Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:46 am BST

PDB ID	:	6DD8
Title	:	Structure of mouse SYCP3, P21 form
Authors	:	Rosenberg, S.C.; Munoz, I.C.; Uson, I.; Corbett, K.D.
Deposited on	:	2018-05-09
Resolution	:	2.60 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 ⓘ) were used in the production of this report:

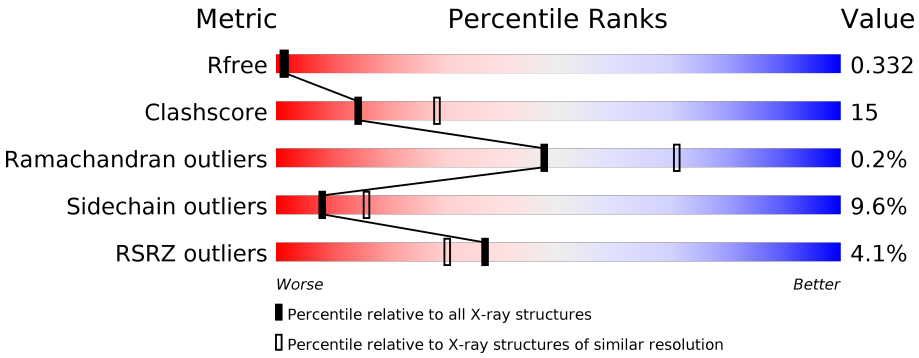
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	144	5% 60% 27% • 9%
1	B	144	3% 53% 30% • 15%
1	C	144	4% 52% 32% • 15%
1	D	144	% 49% 29% • 19%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4123 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 Synaptonemal complex protein 3.

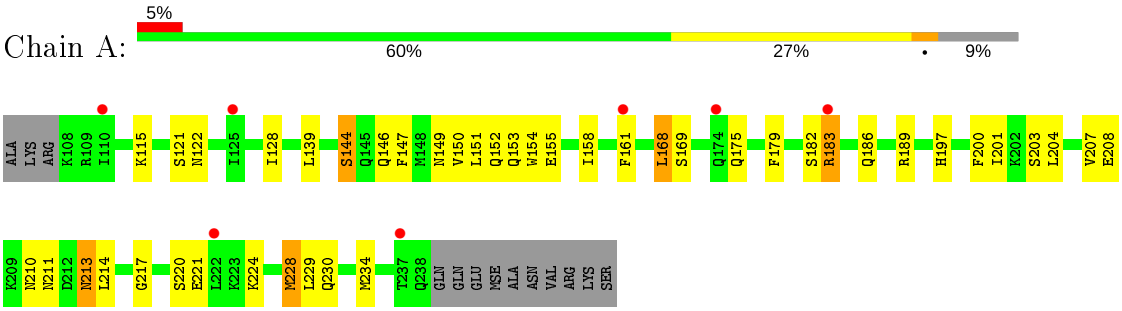
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	131	Total	C	N	O	Se	0	0	0
			1072	673	187	206	6			
1	B	123	Total	C	N	O	Se	0	0	0
			1017	640	179	193	5			
1	C	123	Total	C	N	O	Se	0	0	0
			1048	659	188	195	6			
1	D	117	Total	C	N	O	Se	0	0	0
			986	618	174	188	6			

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 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.

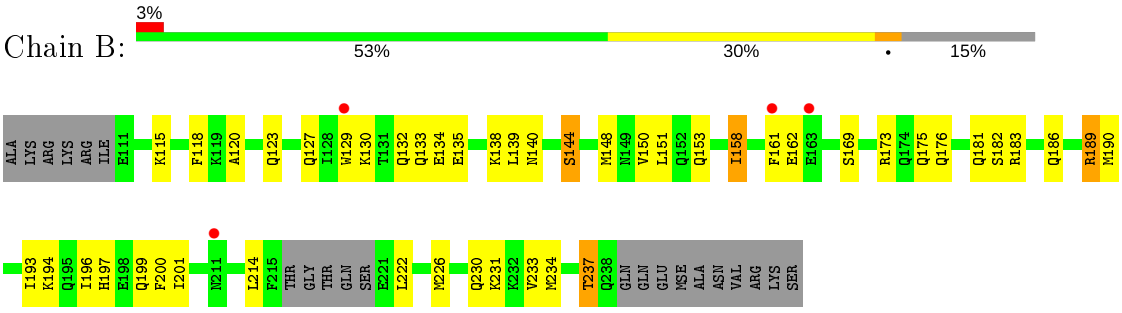
- Molecule 1: Synaptonemal complex protein 3

Chain A:



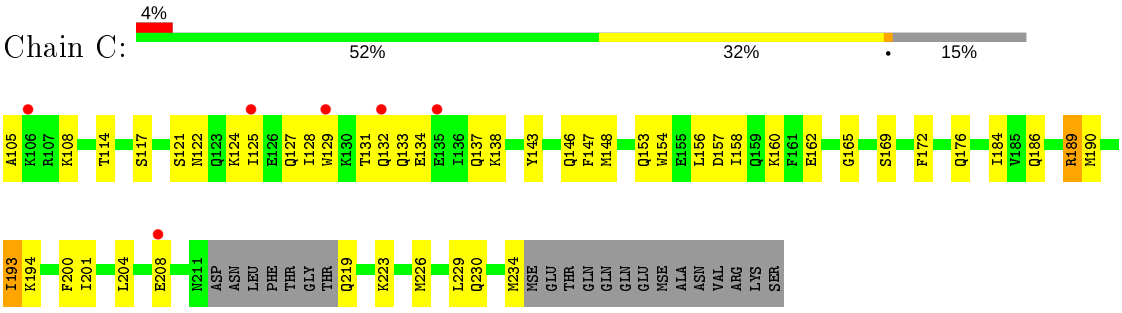
- Molecule 1: Synaptonemal complex protein 3

Chain B:



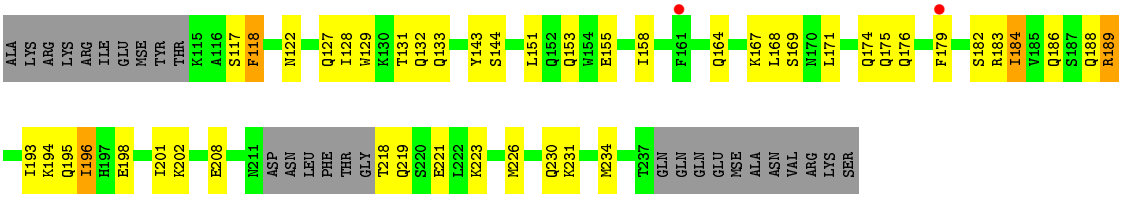
- Molecule 1: Synaptonemal complex protein 3

Chain C:



- Molecule 1: Synaptonemal complex protein 3

Chain D:


ALA LYS ARG LYS ARG ILE GLU MSE TYR THR K115 A116 S117 F118 N122 Q127 I128 W129 K130 T131 Q132 Q133 Y143 S144 L151 Q152 Q153 W154 E155 I158 F161 Q164 K167 L168 S169 N170 L171 Q174 Q175 Q176 F179 S182 R183 I184 V185 Q186 S187 Q188 R189
I193 K194 Q195 I196 H197 E198 I201 K202 E208 N211 ASP ASN LEU PHE THR GLY T218 Q219 S220 E221 L222 K223 M226 Q230 K231 M234 T237 GLN GLN GLN GLU MSE ALA ASN VAL ARG LYS SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	45.81Å 49.40Å 150.26Å 90.00° 90.80° 90.00°	Depositor
Resolution (Å)	46.92 – 2.60 46.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (46.92-2.60) 99.2 (46.93-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.254 , 0.323 0.262 , 0.332	Depositor DCC
R_{free} test set	1127 reflections (5.41%)	wwPDB-VP
Wilson B-factor (Å^2)	65.1	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 67.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4123	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.90% 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	0.45	0/1078	0.54	0/1430
1	B	0.42	0/1021	0.50	0/1349
1	C	0.45	0/1053	0.52	0/1385
1	D	0.50	0/990	0.55	0/1305
All	All	0.45	0/4142	0.53	0/5469

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

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	1072	0	1043	52	0
1	B	1017	0	1001	54	0
1	C	1048	0	1070	45	0
1	D	986	0	991	55	0
All	All	4123	0	4105	127	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 (127) 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:B:233:VAL:HG22	1:C:114:THR:HG22	1.55	0.87
1:C:201:ILE:HD11	1:D:144:SER:HB2	1.63	0.80
1:C:190:MSE:HE2	1:D:155:GLU:HB2	1.62	0.80
1:C:154:TRP:HE1	1:D:186:GLN:HE21	1.27	0.79
1:C:176:GLN:HE21	1:D:169:SER:HB2	1.51	0.76
1:C:121:SER:HA	1:C:124:LYS:HD2	1.76	0.68
1:A:175:GLN:HB3	1:D:168:LEU:HD21	1.75	0.68
1:A:183:ARG:NH2	1:B:158:ILE:O	2.22	0.67
1:B:237:THR:OG1	1:B:237:THR:O	2.13	0.65
1:C:137:GLN:NE2	1:D:208:GLU:OE2	2.30	0.63
1:A:149:ASN:O	1:A:152:GLN:HG2	1.98	0.62
1:A:150:VAL:HG11	1:D:193:ILE:HG13	1.81	0.62
1:D:127:GLN:O	1:D:131:THR:HG23	2.01	0.61
1:A:183:ARG:CZ	1:B:162:GLU:HB2	2.31	0.60
1:C:105:ALA:N	1:C:108:LYS:HZ2	2.01	0.58
1:C:122:ASN:ND2	1:D:223:LYS:HG2	2.18	0.58
1:A:175:GLN:HB3	1:D:168:LEU:CD2	2.33	0.57
1:C:129:TRP:O	1:C:132:GLN:HG3	2.03	0.57
1:A:183:ARG:HH21	1:B:161:PHE:HB3	1.68	0.57
1:B:153:GLN:HB3	1:C:189:ARG:NH1	2.20	0.56
1:A:183:ARG:NE	1:B:162:GLU:HB2	2.21	0.55
1:B:129:TRP:HB2	1:D:129:TRP:CH2	2.41	0.55
1:A:230:GLN:HE21	1:A:234:MSE:HE3	1.71	0.54
1:B:197:HIS:HD2	1:C:143:TYR:OH	1.90	0.54
1:A:221:GLU:HB3	1:D:128:ILE:HD13	1.89	0.54
1:B:186:GLN:NE2	1:D:186:GLN:HG2	2.23	0.54
1:B:169:SER:O	1:B:173:ARG:HD2	2.08	0.54
1:B:161:PHE:HB2	1:C:186:GLN:HE22	1.73	0.54
1:C:108:LYS:HD2	1:C:108:LYS:H	1.72	0.54
1:C:122:ASN:HD21	1:D:223:LYS:HG2	1.73	0.53
1:A:197:HIS:CE1	1:B:144:SER:HB2	2.44	0.53
1:C:134:GLU:O	1:C:138:LYS:HD3	2.09	0.53
1:B:132:GLN:HE22	1:D:133:GLN:HE21	1.55	0.53
1:B:132:GLN:OE1	1:D:133:GLN:NE2	2.42	0.53
1:A:182:SER:O	1:A:186:GLN:HG2	2.09	0.52
1:A:168:LEU:HD11	1:D:174:GLN:HB3	1.90	0.52
1:B:176:GLN:HG3	1:D:175:GLN:HE22	1.74	0.52
1:A:179:PHE:HD1	1:D:164:GLN:HB3	1.74	0.52
1:D:230:GLN:HG2	1:D:234:MSE:HE2	1.90	0.52
1:A:149:ASN:OD1	1:A:152:GLN:NE2	2.42	0.52
1:A:214:LEU:O	1:A:220:SER:OG	2.25	0.52
1:A:201:ILE:HD11	1:B:144:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:OD1	1:B:226:MSE:HG3	2.11	0.51
1:B:189:ARG:HG3	1:C:153:GLN:HE21	1.76	0.51
1:A:155:GLU:N	1:B:190:MSE:HE1	2.26	0.51
1:B:196:ILE:HD13	1:C:146:GLN:HB3	1.92	0.50
1:A:204:LEU:HD13	1:B:140:ASN:ND2	2.27	0.50
1:A:197:HIS:O	1:A:200:PHE:HB3	2.11	0.50
1:B:120:ALA:HA	1:B:123:GLN:OE1	2.12	0.49
1:C:190:MSE:HE1	1:D:151:LEU:HG	1.93	0.49
1:B:139:LEU:HD12	1:C:204:LEU:HD23	1.93	0.49
1:A:168:LEU:HD21	1:D:174:GLN:OE1	2.12	0.49
1:A:154:TRP:CD2	1:B:190:MSE:HE3	2.47	0.49
1:B:189:ARG:NH1	1:C:157:ASP:HB2	2.27	0.49
1:A:144:SER:OG	1:B:197:HIS:HE1	1.94	0.49
1:D:184:ILE:O	1:D:188:GLN:HG3	2.12	0.49
1:C:162:GLU:HA	1:D:179:PHE:HZ	1.78	0.49
1:A:151:LEU:HD23	1:B:194:LYS:HD2	1.95	0.49
1:B:150:VAL:HG11	1:C:193:ILE:HG22	1.95	0.48
1:A:161:PHE:HD1	1:B:183:ARG:HD3	1.78	0.48
1:C:127:GLN:O	1:C:131:THR:HG23	2.12	0.48
1:C:229:LEU:HG	1:D:118:PHE:HZ	1.78	0.48
1:A:155:GLU:HG3	1:B:190:MSE:SE	2.64	0.47
1:A:229:LEU:HD21	1:D:118:PHE:CE1	2.49	0.47
1:A:153:GLN:HB3	1:D:189:ARG:NH1	2.30	0.47
1:C:156:LEU:HB3	1:C:160:LYS:HZ2	1.80	0.47
1:B:175:GLN:OE1	1:D:175:GLN:HB3	2.15	0.46
1:B:190:MSE:HA	1:B:193:ILE:HG22	1.96	0.46
1:C:162:GLU:HG2	1:D:183:ARG:HD3	1.98	0.46
1:D:195:GLN:O	1:D:198:GLU:N	2.49	0.46
1:B:132:GLN:NE2	1:D:133:GLN:HE21	2.14	0.46
1:A:147:PHE:CE1	1:C:147:PHE:HE1	2.33	0.46
1:B:197:HIS:O	1:B:200:PHE:HB3	2.17	0.45
1:B:132:GLN:HG3	1:B:133:GLN:N	2.30	0.45
1:C:200:PHE:O	1:C:204:LEU:HG	2.16	0.45
1:A:144:SER:OG	1:B:197:HIS:CE1	2.69	0.45
1:C:122:ASN:OD1	1:D:226:MSE:HG3	2.17	0.45
1:D:189:ARG:HA	1:D:189:ARG:HD3	1.30	0.45
1:D:194:LYS:HB2	1:D:194:LYS:HE3	1.72	0.45
1:A:230:GLN:HG3	1:A:234:MSE:HE3	1.98	0.44
1:C:200:PHE:CZ	1:C:204:LEU:HD11	2.51	0.44
1:C:176:GLN:NE2	1:D:169:SER:HB2	2.27	0.44
1:C:162:GLU:HA	1:D:179:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LYS:HA	1:B:230:GLN:NE2	2.32	0.44
1:C:230:GLN:HB2	1:D:118:PHE:CE2	2.53	0.44
1:A:161:PHE:CD2	1:D:182:SER:HB2	2.53	0.44
1:A:168:LEU:HD23	1:A:168:LEU:HA	1.76	0.43
1:B:222:LEU:HD12	1:C:125:ILE:HG12	2.00	0.43
1:C:132:GLN:NE2	1:C:133:GLN:HG2	2.32	0.43
1:A:230:GLN:HE21	1:B:115:LYS:HG2	1.83	0.43
1:A:211:ASN:ND2	1:D:132:GLN:HE21	2.17	0.43
1:B:130:LYS:O	1:B:134:GLU:HG3	2.17	0.43
1:D:167:LYS:O	1:D:171:LEU:HG	2.19	0.43
1:A:197:HIS:HA	1:D:143:TYR:CE1	2.53	0.43
1:C:172:PHE:O	1:C:176:GLN:HB2	2.18	0.43
1:C:219:GLN:HG2	1:C:223:LYS:HE3	2.00	0.43
1:C:158:ILE:HD11	1:D:186:GLN:HB3	2.01	0.43
1:B:214:LEU:HD13	1:C:128:ILE:HG23	2.01	0.43
1:B:151:LEU:HD23	1:B:151:LEU:HA	1.83	0.42
1:A:128:ILE:HD13	1:A:128:ILE:HG21	1.78	0.42
1:D:176:GLN:O	1:D:179:PHE:HB3	2.19	0.42
1:D:218:THR:HA	1:D:221:GLU:HB2	2.01	0.42
1:A:213:ASN:O	1:A:217:GLY:N	2.52	0.42
1:A:153:GLN:HB3	1:D:189:ARG:HH12	1.85	0.42
1:A:201:ILE:HD11	1:B:144:SER:CB	2.50	0.42
1:D:151:LEU:HD12	1:D:151:LEU:HA	1.75	0.42
1:A:146:GLN:HB3	1:D:196:ILE:HD13	2.01	0.42
1:A:115:LYS:HA	1:B:230:GLN:HE21	1.85	0.42
1:A:154:TRP:HE1	1:A:158:ILE:HD11	1.85	0.41
1:A:189:ARG:NH1	1:D:153:GLN:OE1	2.53	0.41
1:B:132:GLN:NE2	1:B:133:GLN:OE1	2.53	0.41
1:C:230:GLN:HB2	1:D:118:PHE:CD2	2.55	0.41
1:A:234:MSE:HE1	1:B:115:LYS:HG2	2.02	0.41
1:C:165:GLY:HA3	1:D:179:PHE:CZ	2.55	0.41
1:B:132:GLN:HG3	1:B:133:GLN:H	1.86	0.41
1:A:161:PHE:CD1	1:B:183:ARG:HD3	2.55	0.41
1:B:129:TRP:HD1	1:D:129:TRP:CZ2	2.39	0.41
1:B:231:LYS:HA	1:B:234:MSE:HE2	2.02	0.41
1:A:154:TRP:HE1	1:B:186:GLN:NE2	2.19	0.41
1:B:175:GLN:HE22	1:D:176:GLN:HG3	1.85	0.41
1:C:226:MSE:HG3	1:D:122:ASN:OD1	2.21	0.41
1:C:147:PHE:HZ	1:D:193:ILE:HG23	1.85	0.41
1:B:190:MSE:O	1:B:193:ILE:HG22	2.21	0.40
1:C:132:GLN:HG3	1:C:133:GLN:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:TRP:O	1:A:158:ILE:HG12	2.21	0.40
1:A:197:HIS:HA	1:D:143:TYR:HE1	1.86	0.40
1:A:224:LYS:HG3	1:A:228:MSE:HE2	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	129/144 (90%)	126 (98%)	3 (2%)	0	100 100
1	B	119/144 (83%)	111 (93%)	8 (7%)	0	100 100
1	C	119/144 (83%)	113 (95%)	6 (5%)	0	100 100
1	D	113/144 (78%)	102 (90%)	10 (9%)	1 (1%)	17 35
All	All	480/576 (83%)	452 (94%)	27 (6%)	1 (0%)	47 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	196	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	115/128 (90%)	103 (90%)	12 (10%)	7 13
1	B	109/128 (85%)	96 (88%)	13 (12%)	5 9
1	C	116/128 (91%)	107 (92%)	9 (8%)	12 25
1	D	110/128 (86%)	101 (92%)	9 (8%)	11 22
All	All	450/512 (88%)	407 (90%)	43 (10%)	8 16

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	139	LEU
1	A	144	SER
1	A	168	LEU
1	A	169	SER
1	A	183	ARG
1	A	203	SER
1	A	207	VAL
1	A	208	GLU
1	A	210	ASN
1	A	213	ASN
1	A	228	MSE
1	B	118	PHE
1	B	127	GLN
1	B	135	GLU
1	B	138	LYS
1	B	144	SER
1	B	148	MSE
1	B	158	ILE
1	B	181	GLN
1	B	182	SER
1	B	189	ARG
1	B	199	GLN
1	B	201	ILE
1	B	237	THR
1	C	117	SER
1	C	148	MSE
1	C	169	SER
1	C	184	ILE
1	C	189	ARG
1	C	193	ILE
1	C	194	LYS
1	C	208	GLU

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Mol	Chain	Res	Type
1	C	234	MSE
1	D	117	SER
1	D	118	PHE
1	D	158	ILE
1	D	184	ILE
1	D	189	ARG
1	D	201	ILE
1	D	202	LYS
1	D	219	GLN
1	D	231	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	137	GLN
1	A	149	ASN
1	A	152	GLN
1	A	175	GLN
1	A	211	ASN
1	A	230	GLN
1	B	127	GLN
1	B	132	GLN
1	B	133	GLN
1	B	186	GLN
1	B	197	HIS
1	B	230	GLN
1	C	153	GLN
1	C	186	GLN
1	C	211	ASN
1	D	133	GLN
1	D	152	GLN
1	D	175	GLN
1	D	176	GLN
1	D	186	GLN

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	124/144 (86%)	0.36	7 (5%)	24	19	60, 83, 108, 129	0
1	B	116/144 (80%)	0.47	4 (3%)	45	38	61, 91, 118, 138	0
1	C	117/144 (81%)	0.37	6 (5%)	28	22	61, 92, 121, 132	0
1	D	111/144 (77%)	0.30	2 (1%)	68	64	55, 84, 104, 123	0
All	All	468/576 (81%)	0.38	19 (4%)	37	30	55, 87, 114, 138	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	ARG	4.1
1	D	179	PHE	3.4
1	A	237	THR	3.3
1	C	106	LYS	3.2
1	C	125	ILE	3.1
1	D	161	PHE	3.0
1	B	161	PHE	2.8
1	C	208	GLU	2.7
1	B	163	GLU	2.7
1	A	222	LEU	2.6
1	C	132	GLN	2.5
1	C	135	GLU	2.4
1	A	161	PHE	2.4
1	B	211	ASN	2.3
1	A	110	ILE	2.3
1	C	129	TRP	2.2
1	B	129	TRP	2.1
1	A	174	GLN	2.1
1	A	125	ILE	2.0

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

There are no such residues in this entry.