



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:38 AM UTC

PDB ID : 2HZM / pdb_00002hzm
Title : Structure of the Mediator head subcomplex Med18/20
Authors : Lariviere, L.; Geiger, S.; Hoepfner, S.; Rother, S.; Straesser, K.; Cramer, P.
Deposited on : 2006-08-09
Resolution : 2.40 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

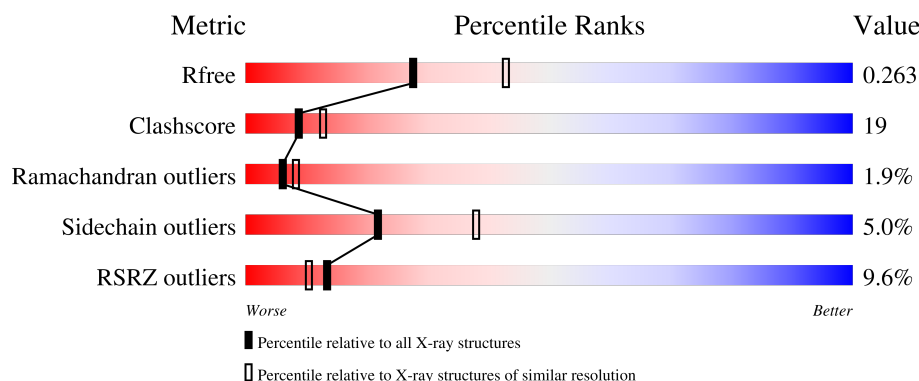
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	212	2% 70% 23% • •
1	C	212	6% 64% 24% • 8%
1	E	212	17% 53% 33% 7% 7%
1	G	212	25% 54% 34% • 8%
2	B	317	3% 48% 21% • • 28%

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Mol	Chain	Length	Quality of chain
2	D	317	4% 49% 21% • • 26%
2	F	317	3% 53% 21% • 25%
2	H	317	9% 44% 24% • • 29%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13587 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA polymerase II mediator complex subunit 20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1574	994	265	310	5			
1	C	195	Total	C	N	O	S	0	0	0
			1504	952	253	294	5			
1	E	197	Total	C	N	O	S	0	0	0
			1520	961	257	297	5			
1	G	196	Total	C	N	O	S	0	0	0
			1511	957	254	295	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	cloning artifact	UNP P34162
A	0	SER	-	cloning artifact	UNP P34162
C	-1	ALA	-	cloning artifact	UNP P34162
C	0	SER	-	cloning artifact	UNP P34162
E	-1	ALA	-	cloning artifact	UNP P34162
E	0	SER	-	cloning artifact	UNP P34162
G	-1	ALA	-	cloning artifact	UNP P34162
G	0	SER	-	cloning artifact	UNP P34162

- Molecule 2 is a protein called RNA polymerase II mediator complex subunit 18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1785	1145	291	342	7			
2	D	233	Total	C	N	O	S	0	0	0
			1820	1165	299	347	9			
2	F	238	Total	C	N	O	S	0	0	0
			1869	1199	302	358	10			
2	H	226	Total	C	N	O	S	0	0	0
			1770	1137	287	337	9			

There are 48 discrepancies between the modelled and reference sequences:

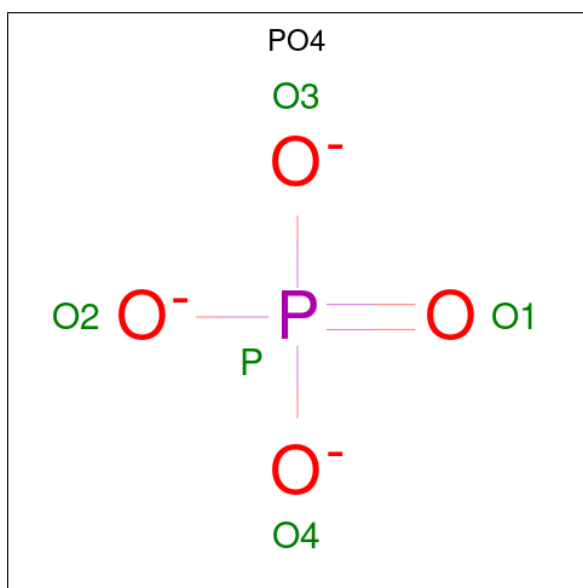
Chain	Residue	Modelled	Actual	Comment	Reference
B	274	VAL	ALA	engineered mutation	UNP P32585
B	308	ALA	-	cloning artifact	UNP P32585
B	309	ALA	-	cloning artifact	UNP P32585
B	310	ALA	-	cloning artifact	UNP P32585
B	311	LEU	-	cloning artifact	UNP P32585
B	312	GLU	-	cloning artifact	UNP P32585
B	313	HIS	-	expression tag	UNP P32585
B	314	HIS	-	expression tag	UNP P32585
B	315	HIS	-	expression tag	UNP P32585
B	316	HIS	-	expression tag	UNP P32585
B	317	HIS	-	expression tag	UNP P32585
B	318	HIS	-	expression tag	UNP P32585
D	274	VAL	ALA	engineered mutation	UNP P32585
D	308	ALA	-	cloning artifact	UNP P32585
D	309	ALA	-	cloning artifact	UNP P32585
D	310	ALA	-	cloning artifact	UNP P32585
D	311	LEU	-	cloning artifact	UNP P32585
D	312	GLU	-	cloning artifact	UNP P32585
D	313	HIS	-	expression tag	UNP P32585
D	314	HIS	-	expression tag	UNP P32585
D	315	HIS	-	expression tag	UNP P32585
D	316	HIS	-	expression tag	UNP P32585
D	317	HIS	-	expression tag	UNP P32585
D	318	HIS	-	expression tag	UNP P32585
F	274	VAL	ALA	engineered mutation	UNP P32585
F	308	ALA	-	cloning artifact	UNP P32585
F	309	ALA	-	cloning artifact	UNP P32585
F	310	ALA	-	cloning artifact	UNP P32585
F	311	LEU	-	cloning artifact	UNP P32585
F	312	GLU	-	cloning artifact	UNP P32585
F	313	HIS	-	expression tag	UNP P32585
F	314	HIS	-	expression tag	UNP P32585
F	315	HIS	-	expression tag	UNP P32585
F	316	HIS	-	expression tag	UNP P32585
F	317	HIS	-	expression tag	UNP P32585
F	318	HIS	-	expression tag	UNP P32585
H	274	VAL	ALA	engineered mutation	UNP P32585
H	308	ALA	-	cloning artifact	UNP P32585
H	309	ALA	-	cloning artifact	UNP P32585
H	310	ALA	-	cloning artifact	UNP P32585
H	311	LEU	-	cloning artifact	UNP P32585
H	312	GLU	-	cloning artifact	UNP P32585

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Chain	Residue	Modelled	Actual	Comment	Reference
H	313	HIS	-	expression tag	UNP P32585
H	314	HIS	-	expression tag	UNP P32585
H	315	HIS	-	expression tag	UNP P32585
H	316	HIS	-	expression tag	UNP P32585
H	317	HIS	-	expression tag	UNP P32585
H	318	HIS	-	expression tag	UNP P32585

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	76	Total	O	0	0
			76	76		
4	B	40	Total	O	0	0
			40	40		
4	C	16	Total	O	0	0
			16	16		
4	D	41	Total	O	0	0
			41	41		
4	E	6	Total	O	0	0
			6	6		

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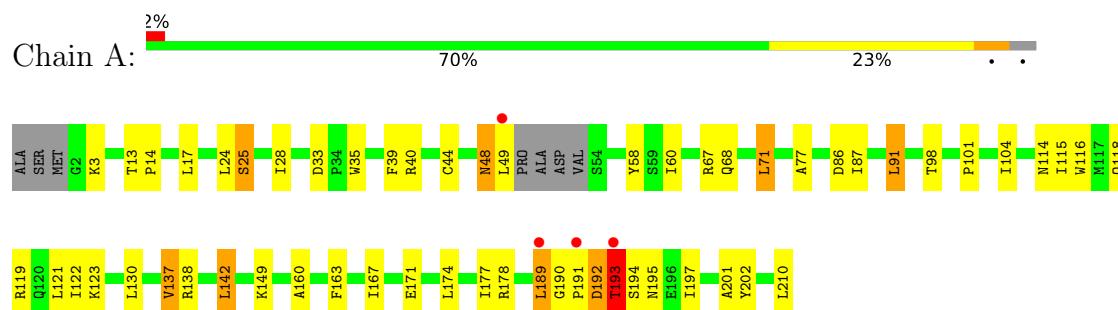
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	40	Total 40	O 40	0	0
4	G	2	Total 2	O 2	0	0
4	H	8	Total 8	O 8	0	0

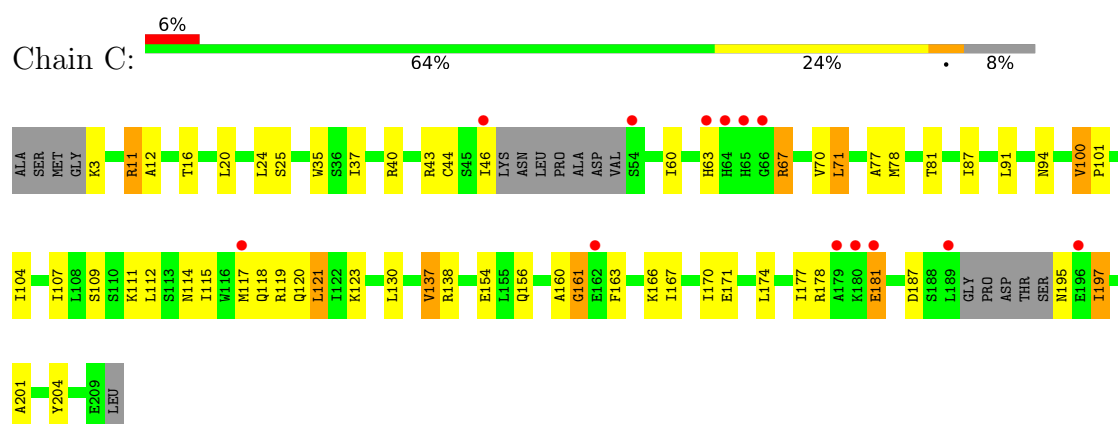
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

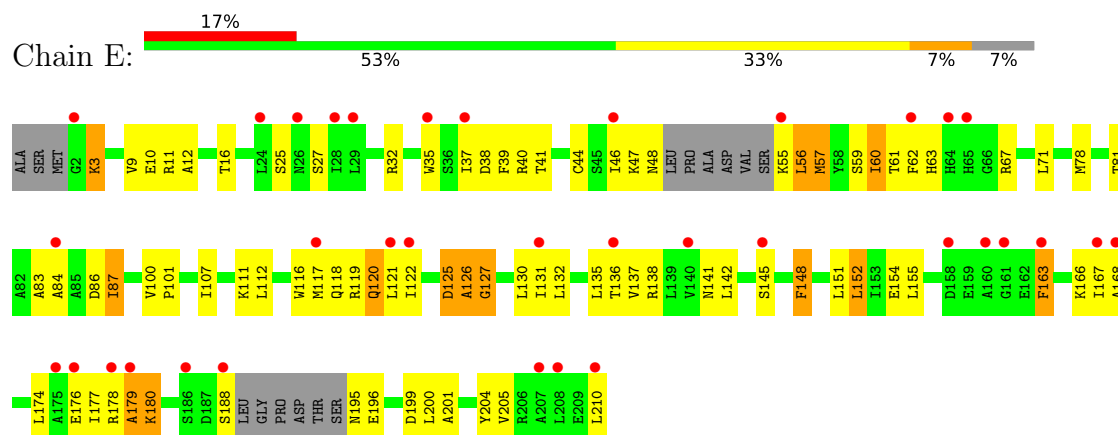
- Molecule 1: RNA polymerase II mediator complex subunit 20



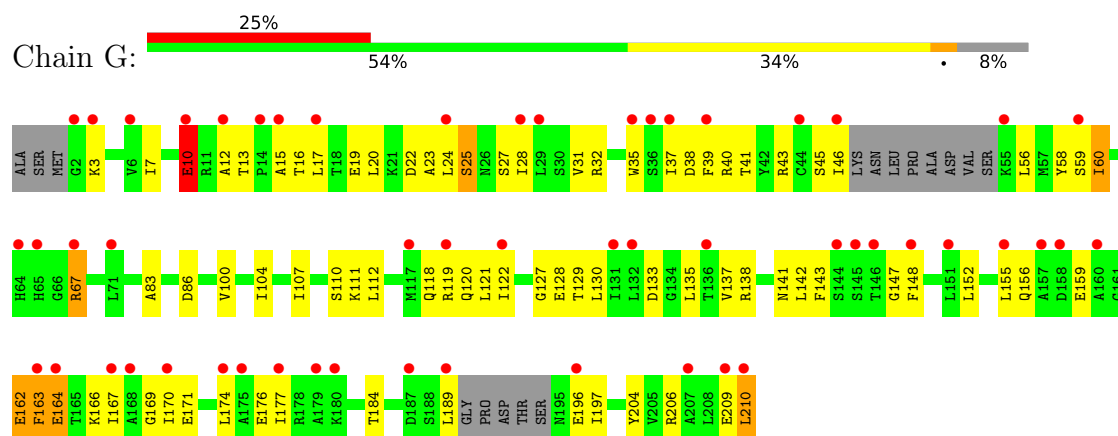
- Molecule 1: RNA polymerase II mediator complex subunit 20



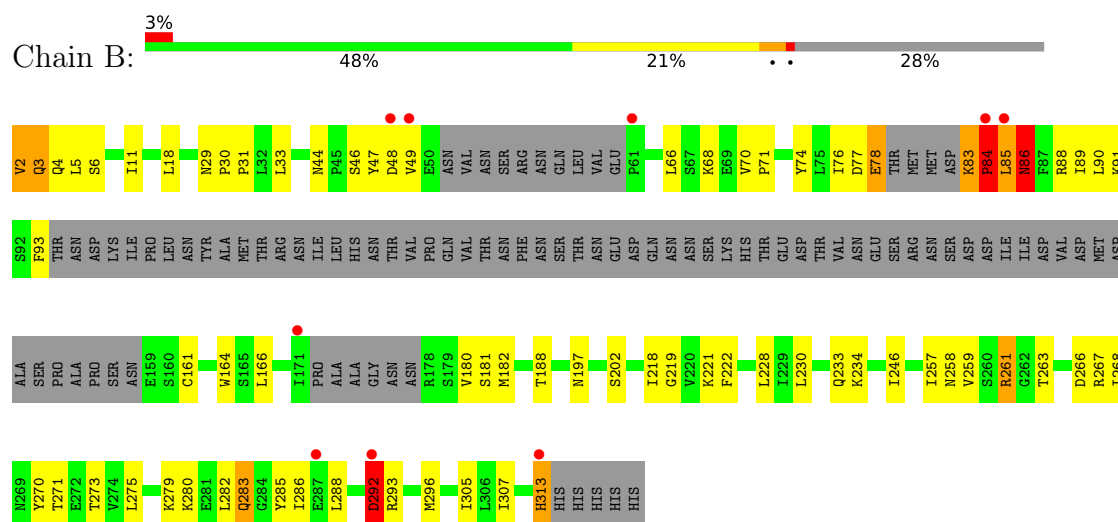
- Molecule 1: RNA polymerase II mediator complex subunit 20



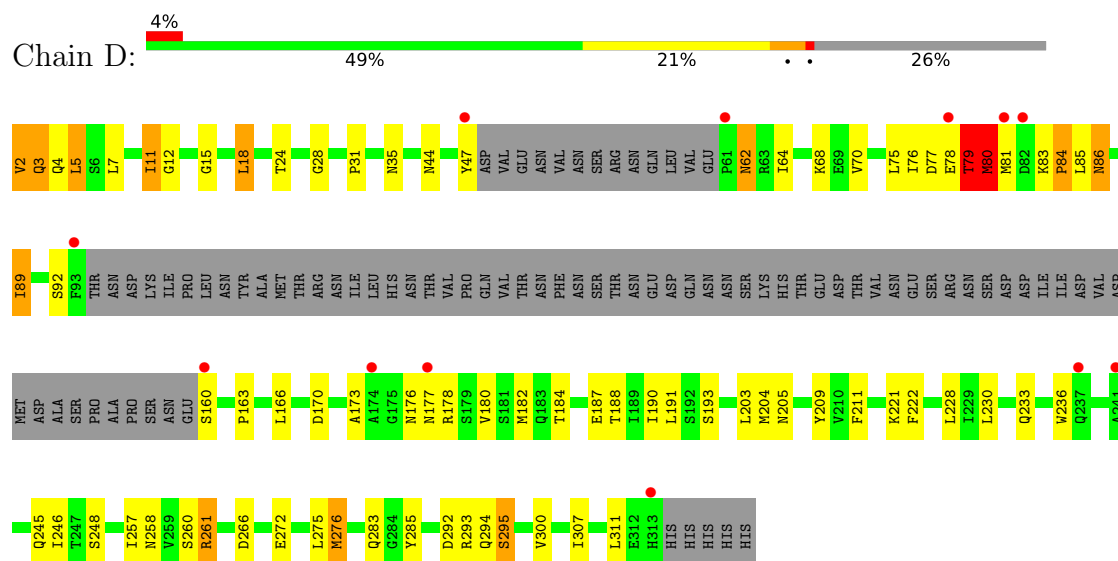
- Molecule 1: RNA polymerase II mediator complex subunit 20



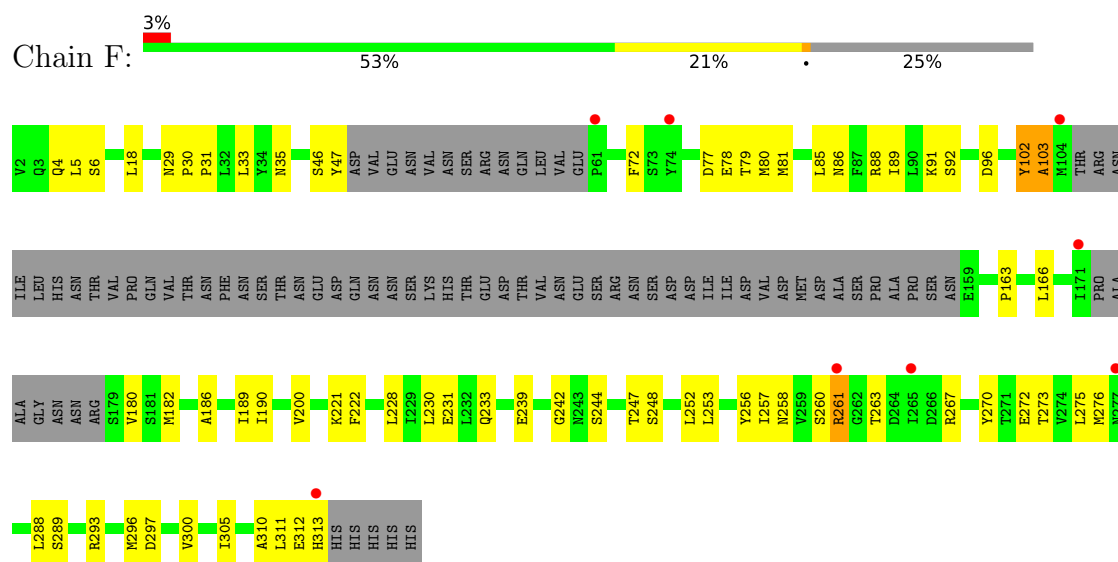
- Molecule 2: RNA polymerase II mediator complex subunit 18



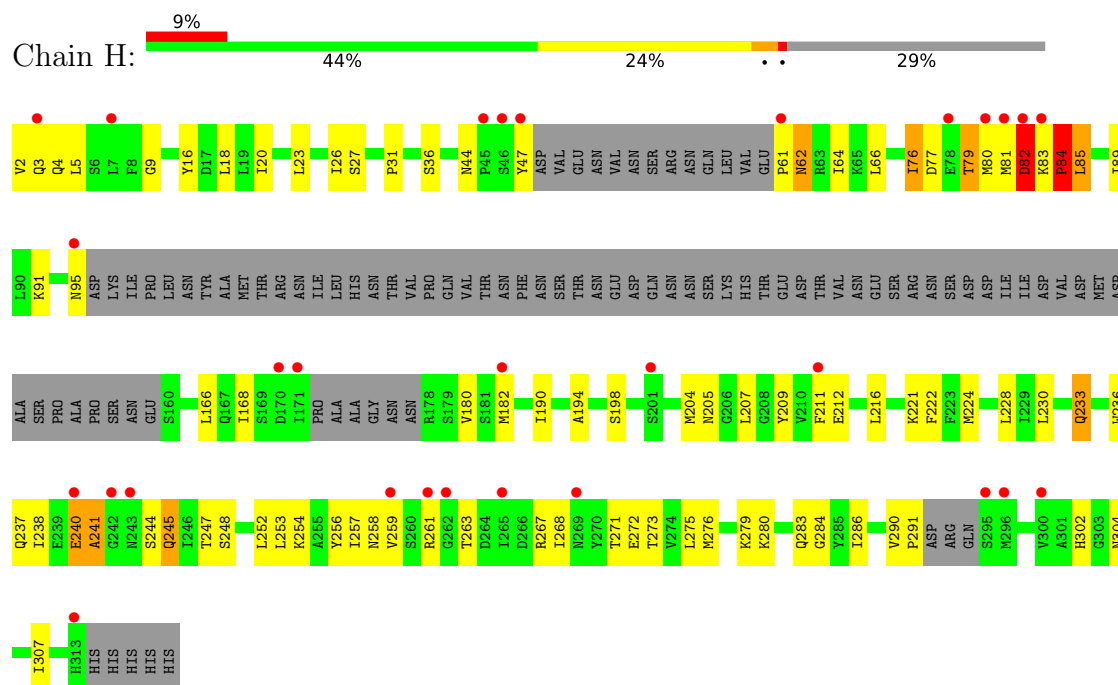
- Molecule 2: RNA polymerase II mediator complex subunit 18



- Molecule 2: RNA polymerase II mediator complex subunit 18



• Molecule 2: RNA polymerase II mediator complex subunit 18



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.90Å 129.35Å 241.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.40) 98.5 (20.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.24 (at 2.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.264 0.228 , 0.263	Depositor DCC
R_{free} test set	4276 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13587	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.61	0/1598	1.06	8/2162 (0.4%)
1	C	0.44	0/1526	0.94	4/2064 (0.2%)
1	E	0.37	0/1542	0.87	4/2083 (0.2%)
1	G	0.40	0/1533	0.88	2/2072 (0.1%)
2	B	0.56	0/1816	1.14	13/2453 (0.5%)
2	D	0.52	1/1854 (0.1%)	0.98	6/2508 (0.2%)
2	F	0.51	0/1903	0.96	3/2573 (0.1%)
2	H	0.39	0/1801	0.95	5/2433 (0.2%)
All	All	0.49	1/13573 (0.0%)	0.98	45/18348 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	276	MET	SD-CE	-5.08	1.66	1.79

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	83	LYS	CA-C-N	14.57	138.05	119.84
2	B	83	LYS	C-N-CA	14.57	138.05	119.84
2	H	82	ASP	N-CA-C	14.00	128.98	109.11
2	B	85	LEU	N-CA-C	9.78	124.15	108.41
1	A	192	ASP	N-CA-C	-9.53	102.45	114.56
2	B	84	PRO	N-CA-C	9.52	132.08	112.47
1	E	163	PHE	N-CA-C	8.66	121.50	111.11
2	H	241	ALA	N-CA-C	-7.78	94.22	110.80
2	D	295	SER	N-CA-C	-7.78	102.84	113.18
1	A	25	SER	N-CA-C	7.12	120.86	111.75
1	A	194	SER	N-CA-C	7.10	120.06	111.82
2	F	233	GLN	N-CA-C	7.00	119.58	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	ASP	N-CA-C	7.00	120.46	110.24
2	H	233	GLN	N-CA-C	6.91	119.26	108.96
2	B	84	PRO	CA-C-N	6.72	131.36	122.42
2	B	84	PRO	C-N-CA	6.72	131.36	122.42
1	C	67	ARG	N-CA-C	6.68	119.61	108.73
2	D	79	THR	N-CA-C	-6.60	96.73	110.80
1	A	163	PHE	N-CA-C	6.44	117.96	111.07
2	H	85	LEU	N-CA-C	-6.36	104.34	111.28
1	G	67	ARG	N-CA-C	6.28	118.53	108.41
2	B	246	ILE	CB-CA-C	-6.27	103.68	112.14
2	H	284	GLY	N-CA-C	-6.01	106.67	115.63
1	A	193	THR	N-CA-C	5.96	123.48	110.80
1	A	123	LYS	N-CA-C	5.95	119.25	109.85
1	E	87	ILE	CB-CA-C	-5.81	105.54	110.94
1	A	98	THR	N-CA-C	-5.79	105.71	112.89
2	D	80	MET	N-CA-C	-5.62	105.55	112.90
2	B	86	ASN	N-CA-C	5.61	115.65	108.24
2	D	233	GLN	N-CA-C	5.59	117.29	108.96
2	B	6	SER	N-CA-C	5.52	117.18	108.96
2	B	233	GLN	N-CA-C	5.50	117.34	109.14
1	C	109	SER	N-CA-C	5.45	117.93	111.33
2	F	256	TYR	N-CA-C	5.44	117.06	108.96
1	E	180	LYS	N-CA-C	5.39	116.96	111.14
2	B	161	CYS	N-CA-C	-5.34	103.64	110.53
2	B	234	LYS	N-CA-C	-5.32	101.21	109.72
1	C	100	VAL	CA-C-N	5.28	125.69	119.99
1	C	100	VAL	C-N-CA	5.28	125.69	119.99
2	F	6	SER	N-CA-C	5.25	116.26	108.60
2	D	205	ASN	N-CA-C	-5.14	105.76	111.36
1	E	145	SER	N-CA-C	-5.13	107.00	113.20
2	B	268	ILE	N-CA-C	-5.11	105.40	110.62
2	D	283	GLN	N-CA-C	5.06	117.53	111.71
1	G	209	GLU	N-CA-C	-5.01	106.74	112.86

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1574	0	1588	39	0
1	C	1504	0	1517	46	0
1	E	1520	0	1534	83	0
1	G	1511	0	1526	86	0
2	B	1785	0	1799	70	0
2	D	1820	0	1837	78	0
2	F	1869	0	1885	49	0
2	H	1770	0	1791	77	0
3	A	5	0	0	0	0
4	A	76	0	0	0	0
4	B	40	0	0	1	0
4	C	16	0	0	0	0
4	D	41	0	0	0	0
4	E	6	0	0	0	0
4	F	40	0	0	1	0
4	G	2	0	0	0	0
4	H	8	0	0	0	0
All	All	13587	0	13477	501	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 19.

All (501) 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)
2:B:83:LYS:HB3	2:B:84:PRO:HD2	1.20	1.07
1:A:114:ASN:HD22	2:B:49:VAL:HG11	1.24	1.02
1:E:40:ARG:HH11	1:E:118:GLN:HE22	1.10	0.95
2:B:83:LYS:CB	2:B:84:PRO:HD2	1.96	0.95
2:B:4:GLN:HE21	2:B:258:ASN:HD21	1.16	0.93
2:B:261:ARG:HD3	2:B:261:ARG:H	1.33	0.91
2:D:77:ASP:OD1	2:D:79:THR:HG22	1.71	0.91
1:G:39:PHE:HZ	1:G:204:TYR:HB3	1.35	0.89
2:D:86:ASN:O	2:D:89:ILE:HG13	1.74	0.88
1:E:142:LEU:HD11	1:E:152:LEU:HD12	1.55	0.87
1:E:41:THR:HB	1:E:120:GLN:HB2	1.57	0.87
2:H:83:LYS:HE2	2:H:83:LYS:HA	1.56	0.86
1:C:40:ARG:HH11	1:C:118:GLN:HE22	1.23	0.85
2:B:5:LEU:HD21	2:B:182:MET:HE2	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:178:ARG:HG3	2:D:182:MET:HE3	1.60	0.83
2:F:263:THR:CG2	2:F:267:ARG:HD3	2.09	0.83
1:G:31:VAL:HG12	1:G:32:ARG:H	1.42	0.83
1:C:163:PHE:O	1:C:167:ILE:HD12	1.81	0.81
1:E:44:CYS:HB3	1:E:55:LYS:HB3	1.63	0.81
1:E:135:LEU:HD12	1:E:166:LYS:HB3	1.61	0.81
1:A:49:LEU:HG	2:B:47:TYR:HE1	1.47	0.80
2:H:5:LEU:HD21	2:H:182:MET:HE2	1.63	0.79
2:D:44:ASN:HB3	2:D:47:TYR:CD2	2.18	0.79
2:F:5:LEU:CD2	2:F:182:MET:HG3	2.13	0.79
1:G:20:LEU:O	1:G:24:LEU:HD13	1.83	0.78
2:D:261:ARG:CD	2:D:261:ARG:H	1.95	0.78
2:B:83:LYS:HB3	2:B:84:PRO:CD	2.09	0.76
2:F:86:ASN:O	2:F:89:ILE:HG12	1.84	0.76
2:D:4:GLN:HE21	2:D:258:ASN:HD21	1.34	0.76
2:D:173:ALA:HA	2:D:176:ASN:ND2	2.01	0.75
1:G:130:LEU:HB2	1:G:137:VAL:HG23	1.69	0.75
2:F:261:ARG:H	2:F:261:ARG:HE	1.31	0.74
2:H:238:ILE:HG23	2:H:240:GLU:OE2	1.86	0.74
1:A:48:ASN:O	1:A:49:LEU:HB2	1.86	0.74
2:D:261:ARG:H	2:D:261:ARG:HD3	1.50	0.74
2:D:85:LEU:HD12	2:D:89:ILE:HD13	1.68	0.74
2:D:11:ILE:HD13	2:D:12:GLY:H	1.53	0.74
1:C:100:VAL:HB	2:D:2:VAL:HG21	1.70	0.73
1:E:135:LEU:HD23	1:E:136:THR:N	2.03	0.73
2:D:76:ILE:HG13	2:D:80:MET:HG2	1.69	0.73
2:H:280:LYS:O	2:H:283:GLN:HG2	1.88	0.73
1:C:20:LEU:O	1:C:24:LEU:HD13	1.89	0.73
2:D:11:ILE:HD13	2:D:12:GLY:N	2.03	0.72
2:D:5:LEU:HD22	2:D:182:MET:HG3	1.71	0.72
1:E:48:ASN:N	1:E:55:LYS:HZ2	1.88	0.72
2:D:178:ARG:HD2	2:D:272:GLU:OE1	1.89	0.71
2:D:261:ARG:HD3	2:D:261:ARG:N	2.04	0.71
1:E:100:VAL:HG11	2:F:261:ARG:HH22	1.55	0.71
2:D:76:ILE:HG23	2:D:80:MET:HB3	1.72	0.71
1:E:117:MET:HE3	1:E:117:MET:HA	1.72	0.70
2:B:85:LEU:HD12	2:B:89:ILE:HD13	1.73	0.70
2:H:240:GLU:OE1	2:H:240:GLU:HA	1.89	0.70
2:H:44:ASN:HB3	2:H:47:TYR:CD2	2.26	0.70
1:C:130:LEU:HB2	1:C:137:VAL:HG13	1.73	0.69
2:D:44:ASN:HB3	2:D:47:TYR:HD2	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4:GLN:HE21	2:H:258:ASN:HD21	1.39	0.69
1:G:39:PHE:CZ	1:G:204:TYR:HB3	2.25	0.69
1:G:60:ILE:N	1:G:60:ILE:HD12	2.08	0.68
2:D:64:ILE:HG21	2:D:204:MET:HE1	1.74	0.68
2:H:4:GLN:HG3	2:H:258:ASN:ND2	2.08	0.68
2:D:160:SER:N	2:D:193:SER:HG	1.90	0.68
1:A:49:LEU:HG	2:B:47:TYR:CE1	2.29	0.68
1:A:114:ASN:HD22	2:B:49:VAL:CG1	2.04	0.68
1:G:135:LEU:HD12	1:G:166:LYS:HE2	1.76	0.68
1:E:119:ARG:O	1:E:120:GLN:HG2	1.94	0.67
1:G:23:ALA:C	1:G:24:LEU:HD12	2.19	0.67
2:D:80:MET:HE1	2:D:92:SER:O	1.93	0.67
2:F:85:LEU:HD23	2:F:88:ARG:HE	1.60	0.67
2:B:85:LEU:HA	2:B:89:ILE:HD11	1.76	0.67
2:B:166:LEU:C	2:B:166:LEU:HD23	2.19	0.67
2:F:263:THR:HG21	2:F:267:ARG:HD3	1.76	0.67
1:C:40:ARG:HH11	1:C:118:GLN:NE2	1.91	0.67
2:B:261:ARG:HD3	2:B:261:ARG:N	2.08	0.66
1:G:25:SER:HA	1:G:28:ILE:HG13	1.75	0.66
1:G:120:GLN:HE21	1:G:122:ILE:HG13	1.60	0.66
1:A:167:ILE:O	1:A:171:GLU:HG3	1.94	0.66
2:B:85:LEU:HD12	2:B:89:ILE:CD1	2.26	0.66
2:D:78:GLU:HA	2:D:81:MET:HG2	1.77	0.65
2:H:4:GLN:HG3	2:H:258:ASN:HD21	1.62	0.65
1:E:67:ARG:HD2	1:E:67:ARG:N	2.12	0.65
1:G:25:SER:HA	1:G:28:ILE:CD1	2.26	0.65
1:G:60:ILE:HD12	1:G:60:ILE:H	1.62	0.65
2:H:263:THR:HB	2:H:267:ARG:HD2	1.79	0.65
2:D:180:VAL:CG1	2:D:276:MET:HE3	2.26	0.65
1:G:137:VAL:HG12	1:G:155:LEU:CD2	2.27	0.64
1:G:31:VAL:HG12	1:G:32:ARG:N	2.10	0.64
1:E:60:ILE:N	1:E:60:ILE:HD12	2.13	0.64
1:E:126:ALA:O	1:E:127:GLY:C	2.41	0.64
1:C:170:ILE:O	1:C:174:LEU:HD13	1.98	0.64
1:G:20:LEU:HD13	1:G:177:ILE:HD13	1.80	0.64
1:G:137:VAL:HG12	1:G:155:LEU:HD22	1.80	0.64
2:D:7:LEU:HD11	2:D:276:MET:CE	2.28	0.64
1:E:56:LEU:N	1:E:56:LEU:HD23	2.12	0.63
2:B:270:TYR:O	2:B:273:THR:HB	1.99	0.63
2:H:77:ASP:OD1	2:H:79:THR:HG23	1.98	0.63
2:F:91:LYS:HD3	4:F:348:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:THR:HG22	1:A:193:THR:O	1.98	0.63
1:A:40:ARG:HE	1:A:118:GLN:HE22	1.46	0.62
2:H:80:MET:HE1	2:H:91:LYS:HD3	1.80	0.62
1:G:25:SER:HA	1:G:28:ILE:CG1	2.29	0.62
2:H:85:LEU:HG	2:H:89:ILE:HD11	1.80	0.62
1:C:114:ASN:ND2	1:C:115:ILE:HG13	2.14	0.62
1:E:87:ILE:HG12	2:F:189:ILE:HG13	1.80	0.62
2:D:178:ARG:HE	2:D:182:MET:HE1	1.64	0.62
2:D:261:ARG:CD	2:D:261:ARG:N	2.62	0.61
1:G:206:ARG:HG3	1:G:206:ARG:HH11	1.65	0.61
1:C:60:ILE:HD13	1:C:201:ALA:HB1	1.81	0.61
1:A:130:LEU:HB2	1:A:137:VAL:HG22	1.83	0.61
1:E:195:ASN:HD22	1:E:196:GLU:N	1.98	0.61
2:D:285:TYR:OH	2:F:80:MET:HE1	2.00	0.61
2:H:80:MET:SD	2:H:91:LYS:HD3	2.41	0.61
2:F:5:LEU:HD22	2:F:182:MET:HG3	1.82	0.61
2:B:71:PRO:HG2	2:B:74:TYR:CD1	2.36	0.61
2:H:253:LEU:HD23	2:H:286:ILE:HD13	1.84	0.60
1:G:58:TYR:HE2	1:G:210:LEU:HD22	1.65	0.60
1:E:11:ARG:HB2	1:E:180:LYS:HB2	1.83	0.60
2:H:64:ILE:HG21	2:H:204:MET:HE1	1.84	0.60
1:A:60:ILE:HD13	1:A:201:ALA:HB1	1.84	0.60
1:G:119:ARG:HH11	1:G:119:ARG:HG3	1.66	0.60
2:B:86:ASN:C	2:B:86:ASN:HD22	2.09	0.60
1:G:163:PHE:O	1:G:164:GLU:C	2.45	0.60
1:C:195:ASN:C	1:C:195:ASN:HD22	2.09	0.59
2:D:178:ARG:NE	2:D:182:MET:HE1	2.17	0.59
1:G:100:VAL:HB	2:H:2:VAL:CG2	2.32	0.59
2:H:23:LEU:O	2:H:27:SER:HB3	2.01	0.59
2:B:261:ARG:H	2:B:261:ARG:CD	2.02	0.59
1:E:135:LEU:CD1	1:E:166:LYS:HB3	2.30	0.59
1:G:100:VAL:HB	2:H:2:VAL:HG21	1.83	0.59
1:G:138:ARG:NH2	1:G:156:GLN:HE21	1.99	0.59
1:G:142:LEU:HD21	1:G:152:LEU:HD12	1.83	0.59
2:F:102:TYR:O	2:F:103:ALA:CB	2.51	0.59
2:D:293:ARG:C	2:D:295:SER:H	2.11	0.58
1:E:174:LEU:HD12	1:E:177:ILE:HD11	1.84	0.58
1:A:142:LEU:HD13	1:A:149:LYS:HD3	1.86	0.58
2:D:85:LEU:HA	2:D:89:ILE:HD11	1.85	0.58
1:E:125:ASP:O	1:E:126:ALA:CB	2.51	0.58
1:G:25:SER:HA	1:G:28:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:ARG:HG3	1:G:119:ARG:NH1	2.19	0.58
1:G:163:PHE:O	1:G:166:LYS:N	2.37	0.58
1:C:40:ARG:NH1	1:C:118:GLN:HE22	1.97	0.58
2:F:4:GLN:HE21	2:F:258:ASN:HD21	1.52	0.58
1:E:3:LYS:HG3	1:E:196:GLU:OE2	2.03	0.57
1:C:63:HIS:CE1	1:C:67:ARG:HE	2.22	0.57
1:E:57:MET:HE2	1:E:116:TRP:CD2	2.40	0.57
1:G:43:ARG:HA	1:G:56:LEU:HD23	1.86	0.57
2:H:64:ILE:HG12	2:H:168:ILE:HG12	1.85	0.57
2:H:23:LEU:HD22	2:H:230:LEU:HD23	1.87	0.57
1:G:40:ARG:NE	1:G:118:GLN:NE2	2.51	0.57
2:B:85:LEU:CA	2:B:89:ILE:HD11	2.35	0.57
1:G:22:ASP:C	1:G:24:LEU:H	2.12	0.57
1:A:35:TRP:CZ2	1:A:138:ARG:HB3	2.40	0.56
2:B:90:LEU:HD11	2:B:219:GLY:HA2	1.87	0.56
2:D:86:ASN:HD22	2:D:86:ASN:C	2.13	0.56
2:H:259:VAL:CG2	2:H:267:ARG:HD3	2.34	0.56
1:C:94:ASN:HD22	2:D:35:ASN:H	1.53	0.56
2:D:3:GLN:NE2	2:D:184:THR:OG1	2.36	0.56
2:D:292:ASP:OD2	2:D:295:SER:HB2	2.05	0.56
2:F:80:MET:HE2	2:F:89:ILE:HG21	1.87	0.56
2:H:304:ASN:CG	2:H:307:ILE:HD13	2.30	0.56
2:H:5:LEU:HD12	2:H:271:THR:CG2	2.35	0.56
1:E:25:SER:C	1:E:27:SER:H	2.14	0.56
2:B:86:ASN:N	2:B:89:ILE:HD11	2.21	0.56
1:C:167:ILE:HD12	1:C:167:ILE:H	1.71	0.56
2:F:46:SER:C	2:F:47:TYR:HD1	2.14	0.56
2:F:221:LYS:HA	2:F:230:LEU:O	2.05	0.56
1:G:111:LYS:C	1:G:112:LEU:HD12	2.31	0.56
1:C:44:CYS:SG	1:C:46:ILE:HD13	2.45	0.56
1:G:100:VAL:CG1	2:H:261:ARG:HH12	2.19	0.56
2:H:257:ILE:HG13	2:H:275:LEU:HD11	1.86	0.56
1:A:114:ASN:ND2	1:A:115:ILE:HG13	2.21	0.56
1:C:87:ILE:HD11	1:C:101:PRO:HG3	1.87	0.56
2:D:85:LEU:HD12	2:D:89:ILE:CD1	2.36	0.56
1:G:130:LEU:HB2	1:G:137:VAL:CG2	2.35	0.55
1:E:44:CYS:SG	1:E:46:ILE:HD13	2.46	0.55
1:A:39:PHE:HB2	1:A:122:ILE:CG1	2.36	0.55
2:D:7:LEU:HD11	2:D:276:MET:HE2	1.88	0.55
2:H:180:VAL:HG22	2:H:272:GLU:HG3	1.87	0.55
2:D:163:PRO:HA	2:D:190:ILE:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:LYS:O	2:H:84:PRO:C	2.50	0.55
2:F:102:TYR:O	2:F:103:ALA:HB3	2.06	0.55
2:H:18:LEU:HD13	2:H:18:LEU:C	2.32	0.55
2:B:263:THR:HG22	2:B:267:ARG:HB3	1.89	0.54
1:E:40:ARG:NH1	1:E:118:GLN:HE22	1.93	0.54
2:B:33:LEU:HD21	2:B:89:ILE:HD12	1.90	0.54
2:F:77:ASP:OD1	2:F:80:MET:HG3	2.07	0.54
2:H:61:PRO:HG2	2:H:62:ASN:H	1.70	0.54
1:C:160:ALA:O	1:C:161:GLY:O	2.25	0.54
1:A:77:ALA:HB2	1:A:189:LEU:HD21	1.88	0.54
2:H:76:ILE:HD11	2:H:89:ILE:HA	1.90	0.54
2:D:5:LEU:CD2	2:D:182:MET:HG3	2.38	0.54
2:D:44:ASN:HB3	2:D:47:TYR:CE2	2.43	0.53
1:A:40:ARG:HE	1:A:118:GLN:NE2	2.06	0.53
1:E:67:ARG:HD2	1:E:67:ARG:H	1.73	0.53
1:C:37:ILE:HD13	1:C:204:TYR:CE1	2.43	0.53
2:D:31:PRO:HB3	2:D:222:PHE:CZ	2.44	0.53
1:E:48:ASN:N	1:E:55:LYS:NZ	2.57	0.53
1:G:40:ARG:HE	1:G:118:GLN:NE2	2.07	0.53
1:G:58:TYR:CE2	1:G:210:LEU:HD22	2.42	0.53
1:G:141:ASN:HB3	1:G:143:PHE:HE1	1.73	0.53
2:H:83:LYS:HA	2:H:83:LYS:CE	2.27	0.53
2:H:254:LYS:HE2	2:H:256:TYR:CD2	2.44	0.53
2:B:86:ASN:HD21	2:B:88:ARG:HB2	1.72	0.53
2:F:252:LEU:HD22	2:F:310:ALA:HB2	1.91	0.53
2:H:194:ALA:C	2:H:198:SER:HB3	2.34	0.53
2:B:44:ASN:HB3	2:B:47:TYR:CD2	2.44	0.53
2:F:180:VAL:HG12	2:F:276:MET:HE2	1.91	0.52
1:E:188:SER:HA	1:E:199:ASP:OD1	2.09	0.52
1:C:78:MET:HB2	2:D:203:LEU:HD22	1.90	0.52
1:C:111:LYS:C	1:C:112:LEU:HD12	2.34	0.52
1:E:163:PHE:O	1:E:166:LYS:HB2	2.09	0.52
2:D:173:ALA:HA	2:D:176:ASN:HD21	1.73	0.52
2:H:166:LEU:HD12	2:H:190:ILE:HD11	1.92	0.52
2:D:24:THR:O	2:D:28:GLY:N	2.42	0.52
1:E:122:ILE:O	1:E:122:ILE:HG13	2.08	0.52
2:D:85:LEU:C	2:D:89:ILE:HD11	2.34	0.52
1:E:100:VAL:HG11	2:F:261:ARG:NH2	2.24	0.52
2:H:36:SER:O	2:H:216:LEU:HD12	2.09	0.52
2:D:166:LEU:C	2:D:166:LEU:HD23	2.35	0.52
2:H:85:LEU:O	2:H:89:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:82:ASP:O	2:H:83:LYS:HG2	2.10	0.51
2:B:5:LEU:CD2	2:B:182:MET:HG3	2.40	0.51
2:B:68:LYS:HE2	2:B:164:TRP:CZ2	2.46	0.51
1:E:11:ARG:CB	1:E:180:LYS:HB2	2.40	0.51
1:G:31:VAL:O	1:G:32:ARG:HG3	2.10	0.51
2:H:259:VAL:HG21	2:H:267:ARG:HD3	1.91	0.51
1:E:10:GLU:OE2	1:E:10:GLU:N	2.34	0.51
1:E:46:ILE:HG22	1:E:47:LYS:N	2.26	0.51
1:G:3:LYS:HG3	1:G:196:GLU:OE2	2.09	0.51
2:H:85:LEU:HG	2:H:89:ILE:CD1	2.39	0.51
1:E:130:LEU:HB2	1:E:137:VAL:CG2	2.41	0.51
2:D:246:ILE:HG23	2:D:311:LEU:HD23	1.93	0.51
2:D:64:ILE:HG21	2:D:204:MET:CE	2.41	0.50
2:D:86:ASN:N	2:D:89:ILE:HD11	2.26	0.50
2:B:221:LYS:HA	2:B:230:LEU:O	2.11	0.50
1:E:46:ILE:HG22	1:E:55:LYS:NZ	2.27	0.50
1:E:138:ARG:HB2	1:E:154:GLU:HB3	1.94	0.50
2:F:239:GLU:HB2	2:F:242:GLY:O	2.11	0.50
1:G:67:ARG:HG3	1:G:67:ARG:HH11	1.76	0.50
1:C:63:HIS:CE1	1:C:67:ARG:NE	2.79	0.50
1:E:56:LEU:HD23	1:E:56:LEU:H	1.75	0.50
2:H:80:MET:CE	2:H:91:LYS:HD3	2.41	0.50
1:G:45:SER:C	1:G:46:ILE:HD12	2.36	0.50
2:H:247:THR:O	2:H:248:SER:C	2.54	0.50
1:A:25:SER:HA	1:A:28:ILE:HG13	1.94	0.50
2:B:29:ASN:HB3	2:B:30:PRO:HD2	1.93	0.50
1:G:171:GLU:HA	1:G:174:LEU:HB2	1.94	0.50
1:A:87:ILE:HD11	1:A:101:PRO:HG3	1.93	0.50
1:E:137:VAL:HG12	1:E:155:LEU:CD2	2.42	0.50
1:E:46:ILE:CG2	1:E:47:LYS:N	2.74	0.49
1:C:71:LEU:O	1:C:77:ALA:HA	2.12	0.49
1:C:167:ILE:O	1:C:171:GLU:HG3	2.12	0.49
1:E:12:ALA:HB1	1:E:16:THR:OG1	2.13	0.49
2:H:9:GLY:O	2:H:252:LEU:HD12	2.11	0.49
2:B:5:LEU:HA	2:B:181:SER:O	2.13	0.49
2:D:221:LYS:HA	2:D:230:LEU:O	2.13	0.49
1:C:43:ARG:HD2	1:C:119:ARG:HD2	1.94	0.49
1:C:117:MET:HE3	1:C:119:ARG:NH1	2.28	0.49
1:E:195:ASN:HD22	1:E:195:ASN:C	2.19	0.49
2:D:261:ARG:H	2:D:261:ARG:NE	2.11	0.49
1:E:135:LEU:HD12	1:E:166:LYS:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:228:LEU:HA	2:F:257:ILE:HG12	1.95	0.49
2:F:300:VAL:HG23	2:F:311:LEU:HD13	1.93	0.49
1:G:40:ARG:CD	1:G:118:GLN:HE21	2.25	0.49
1:E:46:ILE:N	1:E:46:ILE:HD12	2.27	0.49
1:C:11:ARG:HG3	1:C:181:GLU:CB	2.42	0.49
2:H:290:VAL:HG23	2:H:291:PRO:HD2	1.95	0.49
1:G:127:GLY:O	1:G:128:GLU:HG3	2.12	0.48
2:H:221:LYS:HA	2:H:230:LEU:O	2.13	0.48
1:A:58:TYR:CE2	1:A:210:LEU:HB3	2.48	0.48
2:B:68:LYS:HE2	2:B:164:TRP:CH2	2.47	0.48
1:C:12:ALA:HB1	1:C:16:THR:OG1	2.13	0.48
1:E:39:PHE:HB3	1:E:122:ILE:CG1	2.43	0.48
1:E:56:LEU:N	1:E:56:LEU:CD2	2.76	0.48
1:E:87:ILE:HD11	1:E:101:PRO:HD3	1.95	0.48
1:G:22:ASP:C	1:G:24:LEU:N	2.71	0.48
2:B:4:GLN:NE2	2:B:258:ASN:HD21	1.96	0.48
1:G:40:ARG:NE	1:G:118:GLN:HE21	2.12	0.48
2:H:273:THR:O	2:H:276:MET:HB2	2.14	0.48
1:E:176:GLU:O	1:E:178:ARG:HD2	2.14	0.48
1:G:31:VAL:HG13	1:G:129:THR:O	2.13	0.48
2:B:5:LEU:HD21	2:B:182:MET:CE	2.38	0.48
1:C:91:LEU:HD11	2:D:68:LYS:HA	1.96	0.48
2:D:83:LYS:O	2:D:84:PRO:C	2.55	0.48
2:H:240:GLU:OE1	2:H:240:GLU:CA	2.59	0.48
2:H:276:MET:O	2:H:279:LYS:HB3	2.13	0.48
2:F:78:GLU:HA	2:F:81:MET:HE3	1.95	0.48
2:F:231:GLU:O	2:F:253:LEU:HD12	2.12	0.48
2:H:26:ILE:HG22	2:H:224:MET:HE3	1.96	0.48
2:F:96:ASP:HB3	2:F:244:SER:HA	1.96	0.48
2:H:205:ASN:ND2	2:H:209:TYR:O	2.42	0.48
2:B:11:ILE:HG23	2:B:286:ILE:HD12	1.96	0.48
2:B:78:GLU:OE2	2:B:78:GLU:C	2.57	0.48
1:E:107:ILE:CD1	2:F:186:ALA:HB1	2.44	0.48
2:H:5:LEU:HD21	2:H:182:MET:CE	2.38	0.48
2:H:26:ILE:HG22	2:H:224:MET:CE	2.44	0.48
2:B:44:ASN:OD1	2:B:46:SER:HB3	2.13	0.48
1:C:121:LEU:HD22	1:C:123:LYS:HG3	1.96	0.47
1:G:100:VAL:HG12	2:H:261:ARG:HH12	1.78	0.47
2:D:236:TRP:NE1	2:D:245:GLN:HB2	2.29	0.47
2:B:313:HIS:CD2	2:B:313:HIS:H	2.32	0.47
1:A:39:PHE:HB2	1:A:122:ILE:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:ILE:HG13	1:E:168:ALA:N	2.30	0.47
1:G:137:VAL:HG23	1:G:137:VAL:O	2.15	0.47
1:E:125:ASP:O	1:E:126:ALA:HB3	2.15	0.47
1:A:68:GLN:NE2	1:A:197:ILE:CD1	2.78	0.47
1:E:25:SER:C	1:E:27:SER:N	2.71	0.47
1:G:129:THR:O	1:G:130:LEU:HD23	2.15	0.47
1:G:40:ARG:HB2	1:G:59:SER:HB3	1.95	0.47
1:G:163:PHE:HA	1:G:166:LYS:HG3	1.97	0.47
2:B:221:LYS:HE2	4:B:351:HOH:O	2.15	0.47
2:D:180:VAL:HG12	2:D:276:MET:HE3	1.95	0.47
1:E:62:PHE:O	1:E:67:ARG:HA	2.14	0.47
1:G:83:ALA:HB3	1:G:86:ASP:OD2	2.15	0.47
1:A:68:GLN:NE2	1:A:197:ILE:HD13	2.30	0.46
1:C:154:GLU:OE2	1:C:156:GLN:NE2	2.46	0.46
2:D:178:ARG:HG3	2:D:182:MET:CE	2.39	0.46
1:G:31:VAL:CG1	1:G:32:ARG:H	2.21	0.46
1:G:110:SER:O	1:G:111:LYS:HD2	2.15	0.46
2:H:211:PHE:CD1	2:H:212:GLU:N	2.83	0.46
2:D:85:LEU:CA	2:D:89:ILE:HD11	2.44	0.46
1:E:48:ASN:HA	1:E:55:LYS:HE3	1.98	0.46
1:E:67:ARG:H	1:E:67:ARG:CD	2.29	0.46
2:F:166:LEU:C	2:F:166:LEU:HD23	2.39	0.46
2:H:23:LEU:HD22	2:H:230:LEU:CD2	2.45	0.46
1:A:190:GLY:O	1:A:192:ASP:N	2.39	0.46
2:H:307:ILE:N	2:H:307:ILE:HD12	2.31	0.46
2:B:5:LEU:HD12	2:B:271:THR:HG22	1.97	0.46
1:A:44:CYS:HB2	1:A:116:TRP:CZ3	2.50	0.46
1:E:9:VAL:HB	1:E:151:LEU:HB3	1.96	0.46
1:E:35:TRP:CZ2	1:E:138:ARG:HB3	2.51	0.46
1:E:57:MET:HE2	1:E:116:TRP:CE2	2.51	0.46
2:F:88:ARG:HH21	2:F:88:ARG:HG2	1.81	0.46
1:G:167:ILE:O	1:G:170:ILE:N	2.49	0.46
1:C:43:ARG:CD	1:C:119:ARG:HD2	2.45	0.46
2:D:85:LEU:HA	2:D:89:ILE:CD1	2.44	0.46
2:H:236:TRP:NE1	2:H:245:GLN:HG3	2.29	0.46
2:B:83:LYS:HE3	2:F:85:LEU:CD2	2.46	0.46
1:C:11:ARG:HG3	1:C:181:GLU:HB2	1.97	0.46
1:C:35:TRP:CE2	1:C:138:ARG:HB3	2.51	0.46
1:G:41:THR:OG1	1:G:210:LEU:HD21	2.16	0.46
1:G:147:GLY:O	1:G:148:PHE:C	2.59	0.46
1:A:104:ILE:HD13	2:B:188:THR:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ALA:O	1:C:161:GLY:C	2.59	0.46
1:C:177:ILE:O	1:C:178:ARG:HB2	2.14	0.46
1:C:197:ILE:HD13	1:C:197:ILE:O	2.16	0.46
2:F:312:GLU:O	2:F:313:HIS:HB2	2.16	0.46
2:B:5:LEU:HD12	2:B:271:THR:CG2	2.46	0.46
2:D:228:LEU:HA	2:D:257:ILE:HG12	1.97	0.46
1:A:68:GLN:HE21	1:A:197:ILE:CD1	2.29	0.45
2:B:31:PRO:HB3	2:B:222:PHE:CZ	2.51	0.45
2:B:266:ASP:OD2	1:C:3:LYS:HE3	2.15	0.45
2:F:288:LEU:O	2:F:289:SER:HB3	2.16	0.45
2:B:86:ASN:H	2:B:89:ILE:HD11	1.80	0.45
2:D:187:GLU:HG2	2:D:188:THR:N	2.31	0.45
1:E:111:LYS:C	1:E:112:LEU:HD12	2.40	0.45
2:B:83:LYS:CB	2:B:84:PRO:CD	2.79	0.45
2:B:279:LYS:HA	2:B:288:LEU:HD12	1.98	0.45
2:D:11:ILE:HD11	2:D:15:GLY:HA3	1.97	0.45
1:E:141:ASN:HB3	1:E:148:PHE:HE1	1.82	0.45
1:G:15:ALA:O	1:G:19:GLU:HG3	2.16	0.45
2:H:4:GLN:NE2	2:H:258:ASN:HD21	2.11	0.45
1:A:177:ILE:O	1:A:178:ARG:HB2	2.15	0.45
2:B:88:ARG:O	2:B:91:LYS:HG3	2.17	0.45
1:G:60:ILE:N	1:G:60:ILE:CD1	2.79	0.45
1:G:174:LEU:HD12	1:G:177:ILE:HD11	1.97	0.45
2:H:31:PRO:HB3	2:H:222:PHE:CZ	2.52	0.45
1:A:48:ASN:O	1:A:49:LEU:CB	2.61	0.45
2:B:86:ASN:H	2:B:89:ILE:CD1	2.29	0.45
1:G:35:TRP:H	1:G:35:TRP:CD1	2.35	0.45
1:A:71:LEU:O	1:A:77:ALA:HA	2.17	0.45
2:B:5:LEU:HD23	2:B:182:MET:HG3	1.99	0.45
1:G:40:ARG:HG3	1:G:40:ARG:HH11	1.81	0.45
1:G:159:GLU:HB2	1:G:162:GLU:CD	2.41	0.45
2:H:4:GLN:CG	2:H:258:ASN:HD21	2.29	0.45
1:G:7:ILE:HG12	1:G:184:THR:HG23	1.99	0.45
1:A:3:LYS:HG2	1:A:160:ALA:HB2	1.98	0.45
1:C:81:THR:HG21	2:D:191:LEU:HD11	1.99	0.45
2:D:245:GLN:HG2	2:D:248:SER:N	2.32	0.45
2:F:260:SER:O	2:F:263:THR:OG1	2.35	0.45
2:H:180:VAL:CG2	2:H:272:GLU:HG3	2.47	0.45
2:B:292:ASP:O	2:B:296:MET:HG2	2.18	0.44
2:H:237:GLN:CG	2:H:244:SER:HB3	2.48	0.44
1:E:200:LEU:O	1:E:204:TYR:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:ILE:O	1:E:132:LEU:HD23	2.17	0.44
1:E:178:ARG:O	1:E:179:ALA:C	2.60	0.44
2:F:247:THR:O	2:F:248:SER:C	2.59	0.44
2:D:11:ILE:HD12	2:D:12:GLY:O	2.17	0.44
2:D:62:ASN:O	2:D:209:TYR:HE2	2.01	0.44
1:G:12:ALA:HB1	1:G:16:THR:OG1	2.18	0.44
2:B:86:ASN:C	2:B:86:ASN:ND2	2.74	0.44
2:D:18:LEU:HD12	2:F:92:SER:HB3	1.99	0.44
1:E:63:HIS:ND1	1:E:67:ARG:NE	2.66	0.44
1:E:81:THR:HG21	1:E:86:ASP:HB3	1.99	0.44
2:F:296:MET:HE1	2:F:305:ILE:HA	1.99	0.44
1:A:189:LEU:HD13	1:A:202:TYR:CG	2.53	0.44
1:G:39:PHE:HB2	1:G:122:ILE:HB	1.99	0.44
1:G:58:TYR:CD2	1:G:210:LEU:HD13	2.53	0.44
1:G:120:GLN:HG2	1:G:121:LEU:N	2.32	0.44
1:E:37:ILE:HG12	1:E:38:ASP:N	2.33	0.44
1:G:104:ILE:O	1:G:107:ILE:HB	2.18	0.44
2:B:3:GLN:HB3	2:B:259:VAL:HG22	2.00	0.43
1:C:163:PHE:O	1:C:167:ILE:CD1	2.62	0.43
2:F:267:ARG:O	2:F:270:TYR:HB3	2.18	0.43
2:H:3:GLN:OE1	2:H:182:MET:SD	2.76	0.43
2:B:280:LYS:O	2:B:283:GLN:HG2	2.18	0.43
1:C:163:PHE:O	1:C:166:LYS:HB2	2.18	0.43
2:F:31:PRO:HB3	2:F:222:PHE:CZ	2.53	0.43
1:G:23:ALA:O	1:G:24:LEU:HD12	2.18	0.43
2:B:293:ARG:HA	2:B:296:MET:HB2	1.99	0.43
2:D:180:VAL:HG13	2:D:276:MET:HE3	1.99	0.43
1:A:142:LEU:CD1	1:A:149:LYS:HD3	2.48	0.43
2:B:86:ASN:O	2:B:89:ILE:HG13	2.17	0.43
1:E:32:ARG:CD	1:E:131:ILE:HD11	2.48	0.43
1:E:176:GLU:C	1:E:178:ARG:H	2.25	0.43
1:E:67:ARG:N	1:E:67:ARG:CD	2.80	0.43
2:F:29:ASN:HB3	2:F:30:PRO:HD2	2.01	0.43
1:G:167:ILE:C	1:G:169:GLY:N	2.74	0.43
2:B:5:LEU:HD22	2:B:180:VAL:HG23	2.01	0.43
2:B:30:PRO:HB3	2:D:85:LEU:HG	2.00	0.43
2:D:276:MET:HE2	2:D:276:MET:HA	2.00	0.43
1:A:68:GLN:OE1	1:A:86:ASP:OD2	2.36	0.43
2:H:16:TYR:O	2:H:20:ILE:HG12	2.19	0.43
1:G:162:GLU:O	1:G:166:LYS:HG2	2.19	0.43
2:B:228:LEU:HA	2:B:257:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:ILE:HG12	2:F:47:TYR:CD2	2.54	0.42
2:H:272:GLU:O	2:H:276:MET:HG2	2.19	0.42
2:B:5:LEU:CD2	2:B:182:MET:HE2	2.40	0.42
2:B:90:LEU:CD1	2:B:219:GLY:HA2	2.49	0.42
2:F:163:PRO:HA	2:F:190:ILE:O	2.19	0.42
1:G:119:ARG:O	1:G:120:GLN:HB2	2.19	0.42
2:H:44:ASN:HB3	2:H:47:TYR:CE2	2.54	0.42
2:D:89:ILE:HG13	2:D:89:ILE:H	1.58	0.42
1:E:201:ALA:O	1:E:205:VAL:HG23	2.20	0.42
2:D:211:PHE:CD1	2:D:211:PHE:C	2.96	0.42
2:B:86:ASN:N	2:B:89:ILE:CD1	2.83	0.42
2:D:75:LEU:C	2:D:76:ILE:HD12	2.45	0.42
1:E:83:ALA:O	1:E:84:ALA:C	2.63	0.42
1:G:10:GLU:N	1:G:10:GLU:OE1	2.52	0.42
2:H:2:VAL:HG23	2:H:261:ARG:NH1	2.35	0.42
2:H:5:LEU:HD12	2:H:271:THR:HG22	2.01	0.42
2:H:261:ARG:HD2	2:H:261:ARG:N	2.34	0.42
1:A:17:LEU:HD23	1:A:17:LEU:C	2.45	0.42
1:A:91:LEU:HD12	1:A:91:LEU:HA	1.82	0.42
2:B:76:ILE:HD13	2:B:85:LEU:HD11	2.01	0.42
2:B:91:LYS:C	2:B:93:PHE:H	2.28	0.42
2:B:282:LEU:O	2:B:285:TYR:HB2	2.20	0.42
1:E:35:TRP:CE2	1:E:138:ARG:HB3	2.55	0.42
1:E:38:ASP:HB2	1:E:61:THR:HB	2.01	0.42
1:E:39:PHE:HB3	1:E:122:ILE:HG12	2.02	0.42
2:F:263:THR:HG22	2:F:267:ARG:HD3	1.96	0.42
1:G:206:ARG:HH11	1:G:206:ARG:CG	2.31	0.42
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.90	0.41
2:F:77:ASP:OD1	2:F:77:ASP:C	2.62	0.41
2:F:270:TYR:O	2:F:273:THR:HB	2.19	0.41
2:F:300:VAL:CG2	2:F:311:LEU:HD13	2.50	0.41
1:G:138:ARG:NH2	1:G:156:GLN:NE2	2.66	0.41
2:B:197:ASN:HB3	2:B:202:SER:HB3	2.01	0.41
1:C:70:VAL:HG21	1:C:197:ILE:HD12	2.01	0.41
2:D:293:ARG:C	2:D:295:SER:N	2.78	0.41
1:E:10:GLU:H	1:E:10:GLU:CD	2.26	0.41
1:A:39:PHE:HB2	1:A:122:ILE:HG12	2.01	0.41
1:E:40:ARG:HB2	1:E:59:SER:HB3	2.02	0.41
1:E:71:LEU:HD22	1:E:78:MET:HE2	2.02	0.41
1:E:195:ASN:C	1:E:195:ASN:ND2	2.77	0.41
1:E:210:LEU:HD23	1:E:210:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:ASN:OD1	2:F:35:ASN:C	2.64	0.41
1:G:24:LEU:O	1:G:27:SER:N	2.47	0.41
1:G:37:ILE:HG12	1:G:38:ASP:N	2.35	0.41
2:B:296:MET:HE1	2:B:305:ILE:HG12	2.03	0.41
1:E:130:LEU:HB2	1:E:137:VAL:HG23	2.02	0.41
2:F:293:ARG:O	2:F:297:ASP:N	2.46	0.41
2:F:180:VAL:CG1	2:F:272:GLU:HG3	2.51	0.41
2:H:233:GLN:HG2	2:H:252:LEU:O	2.21	0.41
2:B:2:VAL:HA	2:B:261:ARG:HD2	2.01	0.41
2:D:246:ILE:HG23	2:D:311:LEU:CD2	2.51	0.41
1:G:17:LEU:C	1:G:17:LEU:HD23	2.46	0.41
1:E:48:ASN:H	1:E:55:LYS:HZ2	1.64	0.41
1:G:10:GLU:OE1	1:G:10:GLU:CA	2.67	0.41
2:H:44:ASN:HB3	2:H:47:TYR:HD2	1.84	0.41
2:H:82:ASP:O	2:H:83:LYS:CE	2.68	0.41
1:E:163:PHE:HA	1:E:166:LYS:HG3	2.03	0.41
2:H:263:THR:OG1	2:H:268:ILE:HD11	2.21	0.41
1:C:40:ARG:HD3	1:C:118:GLN:NE2	2.35	0.41
2:D:293:ARG:O	2:D:295:SER:N	2.50	0.41
1:A:48:ASN:CG	1:A:49:LEU:H	2.29	0.40
2:B:90:LEU:HD21	2:B:218:ILE:HG22	2.03	0.40
1:C:111:LYS:NZ	2:D:170:ASP:OD2	2.50	0.40
2:D:78:GLU:O	2:D:79:THR:HB	2.21	0.40
1:G:12:ALA:C	1:G:13:THR:CG2	2.93	0.40
1:G:164:GLU:H	1:G:164:GLU:HG3	1.68	0.40
2:H:205:ASN:C	2:H:207:LEU:H	2.29	0.40
1:G:100:VAL:HG11	2:H:261:ARG:HH12	1.87	0.40
2:H:238:ILE:HG23	2:H:240:GLU:CD	2.46	0.40
1:C:100:VAL:HB	2:D:2:VAL:CG2	2.44	0.40
2:D:260:SER:HA	2:D:261:ARG:NH1	2.36	0.40
2:H:228:LEU:HA	2:H:257:ILE:HG12	2.03	0.40
1:G:112:LEU:HD12	1:G:112:LEU:N	2.36	0.40
1:A:13:THR:O	1:A:14:PRO:C	2.62	0.40
1:C:104:ILE:HD12	1:C:107:ILE:HB	2.04	0.40
1:C:163:PHE:HA	1:C:166:LYS:CG	2.51	0.40
1:G:121:LEU:HD23	1:G:121:LEU:C	2.47	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	201/212 (95%)	193 (96%)	5 (2%)	3 (2%)	8	12
1	C	189/212 (89%)	172 (91%)	14 (7%)	3 (2%)	7	11
1	E	191/212 (90%)	163 (85%)	23 (12%)	5 (3%)	4	4
1	G	190/212 (90%)	161 (85%)	23 (12%)	6 (3%)	3	3
2	B	217/317 (68%)	209 (96%)	5 (2%)	3 (1%)	9	13
2	D	227/317 (72%)	209 (92%)	14 (6%)	4 (2%)	6	9
2	F	230/317 (73%)	221 (96%)	8 (4%)	1 (0%)	30	43
2	H	216/317 (68%)	195 (90%)	15 (7%)	6 (3%)	4	3
All	All	1661/2116 (78%)	1523 (92%)	107 (6%)	31 (2%)	6	8

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	193	THR
1	C	161	GLY
1	C	187	ASP
2	D	79	THR
1	E	126	ALA
2	F	103	ALA
1	G	10	GLU
2	H	84	PRO
2	B	292	ASP
1	G	133	ASP
1	G	163	PHE
2	D	62	ASN
2	D	294	GLN
1	E	3	LYS
1	E	148	PHE
1	G	25	SER

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Mol	Chain	Res	Type
2	H	302	HIS
2	B	48	ASP
2	B	84	PRO
2	H	62	ASN
2	H	79	THR
2	H	241	ALA
1	C	25	SER
1	G	164	GLU
1	G	176	GLU
2	H	81	MET
1	E	179	ALA
1	E	127	GLY
1	A	191	PRO
2	D	84	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	174/179 (97%)	163 (94%)	11 (6%)	16	29
1	C	166/179 (93%)	159 (96%)	7 (4%)	26	45
1	E	167/179 (93%)	160 (96%)	7 (4%)	26	45
1	G	166/179 (93%)	160 (96%)	6 (4%)	31	52
2	B	204/288 (71%)	190 (93%)	14 (7%)	14	24
2	D	207/288 (72%)	192 (93%)	15 (7%)	13	23
2	F	214/288 (74%)	206 (96%)	8 (4%)	30	51
2	H	203/288 (70%)	196 (97%)	7 (3%)	32	54
All	All	1501/1868 (80%)	1426 (95%)	75 (5%)	22	38

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU

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Mol	Chain	Res	Type
1	A	67	ARG
1	A	71	LEU
1	A	91	LEU
1	A	119	ARG
1	A	121	LEU
1	A	137	VAL
1	A	142	LEU
1	A	174	LEU
1	A	189	LEU
1	A	195	ASN
2	B	2	VAL
2	B	3	GLN
2	B	18	LEU
2	B	66	LEU
2	B	70	VAL
2	B	77	ASP
2	B	78	GLU
2	B	86	ASN
2	B	261	ARG
2	B	275	LEU
2	B	283	GLN
2	B	292	ASP
2	B	307	ILE
2	B	313	HIS
1	C	11	ARG
1	C	71	LEU
1	C	120	GLN
1	C	121	LEU
1	C	137	VAL
1	C	181	GLU
1	C	197	ILE
2	D	2	VAL
2	D	3	GLN
2	D	5	LEU
2	D	11	ILE
2	D	18	LEU
2	D	70	VAL
2	D	80	MET
2	D	86	ASN
2	D	89	ILE
2	D	177	ASN
2	D	261	ARG

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Mol	Chain	Res	Type
2	D	266	ASP
2	D	275	LEU
2	D	300	VAL
2	D	307	ILE
1	E	56	LEU
1	E	57	MET
1	E	60	ILE
1	E	120	GLN
1	E	121	LEU
1	E	125	ASP
1	E	152	LEU
2	F	18	LEU
2	F	33	LEU
2	F	72	PHE
2	F	79	THR
2	F	102	TYR
2	F	200	VAL
2	F	261	ARG
2	F	275	LEU
1	G	10	GLU
1	G	60	ILE
1	G	162	GLU
1	G	189	LEU
1	G	197	ILE
1	G	210	LEU
2	H	66	LEU
2	H	76	ILE
2	H	82	ASP
2	H	84	PRO
2	H	95	ASN
2	H	240	GLU
2	H	245	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	65	HIS
1	A	68	GLN
1	A	114	ASN
1	A	118	GLN
1	A	203	GLN

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Mol	Chain	Res	Type
2	B	86	ASN
2	B	183	GLN
2	B	205	ASN
2	B	226	HIS
2	B	258	ASN
2	B	269	ASN
2	B	283	GLN
2	B	294	GLN
2	B	313	HIS
1	C	63	HIS
1	C	68	GLN
1	C	94	ASN
1	C	118	GLN
1	C	195	ASN
2	D	3	GLN
2	D	86	ASN
2	D	176	ASN
2	D	177	ASN
2	D	183	GLN
2	D	197	ASN
2	D	205	ASN
2	D	226	HIS
2	D	258	ASN
2	D	294	GLN
1	E	68	GLN
1	E	118	GLN
1	E	195	ASN
2	F	3	GLN
2	F	101	ASN
2	F	205	ASN
2	F	214	GLN
2	F	233	GLN
2	F	237	GLN
2	F	258	ASN
1	G	65	HIS
1	G	68	GLN
1	G	118	GLN
1	G	120	GLN
1	G	156	GLN
1	G	195	ASN
2	H	62	ASN
2	H	95	ASN

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Mol	Chain	Res	Type
2	H	167	GLN
2	H	237	GLN
2	H	243	ASN
2	H	258	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	A	211	-	4,4,4	1.68	1 (25%)	6,6,6	0.48	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	211	PO4	P-O3	-2.07	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	205/212 (96%)	-0.31	4 (1%) 65 60	20, 31, 57, 91	0
1	C	195/212 (91%)	0.43	13 (6%) 24 20	29, 58, 84, 91	0
1	E	197/212 (92%)	1.22	35 (17%) 4 3	30, 88, 100, 100	0
1	G	196/212 (92%)	1.44	54 (27%) 1 1	36, 91, 100, 100	0
2	B	227/317 (71%)	-0.06	9 (3%) 42 38	20, 39, 71, 94	0
2	D	233/317 (73%)	0.22	12 (5%) 33 29	24, 45, 82, 91	0
2	F	238/317 (75%)	0.01	8 (3%) 48 44	21, 43, 77, 95	0
2	H	226/317 (71%)	0.93	29 (12%) 7 6	35, 74, 99, 100	0
All	All	1717/2116 (81%)	0.46	164 (9%) 13 10	20, 55, 99, 100	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	210	LEU	5.4
1	E	175	ALA	5.1
1	E	160	ALA	4.8
2	H	265	ILE	4.6
1	G	39	PHE	4.6
2	H	61	PRO	4.5
2	H	171	ILE	4.5
2	F	171	ILE	4.4
1	C	46	ILE	4.3
1	A	49	LEU	4.2
1	C	63	HIS	3.7
1	G	160	ALA	3.6
2	H	47	TYR	3.6
1	E	167	ILE	3.6
2	D	82	ASP	3.6
2	H	81	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	189	LEU	3.5
2	H	295	SER	3.5
1	G	117	MET	3.4
2	F	61	PRO	3.3
1	G	196	GLU	3.3
1	G	163	PHE	3.2
2	B	313	HIS	3.2
2	H	262	GLY	3.1
2	B	85	LEU	3.1
2	D	174	ALA	3.1
1	E	62	PHE	3.1
1	C	65	HIS	3.1
1	G	55	LYS	3.0
1	G	17	LEU	3.0
1	G	64	HIS	3.0
2	D	61	PRO	3.0
2	F	265	ILE	3.0
1	G	167	ILE	2.9
2	H	300	VAL	2.9
1	E	64	HIS	2.9
1	E	161	GLY	2.9
2	H	259	VAL	2.9
1	C	64	HIS	2.9
1	G	145	SER	2.8
1	G	44	CYS	2.8
2	H	240	GLU	2.8
1	E	117	MET	2.8
1	G	65	HIS	2.8
1	G	46	ILE	2.7
2	B	49	VAL	2.7
1	G	180	LYS	2.7
2	H	78	GLU	2.7
2	B	171	ILE	2.7
2	D	93	PHE	2.7
2	D	160	SER	2.7
1	G	2	GLY	2.6
1	E	28	ILE	2.6
1	E	122	ILE	2.6
1	E	168	ALA	2.6
2	D	81	MET	2.6
1	G	151	LEU	2.6
1	G	136	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	179	ALA	2.6
1	E	188	SER	2.6
1	G	14	PRO	2.5
1	G	131	ILE	2.5
2	H	3	GLN	2.5
1	E	179	ALA	2.5
1	E	207	ALA	2.5
1	G	12	ALA	2.5
1	G	207	ALA	2.5
1	E	2	GLY	2.5
1	G	148	PHE	2.5
2	H	269	ASN	2.5
1	G	174	LEU	2.5
1	E	55	LYS	2.5
1	G	187	ASP	2.5
1	G	132	LEU	2.5
1	G	144	SER	2.5
1	A	191	PRO	2.4
1	E	37	ILE	2.4
2	H	82	ASP	2.4
2	D	241	ALA	2.4
2	H	242	GLY	2.4
1	G	155	LEU	2.4
1	G	210	LEU	2.4
1	E	84	ALA	2.4
1	G	15	ALA	2.4
1	E	136	THR	2.4
1	C	162	GLU	2.4
1	E	176	GLU	2.4
2	D	78	GLU	2.4
1	G	209	GLU	2.4
2	H	201	SER	2.4
1	C	66	GLY	2.4
1	E	131	ILE	2.4
1	E	29	LEU	2.4
2	D	237	GLN	2.4
1	G	3	LYS	2.4
2	B	287	GLU	2.4
1	E	145	SER	2.3
2	B	292	ASP	2.3
1	G	10	GLU	2.3
1	G	168	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	177	ASN	2.3
1	G	157	ALA	2.3
2	H	182	MET	2.3
1	C	196	GLU	2.3
2	D	47	TYR	2.3
1	E	26	ASN	2.3
1	A	193	THR	2.3
2	H	313	HIS	2.3
1	G	71	LEU	2.3
2	B	48	ASP	2.3
1	E	121	LEU	2.2
1	C	189	LEU	2.2
1	G	29	LEU	2.2
1	G	37	ILE	2.2
2	H	261	ARG	2.2
1	G	6	VAL	2.2
1	A	189	LEU	2.2
1	E	208	LEU	2.2
1	G	177	ILE	2.2
2	H	170	ASP	2.2
1	E	35	TRP	2.2
1	E	178	ARG	2.2
2	B	84	PRO	2.2
1	G	28	ILE	2.2
1	G	122	ILE	2.2
1	G	119	ARG	2.2
2	H	45	PRO	2.2
1	E	163	PHE	2.2
1	G	175	ALA	2.1
1	E	158	ASP	2.1
2	H	211	PHE	2.1
1	E	140	VAL	2.1
1	G	35	TRP	2.1
2	H	296	MET	2.1
2	H	95	ASN	2.1
2	H	243	ASN	2.1
2	H	7	LEU	2.1
1	G	170	ILE	2.1
1	C	181	GLU	2.1
2	F	261	ARG	2.1
1	C	54	SER	2.1
1	E	186	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	46	SER	2.1
1	C	180	LYS	2.1
2	D	313	HIS	2.1
2	H	83	LYS	2.1
1	C	117	MET	2.1
1	E	65	HIS	2.1
2	F	104	MET	2.1
1	E	24	LEU	2.1
2	F	277	ASN	2.1
2	F	74	TYR	2.1
1	G	36	SER	2.1
1	G	59	SER	2.1
2	B	61	PRO	2.1
1	G	179	ALA	2.0
1	G	164	GLU	2.0
2	F	313	HIS	2.0
1	G	67	ARG	2.0
1	G	24	LEU	2.0
1	E	46	ILE	2.0
1	G	146	THR	2.0
1	G	158	ASP	2.0
2	H	80	MET	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	A	211	5/5	0.96	0.07	43,44,47,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.