21	1.82	0.44
1:A:285:LYS:C	1:A:286:HIS:ND1	2.70	0.44
1:M:268:ARG:C	1:M:269:LEU:HD22	2.38	0.43
2:B:97:LEU:HD22	2:B:183:TRP:CD2	2.53	0.43
1:M:286:HIS:CD2	1:M:290:ARG:HD3	2.54	0.43
2:B:160:GLU:C	2:B:188:ARG:NH2	2.72	0.43
1:A:216:ASP:OD1	1:A:216:ASP:C	2.57	0.43
2:B:24:GLU:HG3	2:B:25:PRO:CD	2.48	0.43
1:A:287:SER:O	1:A:288:HIS:HB2	2.19	0.43
1:A:304[A]:ARG:NH2	4:A:508:HOH:O	2.51	0.42
1:M:242:VAL:HA	1:M:255:PHE:HB3	2.02	0.42
2:B:160:GLU:C	2:B:188:ARG:HH22	2.23	0.42
1:A:182:LEU:HD13	1:A:190:LEU:HD12	2.02	0.42
2:B:88:SER:CB	2:B:142:CYS:HB2	2.50	0.42
1:A:274:LYS:HG2	1:A:275:PRO:HD2	2.02	0.42
1:A:287:SER:O	1:A:289:SER:N	2.52	0.42
1:A:284:GLU:O	1:A:286:HIS:CE1	2.73	0.41
2:B:90:PHE:HD2	2:B:91:LEU:HD13	1.83	0.41
2:C:79:MET:HA	2:C:120:TYR:CD1	2.55	0.41
1:M:191:ARG:HE	1:M:191:ARG:HB2	1.72	0.41
2:B:155:GLU:HA	2:B:158:LYS:HE2	2.02	0.41
2:C:97:LEU:HD22	2:C:183:TRP:CD2	2.55	0.41
1:A:242:VAL:HA	1:A:255:PHE:HB3	2.02	0.41
1:A:294:MET:HE2	1:A:357:ARG:CD	2.50	0.41
2:B:69:PRO:HD3	1:A:302:LYS:HG3	2.03	0.41
3:D:330:GLN:CG	3:D:330:GLN:O	2.68	0.41
1:A:196:GLY:HA3	1:A:267:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:408:TRP:HB3	3:D:320:TYR:HB3	2.01	0.41
1:M:298:LYS:HB3	1:M:353:GLU:HG3	2.03	0.41
1:A:270:ASN:OD1	1:A:270:ASN:C	2.58	0.41
2:B:161:ASN:OD1	2:B:161:ASN:N	2.53	0.41
2:C:77:ARG:O	2:C:120:TYR:HA	2.21	0.41
2:C:78:PRO:HA	4:C:301:HOH:O	2.21	0.41
2:C:97:LEU:HD22	2:C:183:TRP:CG	2.56	0.41
2:C:110:LEU:HD13	2:C:125:GLN:HE22	1.86	0.41
1:M:185:ALA:CB	1:M:423:GLN:HA	2.42	0.41
1:A:392:VAL:HG11	1:A:409:VAL:CG2	2.45	0.40
1:M:355:LEU:HD23	1:M:355:LEU:HA	1.97	0.40
2:B:148:VAL:CG2	2:B:180:VAL:HG12	2.51	0.40
1:A:210:LEU:CD2	1:A:397:ILE:HG23	2.51	0.40
2:C:101:ILE:HD12	2:C:180:VAL:CG1	2.51	0.40
1:A:291:ILE:O	1:A:359:HIS:HB2	2.21	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)
1:M:352:LYS:NZ	2:B:24:GLU:OE2[4_445]	1.90	0.30

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	252/266 (95%)	240 (95%)	12 (5%)	0	100	100
1	M	252/266 (95%)	238 (94%)	14 (6%)	0	100	100
2	B	143/206 (69%)	138 (96%)	4 (3%)	1 (1%)	22	41
2	C	127/206 (62%)	121 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	10/28 (36%)	10 (100%)	0	0	100	100
3	E	16/28 (57%)	16 (100%)	0	0	100	100
All	All	800/1000 (80%)	763 (95%)	36 (4%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	25	PRO

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	234/242 (97%)	203 (87%)	31 (13%)	4	6
1	M	234/242 (97%)	206 (88%)	28 (12%)	5	9
2	B	131/173 (76%)	118 (90%)	13 (10%)	8	14
2	C	117/173 (68%)	103 (88%)	14 (12%)	5	9
3	D	8/20 (40%)	7 (88%)	1 (12%)	4	8
3	E	11/20 (55%)	10 (91%)	1 (9%)	9	17
All	All	735/870 (84%)	647 (88%)	88 (12%)	5	9

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	160	ARG
1	M	161	SER
1	M	174	ASP
1	M	181	LEU
1	M	184	SER
1	M	190	LEU
1	M	191	ARG
1	M	199	LYS
1	M	209	GLU

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Mol	Chain	Res	Type
1	M	251	ARG
1	M	269	LEU
1	M	285	LYS
1	M	287	SER
1	M	289	SER
1	M	290	ARG
1	M	291	ILE
1	M	292	GLU
1	M	294	MET
1	M	295	VAL
1	M	304	ARG
1	M	310	VAL
1	M	318	ASN
1	M	324	LYS
1	M	326	LYS
1	M	348	PHE
1	M	378	VAL
1	M	401	SER
1	M	417	ASP
2	B	9	SER
2	B	11	ILE
2	B	19	ARG
2	B	66	VAL
2	B	77	ARG
2	B	82	LYS
2	B	91	LEU
2	B	97	LEU
2	B	155	GLU
2	B	161	ASN
2	B	175	ASP
2	B	188	ARG
2	B	198	LEU
2	C	9	SER
2	C	16	VAL
2	C	18	GLU
2	C	19	ARG
2	C	22	ARG
2	C	61	GLN
2	C	62	GLU
2	C	66	VAL
2	C	74	VAL
2	C	77	ARG

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Mol	Chain	Res	Type
2	C	91	LEU
2	C	97	LEU
2	C	110	LEU
2	C	198	LEU
1	A	160	ARG
1	A	161	SER
1	A	164	ILE
1	A	182	LEU
1	A	184	SER
1	A	227	LYS
1	A	240	GLN
1	A	244	LEU
1	A	248	GLU
1	A	249	ASN
1	A	269	LEU
1	A	283	ILE
1	A	285	LYS
1	A	286	HIS
1	A	287	SER
1	A	289	SER
1	A	310	VAL
1	A	318	ASN
1	A	321	ASP
1	A	324	LYS
1	A	325	PHE
1	A	328	THR
1	A	348	PHE
1	A	355	LEU
1	A	360	PHE
1	A	378	VAL
1	A	392	VAL
1	A	398	ILE
1	A	400	LYS
1	A	401	SER
1	A	403	TYR
3	D	319	SER
3	E	315	ARG

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

Mol	Chain	Res	Type
1	M	188	ASN

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Mol	Chain	Res	Type
1	M	286	HIS
1	M	288	HIS
1	M	300	GLN
1	M	313	HIS
1	M	391	GLN
2	B	107	GLN
2	B	125	GLN
2	B	126	ASN
2	B	199	HIS
2	C	61	GLN
2	C	125	GLN
2	C	126	ASN
2	C	199	HIS
1	A	240	GLN
3	D	322	GLN
3	D	330	GLN
3	E	322	GLN

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 monosaccharides 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	255/266 (95%)	0.58	19 (7%) 14 11	49, 70, 119, 153	0
1	M	256/266 (96%)	0.42	13 (5%) 28 24	51, 71, 108, 137	0
2	B	149/206 (72%)	0.53	6 (4%) 38 34	48, 67, 115, 157	0
2	C	133/206 (64%)	0.72	19 (14%) 2 2	55, 81, 155, 210	0
3	D	12/28 (42%)	1.09	2 (16%) 1 1	62, 77, 115, 122	0
3	E	18/28 (64%)	0.44	0 100 100	60, 70, 116, 118	0
All	All	823/1000 (82%)	0.55	59 (7%) 15 13	48, 72, 120, 210	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	329	ALA	6.0
3	D	330	GLN	5.8
2	B	161	ASN	4.7
1	A	360	PHE	4.6
2	C	22	ARG	4.4
1	A	204	LEU	4.1
1	A	289	SER	4.0
2	C	10	VAL	4.0
1	M	288	HIS	3.8
1	A	164	ILE	3.7
2	C	11	ILE	3.5
1	A	325	PHE	3.2
1	M	158	SER	3.2
2	B	178	ARG	3.2
2	C	19	ARG	3.1
2	C	100	LEU	2.9
1	A	163	GLY	2.9
2	C	75	PRO	2.9
2	C	112	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	290	ARG	2.8
2	B	158	LYS	2.7
1	A	285	LYS	2.7
2	C	180	VAL	2.6
1	M	286	HIS	2.6
1	M	398	ILE	2.6
1	M	360	PHE	2.5
2	C	96	GLY	2.5
2	C	65	GLU	2.5
1	A	293	TYR	2.5
1	M	282	VAL	2.5
1	A	291	ILE	2.5
2	B	157	ASN	2.5
2	B	90	PHE	2.5
1	A	398	ILE	2.5
1	A	404	GLN	2.5
1	A	165	LYS	2.5
1	A	403	TYR	2.4
1	A	422	THR	2.4
1	A	405	ALA	2.4
2	C	101	ILE	2.4
2	C	72	PRO	2.3
1	M	187	GLY	2.3
1	M	183	VAL	2.2
1	M	293	TYR	2.2
2	B	176	PRO	2.2
1	M	376	ILE	2.2
1	A	286	HIS	2.2
1	A	288	HIS	2.2
2	C	105	ARG	2.2
1	M	329	VAL	2.1
2	C	13	TRP	2.1
2	C	102	HIS	2.1
1	A	423	GLN	2.1
1	M	297	ALA	2.1
2	C	114	ILE	2.1
1	M	406	LEU	2.1
2	C	57	TRP	2.1
2	C	60	ALA	2.0
2	C	87	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.