Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 11:34 pm BST

PDB ID	:	3VO9
Title	:	Staphylococcus aureus FtsZ apo-form (SeMet)
Authors	:	Matsui, T.; Yamane, J.; Mogi, N.; Yao, M.; Tanaka, I.
Deposited on	:	2012-01-20
Resolution	:	2.71 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.

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 2.71 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.
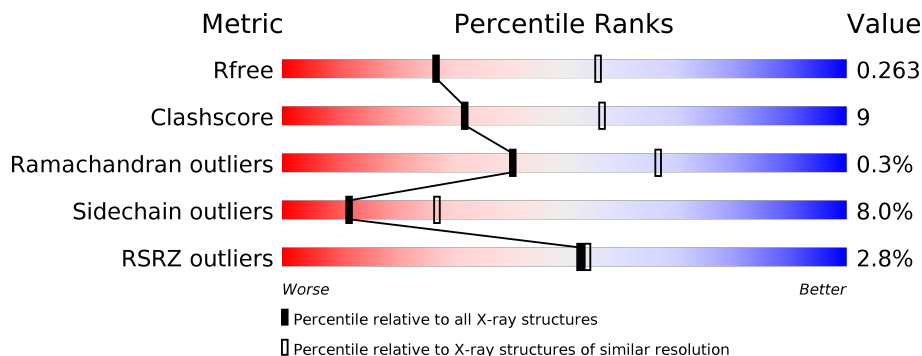
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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	308	2% / 76% / 19% / · ·
1	B	308	2% / 70% / 23% / · 5%
1	C	308	2% / 80% / 16% / · ·
1	D	308	5% / 68% / 22% / · 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8529 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 Cell division protein FtsZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total 2119	C 1315	N 357	O 436	Se 11	0	0	0
1	B	292	Total 2093	C 1298	N 354	O 430	Se 11	0	0	0
1	C	301	Total 2171	C 1344	N 372	O 444	Se 11	0	0	0
1	D	287	Total 2069	C 1284	N 350	O 424	Se 11	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLY	-	EXPRESSION TAG	UNP P0A029
A	10	HIS	-	EXPRESSION TAG	UNP P0A029
A	11	MSE	-	EXPRESSION TAG	UNP P0A029
B	9	GLY	-	EXPRESSION TAG	UNP P0A029
B	10	HIS	-	EXPRESSION TAG	UNP P0A029
B	11	MSE	-	EXPRESSION TAG	UNP P0A029
C	9	GLY	-	EXPRESSION TAG	UNP P0A029
C	10	HIS	-	EXPRESSION TAG	UNP P0A029
C	11	MSE	-	EXPRESSION TAG	UNP P0A029
D	9	GLY	-	EXPRESSION TAG	UNP P0A029
D	10	HIS	-	EXPRESSION TAG	UNP P0A029
D	11	MSE	-	EXPRESSION TAG	UNP P0A029

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	29	Total 29	O 29	0	0
2	B	16	Total 16	O 16	0	0

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![Worldwide Protein Data Bank logo]

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	25	Total 25	O 25	0	0
2	D	7	Total 7	O 7	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 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, or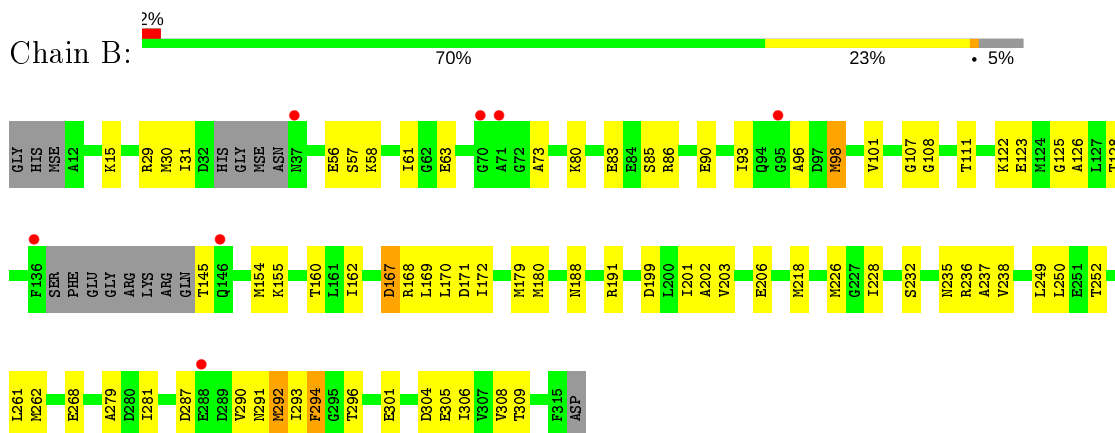ange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
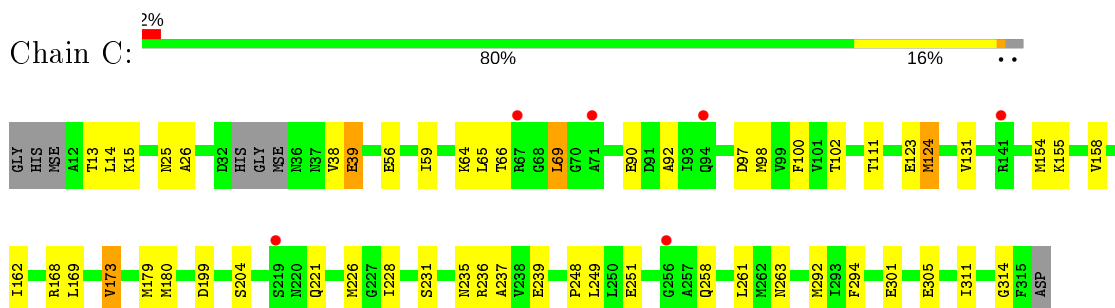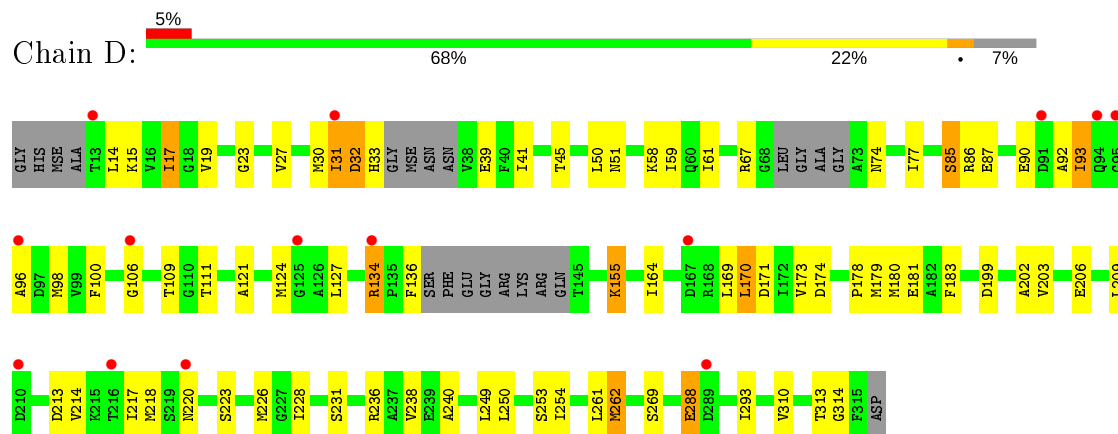
- Molecule 1: Cell division protein FtsZ
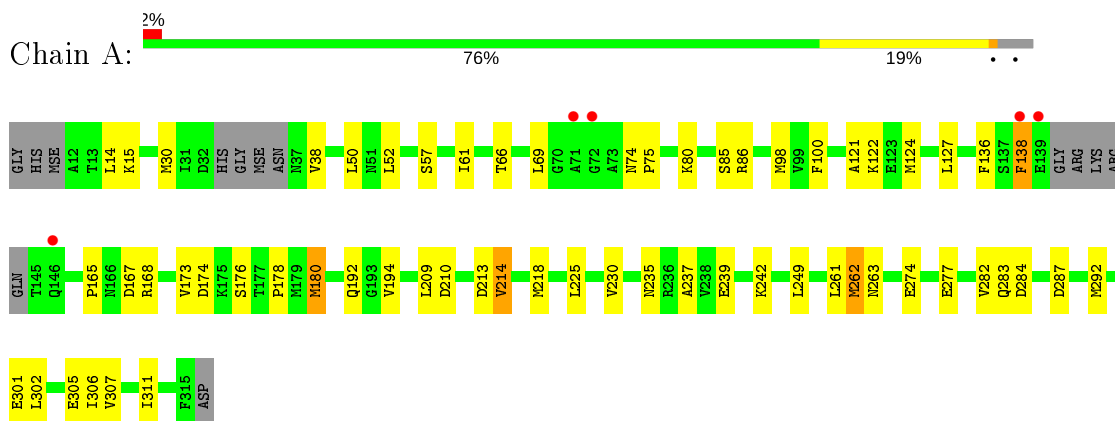
- Molecule 1: Cell division protein FtsZ

- Molecule 1: Cell division protein FtsZ

• Molecule 1: Cell division protein FtsZ

Chain D:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.69Å 79.99Å 225.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.76 – 2.71 31.76 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.8 (31.76-2.71) 96.0 (31.76-2.71)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.99 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.227 , 0.272 0.220 , 0.263	Depositor DCC
R_{free} test set	1688 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.3	EDS
L-test for twinning[2]	$<|L|> = 0.46$, $<L^2> = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8529	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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, 0.333 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	0.60	0/2121	0.62	0/2846
1	B	0.58	0/2094	0.63	0/2810
1	C	0.55	0/2174	0.62	0/2916
1	D	0.60	0/2070	0.61	0/2776
All	All	0.58	0/8459	0.62	0/11348

There are no bond length outliers.

There are no bond angle outliers.

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	2119	0	2141	39	0
1	B	2093	0	2121	40	0
1	C	2171	0	2198	29	0
1	D	2069	0	2094	44	0
2	A	29	0	0	2	0
2	B	16	0	0	2	0
2	C	25	0	0	0	0
2	D	7	0	0	0	0
All	All	8529	0	8554	150	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 9.

All (150) 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:D:93:ILE:HD11	1:D:124:MSE:HG3	1.58	0.86
1:C:90:GLU:HG2	1:C:124:MSE:HE1	1.59	0.84
1:B:98:MSE:SE	1:B:180:MSE:HG2	2.37	0.75
1:C:98:MSE:SE	1:C:180:MSE:HG2	2.37	0.74
1:D:15:LYS:HD2	1:D:96:ALA:HB2	1.73	0.71
1:B:261:LEU:HD23	1:B:293:ILE:HB	1.74	0.68
1:A:14:LEU:HD11	1:A:100:PHE:HD2	1.58	0.68
1:A:52:LEU:HD13	1:C:25:ASN:ND2	2.11	0.66
1:D:30:MSE:HE3	1:D:169:LEU:HG	1.77	0.66
1:D:262:MSE:HG3	1:D:310:VAL:HG22	1.77	0.66
1:B:86:ARG:NH1	1:B:90:GLU:OE2	2.29	0.65
1:B:287:ASP:HB2	1:B:290:VAL:HG23	1.78	0.64
1:D:203:VAL:HG11	1:D:249:LEU:HD23	1.79	0.64
1:C:292:MSE:HE2	1:C:294:PHE:CE1	2.35	0.62
1:A:98:MSE:HE2	1:A:127:LEU:HD23	1.83	0.61
1:D:32:ASP:O	1:D:33:HIS:ND1	2.33	0.61
1:A:138:PHE:H	1:A:213:ASP:HB2	1.64	0.60
1:B:294:PHE:C	1:B:294:PHE:CD2	2.75	0.60
1:D:261:LEU:HD23	1:D:293:ILE:HB	1.83	0.59
1:A:214:VAL:HG13	1:A:218:MSE:HE2	1.86	0.58
1:C:168:ARG:HH11	1:C:168:ARG:HA	1.69	0.57
1:C:98:MSE:HE3	1:C:180:MSE:HE3	1.86	0.57
1:C:90:GLU:CG	1:C:124:MSE:HE1	2.32	0.57
1:B:203:VAL:HG21	1:B:249:LEU:HD23	1.86	0.57
1:D:288:GLU:CD	1:D:288:GLU:H	2.08	0.56
1:A:30:MSE:HE3	1:A:173:VAL:HB	1.86	0.56
1:D:27:VAL:O	1:D:31:ILE:HG12	2.06	0.56
1:D:121:ALA:O	1:D:124:MSE:HB2	2.05	0.56
1:A:178:PRO:HB3	1:A:307:VAL:HG22	1.88	0.56
1:D:45:THR:OG1	1:D:109:THR:HG21	2.06	0.56
1:A:261:LEU:HB2	1:A:311:ILE:HB	1.89	0.55
1:D:61:ILE:HG22	1:D:85:SER:HB2	1.88	0.55
1:A:165:PRO:HG2	1:A:168:ARG:CG	2.37	0.55
1:C:38:VAL:HG21	1:C:173:VAL:HG22	1.88	0.55
1:C:258:GLN:HB2	1:C:314:GLY:HA3	1.89	0.54
1:B:30:MSE:HE2	1:B:169:LEU:HD11	1.90	0.54
1:B:279:ALA:HB2	1:B:294:PHE:CE1	2.42	0.54
1:C:226:MSE:HE3	1:C:228:ILE:HD11	1.90	0.53
1:A:225:LEU:HD22	1:A:249:LEU:HD23	1.90	0.53
1:B:30:MSE:HE2	1:B:169:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:LEU:HD11	1:D:249:LEU:HD22	1.90	0.52
1:B:101:VAL:HG12	1:B:154:MSE:HE1	1.92	0.52
1:D:30:MSE:HE3	1:D:169:LEU:CG	2.38	0.52
1:B:294:PHE:CZ	1:B:296:THR:OG1	2.62	0.51
1:D:50:LEU:HD11	1:D:59:ILE:O	2.10	0.51
1:D:136:PHE:HE2	1:D:217:ILE:HD11	1.75	0.51
1:C:102:THR:HB	1:C:131:VAL:HB	1.91	0.51
1:B:226:MSE:HE3	1:B:228:ILE:HD11	1.92	0.50
1:C:15:LYS:NZ	1:C:39:GLU:HG2	2.27	0.50
1:A:167:ASP:OD1	1:A:167:ASP:N	2.45	0.50
1:D:50:LEU:HD22	1:D:58:LYS:HB3	1.93	0.50
1:B:236:ARG:NH1	1:B:304:ASP:O	2.44	0.49
1:A:274:GLU:O	1:A:277:GLU:HB2	2.13	0.49
1:B:98:MSE:SE	1:B:180:MSE:HE3	2.62	0.49
1:B:15:LYS:HE2	1:B:96:ALA:HB2	1.94	0.48
1:D:32:ASP:OD1	1:D:32:ASP:N	2.46	0.48
1:D:218:MSE:HE3	1:D:223:SER:HB2	1.96	0.48
1:D:209:LEU:CD1	1:D:249:LEU:HD22	2.43	0.48
1:A:283:GLN:HA	1:A:292:MSE:HE1	1.94	0.48
1:B:237:ALA:HA	1:B:306:ILE:HD11	1.96	0.48
1:D:106:GLY:H	1:D:134:ARG:HE	1.62	0.48
1:B:29:ARG:NH1	2:B:415:HOH:O	2.35	0.48
1:C:26:ALA:HB1	1:C:169:LEU:HD21	1.95	0.48
1:D:74:ASN:O	1:D:77:ILE:HG22	2.13	0.48
1:B:292:MSE:HB2	1:B:292:MSE:HE2	1.73	0.47
1:C:14:LEU:HD11	1:C:100:PHE:CE2	2.48	0.47
1:A:14:LEU:HD11	1:A:100:PHE:CD2	2.43	0.47
1:A:176:SER:O	1:A:180:MSE:HE2	2.14	0.47
1:A:209:LEU:HD23	1:A:209:LEU:HA	1.80	0.47
1:B:167:ASP:OD1	1:B:167:ASP:N	2.45	0.47
1:C:155:LYS:NZ	1:C:199:ASP:HB2	2.29	0.47
1:D:179:MSE:HE3	1:D:183:PHE:CZ	2.49	0.47
1:D:19:VAL:N	1:D:23:GLY:HA3	2.29	0.47
1:A:287:ASP:N	1:A:287:ASP:OD1	2.47	0.46
1:D:164:ILE:HD11	1:D:169:LEU:HA	1.97	0.46
1:D:226:MSE:HE3	1:D:228:ILE:HD11	1.96	0.46
1:B:155:LYS:NZ	1:B:199:ASP:OD1	2.41	0.46
1:B:279:ALA:HB2	1:B:294:PHE:HE1	1.80	0.46
1:B:80:LYS:NZ	1:B:83:GLU:OE2	2.38	0.46
1:B:98:MSE:HB2	1:B:180:MSE:HE3	1.97	0.46
1:C:66:THR:O	1:C:69:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLN:HB2	1:A:194:VAL:HG23	1.98	0.45
1:B:122:LYS:O	1:B:125:GLY:N	2.41	0.45
1:B:238:VAL:HG13	1:B:281:ILE:HD11	1.98	0.45
1:D:178:PRO:O	1:D:181:GLU:HB2	2.17	0.45
1:D:231:SER:CB	1:D:240:ALA:HB2	2.47	0.45
1:A:301:GLU:HB2	1:D:51:ASN:HB3	1.97	0.45
1:A:237:ALA:HA	1:A:306:ILE:CD1	2.47	0.45
1:C:155:LYS:HZ3	1:C:199:ASP:HB2	1.81	0.45
1:D:30:MSE:HE2	1:D:173:VAL:HG23	1.99	0.45
1:B:61:ILE:HG22	1:B:85:SER:HB2	1.99	0.45
1:C:248:PRO:HA	1:C:251:GLU:OE2	2.17	0.45
1:D:155:LYS:HE3	1:D:199:ASP:OD1	2.16	0.45
1:A:262:MSE:HG3	1:A:282:VAL:HG11	1.99	0.44
1:C:162:ILE:HD11	1:C:204:SER:HB2	2.00	0.44
1:C:261:LEU:HB2	1:C:311:ILE:HB	1.99	0.44
1:A:74:ASN:HB2	1:A:75:PRO:HD2	2.00	0.44
1:A:86:ARG:NH1	2:A:401:HOH:O	2.39	0.44
1:B:188:ASN:OD1	1:B:191:ARG:NH1	2.51	0.44
1:B:206:GLU:N	1:B:206:GLU:OE1	2.48	0.44
1:C:56:GLU:CD	1:C:56:GLU:H	2.18	0.44
1:D:86:ARG:NH1	1:D:90:GLU:OE2	2.50	0.44
1:A:50:LEU:HD23	1:A:50:LEU:HA	1.83	0.43
1:A:61:ILE:HG22	1:A:85:SER:HB2	2.00	0.43
1:D:231:SER:HB3	1:D:240:ALA:HB2	1.99	0.43
1:A:263:ASN:HB2	2:A:418:HOH:O	2.17	0.43
1:C:154:MSE:O	1:C:158:VAL:HG22	2.18	0.43
1:C:235:ASN:O	1:C:239:GLU:HB2	2.18	0.43
1:B:162:ILE:HD12	1:B:202:ALA:O	2.18	0.43
1:D:313:THR:OG1	1:D:314:GLY:N	2.52	0.43
1:C:236:ARG:HG3	1:C:237:ALA:N	2.33	0.43
1:D:170:LEU:HA	1:D:170:LEU:HD12	1.79	0.43
1:A:165:PRO:HG2	1:A:168:ARG:HG2	2.00	0.43
1:A:210:ASP:HB3	1:A:213:ASP:OD2	2.19	0.43
1:B:262:MSE:HE2	1:B:308:VAL:HG13	2.00	0.43
1:B:30:MSE:HA	1:B:170:LEU:HD21	2.01	0.43
1:B:172:ILE:HG22	1:B:179:MSE:HE3	2.00	0.43
1:A:127:LEU:HA	1:A:127:LEU:HD12	1.84	0.42
1:B:168:ARG:NH1	1:B:171:ASP:OD2	2.52	0.42
1:B:126:ALA:O	1:B:128:THR:HG23	2.19	0.42
1:C:14:LEU:HD11	1:C:100:PHE:CD2	2.54	0.42
1:A:14:LEU:HD12	1:A:15:LYS:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:LEU:HD11	1:D:100:PHE:CE1	2.54	0.42
1:B:107:GLY:HA3	2:B:402:HOH:O	2.19	0.42
1:A:30:MSE:CE	1:A:173:VAL:HB	2.49	0.42
1:A:136:PHE:CZ	1:A:209:LEU:HD11	2.55	0.42
1:B:206:GLU:H	1:B:206:GLU:CD	2.22	0.41
1:C:59:ILE:HD11	1:C:92:ALA:CB	2.50	0.41
1:C:59:ILE:HD11	1:C:92:ALA:HB2	2.01	0.41
1:D:59:ILE:HD11	1:D:92:ALA:HB2	2.01	0.41
1:A:121:ALA:HA	1:A:124:MSE:HG3	2.03	0.41
1:D:98:MSE:HE1	1:D:180:MSE:HB3	2.02	0.41
1:B:58:LYS:HB2	1:B:58:LYS:HE2	1.92	0.41
1:D:17:ILE:HG23	1:D:41:ILE:HB	2.02	0.41
1:A:235:ASN:O	1:A:239:GLU:HG3	2.20	0.41
1:A:80:LYS:HA	1:A:80:LYS:HD3	1.83	0.41
1:B:73:ALA:HB1	1:B:108:GLY:HA2	2.03	0.41
1:D:218:MSE:CE	1:D:223:SER:HB2	2.51	0.41
1:A:237:ALA:HA	1:A:306:ILE:HD11	2.03	0.41
1:A:98:MSE:CE	1:A:180:MSE:HG3	2.51	0.41
1:B:232:SER:HB3	1:B:305:GLU:HG3	2.03	0.41
1:C:249:LEU:HD23	1:C:249:LEU:HA	1.79	0.40
1:D:98:MSE:HE2	1:D:127:LEU:HD23	2.03	0.40
1:A:230:VAL:HG22	1:A:307:VAL:HG13	2.02	0.40
1:D:202:ALA:HB2	1:D:226:MSE:HE2	2.03	0.40
1:A:165:PRO:HG2	1:A:168:ARG:HG3	2.03	0.40
1:B:201:ILE:HG12	1:B:218:MSE:SE	2.72	0.40
1:C:168:ARG:HD2	1:C:168:ARG:HA	1.94	0.40
1:D:171:ASP:HA	1:D:174:ASP:HB3	2.04	0.40
1:D:217:ILE:HG13	1:D:217:ILE:H	1.65	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	289/308 (94%)	280 (97%)	9 (3%)	0	100	100
1	B	286/308 (93%)	270 (94%)	15 (5%)	1 (0%)	41	66
1	C	297/308 (96%)	284 (96%)	13 (4%)	0	100	100
1	D	279/308 (91%)	254 (91%)	23 (8%)	2 (1%)	22	46
All	All	1151/1232 (93%)	1088 (94%)	60 (5%)	3 (0%)	41	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	206	GLU
1	B	291	ASN
1	D	220	ASN

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	223/220 (101%)	209 (94%)	14 (6%)	18	40
1	B	220/220 (100%)	201 (91%)	19 (9%)	10	24
1	C	228/220 (104%)	212 (93%)	16 (7%)	15	35
1	D	219/220 (100%)	197 (90%)	22 (10%)	7	18
All	All	890/880 (101%)	819 (92%)	71 (8%)	12	27

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	57	SER
1	A	66	THR
1	A	69	LEU
1	A	122	LYS
1	A	138	PHE
1	A	174	ASP
1	A	180	MSE

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Mol	Chain	Res	Type
1	A	214	VAL
1	A	242	LYS
1	A	262	MSE
1	A	284	ASP
1	A	302	LEU
1	A	305	GLU
1	B	31	ILE
1	B	56	GLU
1	B	57	SER
1	B	63	GLU
1	B	93	ILE
1	B	98	MSE
1	B	111	THR
1	B	123	GLU
1	B	145	THR
1	B	160	THR
1	B	167	ASP
1	B	235	ASN
1	B	250	LEU
1	B	252	THR
1	B	268	GLU
1	B	292	MSE
1	B	294	PHE
1	B	301	GLU
1	B	309	THR
1	C	13	THR
1	C	39	GLU
1	C	64	LYS
1	C	65	LEU
1	C	69	LEU
1	C	97	ASP
1	C	111	THR
1	C	123	GLU
1	C	124	MSE
1	C	173	VAL
1	C	179	MSE
1	C	221	GLN
1	C	231	SER
1	C	263	ASN
1	C	301	GLU
1	C	305	GLU
1	D	17	ILE

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Mol	Chain	Res	Type
1	D	31	ILE
1	D	32	ASP
1	D	39	GLU
1	D	67	ARG
1	D	85	SER
1	D	87	GLU
1	D	93	ILE
1	D	111	THR
1	D	134	ARG
1	D	155	LYS
1	D	170	LEU
1	D	213	ASP
1	D	214	VAL
1	D	236	ARG
1	D	238	VAL
1	D	250	LEU
1	D	253	SER
1	D	254	ILE
1	D	262	MSE
1	D	269	SER
1	D	288	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	195	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 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	284/308 (92%)	-0.06	5 (1%)	68	70	27, 39, 64, 74	0
1	B	281/308 (91%)	0.04	7 (2%)	57	59	29, 45, 63, 80	0
1	C	290/308 (94%)	0.09	6 (2%)	63	65	28, 45, 66, 74	0
1	D	276/308 (89%)	0.31	14 (5%)	28	26	33, 56, 71, 78	0
All	All	1131/1232 (91%)	0.09	32 (2%)	53	54	27, 46, 68, 80	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	219	SER	4.2
1	B	37	ASN	3.7
1	A	72	GLY	3.7
1	D	134	ARG	3.6
1	C	141	ARG	3.5
1	A	139	GLU	3.4
1	A	138	PHE	3.3
1	D	216	THR	3.2
1	C	94	GLN	3.1
1	B	70	GLY	3.0
1	B	288	GLU	3.0
1	D	106	GLY	2.9
1	B	146	GLN	2.9
1	D	220	ASN	2.8
1	D	94	GLN	2.7
1	D	91	ASP	2.6
1	D	31	ILE	2.6
1	D	13	THR	2.4
1	D	210	ASP	2.4
1	D	167	ASP	2.4
1	A	146	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	71	ALA	2.4
1	B	95	GLY	2.4
1	D	95	GLY	2.2
1	D	125	GLY	2.2
1	C	256	GLY	2.1
1	D	96	ALA	2.1
1	A	71	ALA	2.1
1	C	71	ALA	2.1
1	D	289	ASP	2.0
1	B	136	PHE	2.0
1	C	67	ARG	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.