



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:39 AM UTC

PDB ID : 4GWQ / pdb_00004gwq
Title : Structure of the Mediator Head Module from *S. cerevisiae* in complex with the carboxy-terminal domain (CTD) of RNA Polymerase II Rpb1 subunit
Authors : Robinson, P.J.J.; Bushnell, D.A.; Trnka, M.J.; Burlingame, A.L.; Kornberg, R.D.
Deposited on : 2012-09-03
Resolution : 4.50 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:

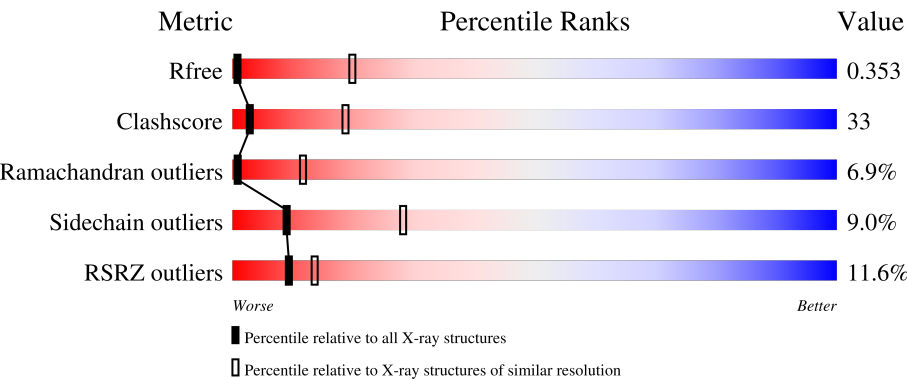
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.50 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	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	A	115	9% 86%11%.
2	B	687	6% 51%17%.28%
3	C	407	3% 33%11%.55%
4	D	121	8% 83%14%.
5	E	307	9% 44%31%7%.18%

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Mol	Chain	Length	Quality of chain
6	F	210	16% 58% 36% 5%
7	G	295	8% 36% 18% • 42%
8	H	35	60% 26% 17% 29% 29%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9217 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 11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	0	0	0
			556	332	112	112			

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	492	Total	C	N	O	0	0	0
			2446	1462	492	492			

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	184	Total	C	N	O	0	0	0
			1004	611	194	199			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	224	SER	-	expression tag	UNP P38304
C	225	MET	-	expression tag	UNP P38304
C	226	GLU	-	expression tag	UNP P38304
C	227	LYS	-	expression tag	UNP P38304
C	228	ARG	-	expression tag	UNP P38304
C	229	ARG	-	expression tag	UNP P38304
C	230	TRP	-	expression tag	UNP P38304
C	231	LYS	-	expression tag	UNP P38304
C	232	LYS	-	expression tag	UNP P38304
C	233	ASN	-	expression tag	UNP P38304
C	234	PHE	-	expression tag	UNP P38304
C	235	ILE	-	expression tag	UNP P38304
C	236	ALA	-	expression tag	UNP P38304
C	237	VAL	-	expression tag	UNP P38304

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Chain	Residue	Modelled	Actual	Comment	Reference
C	238	SER	-	expression tag	UNP P38304
C	239	ALA	-	expression tag	UNP P38304
C	240	ALA	-	expression tag	UNP P38304
C	241	ASN	-	expression tag	UNP P38304
C	242	ARG	-	expression tag	UNP P38304
C	243	PHE	-	expression tag	UNP P38304
C	244	LYS	-	expression tag	UNP P38304
C	245	LYS	-	expression tag	UNP P38304
C	246	ILE	-	expression tag	UNP P38304
C	247	SER	-	expression tag	UNP P38304
C	248	SER	-	expression tag	UNP P38304
C	249	SER	-	expression tag	UNP P38304
C	250	GLY	-	expression tag	UNP P38304
C	251	ALA	-	expression tag	UNP P38304
C	252	LEU	-	expression tag	UNP P38304
C	253	ASP	-	expression tag	UNP P38304
C	254	TYR	-	expression tag	UNP P38304
C	255	ASP	-	expression tag	UNP P38304
C	256	ILE	-	expression tag	UNP P38304
C	257	PRO	-	expression tag	UNP P38304
C	258	THR	-	expression tag	UNP P38304
C	259	THR	-	expression tag	UNP P38304
C	260	ALA	-	expression tag	UNP P38304
C	261	SER	-	expression tag	UNP P38304
C	262	GLU	-	expression tag	UNP P38304
C	263	ASN	-	expression tag	UNP P38304
C	264	LEU	-	expression tag	UNP P38304
C	265	TYR	-	expression tag	UNP P38304
C	266	PHE	-	expression tag	UNP P38304
C	267	GLN	-	expression tag	UNP P38304
C	268	GLY	-	expression tag	UNP P38304
C	269	GLU	-	expression tag	UNP P38304
C	270	LEU	-	expression tag	UNP P38304
C	271	LYS	-	expression tag	UNP P38304
C	272	THR	-	expression tag	UNP P38304
C	273	ALA	-	expression tag	UNP P38304
C	274	ALA	-	expression tag	UNP P38304
C	275	LEU	-	expression tag	UNP P38304
C	276	ALA	-	expression tag	UNP P38304
C	277	GLN	-	expression tag	UNP P38304
C	278	HIS	-	expression tag	UNP P38304
C	279	ASP	-	expression tag	UNP P38304

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Chain	Residue	Modelled	Actual	Comment	Reference
C	280	GLU	-	expression tag	UNP P38304
C	281	ALA	-	expression tag	UNP P38304
C	282	VAL	-	expression tag	UNP P38304
C	283	ASP	-	expression tag	UNP P38304
C	284	ASN	-	expression tag	UNP P38304
C	285	LYS	-	expression tag	UNP P38304
C	286	PHE	-	expression tag	UNP P38304
C	287	ASN	-	expression tag	UNP P38304
C	288	LYS	-	expression tag	UNP P38304
C	289	GLU	-	expression tag	UNP P38304
C	290	GLN	-	expression tag	UNP P38304
C	291	GLN	-	expression tag	UNP P38304
C	292	ASN	-	expression tag	UNP P38304
C	293	ALA	-	expression tag	UNP P38304
C	294	PHE	-	expression tag	UNP P38304
C	295	TYR	-	expression tag	UNP P38304
C	296	GLU	-	expression tag	UNP P38304
C	297	ILE	-	expression tag	UNP P38304
C	298	LEU	-	expression tag	UNP P38304
C	299	HIS	-	expression tag	UNP P38304
C	300	LEU	-	expression tag	UNP P38304
C	301	PRO	-	expression tag	UNP P38304
C	302	ASN	-	expression tag	UNP P38304
C	303	LEU	-	expression tag	UNP P38304
C	304	ASN	-	expression tag	UNP P38304
C	305	GLU	-	expression tag	UNP P38304
C	306	GLU	-	expression tag	UNP P38304
C	307	GLN	-	expression tag	UNP P38304
C	308	ARG	-	expression tag	UNP P38304
C	309	ASN	-	expression tag	UNP P38304
C	310	ALA	-	expression tag	UNP P38304
C	311	PHE	-	expression tag	UNP P38304
C	312	ILE	-	expression tag	UNP P38304
C	313	GLN	-	expression tag	UNP P38304
C	314	SER	-	expression tag	UNP P38304
C	315	LEU	-	expression tag	UNP P38304
C	316	LYS	-	expression tag	UNP P38304
C	317	ASP	-	expression tag	UNP P38304
C	318	ASP	-	expression tag	UNP P38304
C	319	PRO	-	expression tag	UNP P38304
C	320	SER	-	expression tag	UNP P38304
C	321	GLN	-	expression tag	UNP P38304

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Chain	Residue	Modelled	Actual	Comment	Reference
C	322	SER	-	expression tag	UNP P38304
C	323	ALA	-	expression tag	UNP P38304
C	324	ASN	-	expression tag	UNP P38304
C	325	LEU	-	expression tag	UNP P38304
C	326	LEU	-	expression tag	UNP P38304
C	327	ALA	-	expression tag	UNP P38304
C	328	GLU	-	expression tag	UNP P38304
C	329	ALA	-	expression tag	UNP P38304
C	330	LYS	-	expression tag	UNP P38304
C	331	LYS	-	expression tag	UNP P38304
C	332	LEU	-	expression tag	UNP P38304
C	333	ASN	-	expression tag	UNP P38304
C	334	ASP	-	expression tag	UNP P38304
C	335	ALA	-	expression tag	UNP P38304
C	336	GLN	-	expression tag	UNP P38304
C	337	ALA	-	expression tag	UNP P38304
C	338	PRO	-	expression tag	UNP P38304
C	339	LYS	-	expression tag	UNP P38304
C	340	VAL	-	expression tag	UNP P38304
C	341	ASP	-	expression tag	UNP P38304
C	342	ASN	-	expression tag	UNP P38304
C	343	LYS	-	expression tag	UNP P38304
C	344	PHE	-	expression tag	UNP P38304
C	345	ASN	-	expression tag	UNP P38304
C	346	LYS	-	expression tag	UNP P38304
C	347	GLU	-	expression tag	UNP P38304
C	348	GLN	-	expression tag	UNP P38304
C	349	GLN	-	expression tag	UNP P38304
C	350	ASN	-	expression tag	UNP P38304
C	351	ALA	-	expression tag	UNP P38304
C	352	PHE	-	expression tag	UNP P38304
C	353	TYR	-	expression tag	UNP P38304
C	354	GLU	-	expression tag	UNP P38304
C	355	ILE	-	expression tag	UNP P38304
C	356	LEU	-	expression tag	UNP P38304
C	357	HIS	-	expression tag	UNP P38304
C	358	LEU	-	expression tag	UNP P38304
C	359	PRO	-	expression tag	UNP P38304
C	360	ASN	-	expression tag	UNP P38304
C	361	LEU	-	expression tag	UNP P38304
C	362	ASN	-	expression tag	UNP P38304
C	363	GLU	-	expression tag	UNP P38304

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Chain	Residue	Modelled	Actual	Comment	Reference
C	364	GLU	-	expression tag	UNP P38304
C	365	GLN	-	expression tag	UNP P38304
C	366	ARG	-	expression tag	UNP P38304
C	367	ASN	-	expression tag	UNP P38304
C	368	ALA	-	expression tag	UNP P38304
C	369	PHE	-	expression tag	UNP P38304
C	370	ILE	-	expression tag	UNP P38304
C	371	GLN	-	expression tag	UNP P38304
C	372	SER	-	expression tag	UNP P38304
C	373	LEU	-	expression tag	UNP P38304
C	374	LYS	-	expression tag	UNP P38304
C	375	ASP	-	expression tag	UNP P38304
C	376	ASP	-	expression tag	UNP P38304
C	377	PRO	-	expression tag	UNP P38304
C	378	SER	-	expression tag	UNP P38304
C	379	GLN	-	expression tag	UNP P38304
C	380	SER	-	expression tag	UNP P38304
C	381	ALA	-	expression tag	UNP P38304
C	382	ASN	-	expression tag	UNP P38304
C	383	LEU	-	expression tag	UNP P38304
C	384	LEU	-	expression tag	UNP P38304
C	385	ALA	-	expression tag	UNP P38304
C	386	GLU	-	expression tag	UNP P38304
C	387	ALA	-	expression tag	UNP P38304
C	388	LYS	-	expression tag	UNP P38304
C	389	LYS	-	expression tag	UNP P38304
C	390	LEU	-	expression tag	UNP P38304
C	391	ASN	-	expression tag	UNP P38304
C	392	GLY	-	expression tag	UNP P38304
C	393	ALA	-	expression tag	UNP P38304
C	394	GLN	-	expression tag	UNP P38304
C	395	ALA	-	expression tag	UNP P38304
C	396	PRO	-	expression tag	UNP P38304
C	397	LYS	-	expression tag	UNP P38304
C	398	VAL	-	expression tag	UNP P38304
C	399	ASP	-	expression tag	UNP P38304
C	400	ALA	-	expression tag	UNP P38304
C	401	ASN	-	expression tag	UNP P38304
C	402	SER	-	expression tag	UNP P38304
C	403	ALA	-	expression tag	UNP P38304
C	404	GLY	-	expression tag	UNP P38304
C	405	LYS	-	expression tag	UNP P38304

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Chain	Residue	Modelled	Actual	Comment	Reference
C	406	SER	-	expression tag	UNP P38304
C	407	THR	-	expression tag	UNP P38304

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	121	Total	C	N	O	0	0	0
			604	362	121	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	253	Total	C	N	O	S	0	0	0
			1979	1255	330	384	10			

- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 20.

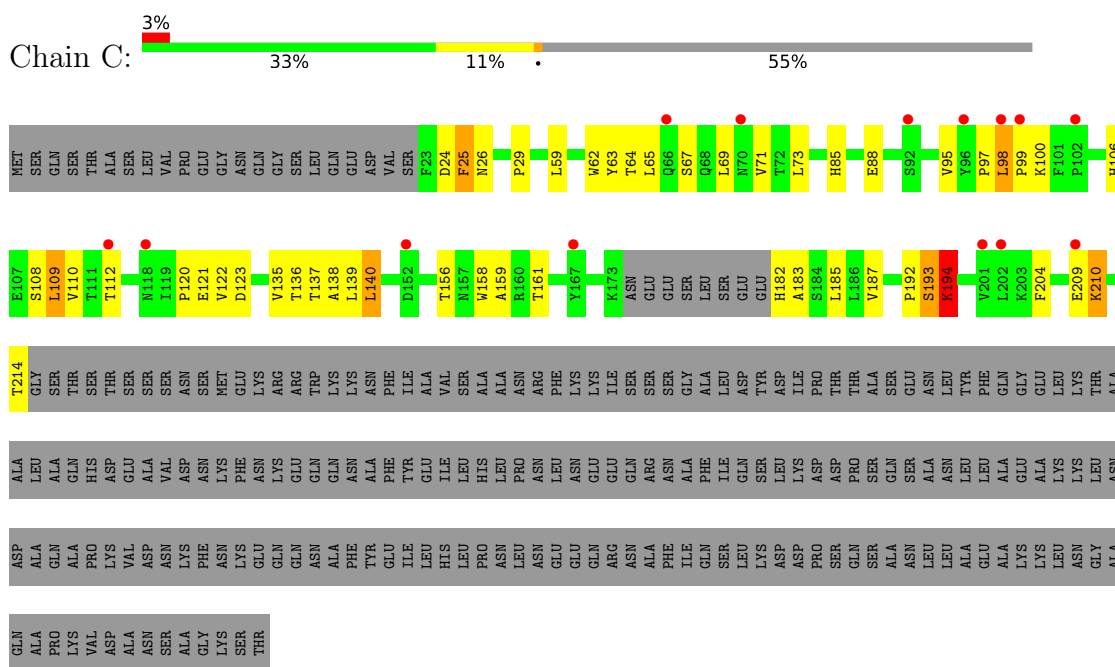
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	209	Total	C	N	O	S	0	0	0
			1600	1011	269	315	5			

- Molecule 7 is a protein called Mediator of RNA polymerase II transcription subunit 6.

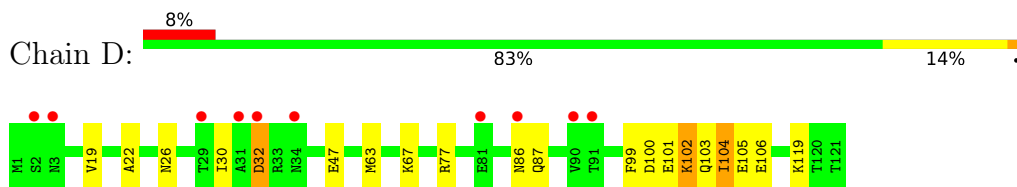
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	170	Total	C	N	O	0	0	0
			844	504	170	170			

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB1.

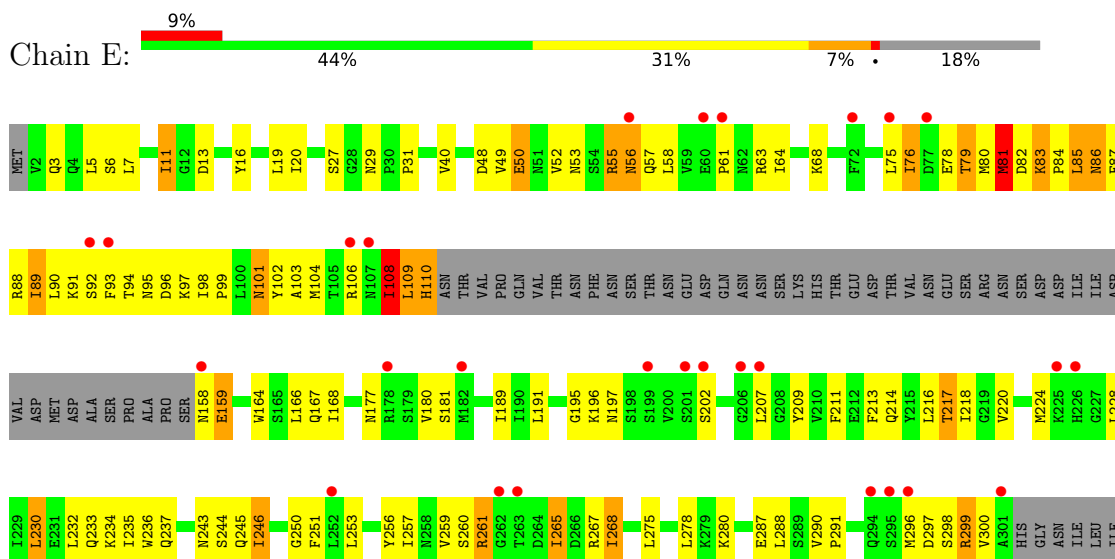
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	25	Total	C	N	O	0	0	0
			184	116	25	43			



- Molecule 4: Mediator of RNA polymerase II transcription subunit 22

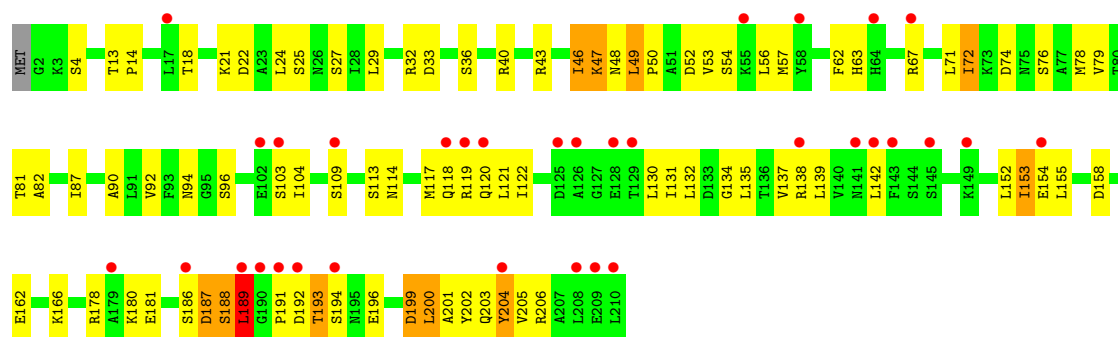


- Molecule 5: Mediator of RNA polymerase II transcription subunit 18

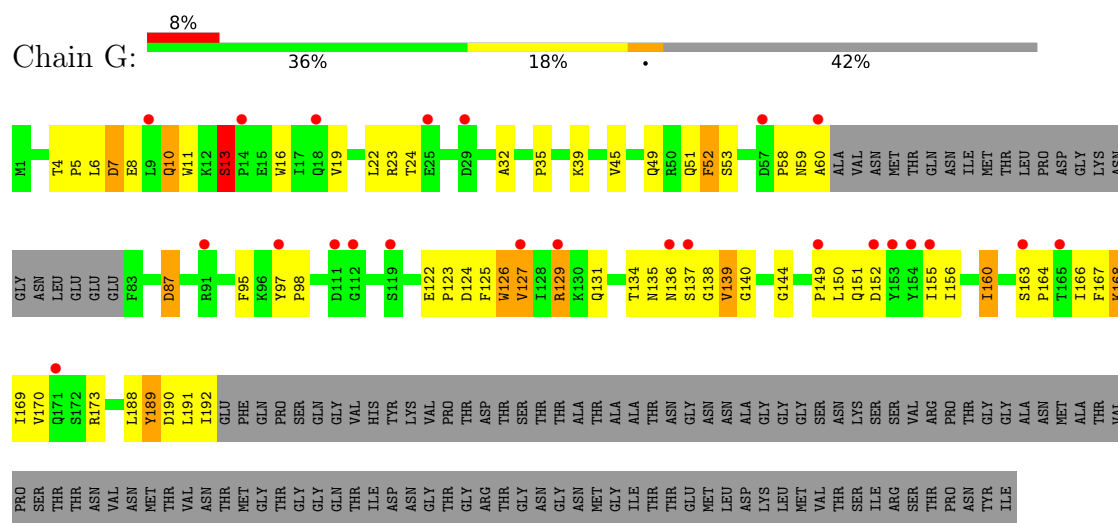


- Molecule 6: Mediator of RNA polymerase II transcription subunit 20

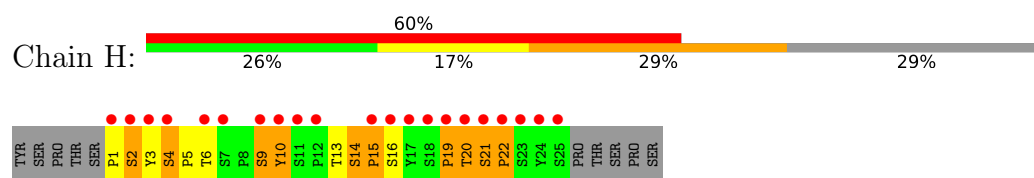




• Molecule 7: Mediator of RNA polymerase II transcription subunit 6



• Molecule 8: DNA-directed RNA polymerase II subunit RPB1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.45Å 142.45Å 305.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.00 – 4.50 45.00 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.00-4.50) 99.8 (45.00-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 4.45Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.286 , 0.345 0.291 , 0.353	Depositor DCC
R_{free} test set	1125 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	207.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 762.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.065 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9217	wwPDB-VP
Average B, all atoms (Å ²)	246.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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	A	0.79	0/555	1.39	6/773 (0.8%)
2	B	0.96	2/2443 (0.1%)	1.54	33/3407 (1.0%)
3	C	0.80	0/1008	1.48	10/1394 (0.7%)
4	D	0.80	0/603	1.31	0/842
5	E	0.67	0/2014	1.02	5/2728 (0.2%)
6	F	0.67	0/1626	0.99	3/2205 (0.1%)
7	G	1.00	2/842 (0.2%)	1.71	17/1172 (1.5%)
8	H	1.08	0/194	1.18	0/270
All	All	0.83	4/9285 (0.0%)	1.34	74/12791 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3
5	E	0	1
7	G	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	342	GLU	CA-C	9.46	1.60	1.52
2	B	343	ASP	N-CA	5.82	1.53	1.46
7	G	8	GLU	CA-C	5.48	1.55	1.52
7	G	126	TRP	N-CA	5.25	1.52	1.46

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	369	ILE	CA-C-N	18.59	143.08	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	369	ILE	C-N-CA	18.59	143.08	119.84
3	C	98	LEU	CA-C-N	15.67	139.42	119.84
3	C	98	LEU	C-N-CA	15.67	139.42	119.84
7	G	97	TYR	CA-C-N	15.08	138.69	119.84
7	G	97	TYR	C-N-CA	15.08	138.69	119.84
7	G	4	THR	CA-C-N	11.61	134.35	119.84
7	G	4	THR	C-N-CA	11.61	134.35	119.84
2	B	526	SER	CA-C-N	10.34	132.77	119.84
2	B	526	SER	C-N-CA	10.34	132.77	119.84
2	B	343	ASP	N-CA-C	9.88	121.64	111.07
3	C	210	LYS	CA-C-N	9.74	132.01	119.84
3	C	210	LYS	C-N-CA	9.74	132.01	119.84
2	B	342	GLU	N-CA-C	9.44	125.06	112.13
2	B	621	LEU	N-CA-C	8.04	115.45	108.22
2	B	612	ILE	CA-C-N	7.68	127.33	119.19
2	B	612	ILE	C-N-CA	7.68	127.33	119.19
7	G	13	SER	CA-C-N	7.62	129.37	119.84
7	G	13	SER	C-N-CA	7.62	129.37	119.84
7	G	39	LYS	N-CA-C	7.54	120.16	111.11
7	G	163	SER	CA-C-N	7.46	129.16	119.84
7	G	163	SER	C-N-CA	7.46	129.16	119.84
7	G	129	ARG	N-CA-C	7.29	120.15	109.07
7	G	87	ASP	CA-C-N	7.24	128.88	119.84
7	G	87	ASP	C-N-CA	7.24	128.88	119.84
7	G	127	VAL	N-CA-C	7.10	120.69	108.90
2	B	459	ILE	N-CA-C	7.06	118.03	107.51
7	G	139	VAL	N-CA-C	6.80	118.52	108.65
2	B	356	ASN	N-CA-C	6.79	120.24	108.76
2	B	457	VAL	N-CA-C	6.79	123.46	109.34
7	G	169	ILE	N-CA-C	-6.72	104.22	110.53
2	B	493	LEU	CA-C-N	6.71	128.23	119.84
2	B	493	LEU	C-N-CA	6.71	128.23	119.84
2	B	569	ILE	CA-C-N	6.62	126.78	120.43
2	B	569	ILE	C-N-CA	6.62	126.78	120.43
2	B	570	VAL	CB-CA-C	-6.49	107.54	113.70
2	B	623	LEU	N-CA-C	6.35	118.72	109.07
2	B	486	ILE	N-CA-C	6.35	117.94	108.23
2	B	533	LEU	N-CA-C	6.33	121.16	112.04
2	B	607	ASP	N-CA-C	6.14	117.64	111.07
6	F	46	ILE	N-CA-C	6.13	116.65	107.51
1	A	87	ASN	N-CA-C	6.09	119.48	109.85
1	A	45	LYS	CA-C-N	6.07	125.46	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	LYS	C-N-CA	6.07	125.46	118.85
3	C	193	SER	N-CA-C	5.92	118.81	110.23
2	B	570	VAL	N-CA-C	5.91	120.05	112.67
5	E	76	ILE	N-CA-C	5.90	117.50	108.71
3	C	26	ASN	N-CA-C	5.88	118.34	109.23
7	G	144	GLY	CA-C-N	5.84	125.98	119.32
7	G	144	GLY	C-N-CA	5.84	125.98	119.32
2	B	632	SER	N-CA-C	5.83	117.27	108.46
3	C	140	LEU	N-CA-C	5.81	123.17	110.80
2	B	338	LYS	N-CA-C	5.79	118.21	109.23
5	E	233	GLN	N-CA-C	5.70	118.35	109.52
1	A	65	GLN	N-CA-C	5.63	117.10	111.07
2	B	627	LYS	N-CA-C	-5.63	98.81	110.80
2	B	628	SER	N-CA-C	5.60	117.74	109.62
6	F	72	ILE	N-CA-C	5.57	116.02	107.77
1	A	91	LEU	N-CA-C	-5.55	106.50	113.72
2	B	339	TYR	N-CA-C	5.54	116.65	107.73
2	B	538	ASP	N-CA-C	-5.49	104.61	112.13
1	A	114	SER	N-CA-C	5.45	115.73	108.38
3	C	59	LEU	CA-C-N	5.35	125.11	119.76
3	C	59	LEU	C-N-CA	5.35	125.11	119.76
3	C	100	LYS	N-CA-C	5.35	115.10	108.19
2	B	612	ILE	CB-CA-C	-5.32	108.65	113.70
5	E	6	SER	N-CA-C	5.19	116.97	109.07
5	E	81	MET	N-CA-C	-5.18	104.89	111.11
6	F	194	SER	N-CA-C	-5.17	107.14	113.50
2	B	615	ARG	N-CA-C	5.16	121.80	110.80
2	B	279	TRP	N-CA-C	5.08	116.51	111.07
2	B	421	GLU	N-CA-C	5.06	117.43	110.35
5	E	85	LEU	N-CA-C	5.01	116.91	109.25
2	B	393	ILE	N-CA-C	5.00	115.06	107.75

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	471	ASN	Peptide
2	B	532	ASN	Peptide
2	B	626	HIS	Peptide
5	E	101	ASN	Peptide
7	G	10	GLN	Peptide

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	556	0	233	7	0
2	B	2446	0	1028	101	0
3	C	1004	0	562	23	0
4	D	604	0	265	12	0
5	E	1979	0	1977	232	0
6	F	1600	0	1614	99	0
7	G	844	0	355	32	0
8	H	184	0	163	24	0
All	All	9217	0	6197	502	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 33.

All (502) 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)
5:E:81:MET:CE	5:E:92:SER:HB3	1.25	1.61
5:E:81:MET:HE2	5:E:92:SER:CB	1.25	1.55
5:E:97:LYS:CE	5:E:243:ASN:HB3	1.37	1.50
6:F:72:ILE:HG21	6:F:202:TYR:CE1	1.52	1.41
5:E:97:LYS:HE2	5:E:243:ASN:CB	1.50	1.40
6:F:43:ARG:NH2	6:F:117:MET:HE1	1.40	1.33
5:E:97:LYS:CD	5:E:243:ASN:HB2	1.59	1.32
5:E:97:LYS:HZ2	5:E:244:SER:N	1.21	1.32
5:E:97:LYS:NZ	5:E:244:SER:N	1.73	1.32
5:E:106:ARG:HH21	5:E:214:GLN:CD	1.35	1.32
5:E:20:ILE:CD1	5:E:87:PHE:CE2	2.13	1.31
7:G:10:GLN:CB	7:G:160:ILE:O	1.79	1.29
5:E:16:TYR:CE2	5:E:87:PHE:HB3	1.53	1.29
5:E:75:LEU:O	5:E:98:ILE:HG23	1.12	1.26
5:E:75:LEU:O	5:E:98:ILE:CG2	1.83	1.26
5:E:16:TYR:HE2	5:E:87:PHE:CB	1.18	1.25
2:B:240:SER:HA	8:H:6:THR:OG1	1.29	1.25
5:E:97:LYS:CG	5:E:243:ASN:HB2	1.66	1.25
6:F:62:PHE:CZ	6:F:201:ALA:HB1	1.70	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:20:ILE:HD11	5:E:87:PHE:CE2	1.73	1.24
2:B:619:ILE:CB	2:B:634:MET:HA	1.67	1.23
5:E:97:LYS:CD	5:E:243:ASN:CB	2.16	1.23
5:E:97:LYS:CE	5:E:243:ASN:CB	2.11	1.22
5:E:97:LYS:HG2	5:E:243:ASN:CB	1.75	1.16
6:F:62:PHE:CE2	6:F:201:ALA:HB1	1.81	1.16
5:E:81:MET:HE2	5:E:92:SER:HB2	1.24	1.14
5:E:85:LEU:O	5:E:89:ILE:HG23	1.47	1.11
5:E:97:LYS:CG	5:E:243:ASN:CB	2.27	1.11
5:E:75:LEU:HA	5:E:98:ILE:HG21	1.20	1.10
5:E:106:ARG:NH2	5:E:214:GLN:OE1	1.85	1.09
2:B:315:SER:CB	2:B:425:ILE:CB	2.28	1.09
5:E:75:LEU:C	5:E:98:ILE:HG23	1.78	1.09
2:B:410:VAL:CB	2:B:502:ASN:HA	1.83	1.08
5:E:90:LEU:CD2	5:E:251:PHE:HE2	1.65	1.07
5:E:106:ARG:NH2	5:E:214:GLN:CD	2.13	1.06
6:F:43:ARG:HB2	6:F:119:ARG:HG3	1.36	1.06
5:E:86:ASN:HA	5:E:89:ILE:HG12	1.38	1.06
5:E:75:LEU:CA	5:E:98:ILE:HG21	1.87	1.05
5:E:86:ASN:ND2	5:E:87:PHE:CD1	2.25	1.05
2:B:410:VAL:CB	2:B:502:ASN:CA	2.34	1.05
2:B:321:VAL:CB	2:B:340:GLY:HA2	1.86	1.04
2:B:321:VAL:CB	2:B:340:GLY:CA	2.37	1.02
5:E:81:MET:CE	5:E:92:SER:CB	2.02	1.02
5:E:48:ASP:O	6:F:47:LYS:HE3	1.60	1.01
5:E:90:LEU:HD22	5:E:251:PHE:HE2	1.22	1.01
2:B:341:TYR:HA	2:B:354:ILE:CB	1.90	1.01
5:E:97:LYS:HZ2	5:E:244:SER:CA	1.73	1.01
5:E:81:MET:HE3	5:E:92:SER:HB3	1.42	1.01
5:E:97:LYS:HD3	5:E:243:ASN:HB2	1.38	1.00
5:E:75:LEU:HA	5:E:98:ILE:CG2	1.91	1.00
6:F:72:ILE:CG2	6:F:202:TYR:CE1	2.44	1.00
8:H:21:SER:H	8:H:22:PRO:HD3	1.23	1.00
6:F:62:PHE:CZ	6:F:201:ALA:CB	2.45	0.98
5:E:97:LYS:NZ	5:E:244:SER:H	1.59	0.98
5:E:98:ILE:HG23	5:E:99:PRO:HD2	1.43	0.98
5:E:16:TYR:HE2	5:E:87:PHE:HB3	0.86	0.98
5:E:90:LEU:CD2	5:E:251:PHE:CE2	2.47	0.97
5:E:106:ARG:NH2	5:E:211:PHE:CZ	2.33	0.97
5:E:75:LEU:HB3	5:E:98:ILE:HD13	1.47	0.96
7:G:129:ARG:CB	7:G:134:THR:CB	2.42	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:98:ILE:CG2	5:E:99:PRO:HD2	1.94	0.96
2:B:323:PHE:CB	2:B:339:TYR:O	2.14	0.96
6:F:4:SER:HB2	6:F:200:LEU:HD23	1.47	0.95
5:E:20:ILE:HD12	5:E:87:PHE:CE2	1.97	0.95
5:E:20:ILE:HD11	5:E:87:PHE:HE2	1.20	0.95
5:E:97:LYS:HZ3	5:E:244:SER:H	1.10	0.94
6:F:43:ARG:NH2	6:F:117:MET:CE	2.30	0.94
5:E:20:ILE:HD12	5:E:87:PHE:CZ	2.02	0.94
5:E:79:THR:O	5:E:82:ASP:HB2	1.68	0.93
3:C:183:ALA:O	3:C:187:VAL:HG23	1.70	0.92
5:E:75:LEU:C	5:E:98:ILE:CG2	2.38	0.92
5:E:86:ASN:ND2	5:E:87:PHE:CE1	2.35	0.91
5:E:85:LEU:HD12	5:E:88:ARG:HB3	1.52	0.91
5:E:97:LYS:HG2	5:E:243:ASN:CG	1.94	0.91
5:E:108:ILE:HD13	5:E:159:GLU:HB2	1.51	0.91
1:A:93:GLN:HA	2:B:345:GLY:H	1.35	0.90
6:F:4:SER:HB2	6:F:200:LEU:CD2	2.00	0.90
2:B:240:SER:HA	8:H:6:THR:CB	2.02	0.89
5:E:20:ILE:HG13	5:E:87:PHE:CD2	2.08	0.89
5:E:90:LEU:HD22	5:E:251:PHE:CE2	2.07	0.88
8:H:4:SER:HB2	8:H:5:PRO:HD3	1.54	0.88
6:F:142:LEU:HD11	6:F:152:LEU:HD12	1.54	0.88
5:E:16:TYR:HE2	5:E:87:PHE:CA	1.87	0.87
2:B:394:PHE:HA	2:B:407:GLY:HA2	1.55	0.85
5:E:16:TYR:CD2	5:E:87:PHE:HB3	2.11	0.85
5:E:85:LEU:CD1	5:E:88:ARG:H	1.90	0.85
5:E:86:ASN:O	5:E:89:ILE:HG13	1.75	0.85
2:B:240:SER:CA	8:H:6:THR:OG1	2.21	0.84
5:E:90:LEU:HD23	5:E:251:PHE:CE2	2.10	0.84
2:B:410:VAL:CB	2:B:502:ASN:N	2.40	0.84
5:E:61:PRO:HG2	5:E:300:VAL:CG2	2.07	0.84
5:E:97:LYS:HG2	5:E:243:ASN:ND2	1.92	0.83
6:F:72:ILE:CG2	6:F:202:TYR:HE1	1.86	0.83
6:F:43:ARG:CZ	6:F:117:MET:HE1	2.08	0.83
5:E:61:PRO:HG2	5:E:300:VAL:HG21	1.60	0.83
5:E:97:LYS:HZ3	5:E:244:SER:N	1.64	0.83
5:E:108:ILE:HG21	5:E:159:GLU:CB	2.08	0.83
5:E:16:TYR:CE2	5:E:87:PHE:CB	2.06	0.82
7:G:45:VAL:O	7:G:49:GLN:N	2.12	0.82
2:B:541:ILE:O	2:B:545:ILE:CB	2.28	0.82
6:F:62:PHE:HZ	6:F:201:ALA:HB1	1.42	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:193:THR:HG22	6:F:196:GLU:HA	1.61	0.81
6:F:46:ILE:HA	6:F:47:LYS:HZ3	1.44	0.81
2:B:362:GLU:O	2:B:423:LYS:HA	1.81	0.80
5:E:27:SER:HB3	5:E:224:MET:HE2	1.62	0.80
2:B:241:MET:CB	8:H:10:TYR:CZ	2.64	0.80
5:E:75:LEU:CA	5:E:98:ILE:CG2	2.54	0.80
8:H:3:TYR:CE1	8:H:5:PRO:HD2	2.16	0.80
2:B:321:VAL:CB	2:B:340:GLY:HA3	2.10	0.79
5:E:97:LYS:HE3	5:E:236:TRP:HB3	1.64	0.79
5:E:265:ILE:HD12	5:E:265:ILE:H	1.45	0.79
6:F:4:SER:CB	6:F:200:LEU:HD23	2.13	0.78
5:E:78:GLU:OE1	5:E:80:MET:HB3	1.83	0.78
5:E:76:ILE:HG23	5:E:93:PHE:HZ	1.49	0.78
2:B:543:ARG:O	2:B:545:ILE:N	2.16	0.78
5:E:97:LYS:NZ	5:E:243:ASN:C	2.41	0.78
2:B:388:PHE:O	2:B:484:ASP:CB	2.33	0.77
5:E:76:ILE:HG23	5:E:93:PHE:CZ	2.18	0.77
4:D:103:GLN:O	4:D:106:GLU:N	2.17	0.77
2:B:380:ASP:O	2:B:383:HIS:O	2.03	0.77
2:B:241:MET:CB	8:H:10:TYR:CE1	2.68	0.76
2:B:341:TYR:CB	2:B:354:ILE:N	2.48	0.76
6:F:130:LEU:HB2	6:F:137:VAL:HG13	1.67	0.76
6:F:4:SER:OG	6:F:200:LEU:HB2	1.85	0.76
5:E:108:ILE:HG21	5:E:159:GLU:HB3	1.66	0.76
5:E:106:ARG:HH21	5:E:214:GLN:CG	1.98	0.76
5:E:97:LYS:HD3	5:E:243:ASN:C	2.10	0.75
6:F:47:LYS:HZ3	6:F:47:LYS:H	1.34	0.75
8:H:21:SER:H	8:H:22:PRO:CD	1.99	0.75
5:E:106:ARG:CZ	5:E:211:PHE:CZ	2.70	0.75
2:B:479:LEU:O	2:B:482:ASP:N	2.19	0.75
7:G:139:VAL:CB	7:G:152:ASP:CB	2.64	0.75
5:E:98:ILE:CG2	5:E:99:PRO:CD	2.65	0.75
6:F:72:ILE:HG21	6:F:202:TYR:HE1	0.95	0.74
2:B:471:ASN:O	2:B:472:GLU:O	2.05	0.74
5:E:97:LYS:HZ2	5:E:243:ASN:C	1.93	0.74
8:H:19:PRO:O	8:H:20:THR:OG1	2.04	0.74
5:E:97:LYS:NZ	5:E:244:SER:C	2.46	0.74
5:E:97:LYS:CB	5:E:243:ASN:HD22	2.01	0.73
7:G:139:VAL:HA	7:G:152:ASP:CB	2.19	0.73
6:F:193:THR:CG2	6:F:196:GLU:HA	2.18	0.73
3:C:120:PRO:C	3:C:122:VAL:H	1.95	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:261:ARG:HD3	5:E:267:ARG:HH21	1.54	0.73
6:F:62:PHE:CE2	6:F:201:ALA:CB	2.65	0.73
5:E:98:ILE:HG22	5:E:99:PRO:CD	2.18	0.72
7:G:22:LEU:O	7:G:24:THR:N	2.22	0.72
5:E:86:ASN:CA	5:E:89:ILE:HG12	2.18	0.72
8:H:4:SER:HB2	8:H:5:PRO:CD	2.19	0.72
5:E:20:ILE:CG1	5:E:87:PHE:CE2	2.72	0.72
5:E:191:LEU:HD11	6:F:81:THR:HB	1.71	0.72
5:E:86:ASN:CG	5:E:220:VAL:HG11	2.14	0.71
5:E:86:ASN:HD22	5:E:87:PHE:N	1.89	0.71
5:E:195:GLY:HA3	6:F:76:SER:HA	1.70	0.71
5:E:86:ASN:OD1	5:E:220:VAL:CG1	2.39	0.70
5:E:7:LEU:HB3	5:E:288:LEU:HB3	1.73	0.70
2:B:619:ILE:CB	2:B:634:MET:CA	2.60	0.70
3:C:62:TRP:O	3:C:65:LEU:N	2.25	0.70
6:F:109:SER:O	6:F:113:SER:HB3	1.91	0.70
5:E:85:LEU:O	5:E:89:ILE:CG2	2.34	0.69
6:F:46:ILE:HA	6:F:47:LYS:NZ	2.07	0.69
6:F:4:SER:CB	6:F:200:LEU:HG	2.22	0.69
5:E:48:ASP:O	6:F:47:LYS:CE	2.40	0.69
7:G:139:VAL:CA	7:G:152:ASP:CB	2.71	0.69
3:C:120:PRO:C	3:C:122:VAL:N	2.49	0.68
6:F:43:ARG:HB2	6:F:119:ARG:CG	2.20	0.68
8:H:4:SER:CB	8:H:5:PRO:HD3	2.22	0.68
7:G:59:ASN:O	7:G:60:ALA:HB2	1.95	0.67
5:E:97:LYS:HB3	5:E:243:ASN:HD22	1.60	0.67
6:F:54:SER:HG	6:F:74:ASP:CG	2.02	0.67
5:E:298:SER:O	5:E:299:ARG:O	2.13	0.67
2:B:380:ASP:O	2:B:381:PHE:C	2.38	0.66
5:E:49:VAL:HG21	6:F:114:ASN:O	1.95	0.66
5:E:16:TYR:CE2	5:E:87:PHE:CA	2.69	0.66
5:E:106:ARG:NH2	5:E:211:PHE:HZ	1.88	0.66
5:E:224:MET:HE1	5:E:230:LEU:HD12	1.78	0.66
8:H:3:TYR:CD1	8:H:5:PRO:HD2	2.30	0.66
7:G:140:GLY:O	7:G:150:LEU:HA	1.95	0.66
5:E:20:ILE:CG1	5:E:87:PHE:CD2	2.78	0.66
5:E:86:ASN:CG	5:E:220:VAL:CG1	2.69	0.66
5:E:97:LYS:HE2	5:E:243:ASN:CA	2.26	0.65
2:B:183:GLU:H	4:D:77:ARG:CB	2.09	0.65
5:E:108:ILE:HG22	5:E:109:LEU:H	1.61	0.65
5:E:3:GLN:HB2	5:E:259:VAL:CG2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:HIS:HA	3:C:88:GLU:CB	2.27	0.65
6:F:53:VAL:HG12	6:F:54:SER:H	1.62	0.65
5:E:81:MET:HE1	5:E:92:SER:HB3	1.62	0.64
6:F:13:THR:HB	6:F:14:PRO:HD2	1.77	0.64
5:E:97:LYS:NZ	5:E:244:SER:CA	2.47	0.64
5:E:86:ASN:O	5:E:89:ILE:CG1	2.45	0.64
5:E:86:ASN:HD22	5:E:87:PHE:H	1.44	0.64
5:E:3:GLN:HB2	5:E:259:VAL:HG22	1.80	0.64
2:B:323:PHE:O	2:B:339:TYR:N	2.30	0.63
6:F:186:SER:O	6:F:187:ASP:HB2	1.98	0.63
5:E:97:LYS:HZ2	5:E:244:SER:C	2.04	0.63
5:E:86:ASN:OD1	5:E:220:VAL:HG12	1.98	0.62
5:E:97:LYS:CE	5:E:243:ASN:CA	2.76	0.62
6:F:187:ASP:OD1	6:F:203:GLN:HG2	1.99	0.62
8:H:3:TYR:O	8:H:4:SER:OG	2.13	0.62
3:C:85:HIS:O	3:C:88:GLU:CB	2.47	0.62
2:B:410:VAL:CB	2:B:502:ASN:CB	2.77	0.62
5:E:64:ILE:HD13	5:E:209:TYR:CE2	2.35	0.62
8:H:1:PRO:O	8:H:2:SER:OG	2.17	0.62
3:C:69:LEU:O	3:C:73:LEU:CB	2.47	0.62
6:F:134:GLY:O	6:F:166:LYS:NZ	2.25	0.62
5:E:52:VAL:HA	5:E:57:GLN:O	2.00	0.62
5:E:97:LYS:HD3	5:E:243:ASN:CB	2.07	0.62
8:H:3:TYR:HE1	8:H:5:PRO:HD2	1.64	0.62
8:H:21:SER:N	8:H:22:PRO:HD3	2.06	0.62
5:E:83:LYS:HG3	5:E:84:PRO:HD2	1.82	0.62
5:E:86:ASN:HA	5:E:89:ILE:CG1	2.24	0.62
6:F:189:LEU:HD13	6:F:189:LEU:H	1.64	0.62
6:F:4:SER:CB	6:F:200:LEU:CG	2.78	0.61
2:B:316:ILE:H	2:B:425:ILE:CB	2.13	0.61
6:F:43:ARG:HH21	6:F:117:MET:HE1	1.56	0.61
2:B:408:GLU:CB	2:B:497:ASN:CB	2.78	0.61
2:B:191:ILE:C	2:B:193:THR:H	2.08	0.61
5:E:104:MET:O	5:E:108:ILE:O	2.18	0.61
6:F:32:ARG:HG2	6:F:33:ASP:H	1.66	0.61
5:E:50:GLU:CD	5:E:50:GLU:H	2.06	0.61
6:F:57:MET:SD	6:F:71:LEU:HD23	2.40	0.61
5:E:16:TYR:CE2	5:E:87:PHE:HA	2.36	0.60
5:E:228:LEU:HD21	5:E:278:LEU:HD22	1.83	0.60
5:E:5:LEU:HA	5:E:181:SER:O	2.00	0.60
5:E:85:LEU:HD13	5:E:88:ARG:H	1.63	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:98:ILE:HD11	5:E:218:ILE:HD11	1.84	0.60
5:E:79:THR:O	5:E:82:ASP:CB	2.46	0.60
6:F:43:ARG:HH22	6:F:117:MET:HE1	1.60	0.60
7:G:126:TRP:O	7:G:137:SER:N	2.33	0.60
2:B:392:ARG:O	2:B:476:ILE:N	2.35	0.60
6:F:72:ILE:HG21	6:F:202:TYR:CZ	2.26	0.60
7:G:127:VAL:HA	7:G:136:ASN:HA	1.84	0.60
3:C:67:SER:O	3:C:71:VAL:CB	2.50	0.59
6:F:90:ALA:O	6:F:94:ASN:OD1	2.20	0.59
2:B:192:GLU:HA	7:G:192:ILE:C	2.27	0.59
2:B:629:PRO:HA	2:B:650:SER:HA	1.83	0.59
2:B:425:ILE:O	2:B:429:ILE:N	2.35	0.59
2:B:631:LEU:HA	2:B:648:LYS:HA	1.83	0.59
5:E:98:ILE:HG22	5:E:99:PRO:N	2.15	0.59
2:B:229:LEU:O	2:B:234:GLU:CB	2.50	0.59
5:E:97:LYS:NZ	5:E:244:SER:O	2.33	0.59
1:A:41:ASN:C	1:A:43:SER:H	2.10	0.59
7:G:136:ASN:N	7:G:155:ILE:O	2.23	0.59
2:B:478:LEU:CB	2:B:483:ASP:HA	2.33	0.59
6:F:4:SER:HB2	6:F:200:LEU:CG	2.33	0.59
6:F:200:LEU:O	6:F:200:LEU:HD22	2.03	0.59
3:C:158:TRP:O	3:C:161:THR:N	2.35	0.59
5:E:167:GLN:NE2	6:F:96:SER:O	2.36	0.58
7:G:188:LEU:C	7:G:190:ASP:H	2.11	0.58
2:B:218:SER:O	2:B:221:ALA:HB3	2.04	0.58
7:G:125:PHE:HA	7:G:138:GLY:HA2	1.85	0.58
6:F:47:LYS:HD2	6:F:48:ASN:N	2.19	0.58
7:G:126:TRP:N	7:G:137:SER:O	2.35	0.58
2:B:229:LEU:CB	2:B:250:LYS:CB	2.82	0.58
6:F:199:ASP:O	6:F:202:TYR:HB3	2.03	0.58
2:B:408:GLU:CB	2:B:498:ASP:N	2.67	0.57
7:G:135:ASN:HA	7:G:156:ILE:HA	1.87	0.57
2:B:543:ARG:C	2:B:545:ILE:H	2.12	0.57
6:F:4:SER:HB2	6:F:200:LEU:HG	1.87	0.57
7:G:11:TRP:CB	7:G:32:ALA:HA	2.35	0.57
2:B:341:TYR:CB	2:B:354:ILE:H	2.18	0.57
2:B:469:LEU:O	2:B:472:GLU:HA	2.04	0.57
5:E:55:ARG:O	5:E:57:GLN:HG3	2.03	0.57
5:E:63:ARG:NH1	5:E:299:ARG:O	2.37	0.57
5:E:75:LEU:O	5:E:98:ILE:HG12	2.05	0.57
6:F:4:SER:CB	6:F:200:LEU:CD2	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:20:ILE:HG13	5:E:87:PHE:CE2	2.35	0.56
6:F:40:ARG:HD3	6:F:118:GLN:NE2	2.20	0.56
6:F:62:PHE:HE2	6:F:201:ALA:HB1	1.64	0.56
6:F:47:LYS:H	6:F:47:LYS:NZ	2.02	0.56
5:E:91:LYS:O	5:E:94:THR:HG22	2.05	0.56
2:B:471:ASN:O	2:B:472:GLU:C	2.48	0.56
6:F:4:SER:OG	6:F:200:LEU:CB	2.54	0.56
5:E:81:MET:HE1	5:E:92:SER:CB	2.23	0.56
5:E:86:ASN:OD1	5:E:220:VAL:HG11	2.02	0.56
5:E:108:ILE:HD13	5:E:159:GLU:CD	2.31	0.56
2:B:363:SER:HA	2:B:423:LYS:H	1.70	0.55
5:E:85:LEU:HD12	5:E:88:ARG:CB	2.32	0.55
3:C:95:VAL:HA	7:G:166:ILE:HA	1.87	0.55
6:F:135:LEU:HD22	6:F:166:LYS:HB3	1.88	0.55
2:B:238:MET:C	2:B:240:SER:H	2.14	0.55
5:E:97:LYS:CE	5:E:243:ASN:C	2.79	0.55
5:E:106:ARG:CZ	5:E:214:GLN:OE1	2.53	0.55
5:E:108:ILE:O	5:E:109:LEU:HB3	2.06	0.55
2:B:402:ASP:O	2:B:404:ILE:N	2.40	0.54
5:E:85:LEU:CD1	5:E:88:ARG:HB3	2.30	0.54
5:E:86:ASN:O	5:E:90:LEU:HD13	2.07	0.54
3:C:156:THR:O	3:C:159:ALA:HB3	2.08	0.54
5:E:106:ARG:NH2	5:E:214:GLN:CG	2.64	0.54
2:B:183:GLU:N	4:D:77:ARG:CB	2.71	0.54
5:E:97:LYS:CB	5:E:243:ASN:HB2	2.34	0.54
5:E:97:LYS:HG2	5:E:243:ASN:HD22	1.73	0.54
5:E:53:ASN:ND2	5:E:57:GLN:HB2	2.23	0.54
5:E:106:ARG:CZ	5:E:211:PHE:CE2	2.90	0.53
2:B:238:MET:C	2:B:240:SER:N	2.65	0.53
7:G:13:SER:HA	7:G:16:TRP:CB	2.38	0.53
5:E:108:ILE:HG21	5:E:159:GLU:CG	2.38	0.53
5:E:31:PRO:HG3	5:E:87:PHE:CE1	2.43	0.53
2:B:593:ASP:CB	2:B:600:ASN:CB	2.86	0.53
2:B:630:ASN:N	2:B:649:PHE:O	2.41	0.53
5:E:75:LEU:O	5:E:98:ILE:CG1	2.56	0.53
4:D:103:GLN:O	4:D:105:GLU:N	2.42	0.53
5:E:97:LYS:HE2	5:E:243:ASN:HB3	0.60	0.53
1:A:92:GLY:C	2:B:344:SER:CB	2.83	0.52
7:G:140:GLY:N	7:G:151:GLN:O	2.41	0.52
5:E:259:VAL:HG21	5:E:268:ILE:CD1	2.39	0.52
6:F:4:SER:HA	6:F:155:LEU:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:203:GLN:O	6:F:205:VAL:N	2.42	0.52
6:F:203:GLN:O	6:F:206:ARG:N	2.41	0.52
6:F:36:SER:HB3	6:F:63:HIS:CD2	2.45	0.52
2:B:362:GLU:O	2:B:423:LYS:CA	2.56	0.52
2:B:380:ASP:O	2:B:383:HIS:C	2.52	0.52
4:D:101:GLU:O	4:D:102:LYS:CB	2.57	0.52
5:E:75:LEU:O	5:E:98:ILE:CB	2.56	0.52
5:E:97:LYS:NZ	5:E:237:GLN:O	2.43	0.52
6:F:49:LEU:HD11	6:F:53:VAL:HB	1.91	0.52
5:E:97:LYS:HD3	5:E:243:ASN:O	2.09	0.52
5:E:64:ILE:HD13	5:E:209:TYR:CZ	2.45	0.52
5:E:197:ASN:HB3	5:E:202:SER:HB3	1.92	0.51
6:F:62:PHE:HZ	6:F:201:ALA:CB	2.08	0.51
2:B:365:ASN:HA	2:B:381:PHE:HA	1.92	0.51
2:B:380:ASP:CB	2:B:384:SER:CB	2.88	0.51
8:H:14:SER:HB3	8:H:15:PRO:CD	2.41	0.51
3:C:193:SER:O	3:C:194:LYS:HB3	2.11	0.51
5:E:97:LYS:CG	5:E:243:ASN:HD22	2.23	0.51
5:E:31:PRO:HB2	5:E:220:VAL:HB	1.92	0.51
5:E:109:LEU:HG	5:E:110:HIS:N	2.26	0.51
6:F:43:ARG:CZ	6:F:117:MET:CE	2.84	0.51
2:B:325:ILE:N	2:B:337:ILE:O	2.37	0.51
2:B:380:ASP:O	2:B:383:HIS:N	2.44	0.51
1:A:83:PRO:CB	4:D:87:GLN:HA	2.41	0.51
5:E:81:MET:HG3	5:E:88:ARG:NH2	2.26	0.51
2:B:566:VAL:O	2:B:569:ILE:CB	2.59	0.50
3:C:120:PRO:O	3:C:122:VAL:N	2.44	0.50
5:E:87:PHE:CE2	5:E:220:VAL:HG21	2.45	0.50
7:G:166:ILE:O	7:G:170:VAL:N	2.43	0.50
5:E:11:ILE:HG12	5:E:19:LEU:CD2	2.41	0.50
6:F:162:GLU:OE1	6:F:162:GLU:HA	2.11	0.50
5:E:97:LYS:HZ1	5:E:244:SER:C	2.15	0.50
2:B:390:ARG:CB	2:B:484:ASP:CB	2.89	0.50
4:D:63:MET:O	4:D:67:LYS:CB	2.59	0.50
5:E:108:ILE:HG21	5:E:159:GLU:HG2	1.94	0.50
5:E:68:LYS:HG2	5:E:164:TRP:CZ3	2.47	0.50
2:B:387:LYS:HA	2:B:484:ASP:O	2.12	0.50
2:B:348:TYR:O	2:B:349:LYS:CB	2.60	0.50
5:E:97:LYS:CD	5:E:243:ASN:HB3	1.99	0.50
2:B:398:GLU:O	2:B:401:ASP:CB	2.60	0.50
6:F:199:ASP:O	6:F:203:GLN:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:97:LYS:CD	5:E:243:ASN:C	2.80	0.49
7:G:59:ASN:O	7:G:60:ALA:CB	2.60	0.49
5:E:108:ILE:HD13	5:E:159:GLU:CB	2.33	0.49
2:B:238:MET:O	2:B:240:SER:N	2.45	0.49
5:E:89:ILE:HG13	5:E:90:LEU:N	2.28	0.49
2:B:566:VAL:HA	2:B:569:ILE:CB	2.43	0.49
2:B:579:GLU:O	2:B:583:GLU:N	2.41	0.49
5:E:13:ASP:OD1	5:E:250:GLY:HA2	2.12	0.49
5:E:189:ILE:HG12	6:F:87:ILE:HG23	1.94	0.49
6:F:203:GLN:O	6:F:204:TYR:C	2.55	0.49
3:C:109:LEU:O	3:C:112:THR:N	2.45	0.48
1:A:93:GLN:N	2:B:344:SER:CB	2.77	0.48
2:B:340:GLY:O	2:B:354:ILE:CB	2.62	0.48
5:E:101:ASN:O	5:E:103:ALA:N	2.46	0.48
6:F:47:LYS:H	6:F:47:LYS:CE	2.26	0.48
2:B:393:ILE:O	2:B:408:GLU:N	2.42	0.48
2:B:566:VAL:C	2:B:569:ILE:H	2.21	0.48
5:E:20:ILE:HG13	5:E:87:PHE:CG	2.46	0.48
5:E:108:ILE:O	5:E:109:LEU:CB	2.61	0.48
6:F:142:LEU:HD11	6:F:152:LEU:CD1	2.35	0.48
5:E:85:LEU:HD11	5:E:88:ARG:H	1.73	0.48
2:B:632:SER:O	2:B:647:ILE:N	2.42	0.48
5:E:224:MET:CE	5:E:230:LEU:HD12	2.44	0.48
2:B:196:THR:CB	2:B:200:PHE:CB	2.91	0.48
4:D:103:GLN:O	4:D:104:ILE:C	2.56	0.48
5:E:256:TYR:O	5:E:257:ILE:HG13	2.14	0.48
6:F:18:THR:HA	6:F:21:LYS:HB3	1.96	0.48
8:H:14:SER:HB3	8:H:15:PRO:HD2	1.95	0.47
2:B:380:ASP:O	2:B:381:PHE:O	2.31	0.47
2:B:582:ARG:O	2:B:585:PRO:O	2.33	0.47
3:C:24:ASP:O	3:C:25:PHE:CB	2.62	0.47
3:C:204:PHE:HA	3:C:209:GLU:O	2.14	0.47
6:F:47:LYS:HZ3	6:F:47:LYS:N	2.05	0.47
8:H:21:SER:N	8:H:22:PRO:CD	2.70	0.47
5:E:299:ARG:HG2	5:E:300:VAL:H	1.78	0.47
3:C:106:HIS:C	3:C:108:SER:H	2.21	0.47
6:F:22:ASP:C	6:F:24:LEU:H	2.23	0.47
2:B:410:VAL:CB	2:B:501:ALA:C	2.87	0.47
2:B:597:THR:CB	5:E:84:PRO:CB	2.93	0.47
5:E:27:SER:HB2	5:E:224:MET:HG2	1.96	0.47
6:F:22:ASP:HA	6:F:25:SER:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:188:LEU:C	7:G:190:ASP:N	2.73	0.47
6:F:29:LEU:HB3	6:F:131:ILE:O	2.15	0.46
5:E:256:TYR:C	5:E:257:ILE:HG13	2.40	0.46
7:G:124:ASP:O	7:G:138:GLY:HA2	2.14	0.46
7:G:189:TYR:C	7:G:191:LEU:H	2.23	0.46
8:H:15:PRO:O	8:H:16:SER:HB2	2.15	0.46
5:E:291:PRO:HG2	5:E:296:MET:SD	2.56	0.46
6:F:200:LEU:HD22	6:F:200:LEU:C	2.41	0.46
2:B:479:LEU:C	2:B:481:LEU:N	2.73	0.46
5:E:55:ARG:O	5:E:56:ASN:C	2.59	0.46
5:E:79:THR:O	5:E:82:ASP:N	2.49	0.46
5:E:98:ILE:HD11	5:E:218:ILE:CD1	2.46	0.46
7:G:6:LEU:O	7:G:7:ASP:O	2.33	0.46
7:G:129:ARG:CA	7:G:134:THR:CB	2.93	0.46
5:E:82:ASP:CG	5:E:83:LYS:H	2.24	0.46
5:E:158:ASN:C	5:E:159:GLU:HG3	2.41	0.46
6:F:178:ARG:HA	6:F:180:LYS:HE2	1.97	0.46
8:H:4:SER:CB	8:H:5:PRO:CD	2.86	0.46
5:E:40:VAL:HG21	5:E:213:PHE:CZ	2.51	0.46
5:E:232:LEU:HD21	5:E:253:LEU:HD13	1.97	0.46
5:E:81:MET:CE	5:E:92:SER:HB2	2.08	0.45
4:D:103:GLN:C	4:D:105:GLU:N	2.73	0.45
5:E:234:LYS:HE2	5:E:251:PHE:CZ	2.52	0.45
3:C:182:HIS:HB2	3:C:185:LEU:HB2	1.97	0.45
6:F:138:ARG:HB2	6:F:154:GLU:HB3	1.99	0.45
6:F:49:LEU:HA	6:F:50:PRO:HD3	1.82	0.45
2:B:494:PRO:O	2:B:495:LYS:CB	2.64	0.45
5:E:31:PRO:HG3	5:E:87:PHE:HE1	1.82	0.45
6:F:27:SER:O	6:F:132:LEU:HD21	2.16	0.45
6:F:46:ILE:HD13	6:F:47:LYS:HZ1	1.82	0.45
4:D:22:ALA:O	4:D:26:ASN:CB	2.65	0.45
7:G:51:GLN:O	7:G:52:PHE:C	2.59	0.45
2:B:394:PHE:CA	2:B:407:GLY:HA2	2.37	0.45
5:E:87:PHE:CZ	5:E:220:VAL:HG21	2.52	0.45
5:E:259:VAL:HG21	5:E:268:ILE:HD11	1.98	0.45
5:E:196:LYS:NZ	6:F:74:ASP:O	2.50	0.44
6:F:72:ILE:HD11	6:F:202:TYR:HB2	1.85	0.44
2:B:618:LYS:O	2:B:619:ILE:CB	2.65	0.44
5:E:98:ILE:O	5:E:99:PRO:C	2.60	0.44
6:F:120:GLN:CD	6:F:122:ILE:HD11	2.43	0.44
4:D:99:PHE:C	4:D:101:GLU:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLN:CA	2:B:345:GLY:H	2.18	0.44
2:B:581:GLU:CB	2:B:618:LYS:O	2.64	0.44
2:B:625:GLU:O	2:B:626:HIS:CB	2.65	0.44
6:F:54:SER:OG	6:F:74:ASP:OD1	2.33	0.44
7:G:167:PHE:O	7:G:168:LYS:CB	2.66	0.44
6:F:200:LEU:HD13	6:F:201:ALA:N	2.33	0.44
6:F:139:LEU:HD23	6:F:153:ILE:HG23	1.98	0.43
2:B:419:GLU:O	2:B:420:ALA:C	2.61	0.43
5:E:86:ASN:C	5:E:89:ILE:HG12	2.43	0.43
6:F:82:ALA:HB2	6:F:103:SER:HA	1.99	0.43
1:A:93:GLN:HA	2:B:344:SER:CB	2.48	0.43
5:E:11:ILE:HG12	5:E:19:LEU:HD22	2.00	0.43
5:E:98:ILE:HD12	5:E:216:LEU:CD2	2.48	0.43
6:F:22:ASP:C	6:F:24:LEU:N	2.74	0.43
5:E:297:ASP:OD2	5:E:299:ARG:NH1	2.52	0.43
2:B:341:TYR:CA	2:B:354:ILE:CB	2.80	0.43
5:E:94:THR:HA	5:E:245:GLN:HE22	1.84	0.43
2:B:252:SER:HA	3:C:98:LEU:HA	2.00	0.43
2:B:596:ILE:O	2:B:600:ASN:CB	2.67	0.43
6:F:71:LEU:HD11	6:F:104:ILE:HG12	2.01	0.43
5:E:78:GLU:CD	5:E:80:MET:HB3	2.44	0.43
5:E:166:LEU:HD23	5:E:166:LEU:C	2.44	0.43
2:B:451:LEU:O	2:B:453:ILE:N	2.51	0.42
3:C:62:TRP:O	3:C:64:THR:N	2.51	0.42
5:E:16:TYR:O	5:E:20:ILE:HG12	2.19	0.42
6:F:188:SER:O	6:F:191:PRO:HD3	2.19	0.42
2:B:387:LYS:CA	2:B:484:ASP:O	2.67	0.42
8:H:9:SER:O	8:H:10:TYR:C	2.62	0.42
2:B:323:PHE:O	2:B:338:LYS:CA	2.67	0.42
5:E:85:LEU:HD21	5:E:87:PHE:HD1	1.83	0.42
5:E:207:LEU:HD21	6:F:78:MET:HE1	2.01	0.42
2:B:392:ARG:H	2:B:476:ILE:HA	1.85	0.42
2:B:524:ILE:HA	5:E:29:ASN:OD1	2.19	0.42
5:E:98:ILE:CG2	5:E:99:PRO:N	2.80	0.42
7:G:167:PHE:HA	7:G:170:VAL:CB	2.50	0.42
2:B:355:ALA:O	2:B:367:ASP:N	2.52	0.42
5:E:20:ILE:HD13	5:E:20:ILE:HA	1.84	0.42
5:E:79:THR:O	5:E:82:ASP:CA	2.68	0.42
5:E:167:GLN:O	5:E:168:ILE:HG13	2.19	0.42
6:F:203:GLN:C	6:F:205:VAL:N	2.78	0.42
2:B:451:LEU:C	2:B:453:ILE:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:109:LEU:HG	5:E:110:HIS:H	1.84	0.42
5:E:232:LEU:CD2	5:E:253:LEU:HD13	2.49	0.42
6:F:52:ASP:OD1	6:F:53:VAL:N	2.53	0.42
2:B:341:TYR:CB	2:B:353:GLY:HA2	2.49	0.41
5:E:298:SER:C	5:E:299:ARG:O	2.63	0.41
8:H:13:THR:O	8:H:14:SER:O	2.38	0.41
5:E:97:LYS:CE	5:E:237:GLN:O	2.69	0.41
5:E:181:SER:HB2	5:E:290:VAL:HG13	2.01	0.41
5:E:217:THR:HB	5:E:235:ILE:HG12	2.01	0.41
5:E:83:LYS:CG	5:E:84:PRO:HD2	2.47	0.41
5:E:259:VAL:HG21	5:E:268:ILE:HD12	2.03	0.41
2:B:341:TYR:CB	2:B:353:GLY:C	2.94	0.41
5:E:97:LYS:CG	5:E:243:ASN:HB3	2.25	0.41
6:F:49:LEU:HA	6:F:49:LEU:HD22	1.94	0.41
6:F:62:PHE:HZ	6:F:201:ALA:CA	2.32	0.41
7:G:138:GLY:O	7:G:152:ASP:CB	2.69	0.41
3:C:109:LEU:O	3:C:110:VAL:C	2.64	0.41
4:D:30:ILE:C	4:D:32:ASP:H	2.29	0.41
5:E:52:VAL:CG2	5:E:56:ASN:HA	2.51	0.41
5:E:81:MET:HG3	5:E:88:ARG:CZ	2.50	0.41
3:C:204:PHE:CE2	5:E:246:ILE:HG12	2.55	0.41
6:F:43:ARG:CB	6:F:119:ARG:HG3	2.27	0.41
5:E:86:ASN:C	5:E:89:ILE:CG1	2.94	0.41
5:E:236:TRP:NE1	5:E:245:GLN:HB2	2.36	0.41
2:B:196:THR:CB	2:B:200:PHE:H	2.34	0.40
3:C:85:HIS:O	3:C:88:GLU:N	2.46	0.40
5:E:88:ARG:C	5:E:88:ARG:HD3	2.47	0.40
5:E:108:ILE:HG22	5:E:109:LEU:N	2.34	0.40
5:E:27:SER:CB	5:E:224:MET:HG2	2.51	0.40
6:F:43:ARG:HH21	6:F:117:MET:CE	2.22	0.40
5:E:78:GLU:HG2	5:E:80:MET:N	2.37	0.40
5:E:228:LEU:HA	5:E:257:ILE:HG12	2.04	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	A	110/115 (96%)	102 (93%)	5 (4%)	3 (3%)	4	25
2	B	486/687 (71%)	391 (80%)	58 (12%)	37 (8%)	1	10
3	C	180/407 (44%)	147 (82%)	17 (9%)	16 (9%)	0	9
4	D	119/121 (98%)	99 (83%)	12 (10%)	8 (7%)	1	12
5	E	249/307 (81%)	216 (87%)	25 (10%)	8 (3%)	3	21
6	F	207/210 (99%)	189 (91%)	14 (7%)	4 (2%)	6	32
7	G	166/295 (56%)	122 (74%)	23 (14%)	21 (13%)	0	4
8	H	23/35 (66%)	7 (30%)	6 (26%)	10 (44%)	0	0
All	All	1540/2177 (71%)	1273 (83%)	160 (10%)	107 (7%)	1	12

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	VAL
1	A	94	ASP
2	B	231	SER
2	B	251	PRO
2	B	349	LYS
2	B	369	ILE
2	B	370	PRO
2	B	476	ILE
2	B	487	VAL
2	B	493	LEU
2	B	494	PRO
2	B	495	LYS
2	B	544	PRO
2	B	615	ARG
2	B	619	ILE
2	B	622	PRO
2	B	626	HIS
3	C	25	PHE
3	C	29	PRO
3	C	99	PRO
3	C	109	LEU
3	C	121	GLU
3	C	135	VAL

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Mol	Chain	Res	Type
3	C	140	LEU
3	C	194	LYS
4	D	19	VAL
4	D	47	GLU
4	D	102	LYS
5	E	56	ASN
5	E	108	ILE
5	E	177	ASN
5	E	299	ARG
6	F	204	TYR
7	G	5	PRO
7	G	7	ASP
7	G	13	SER
7	G	23	ARG
7	G	35	PRO
7	G	58	PRO
7	G	98	PRO
7	G	123	PRO
7	G	164	PRO
7	G	173	ARG
8	H	4	SER
8	H	14	SER
8	H	21	SER
1	A	42	GLU
2	B	239	SER
2	B	252	SER
2	B	315	SER
2	B	381	PHE
2	B	403	TYR
2	B	420	ALA
2	B	472	GLU
2	B	585	PRO
2	B	638	PRO
3	C	63	TYR
3	C	137	THR
4	D	104	ILE
5	E	109	LEU
5	E	261	ARG
6	F	187	ASP
7	G	19	VAL
7	G	52	PHE
7	G	95	PHE

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Mol	Chain	Res	Type
7	G	131	GLN
7	G	149	PRO
7	G	189	TYR
8	H	2	SER
8	H	10	TYR
8	H	15	PRO
8	H	19	PRO
8	H	20	THR
2	B	247	LYS
2	B	392	ARG
2	B	627	LYS
3	C	139	LEU
6	F	56	LEU
7	G	160	ILE
8	H	9	SER
2	B	192	GLU
2	B	452	LEU
2	B	457	VAL
2	B	574	SER
3	C	138	ALA
3	C	192	PRO
6	F	189	LEU
7	G	53	SER
2	B	320	ASP
2	B	478	LEU
2	B	551	PHE
2	B	552	ALA
3	C	97	PRO
3	C	123	ASP
3	C	136	THR
4	D	32	ASP
4	D	86	ASN
5	E	102	TYR
7	G	168	LYS
8	H	22	PRO
4	D	100	ASP
4	D	119	LYS
2	B	337	ILE
7	G	87	ASP
7	G	122	GLU
2	B	248	VAL
5	E	83	LYS

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	
3	C	28/362 (8%)	25 (89%)	3 (11%)	6	22
5	E	226/280 (81%)	203 (90%)	23 (10%)	7	23
6	F	177/178 (99%)	162 (92%)	15 (8%)	10	30
8	H	25/35 (71%)	25 (100%)	0	100	100
All	All	456/855 (53%)	415 (91%)	41 (9%)	9	28

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	194	LYS
3	C	210	LYS
3	C	214	THR
5	E	11	ILE
5	E	50	GLU
5	E	55	ARG
5	E	58	LEU
5	E	79	THR
5	E	81	MET
5	E	86	ASN
5	E	89	ILE
5	E	95	ASN
5	E	96	ASP
5	E	108	ILE
5	E	110	HIS
5	E	159	GLU
5	E	180	VAL
5	E	217	THR
5	E	230	LEU
5	E	246	ILE
5	E	260	SER
5	E	265	ILE
5	E	268	ILE
5	E	275	LEU

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Mol	Chain	Res	Type
5	E	280	LYS
5	E	287	GLU
6	F	47	LYS
6	F	49	LEU
6	F	67	ARG
6	F	79	VAL
6	F	92	VAL
6	F	121	LEU
6	F	153	ILE
6	F	158	ASP
6	F	181	GLU
6	F	188	SER
6	F	189	LEU
6	F	192	ASP
6	F	193	THR
6	F	199	ASP
6	F	200	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	53	ASN
5	E	56	ASN
5	E	57	GLN
5	E	86	ASN
5	E	176	ASN
5	E	205	ASN
5	E	243	ASN
5	E	269	ASN
6	F	26	ASN
6	F	68	GLN
6	F	118	GLN
6	F	141	ASN

5.3.3 RNA ⓘ

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 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	A	112/115 (97%)	0.41	10 (8%)	15 19	130, 215, 308, 357	0
2	B	492/687 (71%)	0.55	42 (8%)	16 20	130, 224, 382, 471	0
3	C	184/407 (45%)	0.51	14 (7%)	20 23	130, 207, 410, 500	0
4	D	121/121 (100%)	0.42	10 (8%)	17 21	122, 213, 366, 442	1 (0%)
5	E	253/307 (82%)	0.78	27 (10%)	11 15	124, 206, 324, 426	0
6	F	209/210 (99%)	0.98	33 (15%)	5 10	157, 292, 395, 487	0
7	G	170/295 (57%)	0.75	24 (14%)	6 11	123, 218, 392, 457	0
8	H	25/35 (71%)	3.45	21 (84%)	0 1	208, 403, 412, 415	2 (8%)
All	All	1566/2177 (71%)	0.69	181 (11%)	9 13	122, 224, 391, 500	3 (0%)

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	481	LEU	8.5
8	H	17	TYR	6.4
8	H	20	THR	6.1
2	B	458	SER	6.1
2	B	595	ASN	5.9
3	C	99	PRO	5.5
2	B	480	SER	5.3
6	F	141	ASN	5.3
2	B	252	SER	5.2
8	H	25	SER	5.2
8	H	21	SER	5.1
5	E	60	GLU	5.0
8	H	18	SER	4.9
8	H	23	SER	4.9
7	G	9	LEU	4.8
7	G	154	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	482	ASP	4.3
8	H	22	PRO	4.3
2	B	461	ASN	4.3
8	H	9	SER	4.2
1	A	91	LEU	4.2
8	H	12	PRO	4.2
2	B	264	PRO	4.1
2	B	593	ASP	4.1
4	D	32	ASP	4.0
2	B	594	GLU	3.9
8	H	7	SER	3.9
7	G	14	PRO	3.9
8	H	2	SER	3.9
2	B	475	GLU	3.8
7	G	153	TYR	3.7
2	B	312	ILE	3.7
2	B	653	THR	3.7
5	E	158	ASN	3.7
2	B	661	ASP	3.6
2	B	382	VAL	3.6
4	D	34	ASN	3.5
8	H	19	PRO	3.5
2	B	251	PRO	3.5
6	F	120	GLN	3.4
2	B	642	ASN	3.4
2	B	182	ASN	3.4
8	H	24	TYR	3.4
5	E	107	ASN	3.4
2	B	462	GLU	3.3
5	E	262	GLY	3.3
2	B	455	TYR	3.2
5	E	92	SER	3.2
7	G	165	THR	3.2
2	B	624	THR	3.1
3	C	202	LEU	3.1
4	D	2	SER	3.1
6	F	209	GLU	3.1
7	G	171	GLN	3.1
5	E	263	THR	3.0
4	D	31	ALA	3.0
6	F	191	PRO	3.0
7	G	136	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
6	F	194	SER	2.9
6	F	204	TYR	2.9
6	F	186	SER	2.9
6	F	109	SER	2.9
6	F	129	THR	2.9
8	H	10	TYR	2.9
8	H	15	PRO	2.9
6	F	210	LEU	2.9
7	G	129	ARG	2.9
7	G	18	GLN	2.8
2	B	466	ILE	2.8
8	H	3	TYR	2.8
4	D	86	ASN	2.8
3	C	92	SER	2.8
6	F	126	ALA	2.8
1	A	95	THR	2.8
6	F	125	ASP	2.8
3	C	201	VAL	2.8
7	G	155	ILE	2.8
3	C	66	GLN	2.8
6	F	102	GLU	2.8
2	B	477	GLU	2.7
7	G	111	ASP	2.7
1	A	77	VAL	2.7
4	D	81	GLU	2.7
8	H	4	SER	2.7
5	E	178	ARG	2.7
2	B	259	ILE	2.7
5	E	226	HIS	2.7
2	B	586	GLN	2.7
5	E	301	ALA	2.6
5	E	252	LEU	2.6
5	E	77	ASP	2.6
3	C	209	GLU	2.6
6	F	208	LEU	2.6
2	B	189	ASP	2.6
2	B	529	GLY	2.6
5	E	225	LYS	2.6
2	B	592	ASP	2.6
6	F	55	LYS	2.6
5	E	56	ASN	2.6
6	F	17	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
5	E	296	MET	2.5
4	D	3	ASN	2.5
1	A	75	GLU	2.5
5	E	294	GLN	2.5
1	A	94	ASP	2.5
5	E	199	SER	2.5
5	E	295	SER	2.5
5	E	93	PHE	2.5
7	G	152	ASP	2.5
4	D	90	VAL	2.4
1	A	78	GLY	2.4
6	F	67	ARG	2.4
3	C	70	ASN	2.4
8	H	1	PRO	2.4
5	E	206	GLY	2.4
6	F	142	LEU	2.4
2	B	639	ASN	2.4
6	F	118	GLN	2.4
5	E	207	LEU	2.4
3	C	152	ASP	2.4
5	E	72	PHE	2.3
8	H	16	SER	2.3
7	G	112	GLY	2.3
6	F	179	ALA	2.3
2	B	188	ASP	2.3
2	B	409	SER	2.3
8	H	11	SER	2.3
6	F	138	ARG	2.3
6	F	189	LEU	2.3
7	G	57	ASP	2.3
2	B	317	SER	2.3
6	F	192	ASP	2.3
7	G	91	ARG	2.3
3	C	96	TYR	2.2
5	E	75	LEU	2.2
6	F	58	TYR	2.2
1	A	4	PRO	2.2
5	E	201	SER	2.2
6	F	190	GLY	2.2
2	B	187	THR	2.2
2	B	265	THR	2.2
2	B	232	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
5	E	182	MET	2.2
4	D	29	THR	2.2
4	D	91	THR	2.2
2	B	239	SER	2.2
3	C	98	LEU	2.2
7	G	25	GLU	2.2
3	C	118	ASN	2.2
6	F	149	LYS	2.2
7	G	97	TYR	2.2
6	F	154	GLU	2.2
7	G	60	ALA	2.1
2	B	424	ASP	2.1
2	B	588	ASN	2.1
7	G	127	VAL	2.1
1	A	115	LYS	2.1
5	E	61	PRO	2.1
7	G	149	PRO	2.1
2	B	364	GLN	2.1
2	B	459	ILE	2.1
6	F	103	SER	2.1
7	G	163	SER	2.1
3	C	102	PRO	2.1
7	G	29	ASP	2.1
5	E	202	SER	2.1
7	G	137	SER	2.1
2	B	582	ARG	2.1
8	H	6	THR	2.1
5	E	106	ARG	2.0
6	F	119	ARG	2.0
2	B	381	PHE	2.0
6	F	64	HIS	2.0
3	C	167	TYR	2.0
1	A	14	ASN	2.0
6	F	145	SER	2.0
7	G	119	SER	2.0
1	A	38	LYS	2.0
3	C	112	THR	2.0
6	F	128	GLU	2.0
6	F	143	PHE	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.