



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:50 PM UTC

PDB ID : 4H63 / pdb_00004h63
Title : Structure of the Schizosaccharomyces pombe Mediator head module
Authors : Lariviere, L.; Plaschka, C.; Seizl, M.; Wenzek, 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 ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

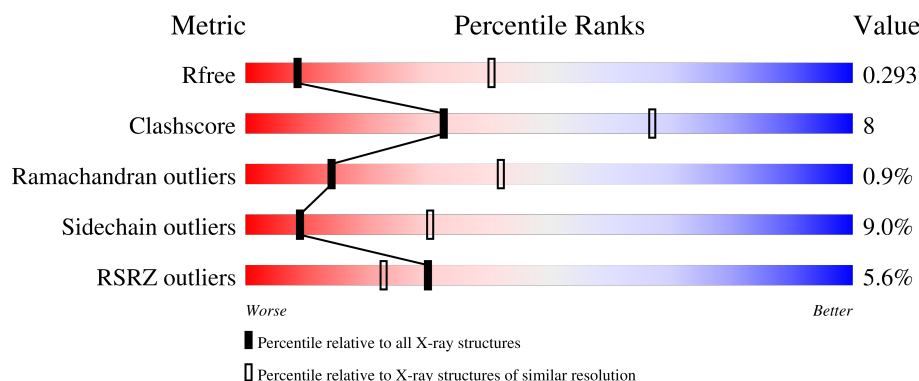
1 Overall quality at a glance ⓘ

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 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 $\leq 5\%$. 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	2% 55% 17% • 26%
2	H	200	2% 68% 14% 5% 13%
3	K	112	2% 61% 23% • • 12%
4	Q	469	2% 59% 24% • • 13%
5	R	209	21% 78% 17% • •

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Mol	Chain	Length	Quality of chain
6	V	135	 2% 63% 22% 13%

2 Entry composition

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	C	N	O	S	0	0	0
			1649	1053	281	307	8			

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

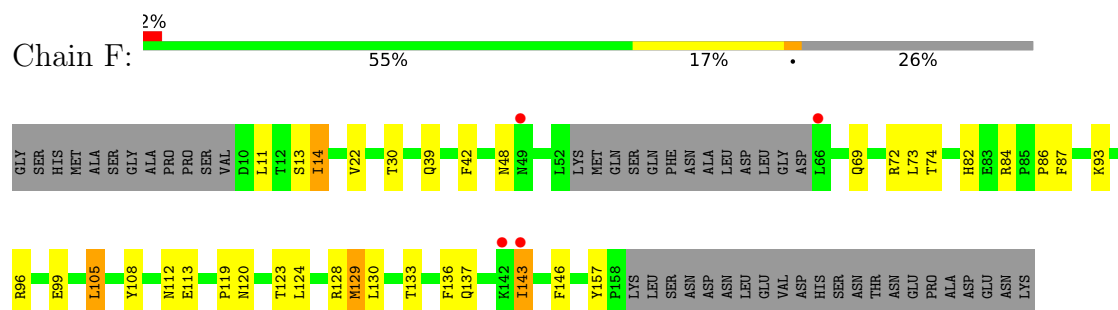
- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	V	117	Total	C	N	O	S	0	0	0
			945	595	160	188	2			

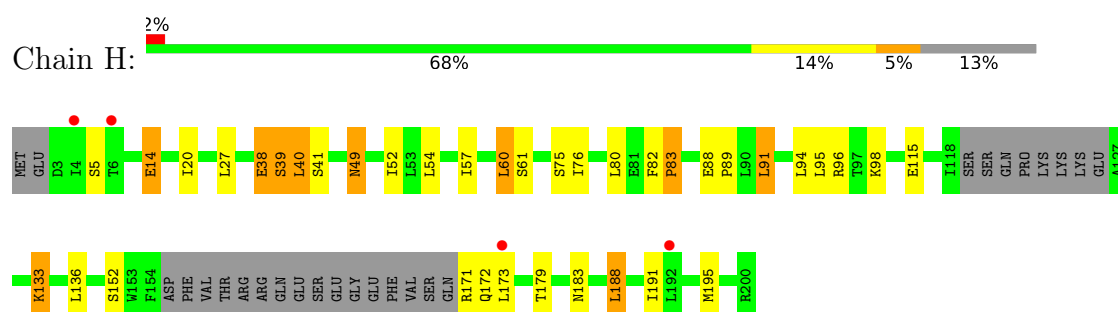
3 Residue-property plots [i](#)

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.

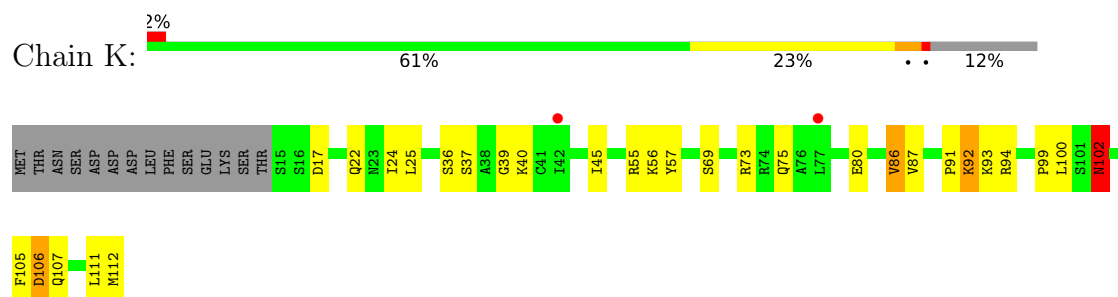
- Molecule 1: Mediator of RNA polymerase II transcription subunit 6



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

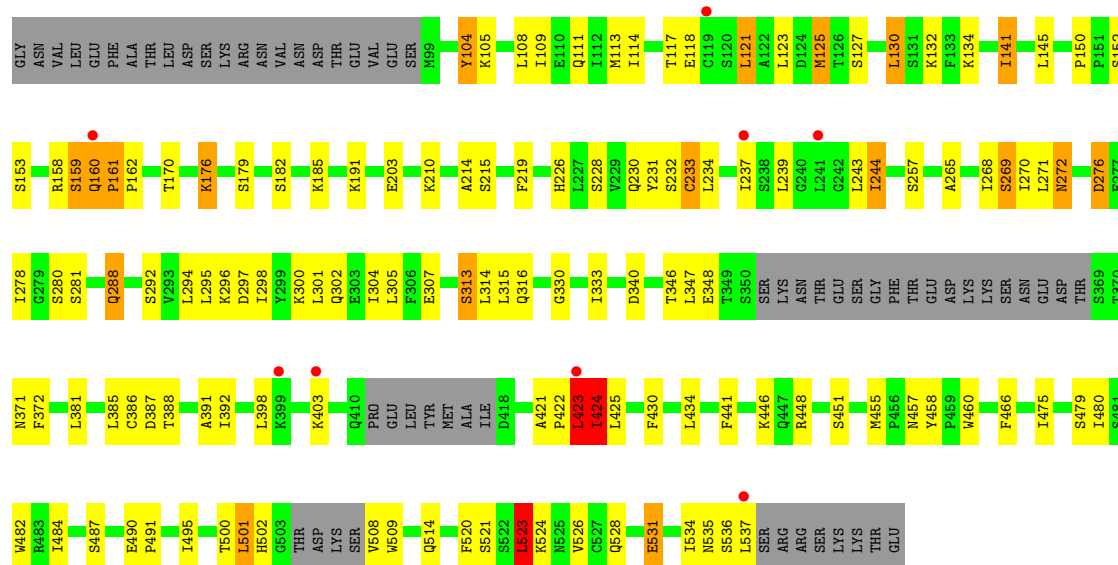


- Molecule 3: Mediator of RNA polymerase II transcription subunit 11

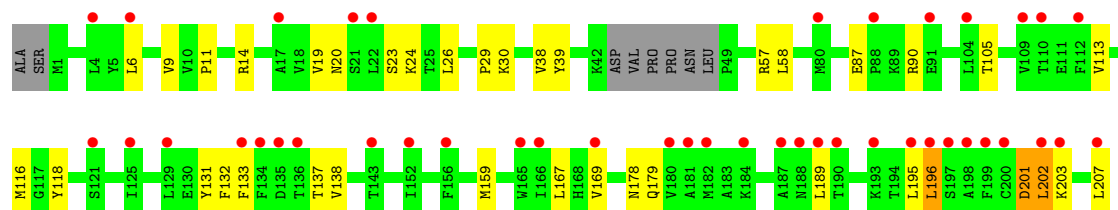
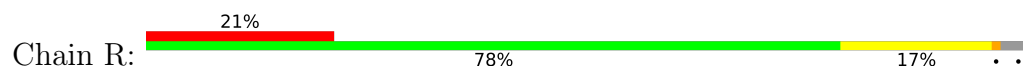


- Molecule 4: Mediator of RNA polymerase II transcription subunit 17

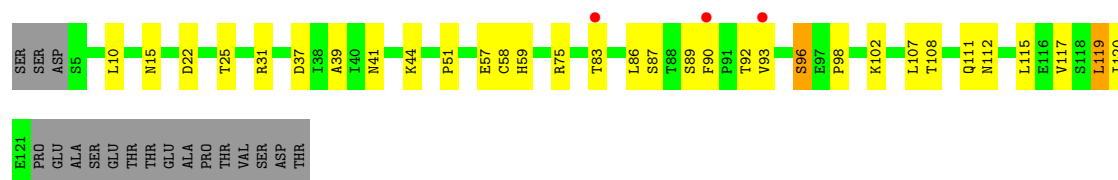




• Molecule 5: Mediator of RNA polymerase II transcription subunit 18



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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.41Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.232 , 0.258 0.256 , 0.293	Depositor DCC
R_{free} test set	2100 reflections (4.53%)	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)	0.35 , 174.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	F	0.82	0/1169	1.27	1/1587 (0.1%)
2	H	0.85	0/1457	1.47	10/1975 (0.5%)
3	K	0.85	0/786	1.49	6/1057 (0.6%)
4	Q	0.83	1/3384 (0.0%)	1.41	25/4570 (0.5%)
5	R	0.90	0/1691	1.23	1/2291 (0.0%)
6	V	0.88	1/958 (0.1%)	1.57	16/1301 (1.2%)
All	All	0.85	2/9445 (0.0%)	1.40	59/12781 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	93	VAL	CA-C	5.37	1.57	1.52
4	Q	424	ILE	CA-C	5.07	1.59	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	520	PHE	CA-C-N	7.83	131.10	120.54
4	Q	520	PHE	C-N-CA	7.83	131.10	120.54
6	V	102	LYS	CA-C-N	6.80	129.13	120.56
6	V	102	LYS	C-N-CA	6.80	129.13	120.56
6	V	96	SER	CA-C-N	6.46	129.87	120.51
6	V	96	SER	C-N-CA	6.46	129.87	120.51
3	K	106	ASP	CA-CB-CG	6.44	119.04	112.60
6	V	119	LEU	N-CA-C	-6.16	105.07	112.58
3	K	102	ASN	CA-CB-CG	6.14	118.74	112.60
5	R	201	ASP	CA-CB-CG	5.98	118.58	112.60
2	H	38	GLU	CA-C-N	5.97	132.94	121.54
2	H	38	GLU	C-N-CA	5.97	132.94	121.54
2	H	172	GLN	N-CA-C	-5.94	105.99	113.18
4	Q	446	LYS	CA-C-N	5.94	128.56	120.54
4	Q	446	LYS	C-N-CA	5.94	128.56	120.54
4	Q	423	LEU	CA-C-N	5.92	132.63	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	423	LEU	C-N-CA	5.92	132.63	121.97
4	Q	272	ASN	CA-CB-CG	5.82	118.42	112.60
4	Q	276	ASP	CA-CB-CG	5.72	118.33	112.60
6	V	44	LYS	CA-C-N	5.62	129.46	121.42
6	V	44	LYS	C-N-CA	5.62	129.46	121.42
4	Q	159	SER	CA-C-N	5.55	135.34	121.80
4	Q	159	SER	C-N-CA	5.55	135.34	121.80
1	F	48	ASN	CA-CB-CG	5.53	118.13	112.60
2	H	172	GLN	CA-C-N	5.52	128.70	120.31
2	H	172	GLN	C-N-CA	5.52	128.70	120.31
2	H	183	ASN	CA-CB-CG	5.46	118.06	112.60
6	V	39	ALA	CA-C-N	5.45	127.88	120.63
6	V	39	ALA	C-N-CA	5.45	127.88	120.63
4	Q	271	LEU	CA-C-N	5.45	130.64	120.95
4	Q	271	LEU	C-N-CA	5.45	130.64	120.95
4	Q	296	LYS	CA-C-N	5.43	127.50	120.44
4	Q	296	LYS	C-N-CA	5.43	127.50	120.44
4	Q	457	ASN	CA-CB-CG	5.42	118.02	112.60
3	K	39	GLY	CA-C-N	5.29	127.36	120.28
3	K	39	GLY	C-N-CA	5.29	127.36	120.28
4	Q	233	CYS	CA-C-N	5.27	127.34	120.28
4	Q	233	CYS	C-N-CA	5.27	127.34	120.28
2	H	179	THR	CA-C-N	5.24	127.73	120.29
2	H	179	THR	C-N-CA	5.24	127.73	120.29
4	Q	524	LYS	CA-C-N	5.22	127.27	120.28
4	Q	524	LYS	C-N-CA	5.22	127.27	120.28
6	V	57	GLU	CA-C-N	5.20	127.50	120.38
6	V	57	GLU	C-N-CA	5.20	127.50	120.38
2	H	83	PRO	CA-C-N	5.17	127.83	120.53
2	H	83	PRO	C-N-CA	5.17	127.83	120.53
4	Q	526	VAL	CA-C-N	5.14	127.42	120.38
4	Q	526	VAL	C-N-CA	5.14	127.42	120.38
4	Q	340	ASP	CA-CB-CG	5.13	117.73	112.60
6	V	117	VAL	CA-C-N	5.12	130.52	120.99
6	V	117	VAL	C-N-CA	5.12	130.52	120.99
6	V	119	LEU	CA-C-N	5.08	131.12	121.97
6	V	119	LEU	C-N-CA	5.08	131.12	121.97
4	Q	141	ILE	N-CA-CB	5.08	117.56	110.56
4	Q	523	LEU	CA-C-N	5.03	127.33	120.54
4	Q	523	LEU	C-N-CA	5.03	127.33	120.54
6	V	37	ASP	CA-CB-CG	5.03	117.63	112.60
3	K	55	ARG	CA-C-N	5.01	127.75	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	55	ARG	C-N-CA	5.01	127.75	120.79

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	F	1138	0	1118	24	0
2	H	1429	0	1396	31	0
3	K	777	0	796	28	0
4	Q	3316	0	3302	80	0
5	R	1649	0	1626	17	0
6	V	945	0	956	22	0
All	All	9254	0	9194	145	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 (145) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:129:MET:HE1	2:H:61:SER:HB3	1.77	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:92:LYS:HZ2	5:R:24:LYS:HA	1.69	0.57
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
3:K:80:GLU:HG3	6:V:10:LEU:HB3	1.87	0.56
4:Q:295:LEU:HD23	4:Q:298:ILE:HD12	1.87	0.56
1:F:146:PHE:HB2	4:Q:104:TYR:HE2	1.71	0.55
3:K:112:MET:HE3	4:Q:391:ALA:CB	2.36	0.55
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
3:K:112:MET:HE3	4:Q:391:ALA:HB3	1.88	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:424:ILE:HG13	4:Q:425:LEU:N	2.22	0.53
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
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
4:Q:161:PRO:HB2	4:Q:162:PRO:C	2.36	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:113:VAL:HA	5:R:116:MET:HE2	1.94	0.49
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
2:H:188:LEU:HD13	5:R:9:VAL:HB	1.94	0.49
5:R:26:LEU:HB3	5:R:133:PHE:HB2	1.93	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
2:H:191:ILE:HG13	2:H:195:MET:HE2	1.94	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
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
2:H:39:SER:O	2:H:40:LEU:C	2.59	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
3:K:69:SER:CB	6:V:25:THR:HG21	2.46	0.46
4:Q:466:PHE:CE1	6:V:98:PRO:HB2	2.51	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: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
3:K:73:ARG:NH1	6:V:22:ASP:OD1	2.49	0.46
4:Q:434:LEU:HD11	4:Q:480:ILE:HD13	1.97	0.46
2:H:76:ILE:HG21	4:Q:125:MET:HE3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:171:ARG:NH1	6:V:15:ASN:OD1	2.40	0.43
5:R:29:PRO:HB3	5:R:131:TYR:CZ	2.53	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: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
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
1:F:129:MET:CE	2:H:61:SER:HB3	2.49	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:N	3:K:57:TYR:CD1	2.89	0.41
4:Q:281:SER:CB	4:Q:386:CYS:HB3	2.50	0.41
4:Q:315:LEU:HA	4:Q:333:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:134:LYS:HD3	4:Q:134:LYS:HA	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
1:F:129:MET:HE1	6:V:51:PRO:HG3	2.03	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

5.3.1 Protein backbone

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
2	H	168/200 (84%)	159 (95%)	7 (4%)	2 (1%)	10	35
3	K	96/112 (86%)	96 (100%)	0	0	100	100
4	Q	402/469 (86%)	381 (95%)	14 (4%)	7 (2%)	7	28
5	R	197/209 (94%)	189 (96%)	8 (4%)	0	100	100
6	V	115/135 (85%)	109 (95%)	5 (4%)	1 (1%)	14	42
All	All	1110/1308 (85%)	1059 (95%)	41 (4%)	10 (1%)	14	42

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	Q	424	ILE
2	H	39	SER
4	Q	160	GLN

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Mol	Chain	Res	Type
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 ⓘ

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%)	113 (89%)	14 (11%)	6	22
2	H	160/185 (86%)	148 (92%)	12 (8%)	12	38
3	K	90/104 (86%)	83 (92%)	7 (8%)	11	37
4	Q	384/439 (88%)	341 (89%)	43 (11%)	6	21
5	R	185/192 (96%)	172 (93%)	13 (7%)	14	40
6	V	112/128 (88%)	106 (95%)	6 (5%)	20	47
All	All	1058/1215 (87%)	963 (91%)	95 (9%)	9	30

All (95) 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	69	GLN
1	F	72	ARG
1	F	73	LEU
1	F	93	LYS
1	F	99	GLU
1	F	105	LEU
1	F	124	LEU

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Mol	Chain	Res	Type
1	F	129	MET
1	F	137	GLN
1	F	143	ILE
2	H	14	GLU
2	H	41	SER
2	H	49	ASN
2	H	57	ILE
2	H	60	LEU
2	H	75	SER
2	H	91	LEU
2	H	115	GLU
2	H	133	LYS
2	H	152	SER
2	H	173	LEU
2	H	188	LEU
3	K	17	ASP
3	K	45	ILE
3	K	86	VAL
3	K	92	LYS
3	K	102	ASN
3	K	106	ASP
3	K	107	GLN
4	Q	104	TYR
4	Q	113	MET
4	Q	121	LEU
4	Q	125	MET
4	Q	130	LEU
4	Q	159	SER
4	Q	170	THR
4	Q	176	LYS
4	Q	179	SER
4	Q	203	GLU
4	Q	226	HIS
4	Q	244	ILE
4	Q	268	ILE
4	Q	269	SER
4	Q	278	ILE
4	Q	288	GLN
4	Q	297	ASP
4	Q	313	SER
4	Q	316	GLN
4	Q	346	THR

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Mol	Chain	Res	Type
4	Q	347	LEU
4	Q	348	GLU
4	Q	372	PHE
4	Q	381	LEU
4	Q	385	LEU
4	Q	392	ILE
4	Q	398	LEU
4	Q	403	LYS
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	484	ILE
4	Q	500	THR
4	Q	501	LEU
4	Q	502	HIS
4	Q	521	SER
4	Q	523	LEU
4	Q	531	GLU
4	Q	534	ILE
4	Q	537	LEU
5	R	19	VAL
5	R	20	ASN
5	R	105	THR
5	R	137	THR
5	R	167	LEU
5	R	178	ASN
5	R	179	GLN
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	75	ARG
6	V	83	THR
6	V	87	SER
6	V	107	LEU
6	V	119	LEU
6	V	120	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	48	ASN
1	F	77	GLN
1	F	94	GLN
1	F	95	ASN
1	F	114	ASN
2	H	36	GLN
2	H	49	ASN
2	H	87	GLN
2	H	182	GLN
3	K	48	ASN
3	K	90	GLN
3	K	102	ASN
4	Q	111	GLN
4	Q	220	ASN
4	Q	230	GLN
4	Q	272	ASN
4	Q	312	ASN
4	Q	341	HIS
4	Q	488	ASN
4	Q	496	GLN
4	Q	519	GLN
5	R	2	GLN
5	R	61	ASN
5	R	127	GLN
5	R	148	GLN
5	R	160	ASN
5	R	188	ASN
5	R	204	ASN
6	V	7	GLN
6	V	9	GLN
6	V	55	GLN
6	V	59	HIS

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 [i](#)

There are no oligosaccharides 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

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, 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	F	136/183 (74%)	0.20	4 (2%)	53	39	99, 149, 196, 212	0
2	H	174/200 (87%)	0.11	4 (2%)	61	46	107, 145, 256, 264	0
3	K	98/112 (87%)	0.13	2 (2%)	65	49	118, 146, 184, 205	0
4	Q	410/469 (87%)	0.14	8 (1%)	65	49	101, 140, 192, 231	0
5	R	201/209 (96%)	1.17	43 (21%)	2	4	204, 246, 260, 266	0
6	V	117/135 (86%)	-0.05	3 (2%)	57	42	108, 134, 193, 217	0
All	All	1136/1308 (86%)	0.30	64 (5%)	30	23	99, 149, 254, 266	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	R	109	VAL	5.6
5	R	188	ASN	5.1
5	R	196	LEU	4.6
1	F	66	LEU	4.2
5	R	197	SER	4.1
4	Q	241	LEU	4.1
4	Q	537	LEU	3.9
5	R	195	LEU	3.8
5	R	134	PHE	3.8
3	K	77	LEU	3.7
5	R	169	VAL	3.6
5	R	110	THR	3.6
1	F	143	ILE	3.5
5	R	133	PHE	3.4
5	R	202	LEU	3.4
5	R	21	SER	3.3
4	Q	423	LEU	3.2
2	H	173	LEU	3.2
5	R	135	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	4	ILE	3.0
4	Q	119	CYS	3.0
5	R	180	VAL	2.9
5	R	190	THR	2.9
6	V	90	PHE	2.9
5	R	6	LEU	2.9
6	V	83	THR	2.9
2	H	192	LEU	2.8
5	R	4	LEU	2.8
5	R	80	MET	2.7
5	R	200	CYS	2.7
5	R	143	THR	2.7
1	F	142	LYS	2.7
5	R	207	LEU	2.6
4	Q	403	LYS	2.6
5	R	182	MET	2.5
5	R	198	ALA	2.5
5	R	166	ILE	2.5
5	R	193	LYS	2.5
5	R	184	LYS	2.5
5	R	22	LEU	2.4
5	R	125	ILE	2.4
5	R	121	SER	2.4
5	R	199	PHE	2.4
5	R	129	LEU	2.4
6	V	93	VAL	2.4
5	R	156	PHE	2.4
5	R	203	LYS	2.3
1	F	49	ASN	2.3
5	R	181	ALA	2.2
5	R	152	ILE	2.2
5	R	17	ALA	2.2
4	Q	399	LYS	2.2
2	H	6	THR	2.2
5	R	189	LEU	2.2
5	R	88	PRO	2.2
5	R	112	PHE	2.1
5	R	165	TRP	2.1
4	Q	237	ILE	2.1
5	R	136	THR	2.1
5	R	187	ALA	2.1
5	R	91	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	K	42	ILE	2.1
5	R	104	LEU	2.1
4	Q	160	GLN	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 oligosaccharides 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.