Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 06:26 AM EST

PDB ID	:	1YKE
Title	:	Structure of the mediator MED7/MED21 subcomplex
Authors	:	Baumli, S.; Hoeppner, S.; Cramer, P.
Deposited on	:	2005-01-18
Resolution	:	3.30 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

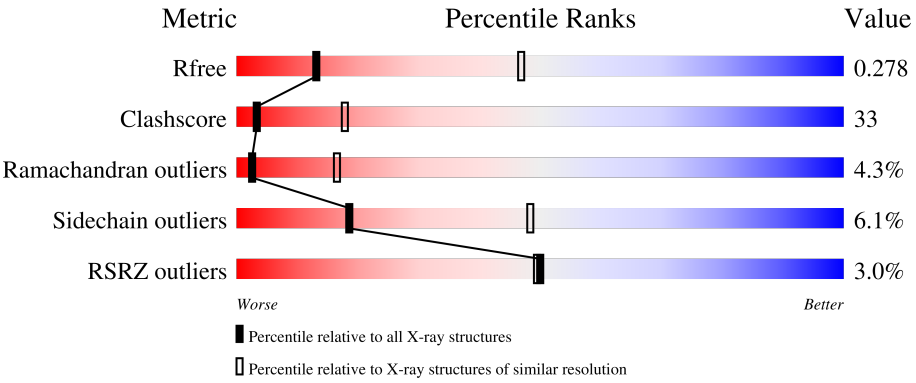
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	108	3% 31% 55% 6% 9%
1	C	108	2% 35% 47% 8% 9%
2	B	151	3% 40% 35% • 21%
2	D	151	3% 33% 36% 6% 25%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3548 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 RNA polymerase II mediator complex protein MED7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			832	527	146	156	3			
1	C	98	Total	C	N	O	S	0	0	0
			832	527	146	156	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	MET	-	cloning artifact	UNP Q08278
A	99	ALA	-	cloning artifact	UNP Q08278
A	100	SER	-	cloning artifact	UNP Q08278
A	101	MET	-	cloning artifact	UNP Q08278
C	98	MET	-	cloning artifact	UNP Q08278
C	99	ALA	-	cloning artifact	UNP Q08278
C	100	SER	-	cloning artifact	UNP Q08278
C	101	MET	-	cloning artifact	UNP Q08278

- Molecule 2 is a protein called RNA polymerase II holoenzyme component SRB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	119	Total	C	N	O	S	0	0	0
			965	608	160	193	4			
2	D	113	Total	C	N	O	S	0	0	0
			919	580	151	184	4			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	141	ALA	-	expression tag	UNP P47822
B	142	ALA	-	expression tag	UNP P47822
B	143	ALA	-	expression tag	UNP P47822
B	144	LEU	-	expression tag	UNP P47822

Continued on next page...

Continued from previous page...

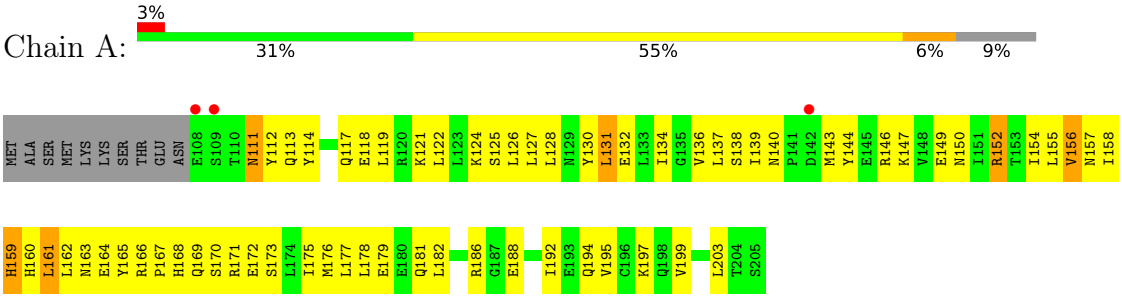
Chain	Residue	Modelled	Actual	Comment	Reference
B	145	GLU	-	expression tag	UNP P47822
B	146	HIS	-	expression tag	UNP P47822
B	147	HIS	-	expression tag	UNP P47822
B	148	HIS	-	expression tag	UNP P47822
B	149	HIS	-	expression tag	UNP P47822
B	150	HIS	-	expression tag	UNP P47822
B	151	HIS	-	expression tag	UNP P47822
D	141	ALA	-	expression tag	UNP P47822
D	142	ALA	-	expression tag	UNP P47822
D	143	ALA	-	expression tag	UNP P47822
D	144	LEU	-	expression tag	UNP P47822
D	145	GLU	-	expression tag	UNP P47822
D	146	HIS	-	expression tag	UNP P47822
D	147	HIS	-	expression tag	UNP P47822
D	148	HIS	-	expression tag	UNP P47822
D	149	HIS	-	expression tag	UNP P47822
D	150	HIS	-	expression tag	UNP P47822
D	151	HIS	-	expression tag	UNP P47822

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.

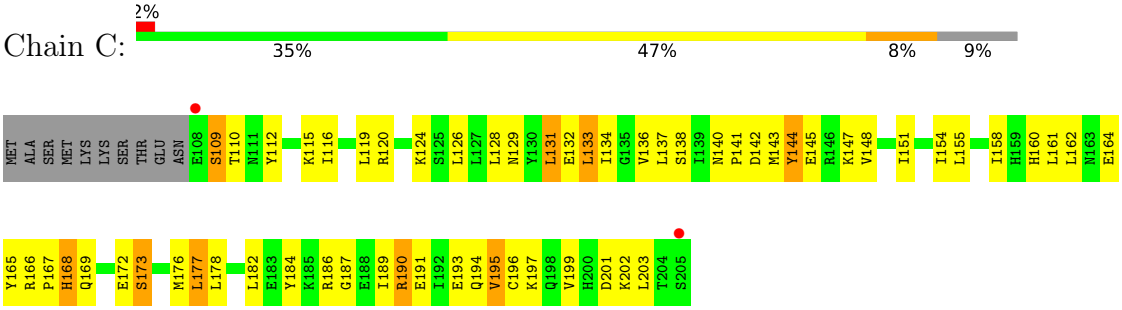
• Molecule 1: RNA polymerase II mediator complex protein MED7

Chain A:



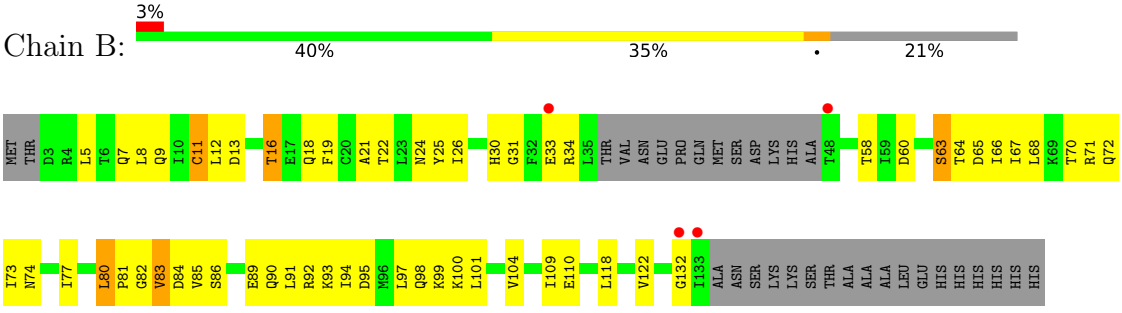
• Molecule 1: RNA polymerase II mediator complex protein MED7

Chain C:



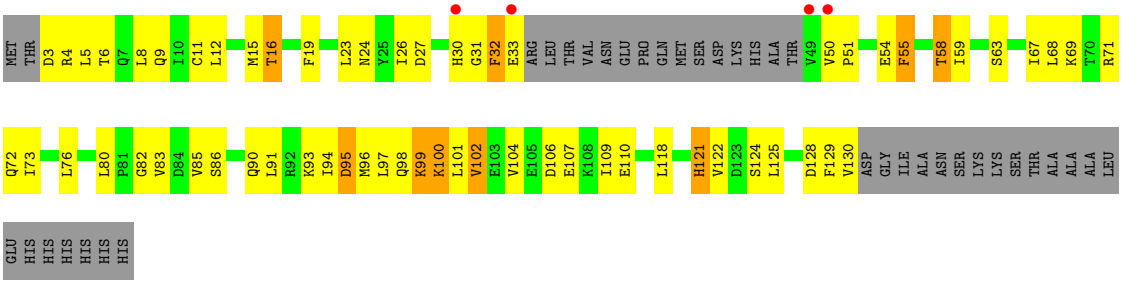
• Molecule 2: RNA polymerase II holoenzyme component SRB7

Chain B:



• Molecule 2: RNA polymerase II holoenzyme component SRB7

Chain D:


MET THR D3 R4 L5 T6 Q7 L8 Q9 I10 C11 L12 M15 T16 F19 L23 N24 Y25 I26 D27 H30 G31 F32 E33 ARG LEU THR VAL ASN GLU PRO GLN MET SER ASP LYS HIS ALA THR V49 V50 P51 E54 F55 T58 I59 S63 I67 L68 K69 T70 R71
Q72 I73 L76 L80 P81 G82 V83 D84 V85 S86 Q90 L91 R92 K93 I94 D95 M96 L97 Q98 K99 K100 L101 V102 E103 V104 E105 D106 E107 K108 I109 E110 L118 H121 V122 D123 S124 L125 D128 F129 V130 ASP GLY ILE ALA ASN SER LYS LYS SER THR ALA ALA ALA LEU
GLU HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	121.46Å 128.86Å 170.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 19.81 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-3.30) 99.8 (19.81-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 3.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.279 , 0.314 0.250 , 0.278	Depositor DCC
R_{free} test set	982 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	104.0	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 38.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3548	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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	0.47	0/843	0.66	0/1132
1	C	0.46	0/843	0.64	0/1132
2	B	0.46	0/973	0.64	0/1308
2	D	0.47	0/927	0.66	0/1246
All	All	0.47	0/3586	0.65	0/4818

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	832	0	858	91	1
1	C	832	0	858	76	0
2	B	965	0	987	67	0
2	D	919	0	938	66	0
All	All	3548	0	3641	236	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 33.

All (236) 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:124:LYS:HD2	1:C:128:LEU:HD11	1.36	1.07
1:A:139:ILE:HD13	1:A:147:LYS:HE3	1.39	1.00
1:A:130:TYR:CE2	1:A:134:ILE:HD11	1.99	0.98
1:C:155:LEU:HD13	2:D:16:THR:HG22	1.46	0.97
1:A:132:GLU:HB3	1:A:139:ILE:HD12	1.49	0.92
1:A:132:GLU:CD	1:A:139:ILE:HD11	1.92	0.90
1:A:134:ILE:HD13	2:B:63:SER:HB2	1.54	0.90
1:A:126:LEU:HB2	1:A:154:ILE:HG21	1.56	0.88
1:A:150:ASN:O	1:A:154:ILE:HG12	1.76	0.86
1:A:175:ILE:O	1:A:179:GLU:HG3	1.77	0.85
1:C:172:GLU:O	1:C:176:MET:HG3	1.77	0.85
1:C:166:ARG:HH21	2:D:9:GLN:HE22	1.21	0.84
2:D:95:ASP:C	2:D:97:LEU:H	1.81	0.82
1:A:139:ILE:CD1	1:A:147:LYS:HE3	2.10	0.81
2:D:6:THR:HA	2:D:9:GLN:HE21	1.44	0.80
2:B:94:ILE:HG13	2:B:95:ASP:N	1.96	0.79
1:A:137:LEU:HD13	1:C:124:LYS:HG3	1.64	0.79
1:C:133:LEU:HD21	2:D:23:LEU:HD21	1.65	0.79
1:C:166:ARG:NH2	2:D:9:GLN:HE22	1.81	0.78
1:C:182:LEU:HD21	1:C:186:ARG:CZ	2.13	0.78
1:A:155:LEU:HD13	2:B:16:THR:HG23	1.63	0.78
1:A:160:HIS:O	1:A:164:GLU:HG3	1.82	0.78
2:B:97:LEU:O	2:B:101:LEU:HB2	1.84	0.77
2:B:83:VAL:HG23	2:B:84:ASP:H	1.48	0.77
1:C:116:ILE:HG13	2:D:83:VAL:HG23	1.66	0.77
1:A:168:HIS:HE1	2:B:82:GLY:O	1.68	0.76
2:D:95:ASP:O	2:D:97:LEU:N	2.20	0.75
1:C:160:HIS:O	1:C:164:GLU:HG3	1.87	0.74
1:A:186:ARG:HH22	2:B:100:LYS:HE3	1.53	0.74
2:B:80:LEU:HD23	2:B:81:PRO:HD2	1.69	0.74
2:D:69:LYS:O	2:D:73:ILE:HG12	1.89	0.72
1:A:134:ILE:CD1	2:B:63:SER:HB2	2.20	0.72
1:C:133:LEU:HD21	2:D:23:LEU:CD2	2.20	0.71
2:D:90:GLN:O	2:D:93:LYS:HB3	1.91	0.71
1:A:182:LEU:HB2	2:B:101:LEU:HD13	1.73	0.71
1:C:172:GLU:HG2	2:D:90:GLN:NE2	2.07	0.70
1:A:132:GLU:OE2	1:A:139:ILE:HD11	1.91	0.70
1:A:130:TYR:CE2	1:A:134:ILE:CD1	2.74	0.70
2:B:68:LEU:O	2:B:72:GLN:HG3	1.92	0.68
1:C:136:VAL:HG12	1:C:137:LEU:HG	1.76	0.68
1:A:130:TYR:CZ	1:A:134:ILE:HD11	2.28	0.68
2:B:60:ASP:O	2:B:64:THR:HG22	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:SER:O	2:B:90:GLN:HG3	1.95	0.67
2:D:63:SER:O	2:D:67:ILE:HG13	1.95	0.66
2:D:6:THR:HA	2:D:9:GLN:NE2	2.11	0.65
1:A:165:TYR:HE2	2:B:80:LEU:HD21	1.60	0.65
1:A:156:VAL:HG12	1:A:157:ASN:N	2.11	0.65
2:D:99:LYS:O	2:D:101:LEU:N	2.31	0.64
1:A:172:GLU:O	1:A:176:MET:HG3	1.98	0.63
1:A:175:ILE:HG13	2:B:94:ILE:HG22	1.80	0.63
2:B:83:VAL:HG23	2:B:84:ASP:N	2.13	0.63
1:A:158:ILE:HG21	2:B:12:LEU:HD11	1.81	0.63
2:D:3:ASP:HA	2:D:6:THR:HB	1.80	0.63
1:A:175:ILE:CG1	2:B:94:ILE:HG22	2.29	0.63
2:B:73:ILE:O	2:B:77:ILE:HG13	1.98	0.63
1:C:194:GLN:O	1:C:197:LYS:N	2.32	0.62
1:C:162:LEU:HD11	2:D:8:LEU:HD23	1.81	0.61
1:A:132:GLU:HB3	1:A:139:ILE:CD1	2.25	0.61
2:B:70:THR:O	2:B:73:ILE:HG22	2.01	0.61
2:B:25:TYR:CZ	2:B:58:THR:HG21	2.36	0.60
2:D:19:PHE:O	2:D:23:LEU:HG	2.01	0.60
1:C:166:ARG:NH2	2:D:9:GLN:NE2	2.49	0.60
2:D:26:ILE:HG22	2:D:26:ILE:O	2.02	0.60
1:A:158:ILE:HG21	2:B:12:LEU:CD1	2.32	0.60
1:C:155:LEU:HD22	2:D:16:THR:HG23	1.83	0.60
1:C:182:LEU:HD21	1:C:186:ARG:NH1	2.17	0.59
1:C:169:GLN:O	1:C:173:SER:HB2	2.01	0.59
2:B:74:ASN:O	2:B:77:ILE:N	2.36	0.59
2:B:100:LYS:O	2:B:104:VAL:HG23	2.03	0.58
1:A:169:GLN:HG2	2:B:5:LEU:HB3	1.84	0.58
1:C:166:ARG:NH2	2:D:6:THR:OG1	2.30	0.58
1:A:159:HIS:O	1:A:163:ASN:HB2	2.04	0.58
1:A:165:TYR:CE2	2:B:80:LEU:HD21	2.39	0.57
1:A:171:ARG:HD2	2:B:90:GLN:OE1	2.03	0.57
2:D:94:ILE:O	2:D:98:GLN:HG3	2.04	0.57
1:C:155:LEU:HD13	2:D:16:THR:CG2	2.29	0.57
1:A:195:VAL:O	1:A:199:VAL:HG23	2.04	0.57
1:C:162:LEU:HD11	2:D:8:LEU:CD2	2.35	0.56
2:D:32:PHE:CE1	2:D:33:GLU:HG3	2.41	0.56
1:A:132:GLU:CB	1:A:139:ILE:HD12	2.30	0.56
2:B:94:ILE:CG1	2:B:95:ASP:N	2.69	0.56
1:A:134:ILE:HG22	2:D:71:ARG:HH22	1.71	0.56
1:C:132:GLU:OE1	1:C:147:LYS:HE3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:HIS:CE1	2:B:82:GLY:O	2.55	0.55
1:A:128:LEU:O	1:A:131:LEU:N	2.40	0.55
2:B:91:LEU:O	2:B:94:ILE:HG12	2.07	0.55
1:A:182:LEU:HD11	2:B:104:VAL:HG21	1.87	0.55
2:D:99:LYS:O	2:D:100:LYS:C	2.45	0.55
1:C:166:ARG:HB2	1:C:167:PRO:HD3	1.89	0.55
1:A:199:VAL:O	1:A:203:LEU:HB2	2.07	0.55
1:A:134:ILE:O	2:D:71:ARG:NH2	2.41	0.54
1:A:172:GLU:OE2	2:B:90:GLN:NE2	2.33	0.54
2:D:121:HIS:O	2:D:124:SER:HB3	2.07	0.54
1:C:110:THR:HG22	1:C:110:THR:O	2.07	0.54
2:D:68:LEU:O	2:D:72:GLN:HG3	2.07	0.53
1:A:127:LEU:HG	1:A:131:LEU:HD23	1.91	0.53
2:B:19:PHE:CE1	2:B:66:ILE:HD13	2.44	0.53
1:C:131:LEU:HG	1:C:136:VAL:HG11	1.90	0.53
2:D:50:VAL:HG13	2:D:51:PRO:HD2	1.89	0.53
1:C:132:GLU:C	1:C:134:ILE:H	2.11	0.53
1:C:140:ASN:ND2	1:C:142:ASP:OD1	2.42	0.53
1:A:143:MET:O	1:A:146:ARG:N	2.42	0.53
1:A:127:LEU:HG	1:A:131:LEU:CD2	2.39	0.53
2:D:128:ASP:C	2:D:130:VAL:H	2.11	0.52
1:A:146:ARG:NH1	1:A:149:GLU:OE1	2.42	0.52
1:A:137:LEU:CD1	1:C:124:LYS:HG3	2.36	0.52
1:A:162:LEU:HD23	2:B:9:GLN:HG2	1.90	0.52
2:B:33:GLU:O	2:B:33:GLU:HG3	2.08	0.52
1:C:182:LEU:HD21	1:C:186:ARG:NE	2.24	0.52
1:C:168:HIS:CE1	2:D:82:GLY:O	2.63	0.51
1:A:124:LYS:HB2	1:C:137:LEU:HD13	1.92	0.51
1:A:128:LEU:HD13	1:C:124:LYS:HE2	1.93	0.51
1:C:110:THR:HG22	1:C:112:TYR:CE1	2.46	0.51
2:B:85:VAL:HG12	2:B:86:SER:O	2.11	0.51
2:B:118:LEU:O	2:B:122:VAL:HG23	2.10	0.50
1:C:136:VAL:HG12	1:C:137:LEU:N	2.27	0.50
1:C:195:VAL:O	1:C:199:VAL:HG23	2.12	0.50
2:B:63:SER:O	2:B:67:ILE:HG13	2.13	0.49
1:C:165:TYR:CE2	2:D:80:LEU:HD13	2.47	0.49
2:D:91:LEU:C	2:D:93:LYS:H	2.16	0.49
2:D:102:VAL:O	2:D:106:ASP:HB2	2.13	0.49
1:A:138:SER:O	1:A:139:ILE:HG13	2.13	0.49
1:C:148:VAL:HG13	2:D:23:LEU:HD13	1.95	0.48
2:D:32:PHE:CG	2:D:33:GLU:N	2.81	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:SER:HB3	1:C:120:ARG:HG2	1.94	0.48
2:B:71:ARG:NH2	1:C:134:ILE:O	2.47	0.48
1:C:184:TYR:O	1:C:187:GLY:N	2.45	0.48
1:A:121:LYS:O	1:A:122:LEU:C	2.53	0.47
1:A:165:TYR:HE2	2:B:80:LEU:CD2	2.27	0.47
1:A:169:GLN:HE21	2:B:5:LEU:H	1.62	0.47
1:A:132:GLU:CD	1:A:139:ILE:CD1	2.75	0.47
1:C:133:LEU:CD2	2:D:23:LEU:HD21	2.42	0.47
1:A:114:TYR:O	1:A:117:GLN:HB2	2.14	0.47
1:A:166:ARG:HA	1:A:169:GLN:HB3	1.97	0.47
1:A:114:TYR:O	1:A:117:GLN:N	2.46	0.47
1:A:166:ARG:HG3	2:B:5:LEU:HD23	1.97	0.47
1:C:194:GLN:O	1:C:195:VAL:C	2.53	0.47
1:C:168:HIS:HE1	2:D:82:GLY:O	1.98	0.47
1:A:188:GLU:O	1:A:192:ILE:HG13	2.15	0.47
2:D:109:ILE:O	2:D:110:GLU:C	2.52	0.47
1:C:178:LEU:HB2	2:D:97:LEU:HD13	1.97	0.46
2:B:7:GLN:O	2:B:11:CYS:HB2	2.16	0.46
1:C:172:GLU:HG2	2:D:90:GLN:HE22	1.78	0.46
1:A:127:LEU:CD2	1:C:137:LEU:HD21	2.46	0.46
2:B:64:THR:HG23	2:B:65:ASP:N	2.31	0.46
2:B:94:ILE:HG13	2:B:95:ASP:H	1.76	0.46
1:A:177:LEU:O	1:A:181:GLN:HG2	2.15	0.46
1:C:133:LEU:CD2	1:C:151:ILE:HD12	2.46	0.46
1:A:166:ARG:O	1:A:169:GLN:HB3	2.16	0.46
2:B:12:LEU:HD23	2:B:12:LEU:O	2.16	0.46
1:A:161:LEU:O	1:A:162:LEU:C	2.53	0.46
1:A:162:LEU:HD23	2:B:9:GLN:CG	2.46	0.46
1:C:201:ASP:O	1:C:203:LEU:N	2.49	0.46
2:D:15:MET:CE	2:D:73:ILE:HG13	2.47	0.46
1:A:118:GLU:O	1:A:121:LYS:N	2.48	0.45
1:C:182:LEU:HD23	1:C:182:LEU:C	2.37	0.45
1:A:134:ILE:HG22	2:D:71:ARG:NH2	2.32	0.45
1:A:127:LEU:O	1:A:131:LEU:HD23	2.17	0.45
1:C:131:LEU:HD12	1:C:131:LEU:HA	1.78	0.45
2:D:100:LYS:O	2:D:104:VAL:HG23	2.16	0.45
1:A:112:TYR:HD2	1:A:165:TYR:HD1	1.65	0.45
2:D:32:PHE:H	2:D:32:PHE:HD2	1.65	0.45
1:C:154:ILE:O	1:C:155:LEU:C	2.55	0.45
1:A:111:ASN:OD1	1:A:113:GLN:HG2	2.17	0.44
1:A:162:LEU:HG	2:B:8:LEU:HD23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:LEU:HD13	2:D:76:LEU:HB2	1.99	0.44
1:A:166:ARG:O	1:A:169:GLN:N	2.50	0.44
1:C:133:LEU:HD23	1:C:151:ILE:CD1	2.48	0.44
1:C:158:ILE:CG2	2:D:12:LEU:HD21	2.47	0.44
2:B:30:HIS:O	2:B:33:GLU:N	2.50	0.44
2:D:24:ASN:C	2:D:26:ILE:H	2.20	0.44
1:C:187:GLY:O	1:C:190:ARG:HG2	2.17	0.44
2:B:18:GLN:HA	2:B:21:ALA:HB3	1.99	0.43
1:C:165:TYR:CD2	2:D:5:LEU:HD13	2.53	0.43
1:C:177:LEU:HA	1:C:177:LEU:HD23	1.85	0.43
2:B:95:ASP:O	2:B:98:GLN:HB2	2.18	0.43
1:C:133:LEU:HG	1:C:133:LEU:O	2.19	0.43
2:D:99:LYS:O	2:D:102:VAL:N	2.51	0.43
1:A:126:LEU:HD11	2:B:19:PHE:CE2	2.53	0.43
1:C:134:ILE:HD13	1:C:134:ILE:HA	1.88	0.43
2:D:128:ASP:O	2:D:130:VAL:N	2.44	0.43
2:B:99:LYS:C	2:B:101:LEU:N	2.72	0.43
1:C:158:ILE:HG22	2:D:12:LEU:CD2	2.49	0.43
2:D:55:PHE:O	2:D:58:THR:N	2.52	0.43
1:A:166:ARG:O	1:A:167:PRO:C	2.57	0.43
1:C:115:LYS:HD3	1:C:164:GLU:HB2	2.01	0.43
1:C:190:ARG:HA	1:C:193:GLU:HG3	2.01	0.43
1:C:194:GLN:O	1:C:196:CYS:N	2.52	0.43
2:D:51:PRO:HG2	2:D:54:GLU:HB3	2.01	0.43
2:D:24:ASN:C	2:D:26:ILE:N	2.72	0.42
1:C:129:ASN:OD1	1:C:147:LYS:HD3	2.19	0.42
2:D:118:LEU:O	2:D:122:VAL:HG23	2.19	0.42
2:B:85:VAL:HG13	2:B:89:GLU:HB3	2.00	0.42
2:D:99:LYS:C	2:D:101:LEU:N	2.71	0.42
1:C:126:LEU:HB2	1:C:154:ILE:HG21	2.02	0.42
1:C:166:ARG:HD3	1:C:166:ARG:HA	1.80	0.42
1:A:144:TYR:OH	2:B:26:ILE:CG2	2.68	0.42
1:A:178:LEU:HB2	2:B:97:LEU:HD13	2.00	0.42
2:B:22:THR:O	2:B:24:ASN:N	2.53	0.42
2:B:92:ARG:O	2:B:95:ASP:N	2.53	0.42
1:A:146:ARG:HD2	1:A:149:GLU:OE1	2.20	0.42
1:A:147:LYS:HA	1:A:147:LYS:HD3	1.62	0.42
1:C:189:ILE:O	1:C:191:GLU:N	2.53	0.42
1:C:166:ARG:O	1:C:167:PRO:C	2.58	0.42
1:A:113:GLN:OE1	2:B:83:VAL:O	2.38	0.41
2:D:12:LEU:HD12	2:D:12:LEU:HA	1.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:O	1:A:186:ARG:HG3	2.20	0.41
1:C:144:TYR:O	1:C:148:VAL:HG23	2.20	0.41
1:C:182:LEU:HD21	1:C:186:ARG:CD	2.49	0.41
2:B:92:ARG:O	2:B:93:LYS:C	2.58	0.41
2:D:59:ILE:HD13	2:D:59:ILE:HA	1.94	0.41
2:B:22:THR:C	2:B:24:ASN:N	2.74	0.41
2:B:92:ARG:HG3	2:B:93:LYS:N	2.35	0.41
1:C:112:TYR:CD1	1:C:168:HIS:CD2	3.09	0.41
1:C:147:LYS:O	1:C:151:ILE:HG13	2.20	0.41
2:D:122:VAL:O	2:D:125:LEU:N	2.54	0.41
1:A:124:LYS:CG	1:A:125:SER:N	2.83	0.41
1:A:136:VAL:HA	2:D:71:ARG:HB2	2.03	0.41
2:D:85:VAL:HG12	2:D:86:SER:N	2.36	0.41
2:B:31:GLY:HA2	2:B:34:ARG:HG2	2.02	0.41
2:B:83:VAL:CG2	2:B:84:ASP:H	2.26	0.41
1:A:146:ARG:O	1:A:149:GLU:HB3	2.20	0.41
2:B:109:ILE:HG22	2:B:110:GLU:N	2.35	0.41
1:A:144:TYR:OH	2:B:26:ILE:HG22	2.21	0.40
1:A:146:ARG:HD3	1:A:146:ARG:HA	1.76	0.40
1:C:143:MET:O	1:C:145:GLU:N	2.54	0.40
1:C:161:LEU:HD12	1:C:161:LEU:HA	1.81	0.40
2:D:104:VAL:O	2:D:107:GLU:HG2	2.20	0.40
1:A:118:GLU:O	1:A:119:LEU:C	2.59	0.40
1:A:170:SER:O	1:A:173:SER:HB2	2.22	0.40
1:A:182:LEU:HG	1:A:186:ARG:NH1	2.36	0.40
1:A:194:GLN:O	1:A:197:LYS:N	2.53	0.40
1:A:143:MET:O	1:A:144:TYR:C	2.60	0.40
1:A:182:LEU:HA	2:B:101:LEU:CD1	2.51	0.40
1:C:109:SER:O	1:C:110:THR:HB	2.22	0.40
1:C:190:ARG:O	1:C:194:GLN:HG3	2.22	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:A:152:ARG:NH1	1:A:152:ARG:NH1[4_555]	2.09	0.11

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	96/108 (89%)	78 (81%)	17 (18%)	1 (1%)	15 46
1	C	96/108 (89%)	78 (81%)	11 (12%)	7 (7%)	1 7
2	B	115/151 (76%)	95 (83%)	18 (16%)	2 (2%)	9 35
2	D	109/151 (72%)	82 (75%)	19 (17%)	8 (7%)	1 7
All	All	416/518 (80%)	333 (80%)	65 (16%)	18 (4%)	2 16

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	96	MET
1	C	109	SER
1	C	141	PRO
1	C	202	LYS
2	D	31	GLY
2	D	100	LYS
1	C	144	TYR
1	C	195	VAL
2	D	4	ARG
2	D	32	PHE
2	D	55	PHE
2	D	129	PHE
1	C	133	LEU
2	D	99	LYS
1	A	111	ASN
1	C	190	ARG
2	B	132	GLY
2	B	83	VAL

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	96/105 (91%)	90 (94%)	6 (6%)	18 47
1	C	96/105 (91%)	90 (94%)	6 (6%)	18 47
2	B	113/140 (81%)	108 (96%)	5 (4%)	28 59
2	D	108/140 (77%)	100 (93%)	8 (7%)	13 40
All	All	413/490 (84%)	388 (94%)	25 (6%)	18 48

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LEU
1	A	140	ASN
1	A	152	ARG
1	A	156	VAL
1	A	159	HIS
1	A	161	LEU
2	B	11	CYS
2	B	13	ASP
2	B	16	THR
2	B	63	SER
2	B	80	LEU
1	C	119	LEU
1	C	131	LEU
1	C	138	SER
1	C	168	HIS
1	C	173	SER
1	C	177	LEU
2	D	11	CYS
2	D	16	THR
2	D	27	ASP
2	D	30	HIS
2	D	58	THR
2	D	95	ASP
2	D	102	VAL
2	D	121	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	169	GLN
1	A	198	GLN
2	B	74	ASN
1	C	111	ASN
1	C	157	ASN
1	C	168	HIS
1	C	181	GLN
2	D	9	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 monosaccharides 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	98/108 (90%)	-0.42	3 (3%) 49 48	45, 71, 104, 133	0
1	C	98/108 (90%)	-0.25	2 (2%) 65 64	52, 77, 121, 151	0
2	B	119/151 (78%)	-0.28	4 (3%) 45 43	50, 81, 171, 188	0
2	D	113/151 (74%)	-0.30	4 (3%) 44 42	48, 77, 154, 181	0
All	All	428/518 (82%)	-0.31	13 (3%) 50 49	45, 77, 149, 188	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	133	ILE	6.5
2	B	132	GLY	5.2
2	B	48	THR	4.2
2	D	33	GLU	3.7
1	C	205	SER	3.5
1	C	108	GLU	3.3
2	D	49	VAL	3.2
2	D	30	HIS	2.6
1	A	108	GLU	2.2
1	A	109	SER	2.1
1	A	142	ASP	2.0
2	B	33	GLU	2.0
2	D	50	VAL	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 (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.