Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:51 pm BST

PDB ID	:	4Y66
Title	:	Crystal structure of Giardia lamblia Hop2-Mnd1 complex
Authors	:	Kang, H.A.; Shin, H.C.; Oh, B.H.
Deposited on	:	2015-02-12
Resolution	:	3.20 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 following versions of software and data (see references ①) were used in the production of this report:

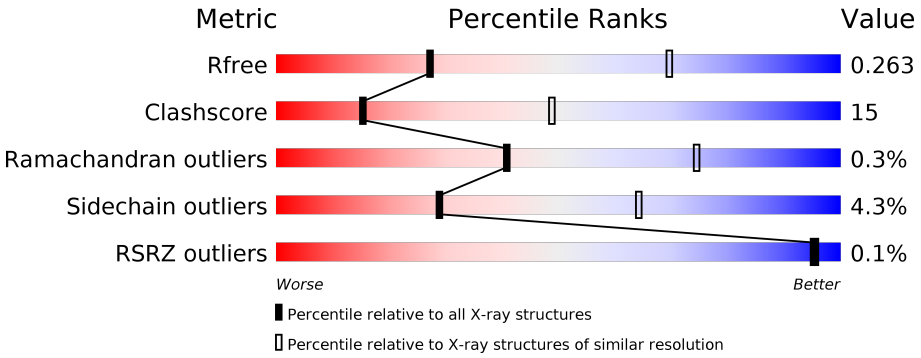
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	203	50% 13% 37%
1	C	203	64% 32%
1	E	203	60% 12% 26%
2	B	231	51% 14% 34%
2	D	231	60% 27% 10%
2	F	231	55% 16% 28%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7211 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 Mnd1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	128	Total	C	N	O	S	0	0	0
			892	566	155	168	3			
1	C	197	Total	C	N	O	S	0	0	0
			1521	957	259	299	6			
1	E	150	Total	C	N	O	S	0	0	0
			1027	638	179	208	2			

- Molecule 2 is a protein called Putative tbpip family protein.

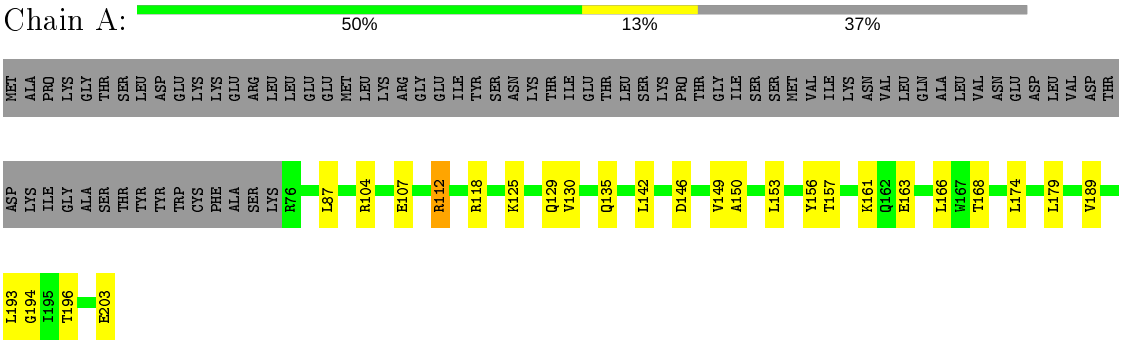
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	152	Total	C	N	O	S	0	0	0
			1062	659	189	207	7			
2	D	208	Total	C	N	O	S	0	0	0
			1547	955	272	310	10			
2	F	167	Total	C	N	O	S	0	0	0
			1162	727	199	230	6			

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 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.

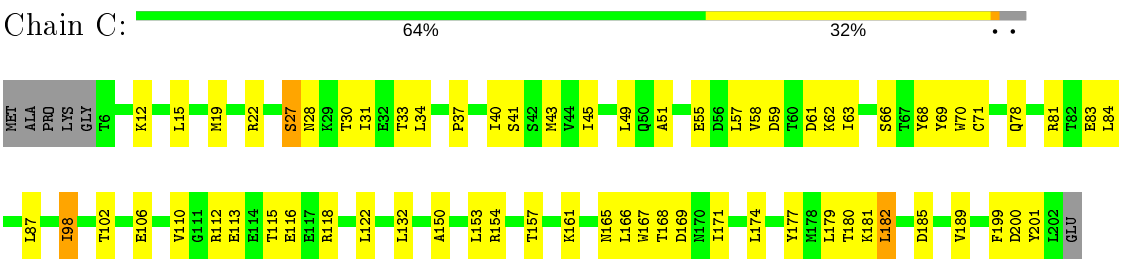
- Molecule 1: Mnd1

Chain A:



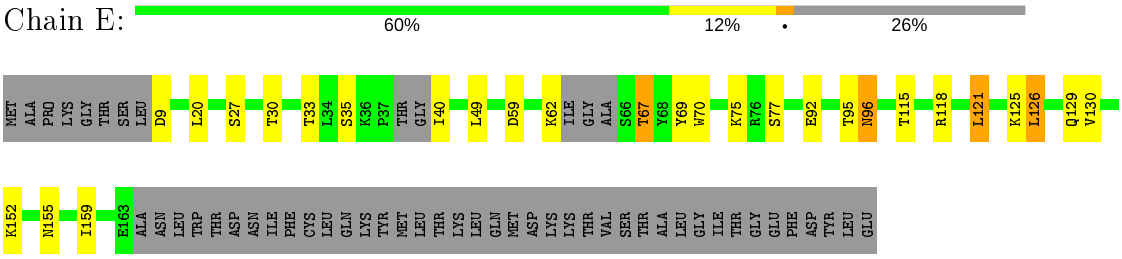
- Molecule 1: Mnd1

Chain C:



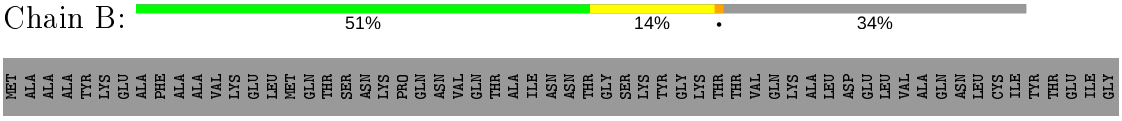
- Molecule 1: Mnd1

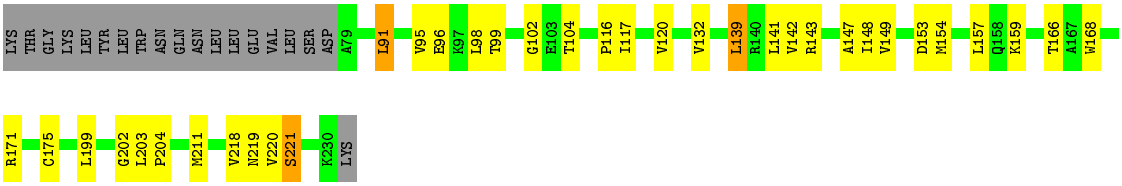
Chain E:



- Molecule 2: Putative tbpip family protein

Chain B:



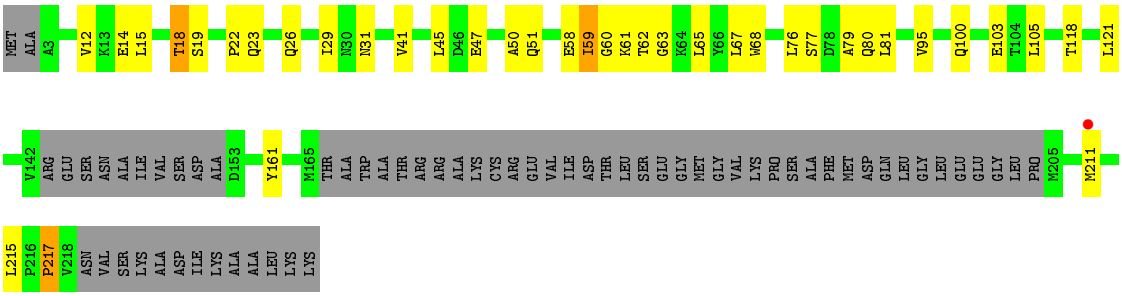


• Molecule 2: Putative tbpip family protein

Chain D:

• Molecule 2: Putative tbpip family protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.85Å 69.07Å 292.14Å 90.00° 95.34° 90.00°	Depositor
Resolution (Å)	40.65 – 3.20 45.03 – 3.18	Depositor EDS
% Data completeness (in resolution range)	87.5 (40.65-3.20) 86.8 (45.03-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 3.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.239 , 0.286 0.247 , 0.263	Depositor DCC
R_{free} test set	1800 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	70.0	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.055 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l 0.054 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	7211	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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

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	0.49	0/900	0.62	0/1228
1	C	0.56	0/1537	0.76	1/2077 (0.0%)
1	E	0.47	0/1034	0.60	0/1409
2	B	0.52	0/1071	0.65	0/1461
2	D	0.56	0/1559	0.72	0/2114
2	F	0.56	1/1171 (0.1%)	0.60	0/1603
All	All	0.54	1/7272 (0.0%)	0.67	1/9892 (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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	103	GLU	CG-CD	6.34	1.61	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	169	ASP	CB-CG-OD2	5.22	123.00	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	31	ASN	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	892	0	804	29	0
1	C	1521	0	1509	65	0
1	E	1027	0	857	22	0
2	B	1062	0	1000	34	0
2	D	1547	0	1499	75	0
2	F	1162	0	1038	35	0
All	All	7211	0	6707	207	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (207) 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:A:87:LEU:HB3	2:B:91:LEU:HD11	1.40	1.03
1:C:112:ARG:HH21	2:D:116:PRO:C	1.69	0.94
2:D:70:GLN:HA	2:D:70:GLN:HE21	1.32	0.92
1:E:92:GLU:O	1:E:96:ASN:ND2	2.08	0.86
2:F:77:SER:CB	2:F:80:GLN:HG2	2.06	0.85
1:A:142:LEU:HB3	2:B:148:ILE:HD11	1.56	0.85
1:E:96:ASN:HD22	1:E:96:ASN:N	1.77	0.83
1:A:135:GLN:HE22	2:B:132:VAL:HG13	1.42	0.82
1:C:153:LEU:HD21	2:D:158:GLN:HG3	1.64	0.79
1:C:118:ARG:NH2	2:D:116:PRO:O	2.19	0.76
2:D:45:LEU:HA	2:D:48:LEU:HD12	1.67	0.75
1:C:132:LEU:HD13	2:D:132:VAL:HG22	1.67	0.74
2:D:27:THR:HA	2:D:30:ASN:ND2	2.01	0.74
2:D:14:GLU:O	2:D:18:THR:OG1	2.06	0.74
1:C:112:ARG:NH2	2:D:116:PRO:C	2.40	0.73
1:C:87:LEU:HD21	2:D:92:LYS:HG3	1.70	0.72
1:C:154:ARG:HG2	2:D:157:LEU:HD11	1.73	0.71
2:D:32:THR:N	2:D:33:GLY:HA2	2.06	0.70
2:D:27:THR:HA	2:D:30:ASN:HD22	1.57	0.70
1:C:81:ARG:NH2	2:D:74:GLU:O	2.26	0.69
1:C:153:LEU:HD23	2:D:157:LEU:HG	1.76	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ARG:HH11	1:C:22:ARG:HG3	1.56	0.68
1:A:118:ARG:NH2	2:B:116:PRO:O	2.26	0.68
1:A:153:LEU:O	1:A:157:THR:HG23	1.92	0.67
1:C:153:LEU:HD12	2:D:215:LEU:HD21	1.77	0.67
1:C:112:ARG:NH2	2:D:117:ILE:N	2.44	0.65
1:E:96:ASN:HD22	1:E:96:ASN:H	1.45	0.64
1:C:168:THR:HA	1:C:171:ILE:HD12	1.80	0.63
1:E:59:ASP:OD1	1:E:75:LYS:HE2	1.98	0.63
1:C:27:SER:HB3	1:C:30:THR:OG1	1.98	0.62
1:A:135:GLN:NE2	2:B:132:VAL:HG13	2.15	0.62
2:D:165:MET:HG3	2:D:208:TYR:HE1	1.65	0.62
2:D:190:PRO:O	2:D:194:MET:HG3	1.99	0.62
1:C:168:THR:HG23	1:C:199:PHE:HE1	1.64	0.62
1:C:98:ILE:HD11	2:D:101:GLN:HB2	1.82	0.62
2:D:117:ILE:HG22	2:D:119:GLU:H	1.65	0.61
1:A:157:THR:O	1:A:161:LYS:HG3	2.01	0.61
1:E:49:LEU:HD21	1:E:69:TYR:CD2	2.35	0.61
2:B:104:THR:HG22	2:F:100:GLN:HG2	1.83	0.61
1:C:122:LEU:HD23	2:D:121:LEU:HD21	1.81	0.61
2:D:33:GLY:O	2:D:35:LYS:HG3	2.02	0.60
2:F:22:PRO:HB2	2:F:65:LEU:HD11	1.82	0.60
1:C:150:ALA:HB2	2:D:154:MET:HE1	1.84	0.60
2:F:161:TYR:HE1	2:F:217:PRO:HB3	1.67	0.59
2:D:22:PRO:O	2:D:23:GLN:HG3	2.02	0.59
2:D:17:GLN:HB2	2:D:68:TRP:CZ3	2.37	0.59
2:D:143:ARG:HG3	2:D:148:ILE:HD12	1.83	0.59
2:D:22:PRO:HA	2:D:67:LEU:HD13	1.84	0.59
2:D:150:SER:OG	2:D:151:ASP:N	2.34	0.59
2:F:58:GLU:HG2	2:F:61:LYS:HA	1.84	0.59
2:D:67:LEU:HD12	2:D:68:TRP:H	1.68	0.58
2:D:90:ASP:O	2:D:93:ALA:HB3	2.02	0.58
2:F:22:PRO:HB3	2:F:67:LEU:HD12	1.84	0.58
1:C:167:TRP:CE2	2:D:172:ARG:HG3	2.39	0.58
1:C:177:TYR:HE1	1:C:182:LEU:HD22	1.68	0.58
1:E:30:THR:HG21	2:F:59:ILE:HG22	1.85	0.58
1:C:84:LEU:HD12	2:D:84:VAL:HG13	1.85	0.57
2:F:12:VAL:HG11	2:F:45:LEU:HD23	1.87	0.57
1:C:12:LYS:NZ	1:C:55:GLU:OE2	2.34	0.57
2:D:128:LEU:O	2:D:132:VAL:HG23	2.05	0.56
2:F:77:SER:H	2:F:80:GLN:CG	2.18	0.56
1:C:112:ARG:HH21	2:D:116:PRO:CA	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:176:ARG:HA	2:D:179:ILE:HB	1.87	0.56
1:A:161:LYS:NZ	1:A:203:GLU:O	2.35	0.56
1:E:96:ASN:ND2	1:E:96:ASN:N	2.51	0.56
2:B:139:LEU:HD22	2:B:143:ARG:NH1	2.21	0.55
2:D:23:GLN:HG2	2:D:27:THR:OG1	2.06	0.55
2:B:203:LEU:HD12	2:B:204:PRO:HD2	1.89	0.55
1:C:102:THR:O	1:C:106:GLU:HG2	2.07	0.55
1:C:112:ARG:HB3	1:C:118:ARG:NH2	2.21	0.55
2:B:117:ILE:HG13	2:B:120:VAL:H	1.72	0.54
2:F:77:SER:H	2:F:80:GLN:HG3	1.73	0.54
2:D:45:LEU:O	2:D:49:VAL:HG23	2.08	0.54
2:F:29:ILE:HG22	2:F:41:VAL:HG21	1.90	0.54
1:C:115:THR:OG1	1:C:116:GLU:N	2.41	0.54
1:C:27:SER:H	1:C:30:THR:HB	1.73	0.53
1:E:70:TRP:CH2	2:F:22:PRO:HD3	2.43	0.53
2:F:47:GLU:O	2:F:51:GLN:HG2	2.09	0.53
2:F:23:GLN:O	2:F:65:LEU:HD12	2.08	0.53
2:D:109:GLN:O	2:D:113:GLU:HG3	2.09	0.53
1:C:115:THR:HG23	1:C:118:ARG:H	1.74	0.53
2:F:76:LEU:HD22	2:F:80:GLN:HB3	1.90	0.52
1:C:177:TYR:CE1	1:C:182:LEU:HD22	2.44	0.52
1:E:126:LEU:O	1:E:130:VAL:HG23	2.10	0.52
2:B:95:VAL:O	2:B:99:THR:HG23	2.08	0.52
2:D:48:LEU:O	2:D:53:LEU:N	2.34	0.52
2:F:19:SER:O	2:F:19:SER:OG	2.28	0.52
2:F:211:MET:O	2:F:215:LEU:N	2.43	0.52
1:A:174:LEU:HD21	2:B:199:LEU:HD11	1.93	0.51
1:C:87:LEU:HD21	2:D:92:LYS:CG	2.40	0.51
1:C:153:LEU:HD21	2:D:158:GLN:CG	2.37	0.51
2:D:55:ILE:O	2:D:66:TYR:HA	2.11	0.51
1:A:146:ASP:HB3	1:A:149:VAL:HG23	1.93	0.51
2:B:98:LEU:O	2:B:102:GLY:N	2.41	0.51
1:C:118:ARG:HH21	2:D:118:THR:N	2.09	0.51
2:D:70:GLN:HA	2:D:70:GLN:NE2	2.14	0.51
2:F:60:GLY:C	2:F:62:THR:H	2.13	0.51
1:C:165:ASN:O	1:C:168:THR:HB	2.11	0.51
1:C:185:ASP:O	1:C:189:VAL:HG23	2.11	0.50
1:E:27:SER:HB3	1:E:30:THR:HB	1.92	0.50
2:F:77:SER:N	2:F:80:GLN:HB2	2.26	0.50
1:A:163:GLU:HB3	2:B:168:TRP:CE2	2.47	0.50
1:A:168:THR:OG1	2:B:171:ARG:NH1	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:NH1	2:B:117:ILE:N	2.59	0.50
1:C:34:LEU:HA	1:C:37:PRO:HD2	1.93	0.50
1:E:118:ARG:HD3	2:F:118:THR:OG1	2.12	0.50
1:A:156:TYR:CE2	2:B:211:MET:HG2	2.47	0.49
1:C:83:GLU:OE2	1:C:87:LEU:HD22	2.12	0.49
1:C:174:LEU:HD21	2:D:199:LEU:HD21	1.93	0.49
2:D:22:PRO:CA	2:D:67:LEU:HD13	2.43	0.49
2:D:213:LYS:HG3	2:D:214:ALA:N	2.28	0.49
1:C:113:GLU:O	1:C:115:THR:HG22	2.13	0.49
2:B:221:SER:HB2	1:C:199:PHE:O	2.12	0.49
1:E:30:THR:O	1:E:33:THR:HG23	2.13	0.48
1:A:135:GLN:HE22	2:B:132:VAL:CG1	2.20	0.48
1:C:30:THR:O	1:C:33:THR:OG1	2.22	0.48
2:F:76:LEU:HB3	2:F:80:GLN:HB2	1.95	0.48
1:E:121:LEU:HD21	2:F:121:LEU:HD22	1.94	0.48
2:D:116:PRO:HG2	2:D:121:LEU:HD13	1.94	0.48
2:D:32:THR:H	2:D:33:GLY:HA2	1.76	0.48
1:C:27:SER:OG	1:C:28:ASN:N	2.47	0.48
2:D:16:MET:HE1	2:D:54:CYS:SG	2.54	0.48
1:C:153:LEU:CD1	2:D:215:LEU:HD21	2.42	0.48
1:A:112:ARG:CZ	2:B:117:ILE:HG22	2.44	0.47
2:F:15:LEU:O	2:F:18:THR:HG22	2.15	0.47
2:B:159:LYS:HB2	2:B:220:VAL:HB	1.95	0.47
1:C:15:LEU:O	1:C:19:MET:HG3	2.15	0.46
1:E:125:LYS:O	1:E:129:GLN:HG2	2.16	0.46
2:D:149:VAL:CG1	2:D:153:ASP:HB3	2.46	0.46
2:D:45:LEU:O	2:D:48:LEU:HB2	2.16	0.46
1:C:177:TYR:CD2	2:D:197:LEU:HD21	2.50	0.46
2:F:47:GLU:O	2:F:50:ALA:HB3	2.15	0.46
1:C:22:ARG:NH1	1:C:22:ARG:HG3	2.26	0.46
1:C:66:SER:HB2	1:C:68:TYR:CZ	2.51	0.46
2:F:105:LEU:HA	2:F:105:LEU:HD12	1.70	0.45
1:A:125:LYS:O	1:A:129:GLN:HB2	2.16	0.45
2:D:179:ILE:HD11	2:D:199:LEU:HD23	1.98	0.45
1:C:63:ILE:HD12	2:D:65:LEU:HD21	1.99	0.45
2:F:15:LEU:HD11	2:F:31:ASN:HB2	1.98	0.45
2:D:56:TYR:HA	2:D:65:LEU:O	2.16	0.45
1:A:112:ARG:CZ	2:B:117:ILE:CG2	2.94	0.45
2:F:14:GLU:O	2:F:18:THR:HB	2.17	0.44
2:D:17:GLN:HB2	2:D:68:TRP:CH2	2.53	0.44
2:D:128:LEU:HA	2:D:128:LEU:HD23	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ASP:OD1	1:C:62:LYS:N	2.48	0.44
2:B:203:LEU:CD1	2:B:204:PRO:HD2	2.48	0.44
2:F:67:LEU:HD23	2:F:68:TRP:O	2.17	0.44
1:A:179:LEU:HD21	1:A:189:VAL:HG11	1.99	0.44
2:D:156:THR:OG1	2:D:157:LEU:N	2.50	0.44
2:B:142:VAL:HG13	2:B:147:ALA:HB3	1.99	0.43
2:D:70:GLN:NE2	2:D:73:LEU:CD1	2.81	0.43
1:E:35:SER:O	1:E:40:ILE:N	2.51	0.43
1:A:166:LEU:HD23	2:B:202:GLY:HA2	2.00	0.43
2:B:117:ILE:HD11	2:B:120:VAL:HG23	2.00	0.43
1:C:49:LEU:HD21	1:C:69:TYR:CG	2.52	0.43
1:A:104:ARG:O	1:A:107:GLU:HG2	2.19	0.43
1:C:167:TRP:O	1:C:171:ILE:HG13	2.18	0.43
1:C:58:VAL:HG22	1:C:71:CYS:HB2	2.00	0.43
2:D:121:LEU:HD12	2:D:121:LEU:HA	1.77	0.43
2:B:141:LEU:HA	2:B:141:LEU:HD23	1.79	0.43
1:C:180:THR:OG1	1:C:181:LYS:N	2.52	0.43
2:D:154:MET:HE3	2:D:154:MET:HB2	1.71	0.43
2:B:171:ARG:O	2:B:175:CYS:HB2	2.19	0.42
2:D:168:TRP:C	2:D:168:TRP:CD1	2.92	0.42
2:F:81:LEU:HD23	2:F:81:LEU:HA	1.81	0.42
1:C:12:LYS:HE2	1:C:51:ALA:HB1	2.01	0.42
2:D:139:LEU:HD23	2:D:139:LEU:HA	1.76	0.42
2:D:161:TYR:O	2:D:165:MET:HB2	2.18	0.42
2:F:58:GLU:HG3	2:F:63:GLY:O	2.19	0.42
1:E:152:LYS:HA	1:E:155:ASN:ND2	2.34	0.42
1:E:20:LEU:HA	1:E:20:LEU:HD23	1.88	0.42
2:F:22:PRO:CB	2:F:67:LEU:HD12	2.48	0.42
1:A:142:LEU:CB	2:B:148:ILE:HD11	2.37	0.42
1:E:27:SER:H	1:E:30:THR:HB	1.84	0.42
1:E:9:ASP:N	1:E:9:ASP:OD1	2.52	0.42
1:A:112:ARG:HG3	2:B:117:ILE:HA	2.01	0.42
1:A:150:ALA:HB2	2:B:154:MET:HE2	2.02	0.42
1:C:59:ASP:HB3	1:C:70:TRP:CZ2	2.55	0.42
1:C:78:GLN:HG3	2:D:73:LEU:HD13	2.01	0.42
2:F:26:GLN:O	2:F:29:ILE:HG12	2.19	0.42
1:C:41:SER:OG	1:C:43:MET:HB3	2.20	0.42
1:C:98:ILE:HD11	2:D:101:GLN:CB	2.49	0.42
1:E:126:LEU:HA	1:E:129:GLN:HE21	1.85	0.42
2:F:121:LEU:HD23	2:F:121:LEU:O	2.20	0.42
1:A:194:GLY:O	1:A:196:THR:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:LEU:HD23	1:C:179:LEU:HA	1.66	0.41
1:C:40:ILE:HB	1:C:45:ILE:HD11	2.02	0.41
1:C:157:THR:O	1:C:161:LYS:HB2	2.20	0.41
1:C:166:LEU:C	1:C:166:LEU:HD23	2.40	0.41
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.83	0.41
1:C:31:ILE:HD12	1:C:34:LEU:HD22	2.02	0.41
2:D:149:VAL:HG12	2:D:153:ASP:HB3	2.02	0.41
2:D:168:TRP:CH2	2:D:208:TYR:HB2	2.56	0.41
1:C:28:ASN:O	1:C:31:ILE:HG22	2.21	0.41
1:C:132:LEU:CD1	2:D:132:VAL:HG22	2.44	0.41
2:D:138:LYS:O	2:D:142:VAL:HG23	2.20	0.41
1:E:62:LYS:HB3	1:E:67:THR:HG22	2.03	0.41
2:D:91:LEU:HA	2:D:91:LEU:HD23	1.66	0.41
1:A:130:VAL:HG13	2:F:79:ALA:HB1	2.03	0.41
2:B:153:ASP:O	2:B:157:LEU:HG	2.20	0.41
1:A:150:ALA:CB	2:B:149:VAL:HG21	2.51	0.40
1:C:200:ASP:OD1	1:C:201:TYR:N	2.45	0.40
1:E:155:ASN:O	1:E:159:ILE:HG13	2.21	0.40
1:A:112:ARG:NH1	2:B:117:ILE:HG23	2.36	0.40
2:D:70:GLN:NE2	2:D:73:LEU:HD12	2.36	0.40
2:F:59:ILE:HG13	2:F:59:ILE:H	1.63	0.40
2:B:95:VAL:HG12	2:B:96:GLU:N	2.35	0.40

There are no symmetry-related clashes.

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	126/203 (62%)	121 (96%)	5 (4%)	0	100 100
1	C	195/203 (96%)	184 (94%)	10 (5%)	1 (0%)	29 67
1	E	144/203 (71%)	139 (96%)	5 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	150/231 (65%)	145 (97%)	5 (3%)	0	100 100
2	D	202/231 (87%)	189 (94%)	12 (6%)	1 (0%)	29 67
2	F	161/231 (70%)	154 (96%)	6 (4%)	1 (1%)	25 64
All	All	978/1302 (75%)	932 (95%)	43 (4%)	3 (0%)	41 74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	110	VAL
2	F	217	PRO
2	D	148	ILE

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	74/180 (41%)	73 (99%)	1 (1%)	67 86
1	C	160/180 (89%)	156 (98%)	4 (2%)	47 77
1	E	81/180 (45%)	74 (91%)	7 (9%)	10 38
2	B	98/196 (50%)	92 (94%)	6 (6%)	18 54
2	D	159/196 (81%)	151 (95%)	8 (5%)	24 60
2	F	102/196 (52%)	99 (97%)	3 (3%)	42 74
All	All	674/1128 (60%)	645 (96%)	29 (4%)	29 64

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ARG
2	B	91	LEU
2	B	139	LEU
2	B	166	THR
2	B	218	VAL

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Mol	Chain	Res	Type
2	B	219	ASN
2	B	221	SER
1	C	27	SER
1	C	57	LEU
1	C	98	ILE
1	C	182	LEU
2	D	18	THR
2	D	47	GLU
2	D	70	GLN
2	D	112	LEU
2	D	143	ARG
2	D	151	ASP
2	D	179	ILE
2	D	215	LEU
1	E	67	THR
1	E	77	SER
1	E	95	THR
1	E	96	ASN
1	E	115	THR
1	E	121	LEU
1	E	126	LEU
2	F	18	THR
2	F	59	ILE
2	F	95	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
2	B	135	ASN
2	D	30	ASN
2	D	52	ASN
2	D	70	GLN
1	E	96	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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

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, 95^{th} 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	128/203 (63%)	-0.49	0	100	100	28, 79, 137, 166	0
1	C	197/203 (97%)	-0.41	0	100	100	24, 48, 85, 129	0
1	E	150/203 (73%)	-0.52	0	100	100	31, 89, 152, 191	0
2	B	152/231 (65%)	-0.45	0	100	100	24, 69, 124, 163	0
2	D	208/231 (90%)	-0.35	0	100	100	26, 63, 110, 144	0
2	F	167/231 (72%)	-0.31	1 (0%)	89	83	29, 79, 151, 208	0
All	All	1002/1302 (76%)	-0.41	1 (0%)	95	95	24, 66, 138, 208	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	211	MET	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.