Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:33 PM GMT

PDB ID	:	4CKP
Title	:	Structure of an N-terminal fragment of Leishmania SAS-6 that contains part of its coiled coil domain
Authors	:	van Breugel, M.
Deposited on	:	2014-01-07
Resolution	:	3.45 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

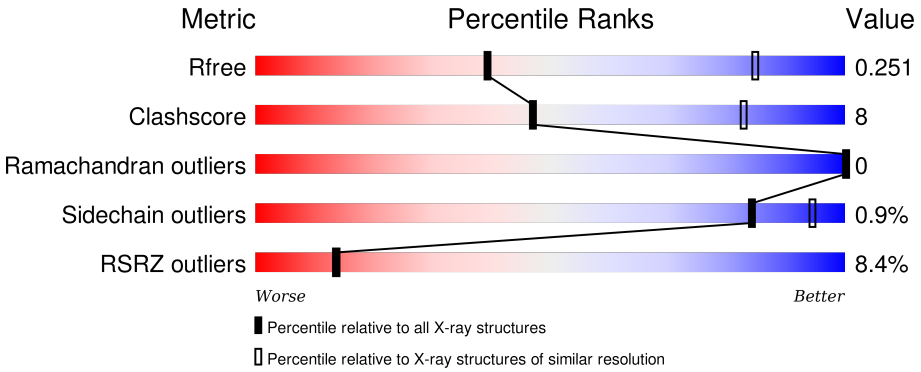
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.45 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	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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	226	7% 64% 13% 22%
1	B	226	6% 63% 15% 22%
1	C	226	7% 70% 13% 16%
1	D	226	6% 69% 15% 17%
1	E	226	6% 69% 15% 16%

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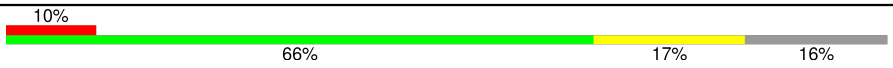
Mol	Chain	Length	Quality of chain
1	F	226	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8777 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 SAS-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	0	0
			1398	889	242	264	3			
1	B	177	Total	C	N	O	S	0	0	0
			1407	894	244	266	3			
1	C	189	Total	C	N	O	S	0	0	0
			1493	945	259	286	3			
1	D	188	Total	C	N	O	S	0	0	0
			1484	940	258	283	3			
1	E	190	Total	C	N	O	S	0	0	0
			1503	952	263	285	3			
1	F	189	Total	C	N	O	S	0	0	0
			1492	946	259	284	3			

There are 12 discrepancies between the modelled and reference sequences:

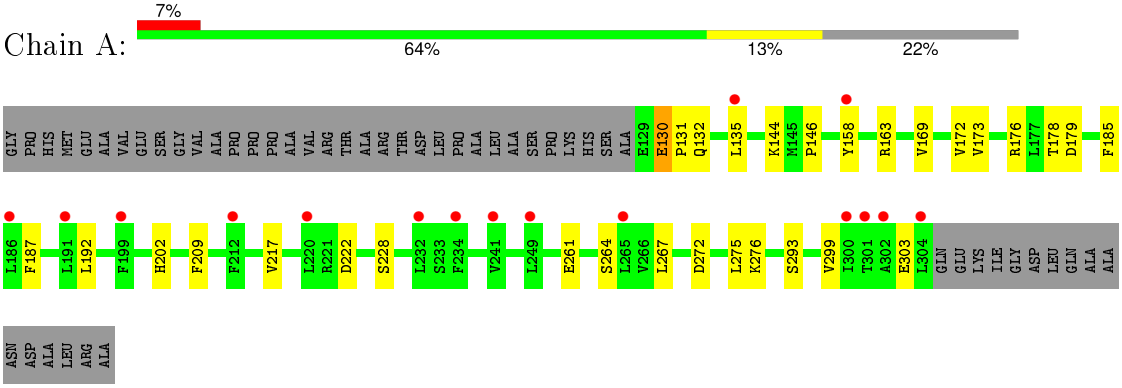
Chain	Residue	Modelled	Actual	Comment	Reference
A	95	GLY	-	EXPRESSION TAG	UNP E9AFQ5
A	96	PRO	-	EXPRESSION TAG	UNP E9AFQ5
B	95	GLY	-	EXPRESSION TAG	UNP E9AFQ5
B	96	PRO	-	EXPRESSION TAG	UNP E9AFQ5
C	95	GLY	-	EXPRESSION TAG	UNP E9AFQ5
C	96	PRO	-	EXPRESSION TAG	UNP E9AFQ5
D	95	GLY	-	EXPRESSION TAG	UNP E9AFQ5
D	96	PRO	-	EXPRESSION TAG	UNP E9AFQ5
E	95	GLY	-	EXPRESSION TAG	UNP E9AFQ5
E	96	PRO	-	EXPRESSION TAG	UNP E9AFQ5
F	95	GLY	-	EXPRESSION TAG	UNP E9AFQ5
F	96	PRO	-	EXPRESSION TAG	UNP E9AFQ5

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.

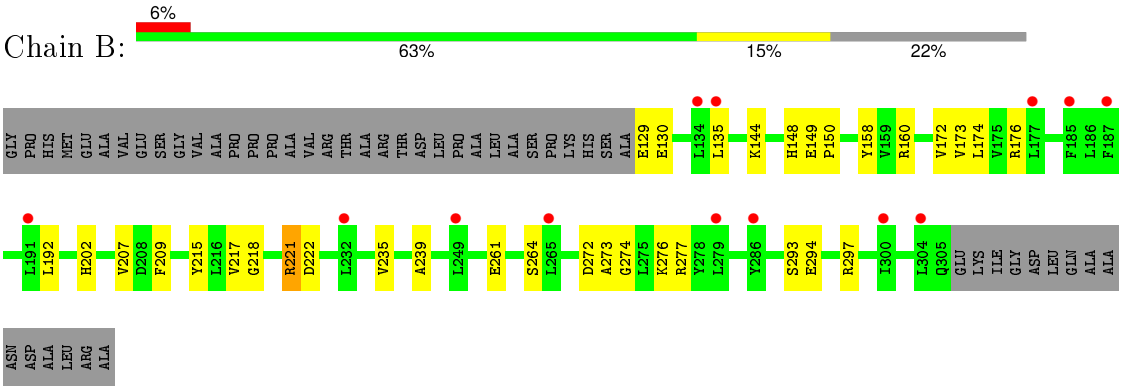
- Molecule 1: SAS-6

Chain A:



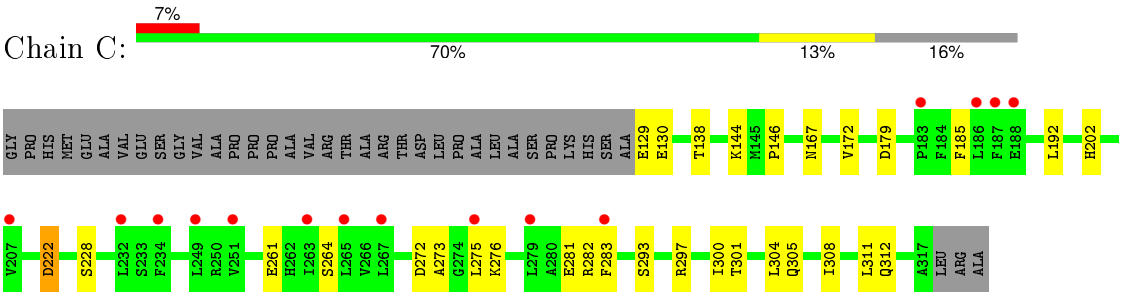
- Molecule 1: SAS-6

Chain B:



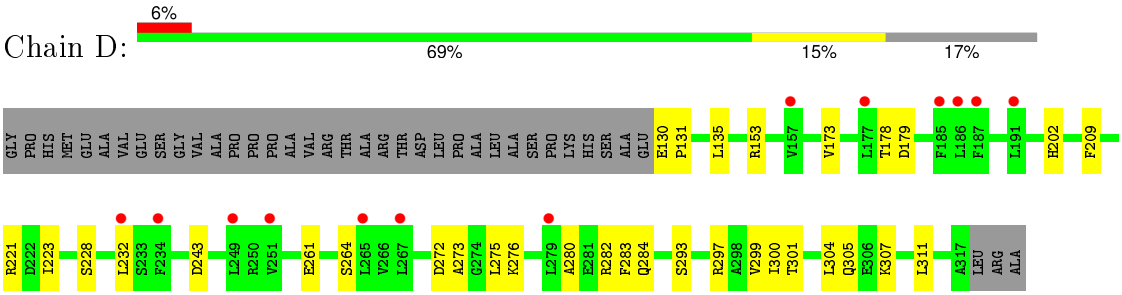
- Molecule 1: SAS-6

Chain C:



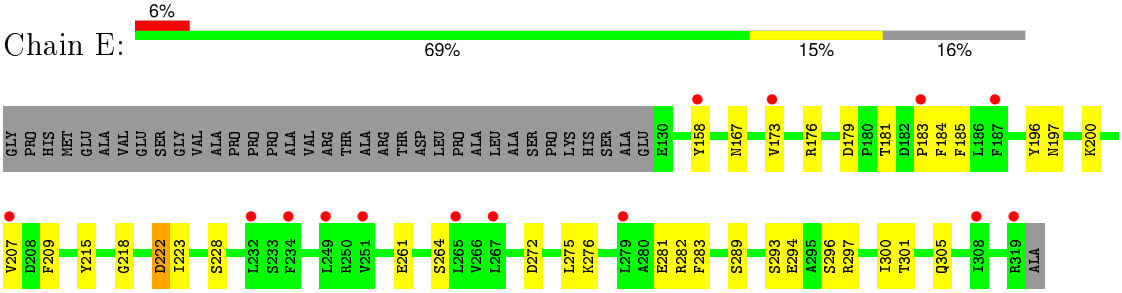
- Molecule 1: SAS-6

Chain D:



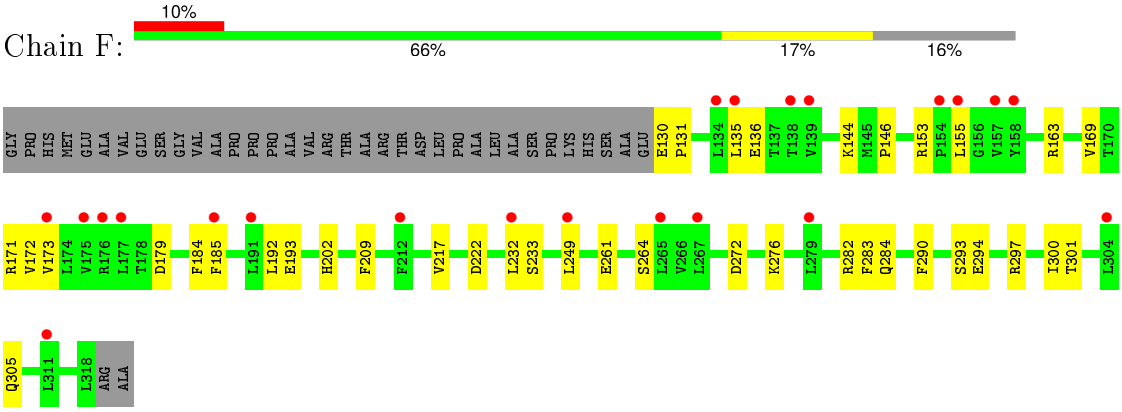
- Molecule 1: SAS-6

Chain E:



- Molecule 1: SAS-6

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	482.68Å 482.68Å 43.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.90 – 3.45 66.94 – 3.45	Depositor EDS
% Data completeness (in resolution range)	97.6 (42.90-3.45) 98.6 (66.94-3.45)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 3.49Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.224 , 0.242 0.234 , 0.251	Depositor DCC
R_{free} test set	4910 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	99.7	Xtriage
Anisotropy	0.829	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 72.2	EDS
Estimated twinning fraction	0.145 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 48650 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8777	wwPDB-VP
Average B, all atoms (Å^2)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, 0.375 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	0.32	0/1427	0.67	1/1937 (0.1%)
1	B	0.32	0/1436	0.68	0/1949
1	C	0.33	0/1522	0.64	0/2065
1	D	0.31	0/1513	0.64	0/2053
1	E	0.33	0/1532	0.69	0/2078
1	F	0.33	0/1521	0.67	0/2064
All	All	0.32	0/8951	0.67	1/12146 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	130	GLU	C-N-CD	5.16	139.23	128.40

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	1398	0	1386	20	0
1	B	1407	0	1394	22	0
1	C	1493	0	1475	28	0
1	D	1484	0	1469	26	0
1	E	1503	0	1493	29	0
1	F	1492	0	1480	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8777	0	8697	131	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 8.

All (131) 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:C:273:ALA:HA	1:C:276:LYS:HE2	1.62	0.80
1:C:308:ILE:HD11	1:D:304:LEU:HD22	1.69	0.75
1:C:311:LEU:HB3	1:D:311:LEU:HB3	1.70	0.73
1:C:300:ILE:HG21	1:D:301:THR:HG22	1.69	0.73
1:D:153:ARG:NH1	1:D:179:ASP:OD2	2.24	0.71
1:C:144:LYS:HZ2	1:C:146:PRO:HG3	1.56	0.71
1:A:222:ASP:HB3	1:A:228:SER:HB2	1.74	0.68
1:A:144:LYS:HZ2	1:A:146:PRO:HG3	1.58	0.68
1:C:293:SER:HB3	1:D:293:SER:HB3	1.75	0.67
1:F:144:LYS:HZ2	1:F:146:PRO:HG3	1.60	0.66
1:C:144:LYS:NZ	1:C:146:PRO:HG3	2.12	0.65
1:F:294:GLU:OE2	1:F:297:ARG:NH2	2.28	0.65
1:A:130:GLU:HG3	1:A:131:PRO:CD	2.28	0.63
1:A:293:SER:HB3	1:B:293:SER:HB3	1.79	0.63
1:C:305:GLN:HA	1:C:308:ILE:HD12	1.81	0.63
1:D:261:GLU:OE2	1:D:264:SER:HB2	1.99	0.63
1:C:129:GLU:HG2	1:C:130:GLU:HG2	1.79	0.62
1:E:293:SER:HB3	1:F:293:SER:HB3	1.81	0.62
1:E:301:THR:HG22	1:F:300:ILE:HG21	1.85	0.59
1:D:272:ASP:O	1:D:276:LYS:HG3	2.02	0.59
1:A:163:ARG:NH1	1:A:169:VAL:O	2.36	0.58
1:D:135:LEU:HD13	1:D:221:ARG:HD3	1.86	0.58
1:C:301:THR:HG22	1:D:300:ILE:HG21	1.86	0.57
1:B:261:GLU:OE2	1:B:264:SER:HB2	2.05	0.57
1:C:272:ASP:O	1:C:276:LYS:HG3	2.05	0.56
1:C:261:GLU:OE2	1:C:264:SER:HB3	2.05	0.56
1:B:272:ASP:O	1:B:276:LYS:HG3	2.05	0.56
1:F:272:ASP:O	1:F:276:LYS:HG3	2.06	0.55
1:E:275:LEU:HD23	1:F:276:LYS:HD3	1.87	0.55
1:A:158:TYR:HB3	1:A:176:ARG:HB3	1.89	0.54
1:F:173:VAL:HG23	1:F:209:PHE:CZ	2.43	0.54
1:F:135:LEU:HB2	1:F:217:VAL:HG13	1.90	0.54
1:A:130:GLU:HG3	1:A:131:PRO:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:TYR:HB3	1:B:176:ARG:HB3	1.91	0.53
1:F:261:GLU:OE2	1:F:264:SER:HB2	2.09	0.53
1:C:304:LEU:HB3	1:D:304:LEU:HB3	1.92	0.52
1:F:301:THR:O	1:F:305:GLN:HB2	2.10	0.52
1:E:294:GLU:OE2	1:E:297:ARG:NH2	2.41	0.51
1:A:272:ASP:O	1:A:276:LYS:HG3	2.11	0.51
1:C:275:LEU:HD23	1:D:276:LYS:HD3	1.91	0.51
1:C:281:GLU:OE2	1:C:282:ARG:NH1	2.44	0.51
1:B:294:GLU:OE2	1:B:297:ARG:NH2	2.44	0.51
1:E:300:ILE:HG21	1:F:301:THR:HG22	1.93	0.50
1:E:158:TYR:HB3	1:E:176:ARG:HB3	1.93	0.50
1:E:282:ARG:HB3	1:F:283:PHE:CE1	2.46	0.50
1:B:149:GLU:HG3	1:B:150:PRO:HD2	1.94	0.50
1:C:202:HIS:C	1:C:202:HIS:HD1	2.16	0.49
1:A:173:VAL:HG23	1:A:209:PHE:CZ	2.47	0.49
1:E:261:GLU:OE2	1:E:264:SER:HB2	2.12	0.49
1:E:301:THR:O	1:E:305:GLN:HB2	2.13	0.49
1:E:179:ASP:HB3	1:E:185:PHE:HB3	1.95	0.49
1:D:301:THR:O	1:D:305:GLN:HB2	2.12	0.49
1:C:129:GLU:N	1:C:129:GLU:OE1	2.45	0.49
1:A:261:GLU:OE2	1:A:264:SER:HB2	2.13	0.49
1:E:184:PHE:HD1	1:E:275:LEU:HD21	1.78	0.48
1:B:135:LEU:HB2	1:B:217:VAL:HG13	1.95	0.48
1:F:171:ARG:HB2	1:F:193:GLU:OE1	2.13	0.48
1:C:282:ARG:HB3	1:D:283:PHE:CE1	2.48	0.48
1:F:153:ARG:HD2	1:F:155:LEU:HD21	1.95	0.48
1:E:196:TYR:CE1	1:E:200:LYS:HB2	2.49	0.48
1:B:207:VAL:HG11	1:B:215:TYR:CE2	2.49	0.47
1:E:272:ASP:O	1:E:276:LYS:HG3	2.13	0.47
1:C:222:ASP:HB3	1:C:228:SER:HB2	1.96	0.47
1:E:167:ASN:OD1	1:E:167:ASN:N	2.36	0.47
1:A:144:LYS:NZ	1:A:146:PRO:HG3	2.28	0.47
1:F:172:VAL:HG12	1:F:192:LEU:HD23	1.97	0.47
1:E:289:SER:HB3	1:F:290:PHE:CE1	2.49	0.46
1:D:202:HIS:C	1:D:202:HIS:HD1	2.18	0.46
1:C:276:LYS:HD2	1:D:275:LEU:HD23	1.97	0.46
1:E:283:PHE:CD1	1:F:282:ARG:HB3	2.51	0.46
1:E:283:PHE:CE1	1:F:282:ARG:HB3	2.51	0.45
1:A:135:LEU:HB2	1:A:217:VAL:HG13	1.98	0.45
1:E:281:GLU:OE2	1:E:282:ARG:NH1	2.49	0.45
1:D:178:THR:HG22	1:D:179:ASP:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:ARG:HB3	1:F:283:PHE:CD1	2.52	0.45
1:E:196:TYR:CD2	1:E:209:PHE:HD1	2.35	0.45
1:E:183:PRO:HG3	1:F:284:GLN:OE1	2.16	0.45
1:E:293:SER:OG	1:F:294:GLU:OE2	2.35	0.45
1:B:160:ARG:HH21	1:B:174:LEU:HD22	1.82	0.44
1:C:172:VAL:HG12	1:C:192:LEU:HD23	1.98	0.44
1:B:217:VAL:O	1:B:221:ARG:HB3	2.18	0.44
1:D:223:ILE:HA	1:D:228:SER:HB3	1.98	0.44
1:E:173:VAL:HG23	1:E:209:PHE:CZ	2.53	0.44
1:A:179:ASP:HB3	1:A:185:PHE:HB3	2.00	0.44
1:E:276:LYS:HD2	1:F:184:PHE:HE2	1.83	0.44
1:C:283:PHE:CE1	1:D:282:ARG:HB3	2.52	0.44
1:A:178:THR:HG22	1:A:179:ASP:N	2.32	0.44
1:C:308:ILE:HG12	1:D:307:LYS:HD2	2.00	0.44
1:C:297:ARG:O	1:C:301:THR:OG1	2.22	0.44
1:C:308:ILE:O	1:C:312:GLN:HB2	2.18	0.44
1:B:149:GLU:CG	1:B:150:PRO:HD2	2.48	0.43
1:D:173:VAL:HG23	1:D:209:PHE:CZ	2.54	0.43
1:F:179:ASP:HB3	1:F:185:PHE:HB3	2.01	0.43
1:B:144:LYS:HB3	1:B:235:VAL:HG22	2.00	0.43
1:A:130:GLU:HG3	1:A:131:PRO:HD3	1.99	0.43
1:E:179:ASP:OD1	1:E:181:THR:OG1	2.24	0.43
1:A:172:VAL:HG12	1:A:192:LEU:HD23	2.00	0.43
1:A:202:HIS:HD1	1:A:202:HIS:C	2.21	0.43
1:D:280:ALA:O	1:D:284:GLN:HG3	2.18	0.42
1:B:202:HIS:C	1:B:202:HIS:HD1	2.23	0.42
1:E:207:VAL:HG11	1:E:215:TYR:CE2	2.54	0.42
1:F:202:HIS:HD1	1:F:202:HIS:C	2.22	0.42
1:B:135:LEU:HB2	1:B:217:VAL:CG1	2.50	0.42
1:C:293:SER:OG	1:D:297:ARG:NH2	2.52	0.42
1:B:172:VAL:CG1	1:B:192:LEU:HD23	2.50	0.42
1:D:273:ALA:HA	1:D:276:LYS:HE3	2.02	0.41
1:B:148:HIS:CE1	1:B:239:ALA:HB1	2.54	0.41
1:F:130:GLU:N	1:F:131:PRO:CD	2.83	0.41
1:D:130:GLU:N	1:D:131:PRO:CD	2.83	0.41
1:B:273:ALA:HA	1:B:276:LYS:HE3	2.01	0.41
1:F:136:GLU:OE2	1:F:282:ARG:NH2	2.54	0.41
1:A:299:VAL:O	1:A:303:GLU:HG3	2.20	0.41
1:A:187:PHE:HB3	1:A:267:LEU:HB3	2.01	0.41
1:E:296:SER:O	1:E:300:ILE:HG13	2.21	0.41
1:B:129:GLU:HB3	1:B:130:GLU:H	1.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:232:LEU:HD23	1:F:232:LEU:HA	1.90	0.41
1:C:304:LEU:O	1:C:308:ILE:HG13	2.21	0.41
1:B:218:GLY:O	1:B:222:ASP:HB2	2.20	0.41
1:F:144:LYS:NZ	1:F:146:PRO:HG3	2.32	0.41
1:F:172:VAL:CG1	1:F:192:LEU:HD23	2.51	0.41
1:D:299:VAL:HG23	1:D:300:ILE:HG13	2.03	0.41
1:F:233:SER:O	1:F:249:LEU:HD12	2.21	0.41
1:B:173:VAL:HG23	1:B:209:PHE:CZ	2.56	0.41
1:E:218:GLY:O	1:E:222:ASP:HB2	2.21	0.41
1:D:232:LEU:HA	1:D:232:LEU:HD23	1.89	0.41
1:C:179:ASP:HB3	1:C:185:PHE:HB3	2.03	0.40
1:A:275:LEU:HD23	1:B:276:LYS:HD3	2.03	0.40
1:F:163:ARG:HD2	1:F:169:VAL:C	2.41	0.40
1:B:274:GLY:O	1:B:277:ARG:HB2	2.22	0.40
1:F:193:GLU:HA	1:F:209:PHE:CE2	2.56	0.40
1:E:223:ILE:HA	1:E:228:SER:HB3	2.03	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	174/226 (77%)	172 (99%)	2 (1%)	0	100	100
1	B	175/226 (77%)	174 (99%)	1 (1%)	0	100	100
1	C	187/226 (83%)	185 (99%)	2 (1%)	0	100	100
1	D	186/226 (82%)	185 (100%)	1 (0%)	0	100	100
1	E	188/226 (83%)	187 (100%)	1 (0%)	0	100	100
1	F	187/226 (83%)	186 (100%)	1 (0%)	0	100	100
All	All	1097/1356 (81%)	1089 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	152/188 (81%)	151 (99%)	1 (1%)	88	95
1	B	153/188 (81%)	152 (99%)	1 (1%)	88	95
1	C	161/188 (86%)	158 (98%)	3 (2%)	65	87
1	D	160/188 (85%)	159 (99%)	1 (1%)	90	97
1	E	162/188 (86%)	160 (99%)	2 (1%)	78	91
1	F	161/188 (86%)	160 (99%)	1 (1%)	90	97
All	All	949/1128 (84%)	940 (99%)	9 (1%)	84	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	B	221	ARG
1	C	138	THR
1	C	167	ASN
1	C	222	ASP
1	D	243	ASP
1	E	197	ASN
1	E	222	ASP
1	F	222	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	176/226 (77%)	0.39	16 (9%)	11	11	100, 152, 226, 289	0
1	B	177/226 (78%)	0.47	13 (7%)	18	17	96, 139, 227, 268	0
1	C	189/226 (83%)	0.35	15 (7%)	15	15	80, 128, 236, 272	0
1	D	188/226 (83%)	0.31	13 (6%)	20	18	86, 148, 236, 277	0
1	E	190/226 (84%)	0.28	14 (7%)	17	17	102, 139, 197, 222	0
1	F	189/226 (83%)	0.47	22 (11%)	6	7	108, 152, 208, 243	0
All	All	1109/1356 (81%)	0.38	93 (8%)	14	14	80, 144, 224, 289	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	304	LEU	5.9
1	A	302	ALA	5.7
1	B	300	ILE	4.6
1	F	304	LEU	4.5
1	F	135	LEU	3.8
1	C	249	LEU	3.7
1	D	251	VAL	3.6
1	F	232	LEU	3.5
1	E	207	VAL	3.5
1	F	157	VAL	3.4
1	C	186	LEU	3.4
1	F	134	LEU	3.4
1	B	177	LEU	3.3
1	D	265	LEU	3.3
1	D	267	LEU	3.3
1	A	241	VAL	3.2
1	B	232	LEU	3.1
1	E	279	LEU	3.1
1	F	265	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	279	LEU	3.1
1	E	267	LEU	3.0
1	E	232	LEU	2.9
1	D	279	LEU	2.9
1	A	249	LEU	2.9
1	B	265	LEU	2.9
1	C	234	PHE	2.9
1	B	185	PHE	2.9
1	F	185	PHE	2.9
1	F	267	LEU	2.9
1	A	234	PHE	2.8
1	B	191	LEU	2.7
1	C	251	VAL	2.7
1	D	232	LEU	2.6
1	A	158	TYR	2.6
1	F	311	LEU	2.6
1	A	191	LEU	2.6
1	C	183	PRO	2.6
1	B	286	TYR	2.6
1	F	249	LEU	2.6
1	D	187	PHE	2.6
1	F	155	LEU	2.6
1	F	158	TYR	2.5
1	A	232	LEU	2.5
1	F	191	LEU	2.5
1	E	249	LEU	2.5
1	C	265	LEU	2.5
1	A	304	LEU	2.5
1	D	186	LEU	2.5
1	A	186	LEU	2.5
1	B	135	LEU	2.5
1	F	154	PRO	2.5
1	A	199	PHE	2.5
1	B	134	LEU	2.5
1	E	319	ARG	2.5
1	C	283	PHE	2.4
1	D	234	PHE	2.4
1	E	234	PHE	2.4
1	C	267	LEU	2.4
1	E	158	TYR	2.4
1	E	308	ILE	2.4
1	B	249	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	183	PRO	2.3
1	F	138	THR	2.3
1	D	249	LEU	2.3
1	E	251	VAL	2.3
1	F	139	VAL	2.3
1	A	212	PHE	2.3
1	A	301	THR	2.3
1	C	187	PHE	2.3
1	F	177	LEU	2.3
1	C	188	GLU	2.3
1	A	265	LEU	2.3
1	B	187	PHE	2.3
1	C	279	LEU	2.2
1	E	187	PHE	2.2
1	F	279	LEU	2.2
1	F	175	VAL	2.2
1	A	220	LEU	2.2
1	C	263	ILE	2.2
1	D	191	LEU	2.1
1	D	185	PHE	2.1
1	E	173	VAL	2.1
1	A	135	LEU	2.1
1	A	300	ILE	2.1
1	F	176	ARG	2.1
1	D	177	LEU	2.1
1	D	157	VAL	2.1
1	F	212	PHE	2.1
1	E	265	LEU	2.0
1	C	207	VAL	2.0
1	C	275	LEU	2.0
1	C	232	LEU	2.0
1	F	173	VAL	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.