Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 12:15 am BST

PDB ID	:	4H63
Title	:	Structure of the Schizosaccharomyces pombe Mediator head module
Authors	:	Lariviere, L.; Plaschka, C.; Seizl, M.; Wenzeck, L.; Kurth, F.; Cramer, P.
Deposited on	:	2012-09-19
Resolution	:	3.40 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.

The following versions of software and data (see references (i)) 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
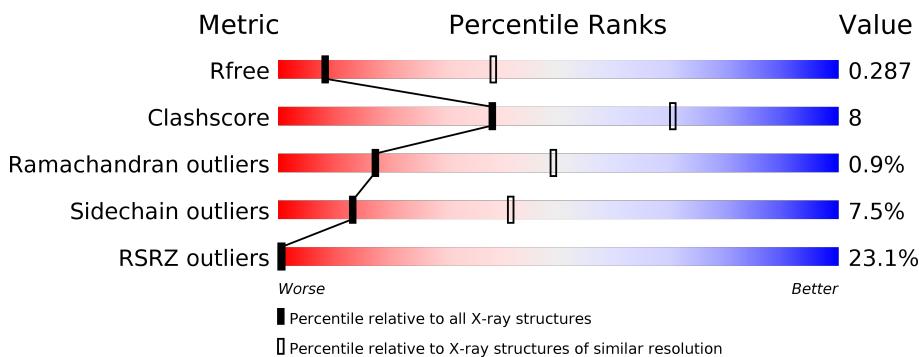
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	Percentile Ranks	Value
Rfree		0.287
Clashscore		8
Ramachandran outliers		0.9%
Sidechain outliers		7.5%
RSRZ outliers		23.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	F	183	15% / 57% / 16% • 26%
2	H	200	18% / 69% / 16% • 13%
3	K	112	23% / 64% / 21% • 13%
4	Q	469	13% / 61% / 23% • 13%
5	R	209	44% / 78% / 17% • •
6	V	135	14% / 69% / 18% / 13%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9254 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 Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	136	Total	C	N	O	S	0	0	0
			1138	736	190	205	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	EXPRESSION TAG	UNP Q9US45
F	-1	SER	-	EXPRESSION TAG	UNP Q9US45
F	0	HIS	-	EXPRESSION TAG	UNP Q9US45

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	174	Total	C	N	O	S	0	0	0
			1429	902	245	279	3			

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	98	Total	C	N	O	S	0	0	0
			777	490	129	156	2			

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Q	410	Total	C	N	O	S	0	0	0
			3316	2111	554	633	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	77	GLY	-	EXPRESSION TAG	UNP P87306

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	R	201	Total 1649	C 1053	N 281	O 307	S 8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
R	-1	ALA	-	EXPRESSION TAG	UNP O14198
R	0	SER	-	EXPRESSION TAG	UNP O14198
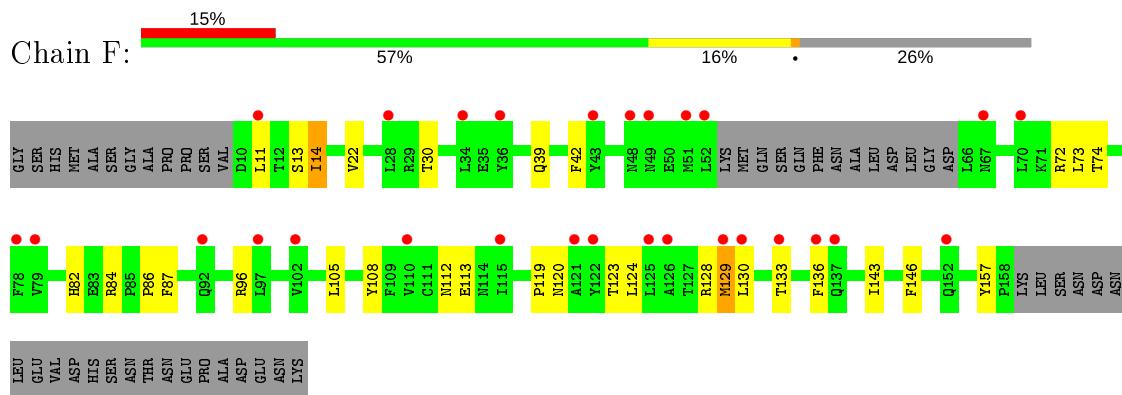
- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 22.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	V	117	Total 945	C 595	N 160	O 188	S 2	0	0	0
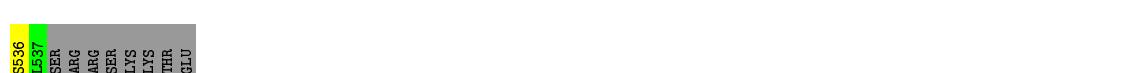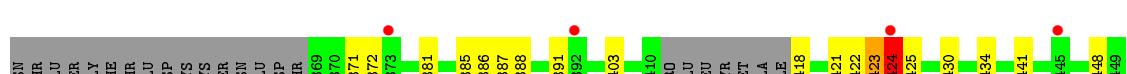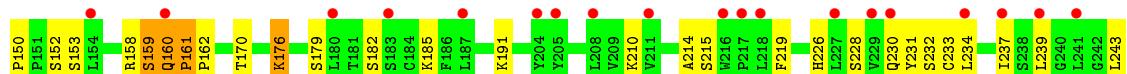
3 Residue-property plots ⓘ

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, 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.
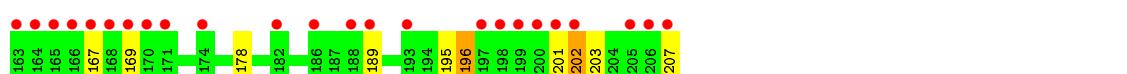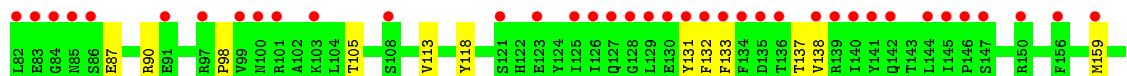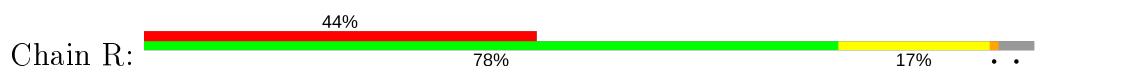
• Molecule 1: Mediator of RNA polymerase II transcription subunit 6


• Molecule 2: Mediator of RNA polymerase II transcription subunit 8

• Molecule 3: Mediator of RNA polymerase II transcription subunit 11
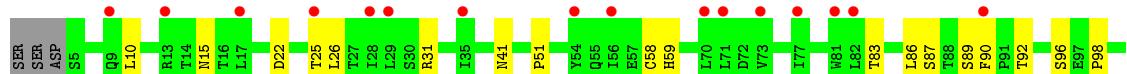
• Molecule 4: Mediator of RNA polymerase II transcription subunit 17

Chain Q:

• Molecule 5: Mediator of RNA polymerase II transcription subunit 18

Chain R:

• Molecule 6: Mediator of RNA polymerase II transcription subunit 22

Chain V:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	145.60Å 145.60Å 241.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	126.09 − 3.40 126.09 − 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (126.09-3.40) 100.0 (126.09-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 3.41Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.232 , 0.258 0.253 , 0.287	Depositor DCC
R_{free} test set	2100 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	132.8	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 150.7	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9254	wwPDB-VP
Average B, all atoms (Å^2)	165.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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	F	0.47	0/1169	0.67	0/1587
2	H	0.48	0/1457	0.65	0/1975
3	K	0.48	0/786	0.66	0/1057
4	Q	0.48	0/3384	0.71	1/4570 (0.0%)
5	R	0.47	0/1691	0.61	0/2291
6	V	0.49	0/958	0.73	0/1301
All	All	0.48	0/9445	0.68	1/12781 (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})
4	Q	159	SER	C-N-CA	5.46	135.34	121.70

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	F	1138	0	1118	23	0
2	H	1429	0	1396	28	0
3	K	777	0	796	27	0
4	Q	3316	0	3302	78	0
5	R	1649	0	1626	16	0
6	V	945	0	956	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9254	0	9194	140	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 (140) 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)
4:Q:214:ALA:O	6:V:90:PHE:HB3	1.60	1.00
3:K:40:LYS:HB3	3:K:57:TYR:HD2	1.31	0.96
3:K:94:ARG:HH12	6:V:89:SER:HB2	1.39	0.85
3:K:40:LYS:HB3	3:K:57:TYR:CD2	2.18	0.77
4:Q:234:LEU:HD12	4:Q:302:GLN:OE1	1.84	0.77
2:H:54:LEU:HD12	6:V:58:CYS:HB3	1.65	0.77
3:K:112:MET:HG2	4:Q:388:THR:HG22	1.65	0.76
3:K:24:ILE:HD11	3:K:75:GLN:HG2	1.67	0.76
3:K:91:PRO:HB3	4:Q:219:PHE:HE2	1.51	0.76
4:Q:460:TRP:HE1	6:V:108:THR:HG23	1.50	0.75
5:R:196:LEU:HD13	5:R:202:LEU:HD13	1.70	0.74
3:K:92:LYS:HD2	3:K:94:ARG:HG3	1.72	0.71
3:K:92:LYS:HE3	5:R:23:SER:O	1.92	0.70
1:F:105:LEU:O	4:Q:160:GLN:HA	1.93	0.69
6:V:31:ARG:HD2	6:V:59:HIS:HD2	1.57	0.67
3:K:91:PRO:HB3	4:Q:219:PHE:CE2	2.29	0.66
4:Q:215:SER:HA	6:V:86:LEU:HD13	1.76	0.66
3:K:36:SER:HB3	4:Q:191:LYS:HG3	1.80	0.64
4:Q:234:LEU:HD11	6:V:90:PHE:HE1	1.63	0.64
4:Q:244:ILE:HG23	4:Q:294:LEU:HD11	1.81	0.63
2:H:38:GLU:HA	4:Q:105:LYS:HE2	1.80	0.62
4:Q:111:GLN:HA	4:Q:114:ILE:HD12	1.84	0.60
2:H:49:ASN:HA	2:H:52:ILE:HD12	1.83	0.60
3:K:100:LEU:HB2	4:Q:234:LEU:HB3	1.83	0.59
5:R:87:GLU:HB2	5:R:90:ARG:HD2	1.83	0.59
4:Q:127:SER:HB2	4:Q:141:ILE:HG23	1.84	0.58
3:K:24:ILE:HD11	3:K:75:GLN:CG	2.33	0.57
4:Q:460:TRP:NE1	6:V:108:THR:HG23	2.21	0.56
2:H:191:ILE:HD13	5:R:159:MET:HG3	1.87	0.56
4:Q:295:LEU:HD23	4:Q:298:ILE:HD12	1.87	0.56
3:K:80:GLU:HG3	6:V:10:LEU:HB3	1.87	0.56
1:F:146:PHE:HB2	4:Q:104:TYR:HE2	1.71	0.55
3:K:112:MET:HE2	4:Q:391:ALA:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:313:SER:HB2	4:Q:422:PRO:HG3	1.89	0.55
3:K:22:GLN:HA	3:K:25:LEU:HD12	1.89	0.55
4:Q:424:ILE:HG13	4:Q:425:LEU:N	2.22	0.54
1:F:129:MET:HE1	6:V:51:PRO:HG3	1.90	0.54
4:Q:491:PRO:HG3	4:Q:514:GLN:HB3	1.89	0.54
4:Q:292:SER:HB3	4:Q:295:LEU:HD12	1.89	0.54
4:Q:176:LYS:HG2	6:V:41:ASN:HB2	1.89	0.53
4:Q:487:SER:HB3	4:Q:490:GLU:HB2	1.91	0.53
6:V:112:ASN:HA	6:V:115:LEU:HD12	1.91	0.53
3:K:56:LYS:HB3	3:K:57:TYR:HD1	1.73	0.53
3:K:92:LYS:HZ2	5:R:24:LYS:HA	1.73	0.53
5:R:39:TYR:HB3	5:R:118:TYR:HB3	1.91	0.52
4:Q:105:LYS:O	4:Q:109:ILE:HG12	2.10	0.52
1:F:42:PHE:HB3	1:F:108:TYR:CE2	2.45	0.52
1:F:112:ASN:O	1:F:113:GLU:HG2	2.11	0.51
2:H:82:PHE:HD1	4:Q:153:SER:HB3	1.76	0.51
1:F:84:ARG:HB2	2:H:80:LEU:HD22	1.92	0.51
3:K:86:VAL:HG13	3:K:87:VAL:HG23	1.93	0.50
3:K:111:LEU:HB3	4:Q:387:ASP:HB3	1.92	0.50
4:Q:182:SER:HA	4:Q:185:LYS:HD2	1.93	0.50
1:F:120:ASN:HB3	1:F:123:THR:OG1	2.11	0.50
4:Q:422:PRO:HB2	4:Q:424:ILE:HG23	1.93	0.50
5:R:30:LYS:HE2	5:R:132:PHE:HZ	1.75	0.50
5:R:138:VAL:HG23	5:R:169:VAL:HG22	1.94	0.49
4:Q:272:ASN:HD22	4:Q:276:ASP:HB2	1.77	0.49
4:Q:314:LEU:HD21	4:Q:424:ILE:HD11	1.95	0.49
4:Q:441:PHE:HB2	4:Q:523:LEU:HD11	1.94	0.49
5:R:26:LEU:HB3	5:R:133:PHE:HB2	1.93	0.49
2:H:188:LEU:HD13	5:R:9:VAL:HB	1.94	0.49
2:H:14:GLU:HA	4:Q:130:LEU:HD21	1.94	0.49
4:Q:288:GLN:HE22	6:V:92:THR:HG22	1.78	0.48
2:H:5:SER:HB2	4:Q:158:ARG:HH22	1.78	0.48
1:F:82:HIS:HB3	2:H:80:LEU:HD21	1.96	0.48
4:Q:300:LYS:O	4:Q:304:ILE:HG12	2.14	0.48
5:R:6:LEU:HD12	5:R:189:LEU:HD22	1.95	0.48
3:K:93:LYS:HA	4:Q:239:LEU:HD12	1.95	0.48
3:K:37:SER:HA	3:K:40:LYS:HD2	1.96	0.48
4:Q:257:SER:HB3	4:Q:301:LEU:HD21	1.94	0.47
4:Q:315:LEU:HD11	4:Q:330:GLY:HA2	1.96	0.47
2:H:133:LYS:HA	2:H:136:LEU:HD12	1.96	0.47
2:H:82:PHE:CE2	2:H:91:LEU:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:269:SER:HB3	4:Q:280:SER:HB2	1.97	0.47
5:R:58:LEU:HD11	5:R:113:VAL:HG11	1.96	0.46
1:F:11:LEU:HA	1:F:14:ILE:HG12	1.97	0.46
3:K:69:SER:HB2	6:V:25:THR:HG21	1.97	0.46
1:F:128:ARG:NH1	4:Q:118:GLU:OE2	2.48	0.46
4:Q:281:SER:HB3	4:Q:386:CYS:HB3	1.95	0.46
5:R:11:PRO:HD2	5:R:14:ARG:HB2	1.97	0.46
4:Q:466:PHE:CE1	6:V:98:PRO:HB2	2.51	0.46
3:K:69:SER:CB	6:V:25:THR:HG21	2.46	0.46
4:Q:270:ILE:HD12	4:Q:386:CYS:SG	2.56	0.46
1:F:143:ILE:HG12	4:Q:108:LEU:HD12	1.97	0.46
4:Q:161:PRO:HB2	4:Q:162:PRO:C	2.36	0.46
4:Q:508:VAL:HG23	4:Q:509:TRP:CD1	2.50	0.46
2:H:54:LEU:HD12	6:V:58:CYS:CB	2.41	0.46
4:Q:434:LEU:HD11	4:Q:480:ILE:HD13	1.97	0.46
3:K:73:ARG:NH1	6:V:22:ASP:OD1	2.49	0.46
1:F:136:PHE:HE1	2:H:27:LEU:HD21	1.81	0.45
5:R:196:LEU:HD13	5:R:202:LEU:CD1	2.43	0.45
1:F:74:THR:HA	1:F:96:ARG:HB3	1.98	0.45
4:Q:430:PHE:CD2	4:Q:475:ILE:HG22	2.51	0.45
4:Q:528:GLN:HA	4:Q:531:GLU:HB2	1.99	0.45
4:Q:132:LYS:HG2	4:Q:152:SER:OG	2.16	0.45
4:Q:231:TYR:CD1	4:Q:301:LEU:HB3	2.52	0.45
1:F:146:PHE:CD2	1:F:157:TYR:HD2	2.35	0.44
4:Q:423:LEU:HD12	4:Q:424:ILE:H	1.82	0.44
1:F:146:PHE:HB2	4:Q:104:TYR:CE2	2.50	0.44
4:Q:232:SER:HB3	4:Q:305:LEU:HD23	1.98	0.44
2:H:88:GLU:N	2:H:89:PRO:CD	2.81	0.43
4:Q:272:ASN:HB2	4:Q:276:ASP:H	1.83	0.43
5:R:38:VAL:HG22	5:R:57:ARG:HG2	2.00	0.43
3:K:99:PRO:HA	3:K:102:ASN:HD21	1.83	0.43
1:F:86:PRO:HD2	1:F:87:PHE:CD2	2.54	0.43
5:R:29:PRO:HB3	5:R:131:TYR:CZ	2.53	0.43
2:H:171:ARG:NH1	6:V:15:ASN:OD1	2.40	0.43
2:H:40:LEU:HD13	4:Q:105:LYS:HA	2.00	0.43
2:H:96:ARG:HE	2:H:98:LYS:HB3	1.82	0.43
1:F:105:LEU:O	4:Q:160:GLN:CA	2.64	0.43
1:F:129:MET:CE	2:H:61:SER:HB3	2.49	0.43
1:F:22:VAL:HG21	1:F:113:GLU:HB2	2.01	0.42
4:Q:210:LYS:HD3	4:Q:292:SER:HB2	2.00	0.42
1:F:129:MET:HG3	2:H:60:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:102:ASN:HA	3:K:105:PHE:HB2	2.01	0.42
4:Q:117:THR:O	4:Q:121:LEU:HB2	2.19	0.42
4:Q:269:SER:HB3	4:Q:280:SER:CB	2.49	0.42
4:Q:458:TYR:HE2	6:V:112:ASN:OD1	2.02	0.42
2:H:20:ILE:HG22	4:Q:123:LEU:HB2	2.00	0.42
2:H:5:SER:CB	4:Q:158:ARG:HH22	2.32	0.42
4:Q:466:PHE:CZ	6:V:98:PRO:HB2	2.55	0.42
2:H:39:SER:O	2:H:40:LEU:C	2.59	0.41
1:F:130:LEU:HA	1:F:133:THR:HG22	2.01	0.41
2:H:83:PRO:HD3	4:Q:150:PRO:HD2	2.03	0.41
4:Q:421:ALA:HB1	4:Q:422:PRO:HD2	2.02	0.41
2:H:94:LEU:HD21	4:Q:145:LEU:HD11	2.02	0.41
4:Q:458:TYR:CZ	6:V:111:GLN:HG3	2.56	0.41
4:Q:482:TRP:HB2	4:Q:495:ILE:HB	2.03	0.41
3:K:57:TYR:CD1	3:K:57:TYR:N	2.89	0.41
4:Q:315:LEU:HA	4:Q:333:ILE:HD11	2.01	0.41
4:Q:281:SER:CB	4:Q:386:CYS:HB3	2.50	0.41
4:Q:134:LYS:HA	4:Q:134:LYS:HD3	1.97	0.41
2:H:188:LEU:HA	2:H:191:ILE:HG22	2.03	0.41
1:F:119:PRO:HG3	2:H:95:LEU:HB3	2.02	0.40
4:Q:265:ALA:HA	4:Q:307:GLU:HG3	2.02	0.40
4:Q:230:GLN:O	4:Q:233:CYS:HB2	2.21	0.40
4:Q:475:ILE:HG12	4:Q:501:LEU:HD23	2.04	0.40
1:F:128:ARG:NH2	2:H:96:ARG:HB3	2.36	0.40
4:Q:228:SER:HB3	4:Q:243:LEU:HG	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	F	132/183 (72%)	125 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	168/200 (84%)	159 (95%)	7 (4%)	2 (1%)	13	41
3	K	96/112 (86%)	96 (100%)	0	0	100	100
4	Q	402/469 (86%)	381 (95%)	14 (4%)	7 (2%)	9	34
5	R	197/209 (94%)	189 (96%)	8 (4%)	0	100	100
6	V	115/135 (85%)	109 (95%)	5 (4%)	1 (1%)	17	49
All	All	1110/1308 (85%)	1059 (95%)	41 (4%)	10 (1%)	17	49

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	Q	424	ILE
2	H	39	SER
4	Q	160	GLN
4	Q	535	ASN
6	V	96	SER
4	Q	161	PRO
4	Q	371	ASN
2	H	40	LEU
4	Q	237	ILE
4	Q	536	SER

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	F	127/167 (76%)	119 (94%)	8 (6%)	18	47
2	H	160/185 (86%)	147 (92%)	13 (8%)	11	38
3	K	90/104 (86%)	86 (96%)	4 (4%)	28	58
4	Q	384/439 (88%)	348 (91%)	36 (9%)	8	30
5	R	185/192 (96%)	172 (93%)	13 (7%)	15	44
6	V	112/128 (88%)	107 (96%)	5 (4%)	27	58
All	All	1058/1215 (87%)	979 (92%)	79 (8%)	13	41

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	13	SER
1	F	14	ILE
1	F	30	THR
1	F	39	GLN
1	F	72	ARG
1	F	73	LEU
1	F	124	LEU
1	F	129	MET
2	H	14	GLU
2	H	17	ARG
2	H	41	SER
2	H	48	LYS
2	H	57	ILE
2	H	60	LEU
2	H	75	SER
2	H	79	SER
2	H	115	GLU
2	H	152	SER
2	H	154	PHE
2	H	173	LEU
2	H	188	LEU
3	K	17	ASP
3	K	92	LYS
3	K	102	ASN
3	K	107	GLN
4	Q	104	TYR
4	Q	113	MET
4	Q	125	MET
4	Q	159	SER
4	Q	170	THR
4	Q	176	LYS
4	Q	179	SER
4	Q	226	HIS
4	Q	244	ILE
4	Q	254	GLU
4	Q	268	ILE
4	Q	269	SER
4	Q	288	GLN
4	Q	297	ASP
4	Q	313	SER
4	Q	346	THR
4	Q	347	LEU

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Mol	Chain	Res	Type
4	Q	348	GLU
4	Q	372	PHE
4	Q	381	LEU
4	Q	385	LEU
4	Q	403	LYS
4	Q	418	ASP
4	Q	423	LEU
4	Q	424	ILE
4	Q	448	ARG
4	Q	451	SER
4	Q	455	MET
4	Q	479	SER
4	Q	500	THR
4	Q	501	LEU
4	Q	502	HIS
4	Q	513	ASP
4	Q	521	SER
4	Q	523	LEU
4	Q	534	ILE
5	R	19	VAL
5	R	20	ASN
5	R	98	PRO
5	R	105	THR
5	R	137	THR
5	R	167	LEU
5	R	178	ASN
5	R	195	LEU
5	R	196	LEU
5	R	201	ASP
5	R	202	LEU
5	R	203	LYS
5	R	207	LEU
6	V	26	LEU
6	V	83	THR
6	V	87	SER
6	V	119	LEU
6	V	120	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	K	102	ASN

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Mol	Chain	Res	Type
4	Q	272	ASN
5	R	204	ASN
6	V	59	HIS

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(Å²)	Q<0.9
1	F	136/183 (74%)	1.14	28 (20%)	1	1	99, 149, 196, 212	0
2	H	174/200 (87%)	1.08	36 (20%)	1	1	107, 145, 256, 264	0
3	K	98/112 (87%)	1.27	26 (26%)	0	0	118, 146, 184, 205	0
4	Q	410/469 (87%)	0.93	60 (14%)	2	3	101, 140, 192, 231	0
5	R	201/209 (96%)	2.26	93 (46%)	0	0	204, 246, 260, 266	0
6	V	117/135 (86%)	0.99	19 (16%)	1	2	108, 134, 193, 217	0
All	All	1136/1308 (86%)	1.25	262 (23%)	0	1	99, 149, 254, 266	0

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	R	199	PHE	11.0
5	R	133	PHE	8.9
5	R	144	LEU	8.2
5	R	202	LEU	8.0
5	R	6	LEU	7.7
5	R	125	ILE	7.5
5	R	166	ILE	7.4
5	R	200	CYS	7.4
5	R	134	PHE	7.0
5	R	4	LEU	6.6
5	R	127	GLN	6.4
5	R	9	VAL	6.1
5	R	141	TYR	5.8
5	R	132	PHE	5.7
5	R	188	ASN	5.7
5	R	164	PRO	5.6
5	R	207	LEU	5.5
5	R	156	PHE	5.4
5	R	167	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
5	R	7	LEU	5.4
5	R	3	GLU	5.4
5	R	100	ASN	5.2
1	F	152	GLN	5.0
5	R	198	ALA	4.9
5	R	65	HIS	4.9
5	R	205	VAL	4.8
5	R	22	LEU	4.8
5	R	140	ILE	4.8
5	R	14	ARG	4.7
5	R	131	TYR	4.7
5	R	174	ALA	4.7
5	R	165	TRP	4.7
3	K	28	GLU	4.7
5	R	126	ILE	4.6
5	R	25	THR	4.6
5	R	121	SER	4.6
5	R	83	GLU	4.5
5	R	103	LYS	4.5
5	R	163	GLN	4.5
2	H	40	LEU	4.5
5	R	138	VAL	4.4
5	R	80	MET	4.4
5	R	11	PRO	4.4
5	R	135	ASP	4.3
5	R	10	VAL	4.2
5	R	97	ARG	4.2
5	R	142	GLN	4.2
4	Q	237	ILE	4.2
4	Q	294	LEU	4.1
5	R	168	HIS	4.1
6	V	81	TRP	4.1
3	K	61	PHE	4.0
5	R	82	LEU	4.0
5	R	56	LEU	4.0
2	H	4	ILE	3.9
5	R	21	SER	3.9
3	K	42	ILE	3.8
1	F	49	ASN	3.8
4	Q	160	GLN	3.8
1	F	136	PHE	3.8
5	R	169	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
5	R	15	PHE	3.8
1	F	52	LEU	3.8
5	R	26	LEU	3.8
5	R	18	VAL	3.8
5	R	145	ILE	3.7
2	H	171	ARG	3.7
1	F	36	TYR	3.7
4	Q	473	LEU	3.6
5	R	123	GLU	3.6
5	R	17	ALA	3.6
5	R	146	PRO	3.6
2	H	172	GLN	3.6
5	R	128	GLY	3.6
5	R	206	ARG	3.6
5	R	39	TYR	3.6
4	Q	208	LEU	3.5
5	R	197	SER	3.5
4	Q	218	LEU	3.4
2	H	90	LEU	3.4
6	V	70	LEU	3.4
4	Q	241	LEU	3.4
2	H	174	GLU	3.4
2	H	184	ALA	3.4
3	K	77	LEU	3.3
5	R	84	GLY	3.3
5	R	139	ARG	3.3
4	Q	126	THR	3.3
3	K	62	LEU	3.3
5	R	130	GLU	3.3
5	R	159	MET	3.3
5	R	129	LEU	3.3
6	V	90	PHE	3.2
2	H	46	ILE	3.2
4	Q	229	VAL	3.2
5	R	101	ARG	3.2
5	R	99	VAL	3.2
5	R	1	MET	3.1
4	Q	424	ILE	3.1
3	K	89	LEU	3.0
3	K	84	VAL	3.0
2	H	194	PHE	3.0
1	F	11	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	53	LEU	3.0
3	K	86	VAL	3.0
2	H	94	LEU	2.9
4	Q	180	LEU	2.9
4	Q	278	ILE	2.9
3	K	112	MET	2.9
2	H	173	LEU	2.9
2	H	144	PHE	2.9
5	R	35	PHE	2.9
5	R	85	ASN	2.8
2	H	186	GLN	2.8
5	R	5	TYR	2.8
5	R	30	LYS	2.8
2	H	27	LEU	2.8
5	R	37	VAL	2.8
5	R	201	ASP	2.8
4	Q	445	LEU	2.8
5	R	170	TYR	2.8
6	V	77	ILE	2.8
4	Q	112	ILE	2.8
2	H	180	GLU	2.8
1	F	51	MET	2.7
1	F	129	MET	2.7
2	H	197	SER	2.7
1	F	48	ASN	2.7
1	F	78	PHE	2.7
1	F	137	GLN	2.7
3	K	72	LEU	2.7
4	Q	211	VAL	2.7
6	V	13	ARG	2.7
1	F	115	ILE	2.7
6	V	54	TYR	2.7
5	R	33	LEU	2.7
2	H	31	LEU	2.6
2	H	188	LEU	2.6
4	Q	217	PRO	2.6
5	R	150	ARG	2.6
4	Q	266	LEU	2.6
1	F	126	ALA	2.6
5	R	171	THR	2.6
4	Q	314	LEU	2.6
3	K	91	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
3	K	35	LEU	2.6
4	Q	259	LEU	2.6
4	Q	475	ILE	2.5
4	Q	253	PHE	2.5
6	V	56	ILE	2.5
1	F	43	TYR	2.5
1	F	133	THR	2.5
4	Q	530	ILE	2.5
2	H	127	ALA	2.5
3	K	31	ILE	2.5
1	F	122	TYR	2.5
4	Q	204	TYR	2.5
5	R	108	SER	2.5
4	Q	293	VAL	2.5
3	K	34	ILE	2.5
4	Q	244	ILE	2.4
4	Q	119	CYS	2.4
1	F	70	LEU	2.4
1	F	130	LEU	2.4
4	Q	183	SER	2.4
3	K	37	SER	2.4
3	K	45	ILE	2.4
2	H	34	LEU	2.4
6	V	35	ILE	2.4
5	R	78	TRP	2.4
3	K	103	LEU	2.4
2	H	82	PHE	2.4
1	F	125	LEU	2.4
3	K	21	VAL	2.4
4	Q	347	LEU	2.4
4	Q	128	LEU	2.4
4	Q	227	LEU	2.4
4	Q	239	LEU	2.4
6	V	115	LEU	2.4
2	H	76	ILE	2.4
3	K	68	ILE	2.4
4	Q	234	LEU	2.4
4	Q	482	TRP	2.4
5	R	136	THR	2.4
1	F	121	ALA	2.3
4	Q	520	PHE	2.3
5	R	8	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	97	LEU	2.3
4	Q	216	TRP	2.3
4	Q	230	GLN	2.3
4	Q	493	ILE	2.3
3	K	81	LYS	2.3
3	K	74	ARG	2.3
4	Q	306	PHE	2.3
6	V	103	VAL	2.3
2	H	111	LEU	2.3
5	R	34	GLU	2.3
2	H	103	VAL	2.3
2	H	131	TYR	2.3
3	K	38	ALA	2.3
5	R	27	ASP	2.3
1	F	102	VAL	2.3
4	Q	460	TRP	2.3
6	V	73	VAL	2.3
6	V	29	LEU	2.3
2	H	57	ILE	2.3
5	R	147	SER	2.3
2	H	60	LEU	2.3
2	H	93	THR	2.2
4	Q	129	LEU	2.2
6	V	17	LEU	2.2
4	Q	345	ILE	2.2
4	Q	470	GLU	2.2
5	R	91	GLU	2.2
2	H	87	GLN	2.2
4	Q	154	LEU	2.2
6	V	28	ILE	2.2
2	H	13	LEU	2.2
4	Q	108	LEU	2.2
5	R	86	SER	2.2
1	F	28	LEU	2.2
6	V	71	LEU	2.2
4	Q	99	MET	2.2
5	R	182	MET	2.2
4	Q	271	LEU	2.2
1	F	79	VAL	2.2
4	Q	205	TYR	2.2
5	R	189	LEU	2.1
3	K	85	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
5	R	32	ILE	2.1
1	F	34	LEU	2.1
3	K	109	SER	2.1
1	F	67	ASN	2.1
1	F	92	GLN	2.1
1	F	110	VAL	2.1
3	K	75	GLN	2.1
4	Q	133	PHE	2.1
2	H	153	TRP	2.1
5	R	186	GLU	2.1
6	V	121	GLU	2.1
2	H	78	PRO	2.1
4	Q	187	LEU	2.1
2	H	97	THR	2.1
4	Q	484	ILE	2.1
4	Q	301	LEU	2.1
6	V	25	THR	2.1
4	Q	299	TYR	2.1
4	Q	373	VAL	2.1
6	V	82	LEU	2.1
4	Q	454	PHE	2.1
2	H	183	ASN	2.1
5	R	193	LYS	2.1
4	Q	450	ILE	2.1
6	V	9	GLN	2.0
4	Q	149	VAL	2.0
4	Q	116	GLN	2.0
4	Q	392	ILE	2.0
5	R	19	VAL	2.0
3	K	100	LEU	2.0
2	H	137	TRP	2.0
4	Q	295	LEU	2.0
4	Q	105	LYS	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.