



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:06 AM UTC

PDB ID : 2HZS / pdb_00002hzs
Title : Structure of the Mediator head submodule Med8C/18/20
Authors : Lariviere, L.; Geiger, S.; Hoepfner, S.; Rother, S.; Straesser, K.; Cramer, P.
Deposited on : 2006-08-09
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

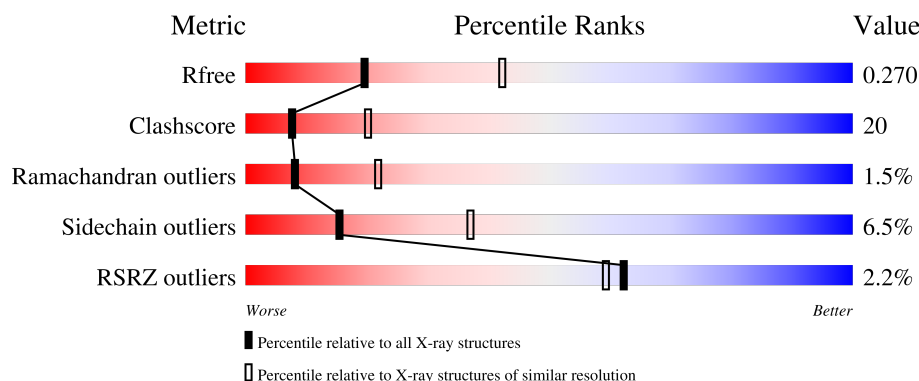
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

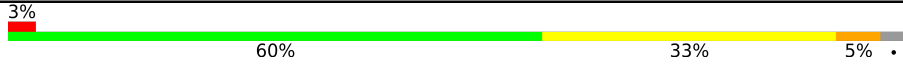
The reported resolution of this entry is 2.70 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	209	
1	C	209	
1	E	209	
1	G	209	
2	B	306	

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Mol	Chain	Length	Quality of chain
2	D	306	% 45%21%••30%
2	F	306	42%30%5%23%
2	H	306	46%24%5%•25%
3	I	27	4% 63%19%19%
3	J	27	52%15%•30%
3	K	27	52%7%41%
3	L	27	56%7%37%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14086 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	203	Total	C	N	O	S	0	0	0
			1560	987	263	305	5			
1	C	202	Total	C	N	O	S	0	0	0
			1554	984	262	303	5			
1	E	203	Total	C	N	O	S	0	0	0
			1560	987	263	305	5			
1	G	203	Total	C	N	O	S	0	0	0
			1560	987	263	305	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	0
			1844	1175	302	358	9			
2	D	214	Total	C	N	O	S	0	0	0
			1671	1065	273	326	7			
2	F	235	Total	C	N	O	S	0	0	0
			1829	1156	298	367	8			
2	H	230	Total	C	N	O	S	0	0	0
			1803	1146	297	351	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	274	VAL	ALA	engineered mutation	UNP P32585
D	274	VAL	ALA	engineered mutation	UNP P32585
F	274	VAL	ALA	engineered mutation	UNP P32585
H	274	VAL	ALA	engineered mutation	UNP P32585

- Molecule 3 is a protein called RNA polymerase II mediator complex subunit 8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	22	Total	C	N	O	0	0	0
			192	123	37	32			
3	J	19	Total	C	N	O	0	0	0
			156	102	25	29			
3	K	16	Total	C	N	O	0	0	0
			131	87	19	25			
3	L	17	Total	C	N	O	0	0	0
			141	93	22	26			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	211	HIS	-	expression tag	UNP P38304
I	212	HIS	-	expression tag	UNP P38304
I	213	HIS	-	expression tag	UNP P38304
I	214	HIS	-	expression tag	UNP P38304
I	215	HIS	-	expression tag	UNP P38304
I	216	HIS	-	expression tag	UNP P38304
J	211	HIS	-	expression tag	UNP P38304
J	212	HIS	-	expression tag	UNP P38304
J	213	HIS	-	expression tag	UNP P38304
J	214	HIS	-	expression tag	UNP P38304
J	215	HIS	-	expression tag	UNP P38304
J	216	HIS	-	expression tag	UNP P38304
K	211	HIS	-	expression tag	UNP P38304
K	212	HIS	-	expression tag	UNP P38304
K	213	HIS	-	expression tag	UNP P38304
K	214	HIS	-	expression tag	UNP P38304
K	215	HIS	-	expression tag	UNP P38304
K	216	HIS	-	expression tag	UNP P38304
L	211	HIS	-	expression tag	UNP P38304
L	212	HIS	-	expression tag	UNP P38304
L	213	HIS	-	expression tag	UNP P38304
L	214	HIS	-	expression tag	UNP P38304
L	215	HIS	-	expression tag	UNP P38304
L	216	HIS	-	expression tag	UNP P38304

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	34	Total	O	0	0
			34	34		

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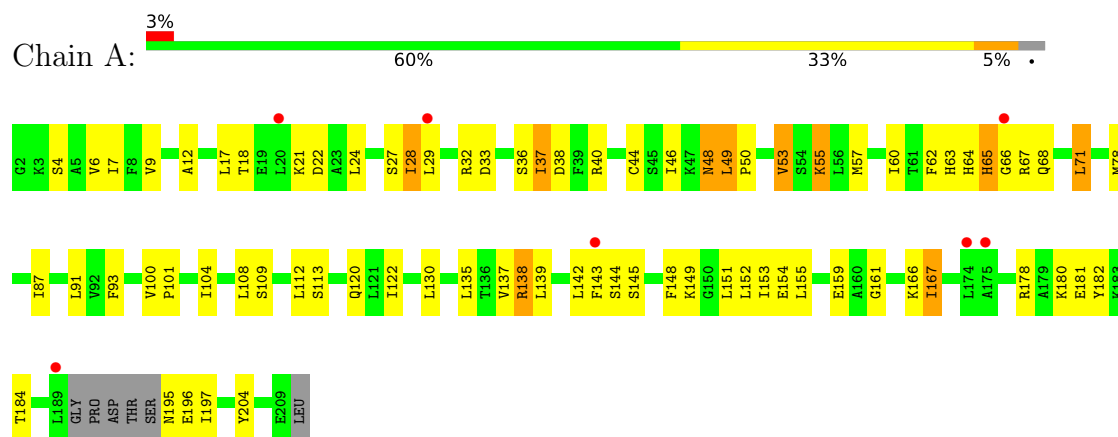
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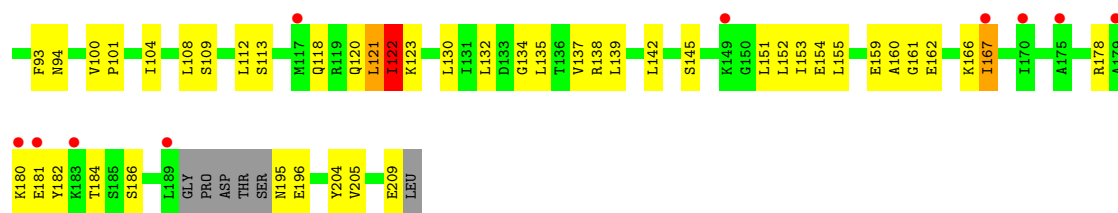
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total 2	O 2	0	0
4	D	12	Total 12	O 12	0	0
4	E	2	Total 2	O 2	0	0
4	F	13	Total 13	O 13	0	0
4	H	15	Total 15	O 15	0	0
4	I	4	Total 4	O 4	0	0

3 Residue-property plots [i](#)

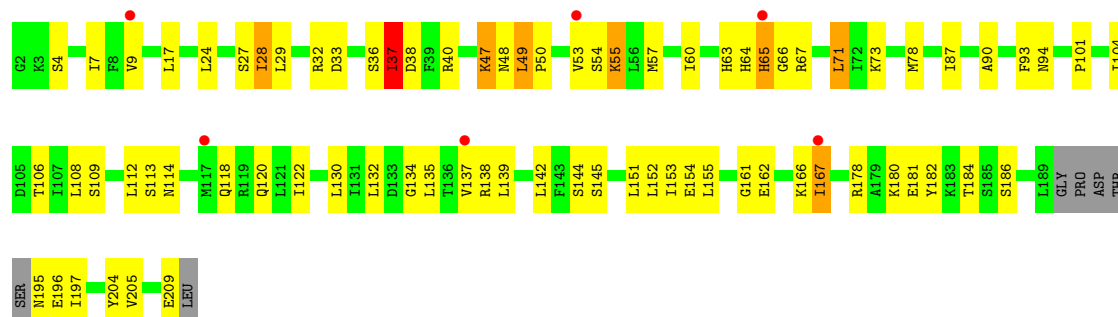
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

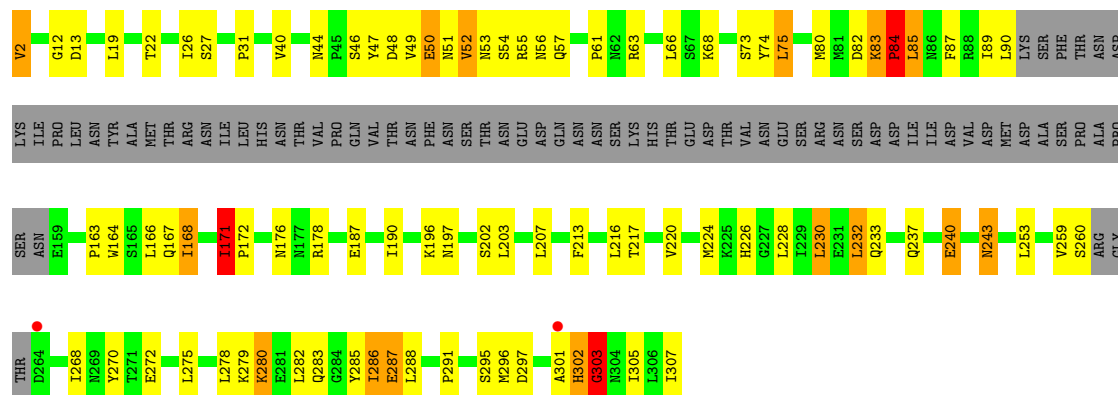




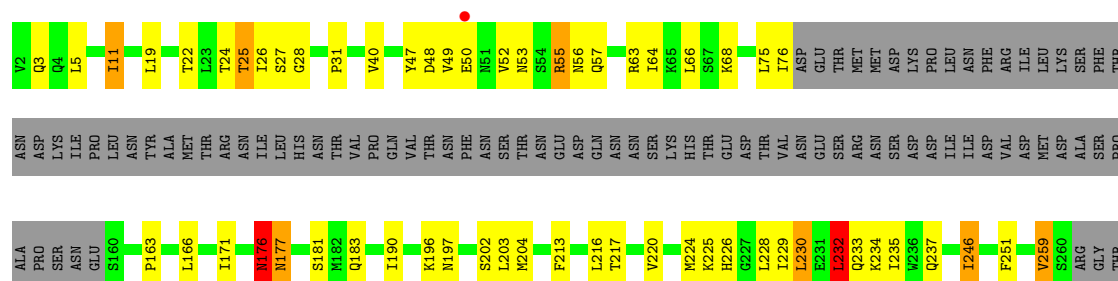
• Molecule 1: RNA polymerase II mediator complex subunit 20



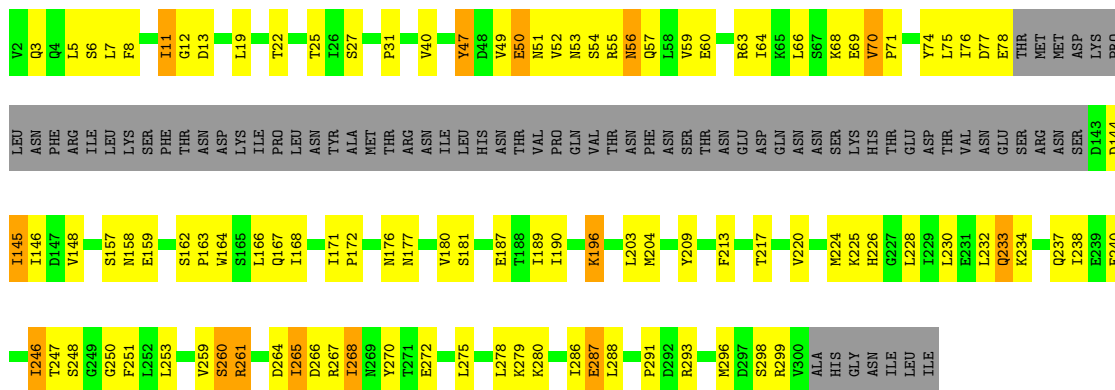
• Molecule 2: RNA polymerase II mediator complex subunit 18



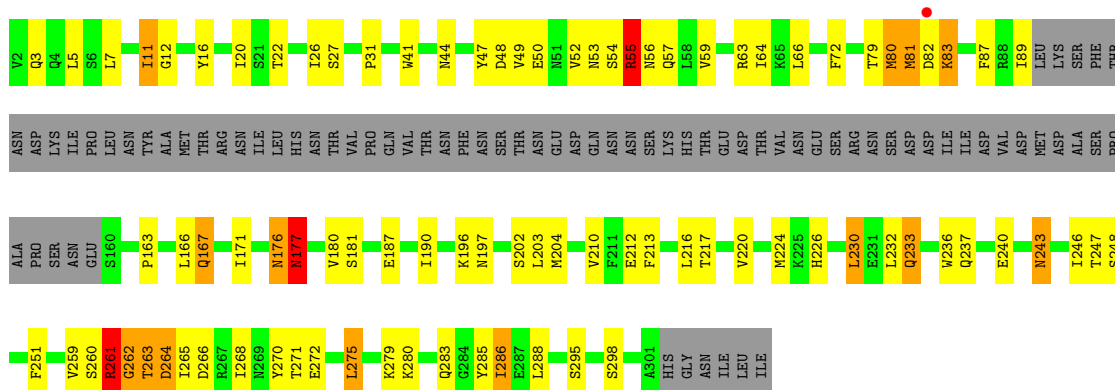
• Molecule 2: RNA polymerase II mediator complex subunit 18



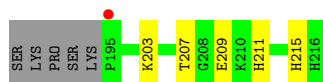
- Molecule 2: RNA polymerase II mediator complex subunit 18



- Molecule 2: RNA polymerase II mediator complex subunit 18



- Molecule 3: RNA polymerase II mediator complex subunit 8



- Molecule 3: RNA polymerase II mediator complex subunit 8



● Molecule 3: RNA polymerase II mediator complex subunit 8



● Molecule 3: RNA polymerase II mediator complex subunit 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.36Å 115.76Å 129.16Å 90.00° 98.49° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.70) 99.6 (20.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.67Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.272 0.232 , 0.270	Depositor DCC
R_{free} test set	3117 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14086	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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	0.47	0/1584	1.09	10/2145 (0.5%)
1	C	0.47	0/1577	0.92	3/2134 (0.1%)
1	E	0.46	0/1584	0.94	7/2145 (0.3%)
1	G	0.45	0/1584	0.90	4/2145 (0.2%)
2	B	0.56	0/1876	1.07	9/2541 (0.4%)
2	D	0.51	0/1700	1.00	7/2304 (0.3%)
2	F	0.53	0/1861	1.02	11/2526 (0.4%)
2	H	0.52	0/1835	1.03	9/2486 (0.4%)
3	I	0.51	0/201	0.85	0/269
3	J	0.44	0/160	1.11	3/214 (1.4%)
3	K	0.58	0/134	0.84	0/179
3	L	0.50	0/145	0.77	0/194
All	All	0.50	0/14241	1.00	63/19282 (0.3%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	HIS	N-CA-C	-13.84	91.64	112.54
1	A	53	VAL	N-CA-C	-9.90	93.02	107.78
2	B	54	SER	N-CA-C	-9.89	100.62	112.89
1	A	67	ARG	N-CA-C	-9.12	100.57	112.24
2	D	176	ASN	N-CA-C	-8.74	96.05	109.85
1	A	138	ARG	NE-CZ-NH2	8.35	126.72	119.20
1	A	138	ARG	NE-CZ-NH1	-8.29	113.21	121.50
1	A	55	LYS	N-CA-C	-8.15	102.38	113.30
2	B	303	GLY	N-CA-C	-8.01	94.19	113.18
3	J	194	LYS	CA-C-N	7.76	127.48	119.56
3	J	194	LYS	C-N-CA	7.76	127.48	119.56
1	E	55	LYS	N-CA-C	-7.66	103.52	113.17
2	B	233	GLN	N-CA-C	7.15	120.61	109.52
2	F	54	SER	N-CA-C	-7.03	104.69	113.20
2	H	233	GLN	N-CA-C	6.95	120.83	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	93	PHE	N-CA-C	6.85	118.82	111.36
2	B	301	ALA	N-CA-C	6.83	125.34	110.80
2	D	233	GLN	N-CA-C	6.74	120.49	109.85
2	F	70	VAL	CA-C-N	-6.34	113.42	119.76
2	F	70	VAL	C-N-CA	-6.34	113.42	119.76
2	F	171	ILE	N-CA-C	-6.31	103.15	109.02
1	E	122	ILE	CB-CA-C	-6.30	102.58	111.21
2	H	55	ARG	N-CA-C	-6.30	99.62	109.25
2	F	47	TYR	N-CA-C	-6.26	102.70	110.41
2	H	47	TYR	N-CA-C	-6.24	102.13	110.55
2	D	177	ASN	N-CA-C	-6.24	103.56	111.92
2	H	261	ARG	N-CA-C	6.23	124.07	110.80
1	A	138	ARG	CD-NE-CZ	6.14	133.00	124.40
2	F	233	GLN	N-CA-C	6.14	119.55	109.85
2	D	225	LYS	N-CA-C	6.11	118.66	110.35
1	A	40	ARG	NE-CZ-NH2	-6.07	113.74	119.20
2	H	171	ILE	N-CA-C	-5.78	103.64	109.02
1	G	37	ILE	N-CA-C	5.78	115.45	108.06
1	C	56	LEU	N-CA-C	5.74	118.82	109.59
2	D	171	ILE	N-CA-C	-5.72	103.70	109.02
2	B	75	LEU	N-CA-C	5.65	117.12	111.07
2	F	12	GLY	N-CA-C	-5.65	105.31	112.54
1	A	93	PHE	N-CA-C	5.62	117.41	111.28
2	D	232	LEU	N-CA-C	-5.60	98.21	108.02
1	E	160	ALA	N-CA-C	-5.54	106.36	113.01
2	B	232	LEU	N-CA-C	-5.54	98.19	107.99
1	E	122	ILE	CB-CG1-CD1	5.52	125.39	113.80
1	E	93	PHE	N-CA-C	5.50	116.96	111.07
2	B	171	ILE	N-CA-C	-5.48	103.92	109.02
2	F	237	GLN	N-CA-C	-5.48	101.54	110.20
2	H	265	ILE	N-CA-C	-5.47	105.82	112.76
1	A	27	SER	N-CA-C	-5.45	107.88	114.75
2	H	72	PHE	N-CA-C	5.41	117.87	111.33
1	G	93	PHE	N-CA-C	5.39	117.16	111.28
2	B	50	GLU	N-CA-C	-5.39	103.78	110.41
3	J	208	GLY	N-CA-C	-5.34	107.88	115.30
2	F	145	ILE	N-CA-C	-5.28	98.36	109.34
1	G	106	THR	N-CA-C	-5.26	105.44	111.07
2	B	168	ILE	N-CA-C	-5.23	100.58	108.12
2	H	12	GLY	N-CA-C	-5.16	105.70	112.82
2	F	240	GLU	N-CA-C	-5.14	105.75	111.36
1	C	186	SER	N-CA-C	-5.14	104.78	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	225	LYS	N-CA-C	5.11	117.71	110.50
1	E	145	SER	N-CA-C	-5.08	106.92	113.02
2	D	183	GLN	N-CA-C	5.06	117.15	108.90
1	G	186	SER	N-CA-C	-5.04	104.93	112.54
1	E	186	SER	N-CA-C	-5.03	104.94	112.54
2	H	167	GLN	N-CA-C	5.02	117.62	109.24

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	1560	0	1576	74	0
1	C	1554	0	1573	72	0
1	E	1560	0	1576	65	0
1	G	1560	0	1576	56	0
2	B	1844	0	1851	84	0
2	D	1671	0	1676	59	1
2	F	1829	0	1811	93	1
2	H	1803	0	1809	79	0
3	I	192	0	168	5	0
3	J	156	0	150	5	0
3	K	131	0	126	2	0
3	L	141	0	133	2	0
4	A	3	0	0	0	0
4	B	34	0	0	2	0
4	C	2	0	0	0	0
4	D	12	0	0	0	0
4	E	2	0	0	0	0
4	F	13	0	0	1	0
4	H	15	0	0	0	0
4	I	4	0	0	0	0
All	All	14086	0	14025	562	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 20.

All (562) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:HD11	1:A:152:LEU:HD12	1.35	1.06
1:G:142:LEU:HD11	1:G:152:LEU:HD12	1.36	1.05
2:F:265:ILE:HD12	2:F:265:ILE:H	1.25	1.02
1:C:142:LEU:HD11	1:C:152:LEU:HD12	1.37	1.01
1:E:142:LEU:HD11	1:E:152:LEU:HD12	1.37	1.00
2:B:83:LYS:O	2:B:84:PRO:C	2.10	0.92
1:C:71:LEU:HD11	1:C:104:ILE:HG12	1.54	0.90
2:B:53:ASN:HD22	2:B:57:GLN:HB2	1.35	0.89
1:A:66:GLY:HA3	1:A:68:GLN:HG3	1.54	0.89
1:E:40:ARG:HD3	1:E:118:GLN:NE2	1.90	0.87
1:A:100:VAL:HB	2:B:2:VAL:HG21	1.55	0.86
1:A:100:VAL:HB	2:B:2:VAL:CG2	2.05	0.86
1:E:27:SER:O	1:E:132:LEU:HD22	1.77	0.84
2:H:11:ILE:HD11	2:H:251:PHE:HB2	1.60	0.83
1:G:71:LEU:HD11	1:G:104:ILE:HG12	1.60	0.82
2:D:75:LEU:HD22	2:D:216:LEU:HD21	1.61	0.82
2:H:263:THR:HG22	2:H:264:ASP:H	1.45	0.82
2:B:53:ASN:HB2	2:B:57:GLN:H	1.44	0.82
2:B:232:LEU:HD13	2:B:253:LEU:HD13	1.62	0.82
1:C:130:LEU:HB2	1:C:137:VAL:HG13	1.60	0.82
1:A:130:LEU:HB2	1:A:137:VAL:HG13	1.61	0.82
1:A:62:PHE:HB3	1:A:65:HIS:HB2	1.62	0.81
1:G:40:ARG:HD3	1:G:118:GLN:NE2	1.96	0.80
1:E:130:LEU:HB2	1:E:137:VAL:HG13	1.63	0.80
2:F:50:GLU:CD	2:F:50:GLU:H	1.90	0.80
1:E:134:GLY:O	1:E:166:LYS:NZ	2.15	0.80
2:F:27:SER:HB3	2:F:224:MET:HE2	1.64	0.79
1:E:178:ARG:HA	1:E:180:LYS:HE2	1.64	0.79
1:A:57:MET:SD	1:A:71:LEU:HD23	2.22	0.79
1:G:130:LEU:HB2	1:G:137:VAL:HG13	1.64	0.79
2:H:83:LYS:H	2:H:83:LYS:HE2	1.46	0.79
1:C:135:LEU:HD22	1:C:166:LYS:HB3	1.64	0.79
1:G:178:ARG:HA	1:G:180:LYS:HE2	1.65	0.78
1:A:49:LEU:HD23	1:A:55:LYS:HD2	1.63	0.78
1:C:178:ARG:HA	1:C:180:LYS:HE2	1.66	0.77
1:C:40:ARG:HD3	1:C:118:GLN:NE2	1.99	0.77
2:F:259:VAL:HG21	2:F:268:ILE:HD11	1.67	0.77
1:A:135:LEU:HD22	1:A:166:LYS:HB3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:LEU:HD23	1:C:55:LYS:HD2	1.66	0.76
2:H:279:LYS:HE2	2:H:288:LEU:O	1.85	0.76
2:B:27:SER:HB3	2:B:224:MET:HE2	1.68	0.76
1:E:57:MET:SD	1:E:71:LEU:HD23	2.25	0.76
2:F:71:PRO:HG2	2:F:74:TYR:HD2	1.49	0.76
1:E:135:LEU:HD22	1:E:166:LYS:HB3	1.69	0.75
2:F:228:LEU:HD21	2:F:278:LEU:HD22	1.68	0.75
3:I:209:GLU:OE1	3:I:211:HIS:HE1	1.69	0.75
2:F:145:ILE:HG13	2:F:146:ILE:HD12	1.69	0.74
2:H:176:ASN:O	2:H:177:ASN:HB2	1.88	0.74
2:F:52:VAL:CG2	2:F:56:ASN:HA	2.17	0.73
1:G:135:LEU:HD22	1:G:166:LYS:HB3	1.71	0.73
1:A:139:LEU:CD2	1:A:153:ILE:HD12	2.18	0.73
2:F:64:ILE:HD13	2:F:209:TYR:CE2	2.24	0.73
2:H:53:ASN:ND2	2:H:55:ARG:HD3	2.05	0.72
2:F:259:VAL:HG21	2:F:268:ILE:CD1	2.21	0.71
1:G:49:LEU:HD12	1:G:55:LYS:HE2	1.71	0.71
1:A:178:ARG:HA	1:A:180:LYS:HE2	1.71	0.70
2:F:224:MET:CE	2:F:230:LEU:HD12	2.22	0.70
1:C:49:LEU:CD2	1:C:55:LYS:HD2	2.21	0.69
2:H:49:VAL:HG22	2:H:50:GLU:H	1.56	0.69
2:B:83:LYS:O	2:B:85:LEU:N	2.25	0.69
2:D:11:ILE:HD11	2:D:232:LEU:HD11	1.75	0.68
2:B:53:ASN:HB3	2:B:55:ARG:H	1.57	0.68
2:H:49:VAL:HG22	2:H:50:GLU:N	2.09	0.68
2:B:83:LYS:HB3	2:B:84:PRO:HD3	1.76	0.68
1:E:71:LEU:HD11	1:E:104:ILE:HG12	1.75	0.68
2:B:90:LEU:N	2:B:90:LEU:HD12	2.08	0.67
2:F:77:ASP:O	2:F:78:GLU:HG3	1.94	0.67
2:F:224:MET:HE1	2:F:230:LEU:HD12	1.76	0.67
2:D:176:ASN:O	2:D:177:ASN:HB3	1.93	0.67
2:D:259:VAL:HG21	2:D:268:ILE:CD1	2.25	0.67
2:B:171:ILE:HG13	2:B:297:ASP:HB2	1.78	0.66
1:G:142:LEU:HD11	1:G:152:LEU:CD1	2.20	0.66
2:H:55:ARG:H	2:H:55:ARG:HD2	1.59	0.66
2:H:11:ILE:HD13	2:H:11:ILE:N	2.10	0.66
1:E:142:LEU:HD11	1:E:152:LEU:CD1	2.23	0.65
2:F:31:PRO:HB2	2:F:220:VAL:HB	1.78	0.65
1:C:142:LEU:HD11	1:C:152:LEU:CD1	2.22	0.65
2:D:53:ASN:HD21	2:D:57:GLN:HB2	1.60	0.65
1:E:44:CYS:SG	1:E:46:ILE:HG12	2.36	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:286:ILE:HD13	2:H:286:ILE:C	2.22	0.65
2:D:259:VAL:HG21	2:D:268:ILE:HD11	1.80	0.64
2:H:11:ILE:HD13	2:H:11:ILE:H	1.62	0.64
2:B:83:LYS:HB3	2:B:84:PRO:CD	2.28	0.64
2:B:83:LYS:CB	2:B:84:PRO:CD	2.75	0.63
1:A:142:LEU:HD11	1:A:152:LEU:CD1	2.19	0.63
2:F:60:GLU:CD	2:F:299:ARG:HH21	2.07	0.63
1:C:138:ARG:HB2	1:C:154:GLU:HB3	1.81	0.62
1:G:71:LEU:CD1	1:G:104:ILE:HG12	2.28	0.62
1:G:205:VAL:O	1:G:209:GLU:HG3	1.99	0.62
1:A:71:LEU:HD11	1:A:104:ILE:HG12	1.81	0.62
1:G:138:ARG:HB2	1:G:154:GLU:HB3	1.82	0.62
1:E:51:ALA:O	1:E:52:ASP:HB2	1.99	0.62
2:F:7:LEU:HG	2:F:180:VAL:HG23	1.81	0.62
1:E:57:MET:SD	1:E:71:LEU:CD2	2.87	0.62
1:E:63:HIS:ND1	1:E:67:ARG:NH2	2.48	0.62
2:B:48:ASP:HB3	4:B:339:HOH:O	1.99	0.62
2:B:31:PRO:HB2	2:B:220:VAL:HB	1.81	0.61
2:D:19:LEU:HD13	2:D:286:ILE:HD12	1.82	0.61
2:F:55:ARG:O	2:F:57:GLN:HG3	2.00	0.61
2:D:53:ASN:HD21	2:D:57:GLN:HE21	1.48	0.61
1:E:138:ARG:HB2	1:E:154:GLU:HB3	1.83	0.61
2:H:3:GLN:HB2	2:H:259:VAL:HG22	1.82	0.61
2:H:31:PRO:HB2	2:H:220:VAL:HB	1.83	0.61
2:B:224:MET:HE1	2:B:230:LEU:HD13	1.83	0.61
1:C:71:LEU:CD1	1:C:104:ILE:HG12	2.30	0.60
2:B:84:PRO:HB2	2:B:87:PHE:HB3	1.84	0.60
2:F:71:PRO:HG2	2:F:74:TYR:CD2	2.34	0.60
1:C:24:LEU:O	1:C:28:ILE:HG12	2.01	0.60
2:D:197:ASN:HB3	2:D:202:SER:HB3	1.82	0.60
1:C:60:ILE:HD12	1:C:60:ILE:N	2.16	0.59
2:B:167:GLN:HG2	2:B:187:GLU:HB2	1.84	0.59
1:C:162:GLU:O	1:C:166:LYS:HE3	2.03	0.59
1:A:49:LEU:HD23	1:A:55:LYS:CD	2.32	0.59
1:A:91:LEU:CD2	2:B:68:LYS:HA	2.33	0.59
1:E:32:ARG:HG2	1:E:33:ASP:H	1.67	0.59
2:B:53:ASN:ND2	2:B:57:GLN:HB2	2.14	0.59
1:C:135:LEU:HB2	1:C:166:LYS:HD3	1.84	0.59
2:D:224:MET:CE	2:D:230:LEU:HD12	2.33	0.59
2:H:79:THR:HG22	2:H:80:MET:N	2.17	0.59
1:A:32:ARG:HG2	1:A:33:ASP:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HB2	1:A:166:LYS:HD3	1.85	0.58
2:D:75:LEU:O	2:D:76:ILE:HB	2.03	0.58
1:G:37:ILE:HG12	1:G:38:ASP:N	2.18	0.58
2:H:259:VAL:HG21	2:H:268:ILE:HD11	1.84	0.58
2:F:52:VAL:HA	2:F:57:GLN:O	2.03	0.58
2:F:265:ILE:H	2:F:265:ILE:CD1	2.04	0.58
1:C:180:LYS:HD2	1:C:180:LYS:N	2.19	0.58
1:C:167:ILE:HD11	1:C:184:THR:HG21	1.86	0.58
2:D:75:LEU:HD22	2:D:216:LEU:CD2	2.33	0.58
1:C:32:ARG:HG2	1:C:33:ASP:H	1.68	0.57
1:C:120:GLN:CD	1:C:122:ILE:HD11	2.29	0.57
1:E:22:ASP:C	1:E:24:LEU:H	2.11	0.57
2:F:68:LYS:HE2	2:F:164:TRP:CH2	2.39	0.57
1:G:180:LYS:N	1:G:180:LYS:HD2	2.18	0.57
1:A:46:ILE:HD13	2:B:49:VAL:HB	1.85	0.57
2:D:273:THR:HG22	2:D:277:ASN:HD21	1.69	0.57
2:H:180:VAL:HG21	2:H:275:LEU:HD23	1.86	0.57
1:G:120:GLN:CD	1:G:122:ILE:HD11	2.29	0.57
1:E:37:ILE:HG12	1:E:38:ASP:N	2.20	0.57
2:F:253:LEU:HD22	2:F:286:ILE:CD1	2.35	0.57
2:D:27:SER:HB3	2:D:224:MET:HE2	1.86	0.57
1:E:167:ILE:HD11	1:E:184:THR:HG21	1.87	0.57
1:A:66:GLY:CA	1:A:68:GLN:HG3	2.31	0.57
1:E:60:ILE:N	1:E:60:ILE:HD12	2.20	0.57
2:D:232:LEU:HD12	2:D:251:PHE:HB3	1.87	0.57
1:G:178:ARG:HA	1:G:180:LYS:CE	2.34	0.57
2:H:53:ASN:HD22	2:H:55:ARG:HD3	1.68	0.57
2:H:55:ARG:O	2:H:57:GLN:N	2.34	0.57
1:A:57:MET:SD	1:A:71:LEU:CD2	2.93	0.56
1:A:120:GLN:CD	1:A:122:ILE:HD11	2.30	0.56
1:C:50:PRO:O	1:C:51:ALA:C	2.46	0.56
1:C:178:ARG:HA	1:C:180:LYS:CE	2.35	0.56
1:E:4:SER:HA	1:E:155:LEU:O	2.06	0.56
1:E:49:LEU:HD12	1:E:55:LYS:HG2	1.87	0.56
1:A:62:PHE:CB	1:A:65:HIS:HB2	2.35	0.56
2:F:64:ILE:HD13	2:F:209:TYR:CZ	2.41	0.56
2:F:60:GLU:OE2	2:F:299:ARG:NH2	2.37	0.56
1:G:32:ARG:HG2	1:G:33:ASP:H	1.70	0.56
1:E:48:ASN:O	1:E:49:LEU:C	2.49	0.56
1:E:178:ARG:HA	1:E:180:LYS:CE	2.34	0.56
1:G:139:LEU:CD2	1:G:153:ILE:HD12	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:279:LYS:HE2	2:F:288:LEU:O	2.05	0.56
2:H:82:ASP:OD2	2:H:83:LYS:HD3	2.05	0.56
1:C:64:HIS:O	1:C:65:HIS:HB2	2.06	0.56
2:F:68:LYS:HE2	2:F:164:TRP:CZ2	2.41	0.56
2:F:69:GLU:OE2	2:F:69:GLU:N	2.36	0.56
1:A:143:PHE:CD2	1:A:148:PHE:HA	2.41	0.55
2:H:197:ASN:HB3	2:H:202:SER:CB	2.36	0.55
2:F:3:GLN:HB2	2:F:259:VAL:HG22	1.87	0.55
2:F:51:ASN:HB3	2:F:59:VAL:O	2.07	0.55
1:A:180:LYS:HD2	1:A:180:LYS:N	2.21	0.55
2:B:68:LYS:HG2	2:B:164:TRP:CZ3	2.42	0.55
2:H:81:MET:HE3	2:H:87:PHE:CE1	2.41	0.55
2:D:232:LEU:HD12	2:D:251:PHE:CB	2.37	0.55
1:A:37:ILE:HD12	1:A:204:TYR:CE1	2.42	0.55
2:B:53:ASN:HD22	2:B:57:GLN:HE21	1.55	0.55
1:A:48:ASN:O	1:A:49:LEU:C	2.51	0.54
1:C:91:LEU:CD2	2:D:68:LYS:HA	2.38	0.54
1:E:40:ARG:HD3	1:E:118:GLN:HE22	1.70	0.54
1:E:71:LEU:CD1	1:E:104:ILE:HG12	2.36	0.54
1:E:27:SER:O	1:E:132:LEU:CD2	2.54	0.54
2:F:224:MET:HE1	2:F:230:LEU:CD1	2.37	0.54
1:E:90:ALA:O	1:E:94:ASN:OD1	2.26	0.54
2:H:7:LEU:HG	2:H:180:VAL:HG23	1.88	0.54
2:B:232:LEU:CD1	2:B:253:LEU:HD13	2.35	0.54
1:E:100:VAL:HG11	2:F:260:SER:HB3	1.88	0.54
1:G:60:ILE:N	1:G:60:ILE:HD12	2.23	0.54
2:H:63:ARG:HG3	2:H:298:SER:O	2.08	0.54
2:H:197:ASN:HB3	2:H:202:SER:HB3	1.90	0.54
2:H:27:SER:HB3	2:H:224:MET:HE2	1.88	0.54
2:D:75:LEU:O	2:D:76:ILE:CB	2.56	0.54
1:E:22:ASP:C	1:E:24:LEU:N	2.62	0.54
2:D:197:ASN:HB3	2:D:202:SER:CB	2.38	0.54
2:F:13:ASP:OD1	2:F:250:GLY:HA2	2.07	0.54
1:A:37:ILE:HG12	1:A:38:ASP:N	2.22	0.53
1:A:48:ASN:N	1:A:48:ASN:ND2	2.56	0.53
1:E:180:LYS:N	1:E:180:LYS:HD2	2.23	0.53
2:H:259:VAL:HG21	2:H:268:ILE:CD1	2.39	0.53
1:A:36:SER:HB3	1:A:63:HIS:HB2	1.89	0.53
2:B:280:LYS:HA	2:B:280:LYS:HE2	1.90	0.53
1:C:139:LEU:CD2	1:C:153:ILE:HD12	2.38	0.53
1:G:49:LEU:HD22	1:G:50:PRO:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:53:ASN:ND2	2:D:57:GLN:HE21	2.06	0.53
1:G:57:MET:SD	1:G:71:LEU:CD2	2.97	0.53
1:G:135:LEU:HB2	1:G:166:LYS:HD3	1.91	0.53
2:H:285:TYR:C	2:H:285:TYR:CD2	2.84	0.53
2:H:224:MET:CE	2:H:230:LEU:HD12	2.39	0.53
1:C:28:ILE:HG22	1:C:29:LEU:N	2.24	0.53
2:H:11:ILE:CD1	2:H:251:PHE:HB2	2.37	0.53
1:A:60:ILE:HD12	1:A:60:ILE:N	2.24	0.53
2:D:3:GLN:HB2	2:D:259:VAL:HG22	1.90	0.53
1:A:149:LYS:O	1:A:149:LYS:HD3	2.09	0.53
1:C:45:SER:OG	1:C:117:MET:HE2	2.08	0.52
2:D:268:ILE:O	2:D:272:GLU:HG3	2.08	0.52
2:F:52:VAL:HG22	2:F:56:ASN:HA	1.91	0.52
2:F:226:HIS:CD2	2:F:270:TYR:OH	2.61	0.52
2:B:224:MET:CE	2:B:230:LEU:HD13	2.39	0.52
1:G:37:ILE:HD12	1:G:204:TYR:CE1	2.44	0.52
1:G:64:HIS:C	1:G:66:GLY:H	2.18	0.52
2:H:268:ILE:O	2:H:272:GLU:HG3	2.09	0.52
1:A:138:ARG:HB2	1:A:154:GLU:HB3	1.91	0.52
1:A:167:ILE:HD11	1:A:184:THR:HG21	1.91	0.52
2:D:31:PRO:HB2	2:D:220:VAL:HB	1.91	0.52
1:C:32:ARG:HH21	1:C:138:ARG:NH2	2.07	0.52
1:G:7:ILE:HG13	1:G:184:THR:OG1	2.10	0.52
2:B:268:ILE:O	2:B:272:GLU:HG3	2.10	0.52
1:E:7:ILE:HG13	1:E:184:THR:OG1	2.10	0.52
2:B:40:VAL:HG21	2:B:213:PHE:CZ	2.45	0.52
1:C:78:MET:HE3	2:D:203:LEU:HB3	1.92	0.52
1:E:28:ILE:HG22	1:E:29:LEU:N	2.25	0.52
1:E:139:LEU:CD2	1:E:153:ILE:HD12	2.40	0.52
2:H:261:ARG:HG2	2:H:262:GLY:N	2.25	0.52
2:D:49:VAL:HG22	2:D:50:GLU:N	2.25	0.51
1:A:71:LEU:CD1	1:A:104:ILE:HG12	2.40	0.51
1:A:100:VAL:CB	2:B:2:VAL:CG2	2.86	0.51
2:B:52:VAL:HG22	2:B:56:ASN:C	2.35	0.51
1:C:133:ASP:C	1:C:135:LEU:H	2.17	0.51
1:A:7:ILE:HG13	1:A:184:THR:OG1	2.10	0.51
1:G:167:ILE:HD11	1:G:184:THR:HG21	1.93	0.51
2:D:53:ASN:ND2	2:D:57:GLN:HB2	2.24	0.51
1:C:37:ILE:HG12	1:C:38:ASP:N	2.23	0.51
1:A:62:PHE:HB3	1:A:65:HIS:CB	2.36	0.51
1:E:32:ARG:HH21	1:E:138:ARG:NH2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ILE:HD12	1:C:204:TYR:CE1	2.46	0.51
2:D:53:ASN:C	2:D:55:ARG:H	2.17	0.51
1:G:36:SER:HB3	1:G:63:HIS:CD2	2.46	0.51
2:F:157:SER:O	2:F:158:ASN:HB2	2.11	0.51
1:A:178:ARG:HA	1:A:180:LYS:CE	2.38	0.51
2:B:203:LEU:O	2:B:207:LEU:HD13	2.10	0.51
2:F:176:ASN:O	2:F:177:ASN:HB3	2.10	0.50
1:G:27:SER:O	1:G:132:LEU:HD22	2.12	0.50
2:H:167:GLN:HG2	2:H:187:GLU:HB2	1.93	0.50
1:A:100:VAL:HB	2:B:2:VAL:HG23	1.88	0.50
2:B:83:LYS:HG3	2:B:240:GLU:HG3	1.93	0.50
1:C:7:ILE:HG13	1:C:184:THR:OG1	2.12	0.50
1:E:120:GLN:HG2	1:E:122:ILE:HD13	1.92	0.50
1:G:108:LEU:HD23	1:G:112:LEU:HD12	1.92	0.50
2:F:75:LEU:HD23	2:F:148:VAL:HG12	1.92	0.50
1:A:28:ILE:HG22	1:A:29:LEU:N	2.26	0.50
1:C:44:CYS:SG	1:C:46:ILE:HG12	2.52	0.50
2:H:52:VAL:HG22	2:H:53:ASN:N	2.26	0.50
3:I:209:GLU:OE1	3:I:211:HIS:CE1	2.58	0.50
1:A:44:CYS:SG	1:A:46:ILE:HG12	2.52	0.50
2:D:296:MET:HA	3:J:206:PHE:CD2	2.46	0.50
1:G:9:VAL:HB	1:G:151:LEU:HB3	1.93	0.50
2:B:197:ASN:HB3	2:B:202:SER:HB3	1.94	0.49
1:G:4:SER:HA	1:G:155:LEU:O	2.12	0.49
1:A:48:ASN:N	1:A:48:ASN:HD22	2.09	0.49
1:C:163:PHE:O	1:C:166:LYS:N	2.45	0.49
2:D:279:LYS:HE2	2:D:288:LEU:O	2.12	0.49
1:E:78:MET:HE3	2:F:203:LEU:HB3	1.94	0.49
1:E:135:LEU:HB2	1:E:166:LYS:HD3	1.94	0.49
1:G:114:ASN:HB3	2:H:59:VAL:HB	1.94	0.49
2:H:49:VAL:CG2	2:H:50:GLU:H	2.24	0.49
1:E:162:GLU:HA	1:E:162:GLU:OE1	2.12	0.49
1:C:87:ILE:HD11	1:C:101:PRO:HD3	1.94	0.49
2:D:64:ILE:HG21	2:D:204:MET:HE1	1.94	0.49
1:G:40:ARG:HD3	1:G:118:GLN:HE22	1.77	0.49
1:A:144:SER:OG	1:A:145:SER:N	2.44	0.49
1:G:28:ILE:HG22	1:G:29:LEU:N	2.26	0.49
1:G:24:LEU:O	1:G:28:ILE:HG12	2.12	0.49
1:G:87:ILE:HD11	1:G:101:PRO:HD3	1.95	0.49
1:A:130:LEU:HB2	1:A:137:VAL:CG1	2.39	0.49
1:C:22:ASP:C	1:C:24:LEU:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:MET:SD	1:C:71:LEU:CD2	3.00	0.49
2:F:68:LYS:HG2	2:F:164:TRP:CZ3	2.47	0.49
2:H:81:MET:HE3	2:H:87:PHE:CZ	2.48	0.49
2:B:166:LEU:C	2:B:166:LEU:HD23	2.38	0.49
1:C:130:LEU:HB2	1:C:137:VAL:CG1	2.38	0.49
1:E:87:ILE:HD11	1:E:101:PRO:HD3	1.93	0.49
2:H:83:LYS:HD2	2:H:240:GLU:OE1	2.13	0.49
2:F:40:VAL:HG21	2:F:213:PHE:CZ	2.48	0.49
2:H:50:GLU:HB2	2:H:52:VAL:HG12	1.95	0.49
2:B:216:LEU:HD23	2:H:80:MET:HE1	1.95	0.49
2:D:24:THR:O	2:D:28:GLY:N	2.45	0.49
1:G:54:SER:O	1:G:73:LYS:NZ	2.46	0.49
1:G:50:PRO:HB2	1:G:53:VAL:HG23	1.96	0.48
2:D:40:VAL:HG11	2:D:63:ARG:HD3	1.94	0.48
2:F:253:LEU:HD22	2:F:286:ILE:HD13	1.96	0.48
2:F:261:ARG:HD3	2:F:267:ARG:HH21	1.78	0.48
2:D:226:HIS:CD2	2:D:270:TYR:OH	2.66	0.48
2:F:70:VAL:HB	2:F:75:LEU:HD11	1.95	0.48
1:G:32:ARG:HH21	1:G:138:ARG:NH2	2.12	0.48
2:H:3:GLN:HB2	2:H:259:VAL:CG2	2.44	0.48
1:A:9:VAL:HB	1:A:151:LEU:HB3	1.96	0.48
2:D:259:VAL:HG21	2:D:268:ILE:HD13	1.95	0.48
2:F:3:GLN:HB2	2:F:259:VAL:CG2	2.44	0.48
2:H:55:ARG:H	2:H:55:ARG:CD	2.25	0.48
1:C:195:ASN:HD21	1:C:197:ILE:HG22	1.78	0.48
2:F:6:SER:O	2:F:180:VAL:HG22	2.13	0.48
2:H:224:MET:SD	2:H:230:LEU:HD12	2.54	0.48
2:D:53:ASN:C	2:D:55:ARG:N	2.71	0.48
1:E:46:ILE:HG23	2:F:47:TYR:HB3	1.96	0.48
2:H:49:VAL:CG2	2:H:50:GLU:N	2.77	0.48
1:G:57:MET:SD	1:G:71:LEU:HD23	2.54	0.48
2:B:83:LYS:HA	2:B:83:LYS:HD3	1.64	0.47
2:B:307:ILE:HG12	3:I:215:HIS:ND1	2.29	0.47
2:B:40:VAL:HG11	2:B:63:ARG:HD3	1.95	0.47
1:E:130:LEU:HB2	1:E:137:VAL:CG1	2.40	0.47
2:B:53:ASN:ND2	2:B:57:GLN:HE21	2.12	0.47
1:C:9:VAL:HB	1:C:151:LEU:HB3	1.97	0.47
1:C:195:ASN:C	1:C:195:ASN:HD22	2.21	0.47
2:F:11:ILE:HG12	2:F:19:LEU:CD2	2.43	0.47
2:H:5:LEU:HA	2:H:181:SER:O	2.14	0.47
2:B:49:VAL:HG22	2:B:50:GLU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:LEU:C	1:C:17:LEU:HD23	2.40	0.47
2:D:26:ILE:HD12	2:D:281:GLU:OE1	2.15	0.47
1:A:87:ILE:HD11	1:A:101:PRO:HD3	1.97	0.47
1:A:195:ASN:C	1:A:195:ASN:HD22	2.22	0.47
1:C:108:LEU:HD23	1:C:112:LEU:HD12	1.95	0.47
1:E:109:SER:O	1:E:113:SER:HB3	2.14	0.47
1:E:134:GLY:O	1:E:135:LEU:HB2	2.15	0.47
1:A:139:LEU:HD22	1:A:153:ILE:HD12	1.92	0.47
1:C:6:VAL:HG13	1:C:152:LEU:HD21	1.94	0.47
2:F:76:ILE:HA	2:F:145:ILE:O	2.15	0.47
1:C:43:ARG:HH12	1:C:55:LYS:NZ	2.12	0.47
2:F:157:SER:C	2:F:159:GLU:H	2.23	0.47
1:A:50:PRO:O	1:A:53:VAL:HG12	2.15	0.47
1:C:163:PHE:C	1:C:165:THR:N	2.72	0.47
2:F:253:LEU:HD22	2:F:286:ILE:HD11	1.97	0.47
1:G:109:SER:O	1:G:113:SER:HB3	2.14	0.47
1:A:53:VAL:CG1	1:A:53:VAL:O	2.62	0.47
2:B:68:LYS:HE2	2:B:164:TRP:CH2	2.49	0.47
2:B:282:LEU:HB3	2:B:286:ILE:HG23	1.96	0.47
2:F:50:GLU:HB2	2:F:52:VAL:HG12	1.97	0.47
2:H:53:ASN:HD22	2:H:55:ARG:HH11	1.63	0.47
1:C:22:ASP:C	1:C:24:LEU:N	2.72	0.46
1:C:122:ILE:CG2	1:C:142:LEU:HB3	2.44	0.46
2:D:52:VAL:CG2	2:D:56:ASN:HA	2.44	0.46
1:E:17:LEU:C	1:E:17:LEU:HD23	2.40	0.46
2:F:166:LEU:C	2:F:166:LEU:HD23	2.40	0.46
2:H:163:PRO:HA	2:H:190:ILE:O	2.15	0.46
2:B:89:ILE:C	2:B:90:LEU:HD12	2.40	0.46
2:B:171:ILE:HG12	2:B:172:PRO:HD2	1.96	0.46
1:E:9:VAL:HB	1:E:151:LEU:HB3	1.97	0.46
1:G:195:ASN:C	1:G:195:ASN:HD22	2.23	0.46
2:H:166:LEU:HD23	2:H:166:LEU:C	2.41	0.46
2:D:273:THR:HG22	2:D:277:ASN:ND2	2.29	0.46
1:A:66:GLY:C	1:A:68:GLN:N	2.70	0.46
2:B:19:LEU:HD23	2:B:232:LEU:HD21	1.96	0.46
1:C:205:VAL:O	1:C:209:GLU:HG2	2.15	0.46
2:D:234:LYS:HE2	2:D:251:PHE:CZ	2.51	0.46
1:E:205:VAL:O	1:E:209:GLU:HG2	2.15	0.46
1:A:24:LEU:O	1:A:28:ILE:HG12	2.16	0.46
2:F:157:SER:HB2	2:F:196:LYS:O	2.16	0.46
2:H:226:HIS:CD2	2:H:270:TYR:OH	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:232:LEU:HD23	2:F:232:LEU:HA	1.80	0.46
1:G:122:ILE:CG2	1:G:142:LEU:HB3	2.45	0.46
2:H:237:GLN:O	2:H:243:ASN:HA	2.15	0.46
1:C:49:LEU:HA	1:C:50:PRO:HD3	1.75	0.46
1:E:120:GLN:CD	1:E:122:ILE:HD11	2.41	0.46
2:F:167:GLN:HG2	2:F:187:GLU:HB2	1.98	0.46
2:H:64:ILE:HG21	2:H:204:MET:HE1	1.98	0.46
1:A:46:ILE:HG23	2:B:47:TYR:HB3	1.98	0.46
2:B:84:PRO:HG2	2:H:251:PHE:CE1	2.51	0.46
2:B:197:ASN:HB3	2:B:202:SER:CB	2.46	0.46
2:D:63:ARG:HG3	2:D:298:SER:O	2.15	0.46
1:A:49:LEU:HD23	1:A:55:LYS:CE	2.45	0.46
2:B:237:GLN:O	2:B:243:ASN:HA	2.16	0.46
2:H:83:LYS:H	2:H:83:LYS:CE	2.23	0.46
1:C:141:ASN:HB3	1:C:148:PHE:HE1	1.80	0.45
2:D:19:LEU:HD13	2:D:286:ILE:CD1	2.46	0.45
2:D:280:LYS:HA	2:D:280:LYS:HE2	1.97	0.45
2:H:53:ASN:HD22	2:H:55:ARG:CD	2.29	0.45
1:C:49:LEU:HD23	1:C:55:LYS:CD	2.41	0.45
1:E:121:LEU:HD22	1:E:123:LYS:HG3	1.98	0.45
2:F:268:ILE:O	2:F:272:GLU:HG3	2.16	0.45
1:G:120:GLN:HG2	1:G:122:ILE:HD12	1.99	0.45
1:A:46:ILE:HB	1:A:49:LEU:HD22	1.98	0.45
2:B:287:GLU:HG3	2:B:287:GLU:O	2.16	0.45
1:G:47:LYS:HD3	1:G:47:LYS:N	2.31	0.45
2:F:224:MET:SD	2:F:230:LEU:HD12	2.56	0.45
1:A:17:LEU:HD23	1:A:17:LEU:C	2.41	0.45
2:B:22:THR:HG22	2:B:26:ILE:HD12	1.99	0.45
1:C:49:LEU:HA	1:C:49:LEU:HD12	1.74	0.45
2:F:50:GLU:CD	2:F:50:GLU:N	2.69	0.45
1:A:4:SER:HA	1:A:155:LEU:O	2.16	0.45
1:A:32:ARG:HH21	1:A:138:ARG:HH22	1.64	0.45
2:F:5:LEU:HA	2:F:181:SER:O	2.17	0.45
2:F:55:ARG:O	2:F:56:ASN:C	2.60	0.45
2:F:259:VAL:HG23	2:F:259:VAL:O	2.15	0.45
2:H:246:ILE:HG13	3:L:204:PHE:CD2	2.52	0.45
2:F:287:GLU:HA	4:F:319:HOH:O	2.17	0.45
2:B:224:MET:CE	2:B:230:LEU:CD1	2.95	0.45
2:B:295:SER:HA	3:I:203:LYS:HD3	1.98	0.45
2:D:246:ILE:CG2	3:J:201:VAL:HG13	2.46	0.45
2:H:79:THR:CG2	2:H:243:ASN:ND2	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:64:ILE:HG21	2:F:204:MET:HE1	1.99	0.45
2:H:264:ASP:C	2:H:266:ASP:N	2.72	0.45
1:A:195:ASN:HD21	1:A:197:ILE:HG22	1.82	0.44
2:D:246:ILE:HG21	3:J:201:VAL:HG13	1.98	0.44
2:F:265:ILE:HD12	2:F:265:ILE:N	2.10	0.44
2:D:40:VAL:HG21	2:D:213:PHE:CZ	2.52	0.44
2:H:5:LEU:HD22	2:H:271:THR:CG2	2.47	0.44
2:B:73:SER:OG	2:D:28:GLY:HA2	2.18	0.44
2:H:232:LEU:HD23	2:H:232:LEU:HA	1.79	0.44
2:B:279:LYS:HE2	2:B:288:LEU:O	2.18	0.44
1:G:90:ALA:O	1:G:94:ASN:OD1	2.35	0.44
2:B:51:ASN:ND2	2:B:61:PRO:HD3	2.32	0.44
1:C:178:ARG:CA	1:C:180:LYS:HE2	2.42	0.44
1:E:195:ASN:C	1:E:195:ASN:HD22	2.26	0.44
2:F:60:GLU:H	2:F:60:GLU:HG2	1.59	0.44
2:B:89:ILE:HB	2:B:90:LEU:HD12	1.99	0.44
2:B:259:VAL:HG11	2:B:268:ILE:HD13	1.98	0.44
2:D:197:ASN:CB	2:D:202:SER:HB3	2.47	0.44
2:B:224:MET:SD	2:B:230:LEU:HD12	2.58	0.44
1:C:46:ILE:HG21	2:D:47:TYR:HB3	2.00	0.44
1:E:6:VAL:HG13	1:E:152:LEU:HD21	1.99	0.44
2:H:11:ILE:N	2:H:11:ILE:CD1	2.79	0.44
2:B:163:PRO:HA	2:B:190:ILE:O	2.18	0.44
2:D:5:LEU:HD12	2:D:5:LEU:N	2.32	0.44
3:J:194:LYS:HE2	3:J:194:LYS:HB3	1.75	0.44
2:F:53:ASN:C	2:F:55:ARG:H	2.26	0.43
2:F:296:MET:HA	3:K:206:PHE:CD2	2.52	0.43
2:D:163:PRO:HA	2:D:190:ILE:O	2.18	0.43
2:F:49:VAL:HG23	2:F:50:GLU:OE2	2.18	0.43
2:F:52:VAL:HG23	2:F:57:GLN:N	2.33	0.43
2:H:44:ASN:HB2	2:H:210:VAL:HG23	2.00	0.43
1:C:57:MET:SD	1:C:71:LEU:HD23	2.59	0.43
2:B:12:GLY:O	2:B:13:ASP:C	2.62	0.43
2:B:280:LYS:HE3	2:B:283:GLN:OE1	2.19	0.43
1:C:109:SER:O	1:C:113:SER:HB3	2.19	0.43
2:F:64:ILE:HG13	2:F:168:ILE:HD11	2.00	0.43
2:F:76:ILE:HG22	2:F:78:GLU:H	1.83	0.43
2:H:81:MET:SD	2:H:89:ILE:HG13	2.58	0.43
1:C:194:SER:O	1:C:195:ASN:HB2	2.17	0.43
2:D:40:VAL:CG1	2:D:63:ARG:HD3	2.49	0.43
1:E:9:VAL:HG12	1:E:12:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:GLU:C	1:E:161:GLY:N	2.75	0.43
2:B:259:VAL:HG11	2:B:268:ILE:CD1	2.48	0.43
2:D:50:GLU:H	2:D:50:GLU:HG3	1.66	0.43
1:E:182:TYR:CD1	1:E:182:TYR:C	2.97	0.43
2:F:11:ILE:HG12	2:F:19:LEU:HD23	2.00	0.43
1:A:9:VAL:HG12	1:A:12:ALA:HB2	2.00	0.43
1:A:122:ILE:CG2	1:A:142:LEU:HB3	2.49	0.43
2:B:228:LEU:HD21	2:B:278:LEU:HD22	2.01	0.43
1:C:149:LYS:O	1:C:149:LYS:HD3	2.17	0.43
2:D:166:LEU:C	2:D:166:LEU:HD23	2.44	0.43
2:F:261:ARG:HD3	2:F:267:ARG:NH2	2.32	0.43
2:F:264:ASP:OD1	2:F:266:ASP:HB2	2.19	0.43
1:A:108:LEU:HD23	1:A:112:LEU:HD12	2.00	0.43
2:B:27:SER:HB2	2:B:224:MET:HG2	2.01	0.43
2:D:19:LEU:CD1	2:D:286:ILE:HD12	2.49	0.43
1:E:37:ILE:CD1	1:E:204:TYR:CE1	3.01	0.43
1:A:182:TYR:C	1:A:182:TYR:CD1	2.97	0.43
2:H:22:THR:O	2:H:26:ILE:HG12	2.18	0.43
2:H:247:THR:O	2:H:248:SER:C	2.62	0.43
1:C:3:LYS:HE3	1:C:163:PHE:HB3	2.01	0.42
1:C:40:ARG:HD3	1:C:118:GLN:HE22	1.81	0.42
1:C:163:PHE:O	1:C:164:GLU:C	2.62	0.42
2:D:228:LEU:HD21	2:D:278:LEU:HD22	2.01	0.42
1:G:17:LEU:C	1:G:17:LEU:HD23	2.44	0.42
2:B:285:TYR:C	2:B:285:TYR:CD2	2.96	0.42
2:H:41:TRP:CD1	2:H:41:TRP:N	2.86	0.42
2:F:63:ARG:HG3	2:F:298:SER:O	2.18	0.42
2:F:172:PRO:O	2:F:293:ARG:HD2	2.19	0.42
1:G:162:GLU:O	1:G:166:LYS:HE3	2.19	0.42
3:I:207:THR:OG1	3:I:209:GLU:HG2	2.19	0.42
1:C:4:SER:HA	1:C:155:LEU:O	2.18	0.42
2:D:224:MET:HE1	2:D:230:LEU:CD1	2.49	0.42
1:E:108:LEU:HD23	1:E:112:LEU:HD12	2.00	0.42
2:F:145:ILE:CG1	2:F:146:ILE:HD12	2.43	0.42
2:F:146:ILE:HD12	2:F:146:ILE:N	2.35	0.42
2:H:83:LYS:HD2	2:H:240:GLU:CD	2.44	0.42
1:A:139:LEU:HD23	1:A:153:ILE:HD12	1.98	0.42
2:B:44:ASN:OD1	2:B:46:SER:N	2.50	0.42
2:D:5:LEU:HA	2:D:181:SER:O	2.18	0.42
1:E:46:ILE:CG2	2:F:47:TYR:HB3	2.50	0.42
2:F:52:VAL:HG22	2:F:53:ASN:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:176:ASN:O	2:H:177:ASN:CB	2.61	0.42
1:G:195:ASN:HD21	1:G:197:ILE:HG22	1.85	0.42
3:J:194:LYS:HA	3:J:195:PRO:HD3	1.71	0.42
1:E:122:ILE:CG2	1:E:142:LEU:HB3	2.49	0.42
2:H:50:GLU:CB	2:H:52:VAL:HG12	2.50	0.42
1:A:6:VAL:HG13	1:A:152:LEU:HD21	2.00	0.42
1:A:100:VAL:CG1	2:B:2:VAL:HG23	2.50	0.42
2:H:286:ILE:C	2:H:286:ILE:CD1	2.92	0.42
1:A:22:ASP:C	1:A:24:LEU:H	2.27	0.42
1:C:159:GLU:HB2	1:C:166:LYS:NZ	2.34	0.42
1:E:24:LEU:O	1:E:28:ILE:HG12	2.19	0.42
1:E:47:LYS:HE3	1:E:47:LYS:HB2	1.92	0.42
2:F:163:PRO:HA	2:F:190:ILE:O	2.20	0.42
2:F:253:LEU:HD23	2:F:288:LEU:HD21	2.02	0.42
2:F:8:PHE:O	2:F:288:LEU:HA	2.20	0.42
1:A:152:LEU:C	1:A:153:ILE:HD13	2.45	0.41
1:C:9:VAL:HG12	1:C:12:ALA:HB2	2.02	0.41
2:H:27:SER:HB3	2:H:224:MET:HG2	2.02	0.41
2:B:291:PRO:HG2	2:B:296:MET:SD	2.60	0.41
1:C:47:LYS:C	1:C:49:LEU:H	2.28	0.41
2:D:177:ASN:O	2:D:177:ASN:CG	2.63	0.41
1:E:71:LEU:O	1:E:77:ALA:HA	2.20	0.41
1:E:167:ILE:HD11	1:E:184:THR:CG2	2.49	0.41
1:G:134:GLY:O	1:G:166:LYS:NZ	2.44	0.41
2:H:264:ASP:OD1	2:H:266:ASP:OD2	2.38	0.41
1:A:78:MET:HE3	2:B:203:LEU:HB3	2.02	0.41
2:B:82:ASP:O	2:B:83:LYS:O	2.39	0.41
1:E:38:ASP:HB2	1:E:61:THR:HB	2.03	0.41
2:F:11:ILE:HD11	2:F:251:PHE:HB2	2.02	0.41
2:F:49:VAL:HG22	2:F:50:GLU:N	2.36	0.41
1:C:47:LYS:HE3	1:C:47:LYS:HB2	1.87	0.41
1:A:49:LEU:CD2	1:A:55:LYS:HD2	2.43	0.41
1:A:109:SER:O	1:A:113:SER:HB3	2.21	0.41
2:B:232:LEU:HA	2:B:232:LEU:HD12	1.75	0.41
2:F:77:ASP:C	2:F:78:GLU:HG3	2.45	0.41
1:A:120:GLN:OE1	1:A:122:ILE:HD11	2.19	0.41
2:B:75:LEU:HA	2:B:75:LEU:HD23	1.86	0.41
2:B:286:ILE:HD12	4:B:332:HOH:O	2.20	0.41
1:C:182:TYR:C	1:C:182:TYR:CD1	2.99	0.41
2:F:259:VAL:CG2	2:F:259:VAL:O	2.69	0.41
1:G:182:TYR:CD1	1:G:182:TYR:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:TYR:CE1	2:B:90:LEU:HD22	2.56	0.41
2:B:226:HIS:CD2	2:B:270:TYR:OH	2.74	0.41
2:B:302:HIS:HB3	2:B:303:GLY:H	1.34	0.41
2:B:305:ILE:HD11	2:F:238:ILE:HG21	2.02	0.41
2:D:292:ASP:O	2:D:293:ARG:C	2.62	0.41
2:F:53:ASN:OD1	2:F:59:VAL:HG21	2.20	0.41
2:F:234:LYS:HE2	2:F:251:PHE:CZ	2.56	0.41
2:F:247:THR:O	2:F:248:SER:C	2.63	0.41
1:G:130:LEU:HB2	1:G:137:VAL:CG1	2.42	0.41
1:C:167:ILE:HD11	1:C:184:THR:CG2	2.49	0.41
1:E:37:ILE:HD12	1:E:204:TYR:CE1	2.56	0.41
2:F:246:ILE:HG12	3:K:204:PHE:CD2	2.56	0.41
1:G:144:SER:OG	1:G:145:SER:N	2.54	0.41
1:A:91:LEU:HD22	2:B:68:LYS:HA	2.02	0.40
1:G:48:ASN:O	1:G:49:LEU:C	2.63	0.40
1:C:120:GLN:OE1	1:C:122:ILE:HD11	2.21	0.40
1:G:71:LEU:HD11	1:G:104:ILE:CG1	2.40	0.40
2:B:80:MET:HE1	2:H:216:LEU:HD23	2.03	0.40
2:H:212:GLU:HG2	2:H:213:PHE:HD2	1.87	0.40
1:A:18:THR:O	1:A:21:LYS:HB3	2.21	0.40
1:E:178:ARG:CA	1:E:180:LYS:HE2	2.43	0.40
2:F:291:PRO:HG2	2:F:296:MET:SD	2.61	0.40
1:G:63:HIS:O	1:G:65:HIS:N	2.54	0.40
1:G:78:MET:HE3	2:H:203:LEU:HB3	2.02	0.40
2:H:16:TYR:CE1	2:H:20:ILE:HD11	2.57	0.40
2:H:54:SER:OG	2:H:55:ARG:HD2	2.21	0.40
2:H:283:GLN:C	2:H:285:TYR:H	2.29	0.40
2:B:80:MET:HE2	2:H:236:TRP:CD2	2.56	0.40
2:B:90:LEU:N	2:B:90:LEU:CD1	2.79	0.40
1:C:46:ILE:HG22	1:C:47:LYS:N	2.36	0.40
1:C:195:ASN:C	1:C:195:ASN:ND2	2.79	0.40
2:H:295:SER:HA	3:L:203:LYS:HD3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:25:THR:OG1	2:F:25:THR:OG1[2_646]	2.06	0.14

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	199/209 (95%)	180 (90%)	17 (8%)	2 (1%)	12	32
1	C	196/209 (94%)	174 (89%)	18 (9%)	4 (2%)	6	16
1	E	199/209 (95%)	180 (90%)	18 (9%)	1 (0%)	24	48
1	G	199/209 (95%)	176 (88%)	21 (11%)	2 (1%)	12	32
2	B	229/306 (75%)	212 (93%)	12 (5%)	5 (2%)	5	14
2	D	208/306 (68%)	196 (94%)	10 (5%)	2 (1%)	12	32
2	F	231/306 (76%)	209 (90%)	19 (8%)	3 (1%)	9	25
2	H	226/306 (74%)	208 (92%)	10 (4%)	8 (4%)	3	6
3	I	20/27 (74%)	20 (100%)	0	0	100	100
3	J	17/27 (63%)	14 (82%)	3 (18%)	0	100	100
3	K	14/27 (52%)	13 (93%)	1 (7%)	0	100	100
3	L	15/27 (56%)	14 (93%)	1 (7%)	0	100	100
All	All	1753/2168 (81%)	1596 (91%)	130 (7%)	27 (2%)	8	22

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	83	LYS
2	B	84	PRO
2	F	56	ASN
2	F	261	ARG
2	H	56	ASN
2	H	261	ARG
1	A	161	GLY
1	C	161	GLY
1	C	195	ASN
1	E	64	HIS
2	H	81	MET
1	A	159	GLU

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Mol	Chain	Res	Type
2	D	196	LYS
1	G	65	HIS
2	H	80	MET
2	H	260	SER
2	B	302	HIS
1	G	161	GLY
1	C	67	ARG
1	C	159	GLU
2	F	196	LYS
2	H	177	ASN
2	H	196	LYS
2	B	196	LYS
2	D	265	ILE
2	H	262	GLY
2	B	303	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/177 (97%)	163 (95%)	9 (5%)	21	47
1	C	172/177 (97%)	163 (95%)	9 (5%)	21	47
1	E	172/177 (97%)	164 (95%)	8 (5%)	23	51
1	G	172/177 (97%)	162 (94%)	10 (6%)	18	42
2	B	213/280 (76%)	195 (92%)	18 (8%)	10	25
2	D	193/280 (69%)	176 (91%)	17 (9%)	9	23
2	F	212/280 (76%)	196 (92%)	16 (8%)	12	31
2	H	208/280 (74%)	192 (92%)	16 (8%)	12	30
3	I	21/26 (81%)	21 (100%)	0	100	100
3	J	18/26 (69%)	18 (100%)	0	100	100
3	K	15/26 (58%)	15 (100%)	0	100	100
3	L	16/26 (62%)	16 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1584/1932 (82%)	1481 (94%)	103 (6%)	15	37

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	37	ILE
1	A	48	ASN
1	A	49	LEU
1	A	64	HIS
1	A	71	LEU
1	A	167	ILE
1	A	181	GLU
1	A	196	GLU
2	B	2	VAL
2	B	52	VAL
2	B	66	LEU
2	B	84	PRO
2	B	85	LEU
2	B	168	ILE
2	B	171	ILE
2	B	176	ASN
2	B	178	ARG
2	B	217	THR
2	B	230	LEU
2	B	240	GLU
2	B	243	ASN
2	B	260	SER
2	B	275	LEU
2	B	280	LYS
2	B	286	ILE
2	B	287	GLU
1	C	3	LYS
1	C	28	ILE
1	C	37	ILE
1	C	54	SER
1	C	71	LEU
1	C	121	LEU
1	C	167	ILE
1	C	181	GLU
1	C	196	GLU
2	D	11	ILE

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Mol	Chain	Res	Type
2	D	22	THR
2	D	25	THR
2	D	48	ASP
2	D	55	ARG
2	D	66	LEU
2	D	176	ASN
2	D	217	THR
2	D	229	ILE
2	D	230	LEU
2	D	232	LEU
2	D	235	ILE
2	D	237	GLN
2	D	246	ILE
2	D	259	VAL
2	D	275	LEU
2	D	280	LYS
1	E	28	ILE
1	E	37	ILE
1	E	71	LEU
1	E	121	LEU
1	E	122	ILE
1	E	167	ILE
1	E	181	GLU
1	E	196	GLU
2	F	11	ILE
2	F	22	THR
2	F	50	GLU
2	F	66	LEU
2	F	144	ASP
2	F	162	SER
2	F	189	ILE
2	F	217	THR
2	F	233	GLN
2	F	246	ILE
2	F	260	SER
2	F	265	ILE
2	F	268	ILE
2	F	275	LEU
2	F	280	LYS
2	F	287	GLU
1	G	28	ILE
1	G	37	ILE

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Mol	Chain	Res	Type
1	G	47	LYS
1	G	49	LEU
1	G	55	LYS
1	G	67	ARG
1	G	71	LEU
1	G	167	ILE
1	G	181	GLU
1	G	196	GLU
2	H	11	ILE
2	H	48	ASP
2	H	55	ARG
2	H	66	LEU
2	H	83	LYS
2	H	176	ASN
2	H	177	ASN
2	H	217	THR
2	H	230	LEU
2	H	233	GLN
2	H	243	ASN
2	H	263	THR
2	H	264	ASP
2	H	275	LEU
2	H	280	LYS
2	H	286	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	48	ASN
1	A	118	GLN
1	A	141	ASN
1	A	195	ASN
2	B	4	GLN
2	B	53	ASN
2	B	56	ASN
2	B	57	GLN
2	B	167	GLN
2	B	226	HIS
2	B	258	ASN
2	B	269	ASN
2	B	294	GLN

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Mol	Chain	Res	Type
2	B	302	HIS
1	C	26	ASN
1	C	63	HIS
1	C	118	GLN
1	C	141	ASN
1	C	195	ASN
1	C	203	GLN
2	D	4	GLN
2	D	57	GLN
2	D	167	GLN
2	D	205	ASN
2	D	243	ASN
2	D	258	ASN
2	D	269	ASN
2	D	277	ASN
2	D	283	GLN
1	E	26	ASN
1	E	68	GLN
1	E	118	GLN
1	E	141	ASN
1	E	173	HIS
1	E	195	ASN
2	F	4	GLN
2	F	57	GLN
2	F	176	ASN
2	F	205	ASN
2	F	214	GLN
2	F	226	HIS
2	F	243	ASN
2	F	258	ASN
2	F	269	ASN
1	G	26	ASN
1	G	68	GLN
1	G	141	ASN
1	G	173	HIS
1	G	195	ASN
2	H	4	GLN
2	H	51	ASN
2	H	57	GLN
2	H	205	ASN
2	H	214	GLN
2	H	226	HIS

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Mol	Chain	Res	Type
2	H	243	ASN
2	H	258	ASN
2	H	283	GLN
3	I	211	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no 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	203/209 (97%)	0.52	7 (3%) 48 44	35, 77, 120, 127	0
1	C	202/209 (96%)	0.51	7 (3%) 47 43	34, 81, 121, 127	0
1	E	203/209 (97%)	0.45	14 (6%) 23 20	34, 74, 117, 122	0
1	G	203/209 (97%)	0.43	6 (2%) 52 49	34, 79, 118, 122	0
2	B	235/306 (76%)	-0.35	2 (0%) 81 80	28, 45, 72, 111	0
2	D	214/306 (69%)	-0.21	2 (0%) 81 80	29, 49, 100, 109	0
2	F	235/306 (76%)	-0.25	0 100 100	29, 48, 91, 108	0
2	H	230/306 (75%)	-0.27	1 (0%) 88 87	30, 47, 92, 104	0
3	I	22/27 (81%)	-0.19	1 (4%) 38 34	35, 44, 61, 82	0
3	J	19/27 (70%)	0.04	0 100 100	40, 50, 83, 93	0
3	K	16/27 (59%)	-0.25	0 100 100	37, 46, 64, 69	0
3	L	17/27 (62%)	-0.27	0 100 100	36, 46, 70, 85	0
All	All	1799/2168 (82%)	0.07	40 (2%) 62 59	28, 57, 115, 127	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	180	LYS	3.7
1	E	64	HIS	3.7
1	G	65	HIS	3.5
1	A	174	LEU	3.3
1	C	51	ALA	3.3
1	E	181	GLU	3.3
1	C	64	HIS	3.2
1	E	29	LEU	3.1
1	A	29	LEU	2.9
1	E	65	HIS	2.9
1	G	137	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	66	GLY	2.6
2	B	301	ALA	2.6
1	E	179	ALA	2.6
1	E	167	ILE	2.5
1	C	94	ASN	2.5
2	H	82	ASP	2.4
1	C	9	VAL	2.4
1	E	189	LEU	2.4
3	I	195	PRO	2.4
1	A	175	ALA	2.4
1	G	167	ILE	2.3
1	G	117	MET	2.3
2	D	50	GLU	2.3
1	E	28	ILE	2.3
2	B	264	ASP	2.3
1	C	160	ALA	2.2
1	E	183	LYS	2.2
1	C	189	LEU	2.1
1	E	175	ALA	2.1
1	A	20	LEU	2.1
1	A	189	LEU	2.1
2	D	265	ILE	2.1
1	A	143	PHE	2.1
1	G	53	VAL	2.1
1	E	117	MET	2.1
1	C	65	HIS	2.1
1	G	9	VAL	2.1
1	E	149	LYS	2.0
1	E	170	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.