



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:12 AM UTC

PDB ID : 1Q5Q / pdb_00001q5q
Title : The Rhodococcus 20S proteasome
Authors : Kwon, Y.D.; Nagy, I.; Adams, P.D.; Baumeister, W.; Jap, B.K.
Deposited on : 2003-08-08
Resolution : 2.60 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

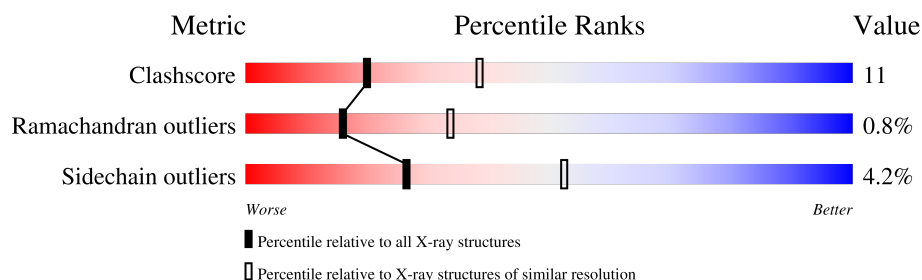
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	259	
1	B	259	
1	C	259	
1	D	259	
1	E	259	
1	F	259	
1	G	259	
2	H	235	

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Mol	Chain	Length	Quality of chain
2	I	235	71%23%5%
2	J	235	71%23%5%
2	K	235	71%24%5%
2	L	235	72%23%5%
2	M	235	71%23%5%
2	N	235	71%23%5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23706 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 proteasome alpha-type subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1695	1057	312	321	5			
1	B	219	Total	C	N	O	S	0	0	0
			1695	1057	312	321	5			
1	C	219	Total	C	N	O	S	0	0	0
			1695	1057	312	321	5			
1	D	219	Total	C	N	O	S	0	0	0
			1695	1057	312	321	5			
1	E	219	Total	C	N	O	S	0	0	0
			1695	1057	312	321	5			
1	F	219	Total	C	N	O	S	0	0	0
			1695	1057	312	321	5			
1	G	219	Total	C	N	O	S	0	0	0
			1695	1057	312	321	5			

- Molecule 2 is a protein called proteasome beta-type subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	0	0	0
			1668	1037	289	340	2			
2	I	224	Total	C	N	O	S	0	0	0
			1668	1037	289	340	2			
2	J	224	Total	C	N	O	S	0	0	0
			1667	1037	289	339	2			
2	K	224	Total	C	N	O	S	0	0	0
			1667	1037	289	339	2			
2	L	224	Total	C	N	O	S	0	0	0
			1668	1037	289	340	2			
2	M	224	Total	C	N	O	S	0	0	0
			1668	1037	289	340	2			
2	N	224	Total	C	N	O	S	0	0	0
			1668	1037	289	340	2			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	230	HIS	-	expression tag	UNP Q53079
H	231	HIS	-	expression tag	UNP Q53079
H	232	HIS	-	expression tag	UNP Q53079
H	233	HIS	-	expression tag	UNP Q53079
H	234	HIS	-	expression tag	UNP Q53079
H	235	HIS	-	expression tag	UNP Q53079
I	230	HIS	-	expression tag	UNP Q53079
I	231	HIS	-	expression tag	UNP Q53079
I	232	HIS	-	expression tag	UNP Q53079
I	233	HIS	-	expression tag	UNP Q53079
I	234	HIS	-	expression tag	UNP Q53079
I	235	HIS	-	expression tag	UNP Q53079
J	230	HIS	-	expression tag	UNP Q53079
J	231	HIS	-	expression tag	UNP Q53079
J	232	HIS	-	expression tag	UNP Q53079
J	233	HIS	-	expression tag	UNP Q53079
J	234	HIS	-	expression tag	UNP Q53079
J	235	HIS	-	expression tag	UNP Q53079
K	230	HIS	-	expression tag	UNP Q53079
K	231	HIS	-	expression tag	UNP Q53079
K	232	HIS	-	expression tag	UNP Q53079
K	233	HIS	-	expression tag	UNP Q53079
K	234	HIS	-	expression tag	UNP Q53079
K	235	HIS	-	expression tag	UNP Q53079
L	230	HIS	-	expression tag	UNP Q53079
L	231	HIS	-	expression tag	UNP Q53079
L	232	HIS	-	expression tag	UNP Q53079
L	233	HIS	-	expression tag	UNP Q53079
L	234	HIS	-	expression tag	UNP Q53079
L	235	HIS	-	expression tag	UNP Q53079
M	230	HIS	-	expression tag	UNP Q53079
M	231	HIS	-	expression tag	UNP Q53079
M	232	HIS	-	expression tag	UNP Q53079
M	233	HIS	-	expression tag	UNP Q53079
M	234	HIS	-	expression tag	UNP Q53079
M	235	HIS	-	expression tag	UNP Q53079
N	230	HIS	-	expression tag	UNP Q53079
N	231	HIS	-	expression tag	UNP Q53079
N	232	HIS	-	expression tag	UNP Q53079
N	233	HIS	-	expression tag	UNP Q53079
N	234	HIS	-	expression tag	UNP Q53079
N	235	HIS	-	expression tag	UNP Q53079

- Molecule 3 is water.

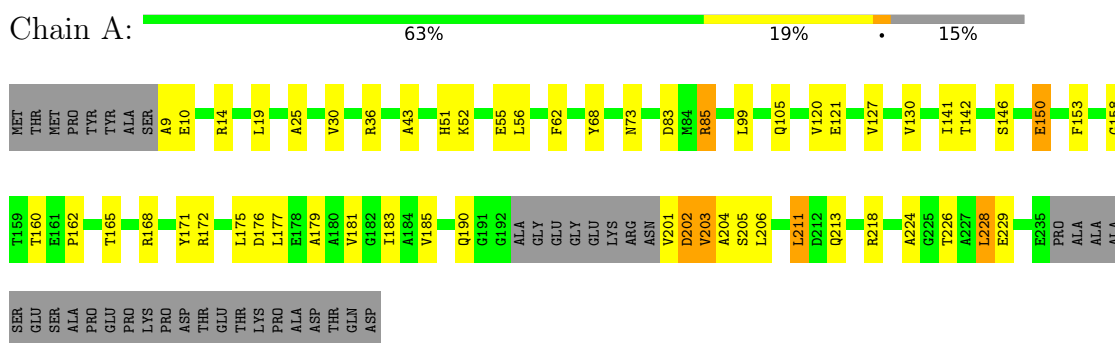
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	17	Total O 17 17	0	0
3	B	11	Total O 11 11	0	0
3	C	9	Total O 9 9	0	0
3	D	3	Total O 3 3	0	0
3	E	6	Total O 6 6	0	0
3	F	3	Total O 3 3	0	0
3	G	8	Total O 8 8	0	0
3	H	22	Total O 22 22	0	0
3	I	27	Total O 27 27	0	0
3	J	17	Total O 17 17	0	0
3	K	10	Total O 10 10	0	0
3	L	10	Total O 10 10	0	0
3	M	13	Total O 13 13	0	0
3	N	11	Total O 11 11	0	0

3 Residue-property plots

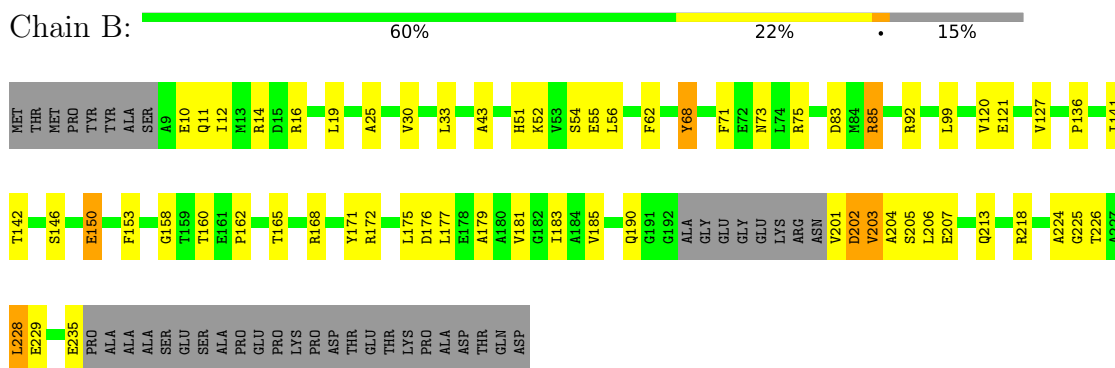
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

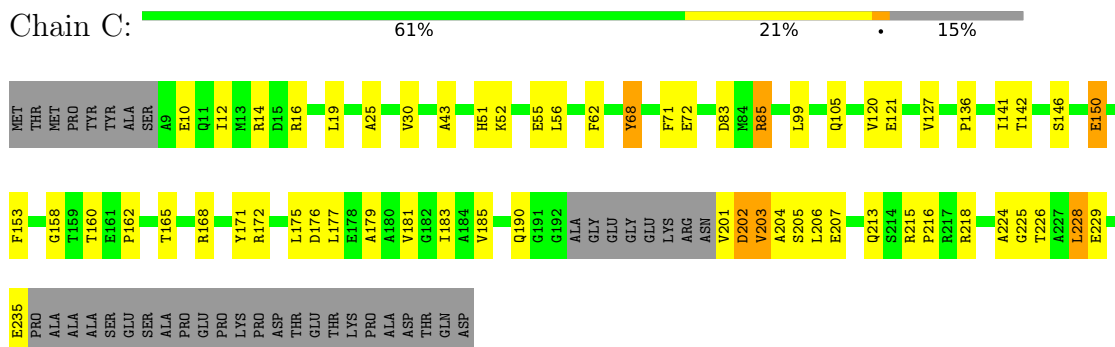
- Molecule 1: proteasome alpha-type subunit 1



- Molecule 1: proteasome alpha-type subunit 1



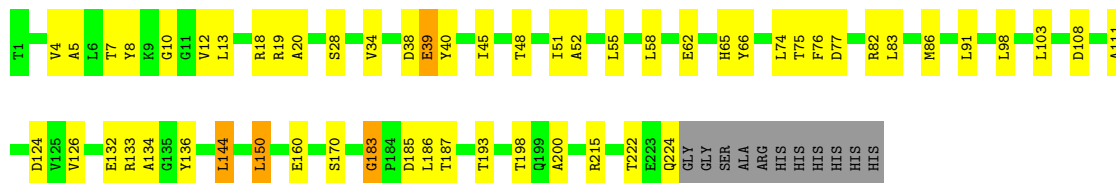
- Molecule 1: proteasome alpha-type subunit 1



ALA	SER	GLU	SER	ALA	PRO	GLU	PRO	PRO	ASP	THR	GLU	THR	LYS	PRO	ALA	ALA	ASP	THR	ASP																													
G158	P162	T165	R168	Y171	L175	D176	L177	E178	A179	V181	G182	I183	A184	V185	Q190	G191	G192	ALA	GLY	GLU	GLY	GLU	LYS	ARG	ASN	V201	D202	V203	A204	S205	L206	E207	Q213	S214	R215	P216	R217	R218	A224	G225	T226	A227	L228	E229	E235	PRO	ALA	ALA
MET	THR	PRO	TTR	ALA	SER	A9	E10	Q11	I12	H13	R14	D15	R16	L19	A25	V30	A43	H51	E55	L56	F62	Y68	F71	E72	N73	D83	H84	R85	L99	Q105	V120	E121	V127	T141	T142	S146	E150	F153										

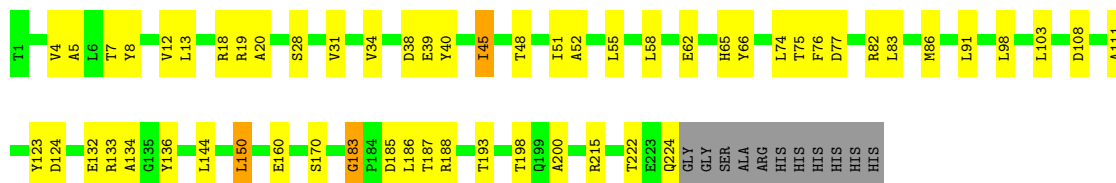
- Molecule 2: proteasome beta-type subunit 1

Chain H:  71% 22% • 5%



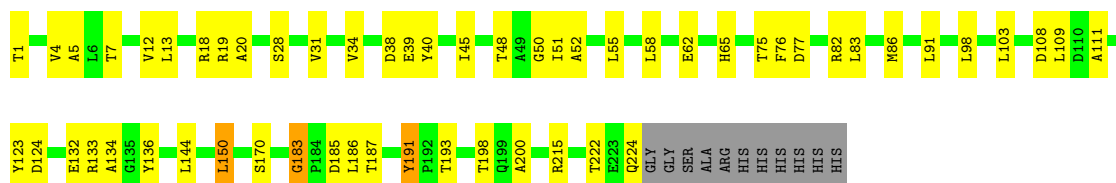
- Molecule 2: proteasome beta-type subunit 1

Chain I:  71% 23% • 5%



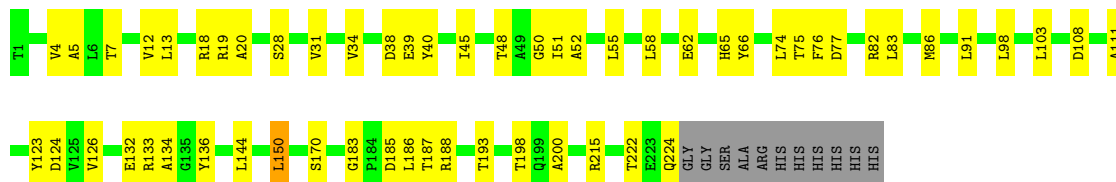
- Molecule 2: proteasome beta-type subunit 1

Chain J:  71% 23% • 5%



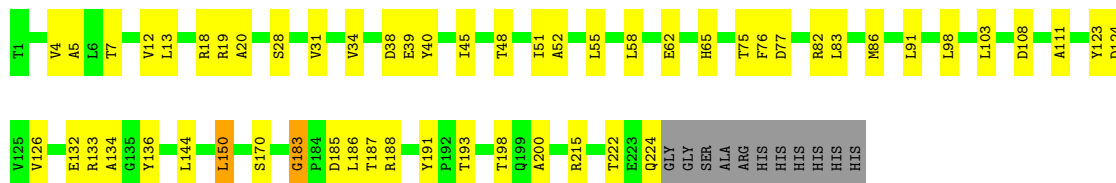
- Molecule 2: proteasome beta-type subunit 1

Chain K:  71% 24% 5%

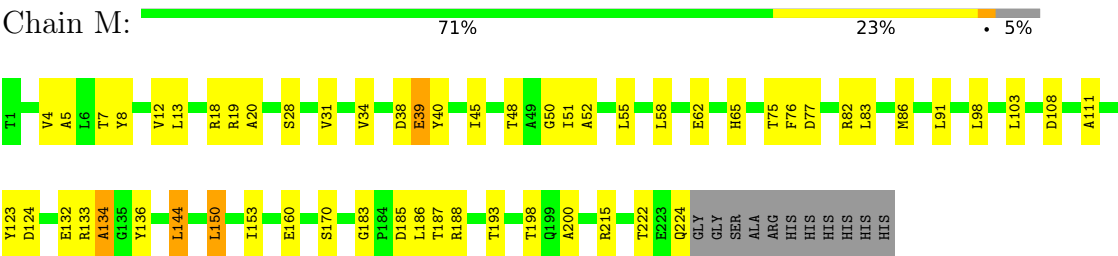


- Molecule 2: proteasome beta-type subunit 1

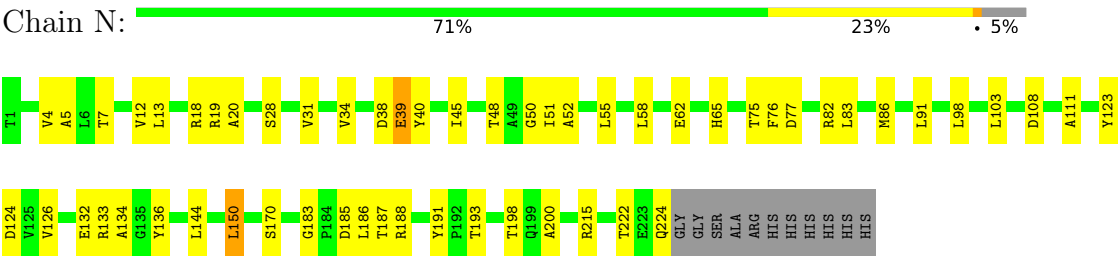
Chain L:  72% 23% • 5%



● Molecule 2: proteasome beta-type subunit 1



● Molecule 2: proteasome beta-type subunit 1



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	150.11Å 215.31Å 251.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.60	Depositor
% Data completeness (in resolution range)	91.7 (19.99-2.60)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23706	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/1720	0.91	5/2325 (0.2%)
1	B	0.49	0/1720	0.91	3/2325 (0.1%)
1	C	0.49	0/1720	0.91	4/2325 (0.2%)
1	D	0.49	0/1720	0.90	2/2325 (0.1%)
1	E	0.48	0/1720	0.91	2/2325 (0.1%)
1	F	0.48	0/1720	0.91	2/2325 (0.1%)
1	G	0.50	0/1720	0.90	2/2325 (0.1%)
2	H	0.55	0/1689	0.96	5/2291 (0.2%)
2	I	0.55	0/1689	0.97	7/2291 (0.3%)
2	J	0.55	0/1688	0.96	6/2290 (0.3%)
2	K	0.53	0/1688	0.96	6/2290 (0.3%)
2	L	0.52	0/1689	0.96	6/2291 (0.3%)
2	M	0.54	0/1689	0.97	7/2291 (0.3%)
2	N	0.54	0/1689	0.96	6/2291 (0.3%)
All	All	0.52	0/23861	0.93	63/32310 (0.2%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	134	ALA	N-CA-C	-8.48	102.09	114.39
2	M	134	ALA	N-CA-C	-8.47	102.11	114.39
2	L	134	ALA	N-CA-C	-8.29	102.37	114.39
2	K	134	ALA	N-CA-C	-8.18	102.53	114.39
2	I	134	ALA	N-CA-C	-7.96	102.85	114.39
2	J	134	ALA	N-CA-C	-7.74	103.17	114.39
2	H	134	ALA	N-CA-C	-7.69	103.24	114.39
2	J	19	ARG	N-CA-C	6.59	120.24	110.48
2	I	19	ARG	N-CA-C	6.54	120.17	110.48
2	N	183	GLY	CA-C-N	6.50	126.45	119.76
2	N	183	GLY	C-N-CA	6.50	126.45	119.76
2	L	183	GLY	CA-C-N	6.13	126.07	119.76
2	L	183	GLY	C-N-CA	6.13	126.07	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	19	ARG	N-CA-C	6.11	119.53	110.48
2	M	183	GLY	CA-C-N	6.11	126.05	119.76
2	M	183	GLY	C-N-CA	6.11	126.05	119.76
2	M	19	ARG	N-CA-C	6.10	119.50	110.48
2	L	19	ARG	N-CA-C	6.07	119.46	110.48
2	L	52	ALA	N-CA-C	6.02	118.34	111.11
2	N	19	ARG	N-CA-C	6.02	119.39	110.48
2	K	183	GLY	CA-C-N	6.01	125.95	119.76
2	K	183	GLY	C-N-CA	6.01	125.95	119.76
2	H	19	ARG	N-CA-C	5.96	119.80	110.32
2	I	183	GLY	CA-C-N	5.79	125.72	119.76
2	I	183	GLY	C-N-CA	5.79	125.72	119.76
2	M	52	ALA	N-CA-C	5.76	118.03	111.11
2	J	183	GLY	CA-C-N	5.73	125.66	119.76
2	J	183	GLY	C-N-CA	5.73	125.66	119.76
2	H	183	GLY	CA-C-N	5.72	125.66	119.76
2	H	183	GLY	C-N-CA	5.72	125.66	119.76
1	A	68	TYR	N-CA-C	5.70	117.97	111.02
1	B	68	TYR	N-CA-C	5.68	117.95	111.02
2	H	52	ALA	N-CA-C	5.66	117.91	111.11
1	C	68	TYR	N-CA-C	5.62	117.88	111.02
2	I	52	ALA	N-CA-C	5.57	117.79	111.11
2	I	123	TYR	N-CA-C	5.56	117.86	109.41
2	J	123	TYR	N-CA-C	5.56	117.86	109.41
2	N	52	ALA	N-CA-C	5.53	117.75	111.11
1	B	52	LYS	N-CA-C	-5.52	106.38	114.39
2	K	52	ALA	N-CA-C	5.47	117.67	111.11
1	E	72	GLU	N-CA-C	-5.42	105.53	111.82
2	L	123	TYR	N-CA-C	5.37	117.58	109.41
2	J	52	ALA	N-CA-C	5.37	117.56	111.11
1	F	68	TYR	N-CA-C	5.36	117.56	111.02
1	G	68	TYR	N-CA-C	5.36	117.55	111.02
1	F	160	THR	N-CA-C	5.34	117.92	111.40
1	B	160	THR	N-CA-C	5.30	117.86	111.40
1	C	72	GLU	N-CA-C	-5.27	105.70	111.82
1	D	160	THR	N-CA-C	5.27	117.83	111.40
1	A	51	HIS	N-CA-C	5.27	118.58	110.42
1	E	68	TYR	N-CA-C	5.26	117.44	111.02
2	M	153	ILE	N-CA-C	5.26	118.04	112.83
1	D	68	TYR	N-CA-C	5.23	117.40	111.02
2	N	123	TYR	N-CA-C	5.23	117.62	109.52
1	C	52	LYS	N-CA-C	-5.22	106.82	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ARG	N-CA-C	5.20	117.62	111.33
2	K	123	TYR	N-CA-C	5.20	117.31	109.41
1	G	51	HIS	N-CA-C	5.14	118.39	110.42
1	C	160	THR	N-CA-C	5.13	118.00	111.69
2	M	123	TYR	N-CA-C	5.12	117.94	109.85
1	A	160	THR	N-CA-C	5.08	117.94	111.69
1	A	52	LYS	N-CA-C	-5.07	107.03	114.39
2	I	45	ILE	N-CA-C	5.01	115.92	108.46

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	1695	0	1693	45	1
1	B	1695	0	1693	52	0
1	C	1695	0	1693	47	0
1	D	1695	0	1693	48	0
1	E	1695	0	1693	47	0
1	F	1695	0	1693	44	0
1	G	1695	0	1693	48	0
2	H	1668	0	1653	35	0
2	I	1668	0	1653	31	0
2	J	1667	0	1653	35	0
2	K	1667	0	1653	34	0
2	L	1668	0	1653	32	0
2	M	1668	0	1653	33	0
2	N	1668	0	1653	32	0
3	A	17	0	0	3	0
3	B	11	0	0	3	0
3	C	9	0	0	1	0
3	D	3	0	0	1	0
3	E	6	0	0	2	0
3	F	3	0	0	1	0
3	G	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	22	0	0	2	0
3	I	27	0	0	1	0
3	J	17	0	0	3	0
3	K	10	0	0	0	0
3	L	10	0	0	1	0
3	M	13	0	0	1	0
3	N	11	0	0	0	0
All	All	23706	0	23422	534	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 11.

All (534) 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:C:85:ARG:HH11	1:C:85:ARG:HB3	1.30	0.97
1:D:85:ARG:HB3	1:D:85:ARG:HH11	1.31	0.95
1:A:85:ARG:HH11	1:A:85:ARG:HB3	1.31	0.94
1:B:85:ARG:HH11	1:B:85:ARG:HB3	1.31	0.94
1:F:85:ARG:HH11	1:F:85:ARG:HB3	1.31	0.93
1:E:85:ARG:HH11	1:E:85:ARG:HB3	1.32	0.93
1:G:85:ARG:HH11	1:G:85:ARG:HB3	1.32	0.92
1:A:203:VAL:HG22	1:A:204:ALA:H	1.41	0.86
1:E:203:VAL:HG22	1:E:204:ALA:H	1.41	0.85
1:F:203:VAL:HG22	1:F:204:ALA:H	1.40	0.85
1:D:203:VAL:HG22	1:D:204:ALA:H	1.43	0.84
1:G:203:VAL:HG22	1:G:204:ALA:H	1.41	0.84
1:C:203:VAL:HG22	1:C:204:ALA:H	1.41	0.82
1:B:203:VAL:HG22	1:B:204:ALA:H	1.42	0.82
2:H:10:GLY:HA3	3:H:253:HOH:O	1.79	0.80
2:I:183:GLY:HA2	3:I:242:HOH:O	1.84	0.76
2:L:198:THR:HG23	2:L:200:ALA:H	1.53	0.73
2:J:183:GLY:HA2	3:J:238:HOH:O	1.88	0.73
1:A:10:GLU:HA	1:B:19:LEU:HD12	1.69	0.73
2:I:198:THR:HG23	2:I:200:ALA:H	1.54	0.73
2:N:198:THR:HG23	2:N:200:ALA:H	1.55	0.72
2:M:198:THR:HG23	2:M:200:ALA:H	1.54	0.71
1:C:10:GLU:HA	1:D:19:LEU:HD12	1.72	0.71
1:F:10:GLU:HA	1:G:19:LEU:HD12	1.73	0.71
2:J:186:LEU:HD22	2:J:215:ARG:HE	1.57	0.70
2:K:198:THR:HG23	2:K:200:ALA:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ARG:HH11	1:C:85:ARG:CB	2.04	0.69
2:J:198:THR:HG23	2:J:200:ALA:H	1.57	0.69
1:F:85:ARG:HH11	1:F:85:ARG:CB	2.05	0.69
1:A:130:VAL:HG23	3:A:269:HOH:O	1.92	0.68
1:A:85:ARG:HH11	1:A:85:ARG:CB	2.06	0.68
1:B:85:ARG:HH11	1:B:85:ARG:CB	2.05	0.67
2:K:186:LEU:HD22	2:K:215:ARG:HE	1.59	0.67
1:G:85:ARG:HH11	1:G:85:ARG:CB	2.07	0.67
2:M:186:LEU:HD22	2:M:215:ARG:HE	1.59	0.67
1:E:85:ARG:HH11	1:E:85:ARG:CB	2.07	0.67
2:L:186:LEU:HD22	2:L:215:ARG:HE	1.59	0.66
2:H:198:THR:HG23	2:H:200:ALA:H	1.59	0.66
1:D:85:ARG:HH11	1:D:85:ARG:CB	2.06	0.66
1:E:150:GLU:HG3	3:E:261:HOH:O	1.95	0.66
2:N:186:LEU:HD22	2:N:215:ARG:HE	1.61	0.65
1:A:165:THR:CG2	1:A:168:ARG:HH21	2.10	0.65
1:E:10:GLU:HA	1:F:19:LEU:HD12	1.79	0.65
1:A:9:ALA:N	3:A:260:HOH:O	2.30	0.65
1:E:127:VAL:CG2	1:E:213:GLN:HB2	2.28	0.64
1:A:14:ARG:HD3	3:A:271:HOH:O	1.98	0.64
1:B:165:THR:CG2	1:B:168:ARG:HH21	2.11	0.64
1:C:165:THR:CG2	1:C:168:ARG:HH21	2.11	0.64
1:D:10:GLU:HA	1:E:19:LEU:HD12	1.79	0.64
1:F:165:THR:CG2	1:F:168:ARG:HH21	2.11	0.64
2:J:39:GLU:HB3	2:J:40:TYR:CD1	2.31	0.64
1:E:165:THR:CG2	1:E:168:ARG:HH21	2.11	0.64
2:H:186:LEU:HD22	2:H:215:ARG:HE	1.62	0.64
1:A:172:ARG:HD2	1:A:175:LEU:HD21	1.81	0.63
1:G:165:THR:CG2	1:G:168:ARG:HH21	2.11	0.63
1:C:127:VAL:HG21	1:C:213:GLN:HB2	1.80	0.62
1:E:127:VAL:HG21	1:E:213:GLN:HB2	1.80	0.62
1:G:127:VAL:CG2	1:G:213:GLN:HB2	2.29	0.62
1:A:105:GLN:NE2	1:B:73:ASN:HD22	1.96	0.62
1:D:127:VAL:HG21	1:D:213:GLN:HB2	1.80	0.62
1:D:165:THR:CG2	1:D:168:ARG:HH21	2.12	0.62
1:F:127:VAL:HG21	1:F:213:GLN:HB2	1.81	0.62
2:H:183:GLY:HA2	3:H:247:HOH:O	1.98	0.62
1:A:83:ASP:OD2	2:H:65:HIS:HD2	1.83	0.62
2:L:39:GLU:HB3	2:L:40:TYR:CD1	2.35	0.62
1:B:127:VAL:HG21	1:B:213:GLN:HB2	1.82	0.61
1:D:127:VAL:CG2	1:D:213:GLN:HB2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:VAL:CG2	1:B:213:GLN:HB2	2.31	0.61
1:G:127:VAL:HG21	1:G:213:GLN:HB2	1.82	0.61
2:I:39:GLU:HB3	2:I:40:TYR:CD1	2.34	0.61
1:A:19:LEU:HD12	1:G:10:GLU:HA	1.80	0.61
2:M:39:GLU:HB3	2:M:40:TYR:CD1	2.35	0.61
2:H:39:GLU:HB3	2:H:40:TYR:CD1	2.35	0.61
2:N:39:GLU:HB3	2:N:40:TYR:CD1	2.35	0.61
1:C:127:VAL:CG2	1:C:213:GLN:HB2	2.30	0.61
1:F:127:VAL:CG2	1:F:213:GLN:HB2	2.31	0.61
1:A:127:VAL:HG21	1:A:213:GLN:HB2	1.82	0.60
2:I:186:LEU:HD22	2:I:215:ARG:HE	1.65	0.60
1:A:127:VAL:CG2	1:A:213:GLN:HB2	2.31	0.60
1:A:165:THR:HG22	1:A:168:ARG:HH21	1.66	0.60
2:K:39:GLU:HB3	2:K:40:TYR:CD1	2.36	0.60
1:C:203:VAL:C	1:C:205:SER:H	2.09	0.60
2:I:13:LEU:C	2:I:13:LEU:HD12	2.27	0.59
2:K:62:GLU:OE2	2:K:82:ARG:HD3	2.02	0.59
2:L:20:ALA:HB3	2:L:28:SER:HB3	1.84	0.59
1:G:14:ARG:HD3	3:G:266:HOH:O	2.02	0.59
2:K:13:LEU:C	2:K:13:LEU:HD12	2.28	0.59
1:E:203:VAL:C	1:E:205:SER:H	2.11	0.59
2:I:62:GLU:OE2	2:I:82:ARG:HD3	2.03	0.59
1:D:56:LEU:HD13	1:D:99:LEU:HD22	1.85	0.58
2:I:20:ALA:HB3	2:I:28:SER:HB3	1.85	0.58
1:B:136:PRO:HD3	3:B:264:HOH:O	2.02	0.58
1:C:165:THR:HG22	1:C:168:ARG:HH21	1.67	0.58
1:G:203:VAL:C	1:G:205:SER:H	2.11	0.58
2:H:13:LEU:C	2:H:13:LEU:HD12	2.28	0.58
2:M:62:GLU:OE2	2:M:82:ARG:HD3	2.03	0.58
1:C:105:GLN:NE2	1:D:73:ASN:HD22	2.01	0.58
1:A:203:VAL:C	1:A:205:SER:H	2.11	0.58
1:E:165:THR:HG22	1:E:168:ARG:HH21	1.67	0.58
1:F:165:THR:HG22	1:F:168:ARG:HH21	1.69	0.58
1:G:83:ASP:OD2	2:N:65:HIS:HD2	1.87	0.58
1:D:83:ASP:OD2	2:K:65:HIS:HD2	1.87	0.58
1:G:165:THR:HG22	1:G:168:ARG:HH21	1.69	0.58
2:L:13:LEU:HD12	2:L:13:LEU:C	2.29	0.58
2:J:13:LEU:HD12	2:J:13:LEU:C	2.28	0.57
1:C:56:LEU:HD13	1:C:99:LEU:HD22	1.85	0.57
1:D:203:VAL:C	1:D:205:SER:H	2.11	0.57
1:B:203:VAL:C	1:B:205:SER:H	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLU:HG3	3:B:261:HOH:O	2.03	0.57
1:B:165:THR:HG22	1:B:168:ARG:HH21	1.68	0.57
1:G:172:ARG:HD2	1:G:175:LEU:HD21	1.87	0.57
1:F:203:VAL:C	1:F:205:SER:H	2.11	0.57
1:D:165:THR:HG22	1:D:168:ARG:HH21	1.69	0.57
2:L:62:GLU:OE2	2:L:82:ARG:HD3	2.05	0.56
1:D:172:ARG:HD2	1:D:175:LEU:HD21	1.86	0.56
1:F:172:ARG:HD2	1:F:175:LEU:HD21	1.87	0.56
2:J:62:GLU:OE2	2:J:82:ARG:HD3	2.06	0.56
2:H:20:ALA:HB3	2:H:28:SER:HB3	1.86	0.56
2:N:20:ALA:HB3	2:N:28:SER:HB3	1.87	0.56
1:E:56:LEU:HD13	1:E:99:LEU:HD22	1.88	0.56
1:F:56:LEU:HD13	1:F:99:LEU:HD22	1.87	0.56
2:M:13:LEU:C	2:M:13:LEU:HD12	2.30	0.56
1:G:56:LEU:HD13	1:G:99:LEU:HD22	1.88	0.56
2:N:13:LEU:C	2:N:13:LEU:HD12	2.31	0.56
2:N:75:THR:HG22	2:N:77:ASP:H	1.70	0.56
2:H:62:GLU:OE2	2:H:82:ARG:HD3	2.05	0.55
1:B:83:ASP:OD2	2:I:65:HIS:HD2	1.89	0.55
1:B:172:ARG:HD2	1:B:175:LEU:HD21	1.88	0.55
2:M:20:ALA:HB3	2:M:28:SER:HB3	1.88	0.55
2:L:55:LEU:HD11	2:L:86:MET:HB3	1.88	0.55
2:M:55:LEU:HD11	2:M:86:MET:HB3	1.87	0.55
2:H:75:THR:HG22	2:H:77:ASP:H	1.71	0.55
2:K:20:ALA:HB3	2:K:28:SER:HB3	1.89	0.55
2:H:55:LEU:HD11	2:H:86:MET:HB3	1.90	0.54
1:F:14:ARG:HG3	1:F:14:ARG:HH11	1.73	0.54
1:A:203:VAL:HG22	1:A:204:ALA:N	2.19	0.54
2:J:20:ALA:HB3	2:J:28:SER:HB3	1.88	0.54
2:J:55:LEU:HD11	2:J:86:MET:HB3	1.90	0.54
1:A:73:ASN:HD22	1:G:105:GLN:NE2	2.05	0.54
1:C:172:ARG:HD2	1:C:175:LEU:HD21	1.89	0.54
2:J:222:THR:C	2:J:224:GLN:H	2.15	0.54
2:N:62:GLU:OE2	2:N:82:ARG:HD3	2.07	0.54
1:E:172:ARG:HD2	1:E:175:LEU:HD21	1.90	0.54
1:C:14:ARG:HG3	1:C:14:ARG:HH11	1.73	0.54
2:J:75:THR:HG22	2:J:77:ASP:H	1.73	0.54
2:N:55:LEU:HD11	2:N:86:MET:HB3	1.89	0.54
1:F:105:GLN:NE2	1:G:73:ASN:HD22	2.06	0.53
2:K:222:THR:C	2:K:224:GLN:H	2.16	0.53
2:M:222:THR:C	2:M:224:GLN:H	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:HD13	1:A:99:LEU:HD22	1.88	0.53
1:G:203:VAL:HG22	1:G:204:ALA:N	2.19	0.53
2:H:185:ASP:OD1	2:H:187:THR:HB	2.08	0.53
2:K:75:THR:HG22	2:K:77:ASP:H	1.74	0.53
1:F:202:ASP:HB3	3:F:262:HOH:O	2.07	0.53
1:C:203:VAL:HG22	1:C:204:ALA:N	2.19	0.53
2:M:75:THR:HG22	2:M:77:ASP:H	1.73	0.53
2:N:222:THR:C	2:N:224:GLN:H	2.17	0.53
1:B:10:GLU:HA	1:C:19:LEU:HD12	1.91	0.53
1:D:105:GLN:NE2	1:E:73:ASN:HD22	2.07	0.53
2:K:55:LEU:HD11	2:K:86:MET:HB3	1.90	0.53
2:J:34:VAL:HG23	2:J:34:VAL:O	2.08	0.53
2:I:55:LEU:HD11	2:I:86:MET:HB3	1.90	0.53
2:I:222:THR:C	2:I:224:GLN:H	2.16	0.53
1:A:14:ARG:HG3	1:A:14:ARG:HH11	1.74	0.53
1:A:56:LEU:HG	1:A:62:PHE:HB2	1.91	0.53
2:J:224:GLN:HA	2:J:224:GLN:HE21	1.75	0.53
1:B:14:ARG:HG3	1:B:14:ARG:HH11	1.73	0.52
1:B:56:LEU:HD13	1:B:99:LEU:HD22	1.90	0.52
1:D:179:ALA:O	1:D:183:ILE:HG12	2.08	0.52
2:L:150:LEU:HD13	2:L:170:SER:HB3	1.91	0.52
2:K:4:VAL:HG21	2:K:150:LEU:HD21	1.91	0.52
2:M:134:ALA:HB2	3:M:236:HOH:O	2.07	0.52
1:A:179:ALA:O	1:A:183:ILE:HG12	2.09	0.52
1:F:56:LEU:HG	1:F:62:PHE:HB2	1.92	0.52
2:L:4:VAL:HG21	2:L:150:LEU:HD21	1.91	0.52
2:I:34:VAL:HG23	2:I:34:VAL:O	2.10	0.52
2:I:75:THR:HG22	2:I:77:ASP:H	1.75	0.52
2:M:34:VAL:HG23	2:M:34:VAL:O	2.09	0.52
1:F:179:ALA:O	1:F:183:ILE:HG12	2.10	0.52
2:K:185:ASP:OD1	2:K:187:THR:HB	2.09	0.52
2:L:75:THR:HG22	2:L:77:ASP:H	1.75	0.52
2:L:222:THR:C	2:L:224:GLN:H	2.17	0.52
1:E:14:ARG:HG3	1:E:14:ARG:HH11	1.75	0.52
1:G:14:ARG:HH11	1:G:14:ARG:HG3	1.75	0.52
1:C:120:VAL:HG12	1:C:121:GLU:N	2.25	0.51
2:H:222:THR:C	2:H:224:GLN:H	2.18	0.51
1:G:179:ALA:O	1:G:183:ILE:HG12	2.10	0.51
1:D:14:ARG:HG3	1:D:14:ARG:HH11	1.75	0.51
2:K:108:ASP:HB3	2:K:111:ALA:HB2	1.92	0.51
2:H:224:GLN:HE21	2:H:224:GLN:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:224:GLN:HE21	2:I:224:GLN:HA	1.76	0.51
2:L:185:ASP:OD1	2:L:187:THR:HB	2.10	0.51
2:N:34:VAL:HG23	2:N:34:VAL:O	2.10	0.51
1:E:179:ALA:O	1:E:183:ILE:HG12	2.11	0.51
2:N:108:ASP:HB3	2:N:111:ALA:HB2	1.93	0.51
1:C:56:LEU:HG	1:C:62:PHE:HB2	1.93	0.50
1:D:56:LEU:HG	1:D:62:PHE:HB2	1.94	0.50
2:H:150:LEU:HD13	2:H:170:SER:HB3	1.92	0.50
2:N:4:VAL:HG21	2:N:150:LEU:HD21	1.93	0.50
1:E:56:LEU:HG	1:E:62:PHE:HB2	1.93	0.50
2:K:75:THR:HG22	2:K:76:PHE:N	2.26	0.50
2:M:224:GLN:HE21	2:M:224:GLN:HA	1.77	0.50
1:F:203:VAL:HG22	1:F:204:ALA:N	2.18	0.50
2:L:224:GLN:HE21	2:L:224:GLN:HA	1.77	0.50
2:J:185:ASP:OD1	2:J:187:THR:HB	2.11	0.50
2:N:224:GLN:HE21	2:N:224:GLN:HA	1.77	0.50
1:A:83:ASP:OD2	2:H:65:HIS:CD2	2.65	0.50
1:C:162:PRO:HB2	1:C:190:GLN:O	2.12	0.50
1:F:19:LEU:C	1:F:19:LEU:HD23	2.37	0.50
2:J:4:VAL:HG21	2:J:150:LEU:HD21	1.94	0.50
2:M:108:ASP:HB3	2:M:111:ALA:HB2	1.94	0.50
1:A:171:TYR:C	1:A:172:ARG:HG3	2.36	0.50
1:B:56:LEU:HG	1:B:62:PHE:HB2	1.94	0.50
1:B:162:PRO:HB2	1:B:190:GLN:O	2.11	0.50
1:B:179:ALA:O	1:B:183:ILE:HG12	2.12	0.50
1:C:179:ALA:O	1:C:183:ILE:HG12	2.11	0.50
1:F:162:PRO:HB2	1:F:190:GLN:O	2.12	0.50
2:M:4:VAL:HG21	2:M:150:LEU:HD21	1.92	0.50
2:M:150:LEU:HD13	2:M:170:SER:HB3	1.93	0.50
2:I:4:VAL:HG21	2:I:150:LEU:HD21	1.95	0.49
2:L:58:LEU:HB3	2:L:86:MET:HE1	1.94	0.49
2:M:185:ASP:OD1	2:M:187:THR:HB	2.12	0.49
1:B:176:ASP:OD2	1:B:177:LEU:N	2.45	0.49
2:K:150:LEU:HD13	2:K:170:SER:HB3	1.93	0.49
2:M:58:LEU:HB3	2:M:86:MET:HE1	1.95	0.49
2:N:150:LEU:HD13	2:N:170:SER:HB3	1.94	0.49
1:A:162:PRO:HB2	1:A:190:GLN:O	2.13	0.49
1:G:56:LEU:HG	1:G:62:PHE:HB2	1.93	0.49
2:I:132:GLU:O	2:I:133:ARG:HG2	2.12	0.49
2:K:224:GLN:HA	2:K:224:GLN:HE21	1.76	0.49
2:L:34:VAL:HG23	2:L:34:VAL:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:VAL:HG22	1:B:43:ALA:HB1	1.95	0.49
1:C:14:ARG:HG3	1:C:14:ARG:NH1	2.27	0.49
1:D:162:PRO:HB2	1:D:190:GLN:O	2.13	0.49
1:F:14:ARG:HG3	1:F:14:ARG:NH1	2.27	0.49
1:D:19:LEU:HD23	1:D:19:LEU:C	2.38	0.49
2:J:75:THR:HG22	2:J:76:PHE:N	2.27	0.49
2:I:185:ASP:OD1	2:I:187:THR:HB	2.12	0.49
2:K:38:ASP:OD2	2:K:38:ASP:C	2.56	0.49
1:B:120:VAL:HG12	1:B:121:GLU:N	2.27	0.49
2:L:108:ASP:HB3	2:L:111:ALA:HB2	1.95	0.49
2:M:75:THR:HG22	2:M:76:PHE:N	2.28	0.49
1:A:120:VAL:HG12	1:A:121:GLU:N	2.28	0.49
1:E:181:VAL:O	1:E:185:VAL:HG23	2.13	0.49
1:D:203:VAL:HG22	1:D:204:ALA:N	2.21	0.48
2:L:38:ASP:C	2:L:38:ASP:OD2	2.56	0.48
1:C:176:ASP:OD2	1:C:177:LEU:N	2.46	0.48
1:E:162:PRO:HB2	1:E:190:GLN:O	2.12	0.48
2:J:132:GLU:O	2:J:133:ARG:HG2	2.13	0.48
1:A:14:ARG:HG3	1:A:14:ARG:NH1	2.29	0.48
1:E:19:LEU:C	1:E:19:LEU:HD23	2.39	0.48
2:J:108:ASP:HB3	2:J:111:ALA:HB2	1.95	0.48
1:D:56:LEU:HD13	1:D:99:LEU:CD2	2.43	0.48
2:H:34:VAL:HG23	2:H:34:VAL:O	2.12	0.48
2:I:224:GLN:HA	2:I:224:GLN:NE2	2.29	0.48
2:J:38:ASP:C	2:J:38:ASP:OD2	2.57	0.48
2:K:224:GLN:HA	2:K:224:GLN:NE2	2.29	0.48
1:F:30:VAL:HG22	1:F:43:ALA:HB1	1.95	0.48
2:N:20:ALA:HB2	2:N:31:VAL:HG21	1.95	0.48
1:D:25:ALA:O	1:D:158:GLY:HA2	2.14	0.48
1:G:162:PRO:HB2	1:G:190:GLN:O	2.13	0.48
2:J:224:GLN:HA	2:J:224:GLN:NE2	2.28	0.48
1:F:120:VAL:HG12	1:F:121:GLU:N	2.29	0.48
2:M:132:GLU:O	2:M:133:ARG:HG2	2.13	0.48
1:E:25:ALA:O	1:E:158:GLY:HA2	2.13	0.48
1:E:30:VAL:HG22	1:E:43:ALA:HB1	1.96	0.48
2:M:38:ASP:OD2	2:M:38:ASP:C	2.57	0.48
1:E:203:VAL:HG22	1:E:204:ALA:N	2.19	0.48
1:B:14:ARG:HG3	1:B:14:ARG:NH1	2.28	0.48
2:I:38:ASP:OD2	2:I:38:ASP:C	2.57	0.48
2:J:150:LEU:HD13	2:J:170:SER:HB3	1.96	0.48
2:N:224:GLN:HA	2:N:224:GLN:NE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ILE:N	1:B:141:ILE:HD12	2.29	0.47
2:J:58:LEU:HB3	2:J:86:MET:HE1	1.96	0.47
1:F:176:ASP:OD2	1:F:177:LEU:N	2.48	0.47
1:G:171:TYR:C	1:G:172:ARG:HG3	2.39	0.47
2:H:4:VAL:HG21	2:H:150:LEU:HD21	1.95	0.47
2:H:75:THR:HG22	2:H:76:PHE:N	2.30	0.47
2:N:185:ASP:OD1	2:N:187:THR:HB	2.14	0.47
2:I:150:LEU:HD13	2:I:170:SER:HB3	1.96	0.47
2:L:75:THR:HG22	2:L:76:PHE:N	2.29	0.47
1:B:92:ARG:NH2	3:B:269:HOH:O	2.47	0.47
1:D:176:ASP:OD2	1:D:177:LEU:N	2.47	0.47
2:H:224:GLN:HA	2:H:224:GLN:NE2	2.29	0.47
2:L:186:LEU:HD22	2:L:215:ARG:NE	2.29	0.47
2:H:108:ASP:HB3	2:H:111:ALA:HB2	1.96	0.47
2:J:186:LEU:HD22	2:J:215:ARG:NE	2.28	0.47
2:N:132:GLU:O	2:N:133:ARG:HG2	2.15	0.47
1:D:120:VAL:HG12	1:D:121:GLU:N	2.29	0.47
2:I:108:ASP:HB3	2:I:111:ALA:HB2	1.96	0.47
2:K:34:VAL:O	2:K:34:VAL:HG23	2.13	0.47
2:M:224:GLN:HA	2:M:224:GLN:NE2	2.29	0.47
1:E:141:ILE:N	1:E:141:ILE:HD12	2.29	0.47
1:G:120:VAL:HG12	1:G:121:GLU:N	2.28	0.47
2:M:51:ILE:HD12	2:M:98:LEU:HB3	1.97	0.47
2:N:5:ALA:O	2:N:136:TYR:HA	2.14	0.47
1:E:120:VAL:HG12	1:E:121:GLU:N	2.29	0.47
2:K:58:LEU:HB3	2:K:86:MET:HE1	1.96	0.47
2:L:224:GLN:HA	2:L:224:GLN:NE2	2.29	0.47
2:L:20:ALA:HB2	2:L:31:VAL:HG21	1.96	0.47
1:E:105:GLN:NE2	1:F:73:ASN:HD22	2.12	0.47
1:E:176:ASP:OD2	1:E:177:LEU:N	2.48	0.47
2:I:51:ILE:HD12	2:I:98:LEU:HB3	1.97	0.47
2:M:50:GLY:HA3	2:N:126:VAL:CG2	2.45	0.47
1:C:83:ASP:OD2	2:J:65:HIS:HD2	1.97	0.46
1:C:171:TYR:C	1:C:172:ARG:HG3	2.40	0.46
1:E:14:ARG:HG3	1:E:14:ARG:NH1	2.29	0.46
2:J:5:ALA:O	2:J:136:TYR:HA	2.15	0.46
2:L:132:GLU:O	2:L:133:ARG:HG2	2.15	0.46
1:D:14:ARG:HG3	1:D:14:ARG:NH1	2.30	0.46
1:E:171:TYR:C	1:E:172:ARG:HG3	2.40	0.46
1:F:171:TYR:C	1:F:172:ARG:HG3	2.41	0.46
2:J:34:VAL:HG22	3:J:236:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:55:LEU:CD1	2:J:86:MET:HE2	2.45	0.46
1:B:224:ALA:O	1:B:228:LEU:HB2	2.16	0.46
1:D:141:ILE:HD12	1:D:141:ILE:N	2.30	0.46
2:N:75:THR:HG22	2:N:76:PHE:N	2.30	0.46
2:I:20:ALA:HB2	2:I:31:VAL:HG21	1.98	0.46
2:L:51:ILE:HD12	2:L:98:LEU:HB3	1.97	0.46
1:C:56:LEU:HD13	1:C:99:LEU:CD2	2.45	0.46
1:C:150:GLU:HG2	1:C:153:PHE:O	2.15	0.46
1:D:150:GLU:HG2	1:D:153:PHE:O	2.16	0.46
1:G:14:ARG:HG3	1:G:14:ARG:NH1	2.30	0.46
1:D:30:VAL:HG22	1:D:43:ALA:HB1	1.97	0.46
2:H:55:LEU:CD1	2:H:86:MET:HE2	2.45	0.46
2:I:5:ALA:O	2:I:136:TYR:HA	2.16	0.46
2:J:20:ALA:HB2	2:J:31:VAL:HG21	1.97	0.46
1:A:19:LEU:C	1:A:19:LEU:HD23	2.41	0.46
1:C:30:VAL:HG22	1:C:43:ALA:HB1	1.98	0.46
2:H:38:ASP:OD2	2:H:38:ASP:C	2.59	0.46
2:H:5:ALA:O	2:H:136:TYR:HA	2.16	0.46
2:K:132:GLU:O	2:K:133:ARG:HG2	2.15	0.46
2:L:183:GLY:HA2	3:L:236:HOH:O	2.16	0.46
2:N:51:ILE:HD12	2:N:98:LEU:HB3	1.98	0.46
2:N:58:LEU:HB3	2:N:86:MET:HE1	1.97	0.46
1:A:226:THR:HA	1:A:229:GLU:HG3	1.98	0.46
1:D:224:ALA:O	1:D:228:LEU:HB2	2.16	0.46
2:L:5:ALA:O	2:L:136:TYR:HA	2.16	0.46
1:E:201:VAL:O	1:E:202:ASP:HB3	2.16	0.45
1:F:83:ASP:OD2	2:M:65:HIS:HD2	2.00	0.45
1:G:201:VAL:O	1:G:202:ASP:HB3	2.16	0.45
1:A:201:VAL:O	1:A:202:ASP:HB3	2.16	0.45
1:A:176:ASP:OD2	1:A:177:LEU:N	2.50	0.45
1:C:19:LEU:C	1:C:19:LEU:HD23	2.41	0.45
1:E:83:ASP:OD2	2:L:65:HIS:HD2	1.99	0.45
1:F:201:VAL:O	1:F:202:ASP:HB3	2.16	0.45
2:I:75:THR:HG22	2:I:76:PHE:N	2.30	0.45
2:K:5:ALA:O	2:K:136:TYR:HA	2.17	0.45
2:K:20:ALA:HB2	2:K:31:VAL:HG21	1.98	0.45
2:M:18:ARG:HD3	2:M:193:THR:HG23	1.98	0.45
1:B:19:LEU:C	1:B:19:LEU:HD23	2.41	0.45
1:B:171:TYR:C	1:B:172:ARG:HG3	2.42	0.45
1:B:203:VAL:HG22	1:B:204:ALA:N	2.20	0.45
1:C:201:VAL:O	1:C:202:ASP:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:GLU:HG2	1:F:153:PHE:O	2.17	0.45
1:G:19:LEU:C	1:G:19:LEU:HD23	2.41	0.45
1:G:68:TYR:HA	1:G:71:PHE:CE2	2.52	0.45
2:K:51:ILE:HD12	2:K:98:LEU:HB3	1.98	0.45
2:M:186:LEU:HD22	2:M:215:ARG:NE	2.30	0.45
1:B:25:ALA:O	1:B:158:GLY:HA2	2.17	0.45
1:B:150:GLU:HG2	1:B:153:PHE:O	2.17	0.45
1:F:25:ALA:O	1:F:158:GLY:HA2	2.16	0.45
1:G:141:ILE:N	1:G:141:ILE:HD12	2.31	0.45
1:A:224:ALA:O	1:A:228:LEU:HB2	2.17	0.45
1:D:201:VAL:O	1:D:202:ASP:HB3	2.17	0.45
1:B:201:VAL:O	1:B:202:ASP:HB3	2.16	0.45
1:E:150:GLU:HG2	1:E:153:PHE:O	2.17	0.45
1:G:30:VAL:HG22	1:G:43:ALA:HB1	1.99	0.45
1:F:226:THR:HA	1:F:229:GLU:HG3	1.98	0.45
2:J:51:ILE:HD12	2:J:98:LEU:HB3	1.98	0.45
2:K:18:ARG:HD3	2:K:193:THR:HG23	1.98	0.45
1:A:181:VAL:O	1:A:185:VAL:HG23	2.17	0.45
1:E:226:THR:HA	1:E:229:GLU:HG3	1.99	0.44
2:L:18:ARG:HD3	2:L:193:THR:HG23	1.99	0.44
1:A:142:THR:OG1	1:A:146:SER:HB2	2.16	0.44
1:C:56:LEU:HD23	1:C:56:LEU:HA	1.88	0.44
1:G:11:GLN:HE22	1:G:14:ARG:HG2	1.82	0.44
2:M:5:ALA:O	2:M:136:TYR:HA	2.17	0.44
1:A:141:ILE:HD12	1:A:141:ILE:N	2.32	0.44
1:E:224:ALA:O	1:E:228:LEU:HB2	2.18	0.44
2:H:51:ILE:HD12	2:H:98:LEU:HB3	1.98	0.44
2:N:38:ASP:OD2	2:N:38:ASP:C	2.59	0.44
1:A:56:LEU:HD13	1:A:99:LEU:CD2	2.47	0.44
1:D:142:THR:OG1	1:D:146:SER:HB2	2.17	0.44
1:B:30:VAL:HG22	1:B:43:ALA:CB	2.48	0.44
1:E:201:VAL:O	1:E:202:ASP:CB	2.66	0.44
1:F:68:TYR:HA	1:F:71:PHE:CE2	2.53	0.44
1:G:150:GLU:HG2	1:G:153:PHE:O	2.17	0.44
2:I:58:LEU:HB3	2:I:86:MET:HE1	2.00	0.44
1:B:11:GLN:HE22	1:B:14:ARG:HG2	1.83	0.44
1:D:226:THR:HA	1:D:229:GLU:HG3	1.99	0.44
1:G:165:THR:HG23	1:G:168:ARG:HH21	1.83	0.44
2:K:50:GLY:HA3	2:L:126:VAL:CG2	2.48	0.44
2:K:55:LEU:CD1	2:K:86:MET:HE2	2.48	0.44
1:D:171:TYR:C	1:D:172:ARG:HG3	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:VAL:O	1:G:185:VAL:HG23	2.17	0.44
1:G:201:VAL:O	1:G:202:ASP:CB	2.66	0.44
1:B:201:VAL:O	1:B:202:ASP:CB	2.66	0.43
1:F:201:VAL:O	1:F:202:ASP:CB	2.66	0.43
1:G:25:ALA:O	1:G:158:GLY:HA2	2.17	0.43
1:G:176:ASP:OD2	1:G:177:LEU:N	2.51	0.43
2:K:186:LEU:HD22	2:K:215:ARG:NE	2.28	0.43
1:A:30:VAL:HG22	1:A:43:ALA:HB1	2.00	0.43
1:B:226:THR:HA	1:B:229:GLU:HG3	2.00	0.43
1:F:141:ILE:HD12	1:F:141:ILE:N	2.33	0.43
1:F:203:VAL:C	1:F:205:SER:N	2.77	0.43
2:H:132:GLU:O	2:H:133:ARG:HG2	2.18	0.43
2:L:55:LEU:CD1	2:L:86:MET:HE2	2.48	0.43
2:M:20:ALA:HB2	2:M:31:VAL:HG21	2.00	0.43
2:N:55:LEU:CD1	2:N:86:MET:HE2	2.47	0.43
1:A:150:GLU:HG2	1:A:153:PHE:O	2.19	0.43
1:D:201:VAL:O	1:D:202:ASP:CB	2.66	0.43
2:J:39:GLU:HB3	2:J:40:TYR:CE1	2.53	0.43
2:N:185:ASP:OD2	2:N:188:ARG:HD2	2.18	0.43
1:A:25:ALA:O	1:A:158:GLY:HA2	2.18	0.43
1:B:165:THR:HG23	1:B:168:ARG:HH21	1.83	0.43
1:C:201:VAL:O	1:C:202:ASP:CB	2.66	0.43
1:C:215:ARG:HA	1:C:216:PRO:HD3	1.91	0.43
1:C:224:ALA:O	1:C:228:LEU:HB2	2.18	0.43
1:D:68:TYR:HA	1:D:71:PHE:CE2	2.53	0.43
1:E:142:THR:OG1	1:E:146:SER:HB2	2.18	0.43
1:E:177:LEU:O	1:E:181:VAL:HG23	2.18	0.43
1:A:211:LEU:HD12	1:A:211:LEU:HA	1.92	0.43
1:B:142:THR:OG1	1:B:146:SER:HB2	2.18	0.43
2:M:55:LEU:CD1	2:M:86:MET:HE2	2.48	0.43
1:A:201:VAL:O	1:A:202:ASP:CB	2.66	0.43
1:B:83:ASP:OD2	2:I:65:HIS:CD2	2.70	0.43
1:B:235:GLU:H	1:B:235:GLU:HG2	1.68	0.43
1:C:25:ALA:O	1:C:158:GLY:HA2	2.18	0.43
1:G:215:ARG:HA	1:G:216:PRO:HD3	1.91	0.43
2:H:18:ARG:HD3	2:H:193:THR:HG23	1.99	0.43
2:H:144:LEU:HD22	2:H:144:LEU:HA	1.91	0.43
2:L:132:GLU:OE1	2:L:132:GLU:HA	2.18	0.43
1:A:203:VAL:C	1:A:205:SER:N	2.77	0.43
1:E:68:TYR:HA	1:E:71:PHE:CE2	2.54	0.43
1:G:226:THR:HA	1:G:229:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:18:ARG:HD3	2:J:193:THR:HG23	2.00	0.43
1:C:136:PRO:HD3	3:C:263:HOH:O	2.19	0.43
1:C:226:THR:HA	1:C:229:GLU:HG3	2.00	0.43
1:F:30:VAL:HG22	1:F:43:ALA:CB	2.49	0.43
1:G:83:ASP:OD2	2:N:65:HIS:CD2	2.69	0.43
2:L:185:ASP:OD2	2:L:188:ARG:HD2	2.18	0.43
2:M:144:LEU:HD22	2:M:144:LEU:HA	1.90	0.43
2:N:18:ARG:HD3	2:N:193:THR:HG23	2.01	0.43
2:H:58:LEU:HB3	2:H:86:MET:HE1	1.99	0.43
1:A:165:THR:HG23	1:A:168:ARG:HH21	1.83	0.42
1:C:120:VAL:CG1	1:C:121:GLU:N	2.81	0.42
1:F:56:LEU:HD13	1:F:99:LEU:CD2	2.49	0.42
1:F:224:ALA:O	1:F:228:LEU:HB2	2.19	0.42
1:C:142:THR:OG1	1:C:146:SER:HB2	2.18	0.42
1:F:181:VAL:O	1:F:185:VAL:HG23	2.19	0.42
1:C:235:GLU:H	1:C:235:GLU:HG2	1.69	0.42
1:G:224:ALA:O	1:G:228:LEU:HB2	2.19	0.42
1:D:215:ARG:HA	1:D:216:PRO:HD3	1.90	0.42
1:E:11:GLN:HE22	1:E:14:ARG:HG2	1.84	0.42
1:E:56:LEU:HD13	1:E:99:LEU:CD2	2.48	0.42
1:G:56:LEU:HD13	1:G:99:LEU:CD2	2.48	0.42
2:I:66:TYR:CD2	2:I:74:LEU:HG	2.55	0.42
1:D:203:VAL:C	1:D:205:SER:N	2.77	0.42
1:E:165:THR:HG23	1:E:168:ARG:HH21	1.85	0.42
1:B:203:VAL:C	1:B:205:SER:N	2.77	0.42
2:J:132:GLU:OE1	2:J:132:GLU:HA	2.19	0.42
1:E:203:VAL:C	1:E:205:SER:N	2.77	0.42
2:I:39:GLU:HB3	2:I:40:TYR:CE1	2.55	0.42
1:D:150:GLU:HG3	3:D:261:HOH:O	2.20	0.41
1:D:165:THR:HG23	1:D:168:ARG:HH21	1.83	0.41
1:F:211:LEU:HD12	1:F:211:LEU:HA	1.92	0.41
1:C:55:GLU:OE2	1:C:218:ARG:HD2	2.20	0.41
1:G:56:LEU:HD23	1:G:56:LEU:HA	1.90	0.41
2:M:185:ASP:OD2	2:M:188:ARG:HD2	2.20	0.41
1:C:105:GLN:HE22	1:D:73:ASN:HB2	1.85	0.41
1:D:83:ASP:OD2	2:K:65:HIS:CD2	2.69	0.41
1:E:85:ARG:HH11	1:E:85:ARG:CG	2.33	0.41
2:J:50:GLY:HA3	2:K:126:VAL:CG2	2.51	0.41
2:H:186:LEU:HD22	2:H:215:ARG:NE	2.33	0.41
2:I:18:ARG:HD3	2:I:193:THR:HG23	2.03	0.41
1:B:51:HIS:HB3	1:B:207:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLU:OE2	1:B:218:ARG:HD2	2.20	0.41
1:C:85:ARG:HH11	1:C:85:ARG:CG	2.32	0.41
1:F:85:ARG:HH11	1:F:85:ARG:CG	2.33	0.41
1:F:165:THR:HG23	1:F:168:ARG:HH21	1.82	0.41
1:G:51:HIS:HB3	1:G:207:GLU:OE1	2.21	0.41
2:K:132:GLU:OE1	2:K:132:GLU:HA	2.20	0.41
2:N:132:GLU:OE1	2:N:132:GLU:HA	2.21	0.41
1:B:85:ARG:HH11	1:B:85:ARG:CG	2.33	0.41
1:G:120:VAL:CG1	1:G:121:GLU:N	2.82	0.41
1:C:141:ILE:N	1:C:141:ILE:HD12	2.35	0.41
1:D:120:VAL:CG1	1:D:121:GLU:N	2.83	0.41
1:G:142:THR:OG1	1:G:146:SER:HB2	2.21	0.41
2:I:8:TYR:CZ	2:I:160:GLU:HG3	2.56	0.41
1:B:120:VAL:CG1	1:B:121:GLU:N	2.83	0.41
1:E:30:VAL:HG22	1:E:43:ALA:CB	2.51	0.41
1:F:120:VAL:CG1	1:F:121:GLU:N	2.84	0.41
2:H:126:VAL:CG2	2:N:50:GLY:HA3	2.50	0.41
1:B:68:TYR:HA	1:B:71:PHE:CE2	2.56	0.41
1:B:181:VAL:O	1:B:185:VAL:HG23	2.21	0.41
1:C:30:VAL:HG22	1:C:43:ALA:CB	2.51	0.41
1:C:68:TYR:HA	1:C:71:PHE:CE2	2.55	0.41
1:D:30:VAL:HG22	1:D:43:ALA:CB	2.51	0.41
1:D:60:LEU:CD2	1:D:126:GLU:HB2	2.51	0.41
1:D:177:LEU:O	1:D:181:VAL:HG23	2.20	0.41
2:I:185:ASP:OD2	2:I:188:ARG:HD2	2.21	0.41
2:J:1:THR:HB	3:J:243:HOH:O	2.20	0.41
2:K:39:GLU:HB3	2:K:40:TYR:CE1	2.56	0.41
2:L:39:GLU:HB3	2:L:40:TYR:CE1	2.56	0.41
1:B:12:ILE:O	1:B:16:ARG:HG2	2.21	0.41
1:G:85:ARG:HH11	1:G:85:ARG:CG	2.34	0.41
1:A:55:GLU:OE2	1:A:218:ARG:HD2	2.21	0.40
1:E:94:VAL:HA	3:E:262:HOH:O	2.20	0.40
1:F:51:HIS:HB3	1:F:207:GLU:OE1	2.21	0.40
1:G:55:GLU:OE2	1:G:218:ARG:HD2	2.20	0.40
1:C:12:ILE:O	1:C:16:ARG:HG2	2.21	0.40
1:D:181:VAL:O	1:D:185:VAL:HG23	2.20	0.40
1:E:232:VAL:O	1:E:232:VAL:HG13	2.21	0.40
1:G:12:ILE:O	1:G:16:ARG:HG2	2.22	0.40
2:H:132:GLU:OE1	2:H:132:GLU:HA	2.21	0.40
2:J:40:TYR:CE2	2:J:109:LEU:HD21	2.57	0.40
2:J:191:TYR:CD1	2:J:191:TYR:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:39:GLU:HB3	2:M:40:TYR:CE1	2.56	0.40
1:C:51:HIS:HB3	1:C:207:GLU:OE1	2.20	0.40
1:C:181:VAL:O	1:C:185:VAL:HG23	2.21	0.40
1:D:11:GLN:HE22	1:D:14:ARG:HG2	1.86	0.40
1:E:215:ARG:HA	1:E:216:PRO:HD3	1.90	0.40
2:M:8:TYR:CZ	2:M:160:GLU:HG3	2.56	0.40
1:B:54:SER:CB	1:B:75:ARG:HD2	2.50	0.40
2:H:39:GLU:HB3	2:H:40:TYR:CE1	2.56	0.40
2:H:66:TYR:CD2	2:H:74:LEU:HG	2.56	0.40
2:K:66:TYR:CD2	2:K:74:LEU:HG	2.56	0.40
2:K:185:ASP:OD2	2:K:188:ARG:HD2	2.21	0.40
1:A:120:VAL:CG1	1:A:121:GLU:N	2.83	0.40
1:B:33:LEU:C	1:B:33:LEU:HD12	2.47	0.40
1:B:56:LEU:HD13	1:B:99:LEU:CD2	2.50	0.40
2:H:8:TYR:CZ	2:H:160:GLU:HG3	2.56	0.40
2:N:186:LEU:HD22	2:N:215:ARG:NE	2.31	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)
1:A:172:ARG:CD	1:A:172:ARG:CD[4_577]	2.15	0.05

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	215/259 (83%)	200 (93%)	13 (6%)	2 (1%)	14	30
1	B	215/259 (83%)	198 (92%)	14 (6%)	3 (1%)	9	19
1	C	215/259 (83%)	199 (93%)	13 (6%)	3 (1%)	9	19
1	D	215/259 (83%)	199 (93%)	14 (6%)	2 (1%)	14	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	215/259 (83%)	200 (93%)	12 (6%)	3 (1%)	9	19
1	F	215/259 (83%)	200 (93%)	12 (6%)	3 (1%)	9	19
1	G	215/259 (83%)	200 (93%)	13 (6%)	2 (1%)	14	30
2	H	222/235 (94%)	212 (96%)	9 (4%)	1 (0%)	24	46
2	I	222/235 (94%)	212 (96%)	9 (4%)	1 (0%)	24	46
2	J	222/235 (94%)	211 (95%)	10 (4%)	1 (0%)	24	46
2	K	222/235 (94%)	211 (95%)	10 (4%)	1 (0%)	24	46
2	L	222/235 (94%)	211 (95%)	10 (4%)	1 (0%)	24	46
2	M	222/235 (94%)	211 (95%)	10 (4%)	1 (0%)	24	46
2	N	222/235 (94%)	211 (95%)	10 (4%)	1 (0%)	24	46
All	All	3059/3458 (88%)	2875 (94%)	159 (5%)	25 (1%)	16	34

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	ASP
1	B	202	ASP
1	C	202	ASP
1	D	202	ASP
1	E	202	ASP
1	F	202	ASP
1	G	202	ASP
2	H	48	THR
2	I	48	THR
2	J	48	THR
2	K	48	THR
2	L	48	THR
2	M	48	THR
2	N	48	THR
1	A	203	VAL
1	B	203	VAL
1	C	203	VAL
1	D	203	VAL
1	E	203	VAL
1	E	225	GLY
1	F	203	VAL
1	G	203	VAL
1	B	225	GLY

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Mol	Chain	Res	Type
1	F	225	GLY
1	C	225	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	174/205 (85%)	169 (97%)	5 (3%)	37	65
1	B	174/205 (85%)	170 (98%)	4 (2%)	44	71
1	C	174/205 (85%)	170 (98%)	4 (2%)	44	71
1	D	174/205 (85%)	169 (97%)	5 (3%)	37	65
1	E	174/205 (85%)	169 (97%)	5 (3%)	37	65
1	F	174/205 (85%)	169 (97%)	5 (3%)	37	65
1	G	174/205 (85%)	170 (98%)	4 (2%)	44	71
2	H	169/177 (96%)	159 (94%)	10 (6%)	18	38
2	I	169/177 (96%)	160 (95%)	9 (5%)	20	43
2	J	169/177 (96%)	159 (94%)	10 (6%)	18	38
2	K	169/177 (96%)	160 (95%)	9 (5%)	20	43
2	L	169/177 (96%)	159 (94%)	10 (6%)	18	38
2	M	169/177 (96%)	159 (94%)	10 (6%)	18	38
2	N	169/177 (96%)	158 (94%)	11 (6%)	15	35
All	All	2401/2674 (90%)	2300 (96%)	101 (4%)	26	52

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ARG
1	A	150	GLU
1	A	206	LEU
1	A	211	LEU
1	A	228	LEU

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Mol	Chain	Res	Type
1	B	85	ARG
1	B	150	GLU
1	B	206	LEU
1	B	228	LEU
1	C	85	ARG
1	C	150	GLU
1	C	206	LEU
1	C	228	LEU
1	D	85	ARG
1	D	150	GLU
1	D	206	LEU
1	D	211	LEU
1	D	228	LEU
1	E	85	ARG
1	E	150	GLU
1	E	206	LEU
1	E	211	LEU
1	E	228	LEU
1	F	85	ARG
1	F	150	GLU
1	F	206	LEU
1	F	211	LEU
1	F	228	LEU
1	G	85	ARG
1	G	150	GLU
1	G	206	LEU
1	G	228	LEU
2	H	7	THR
2	H	12	VAL
2	H	39	GLU
2	H	45	ILE
2	H	83	LEU
2	H	91	LEU
2	H	103	LEU
2	H	124	ASP
2	H	144	LEU
2	H	150	LEU
2	I	7	THR
2	I	12	VAL
2	I	45	ILE
2	I	83	LEU
2	I	91	LEU

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Mol	Chain	Res	Type
2	I	103	LEU
2	I	124	ASP
2	I	144	LEU
2	I	150	LEU
2	J	7	THR
2	J	12	VAL
2	J	45	ILE
2	J	83	LEU
2	J	91	LEU
2	J	103	LEU
2	J	124	ASP
2	J	144	LEU
2	J	150	LEU
2	J	191	TYR
2	K	7	THR
2	K	12	VAL
2	K	45	ILE
2	K	83	LEU
2	K	91	LEU
2	K	103	LEU
2	K	124	ASP
2	K	144	LEU
2	K	150	LEU
2	L	7	THR
2	L	12	VAL
2	L	45	ILE
2	L	83	LEU
2	L	91	LEU
2	L	103	LEU
2	L	124	ASP
2	L	144	LEU
2	L	150	LEU
2	L	191	TYR
2	M	7	THR
2	M	12	VAL
2	M	39	GLU
2	M	45	ILE
2	M	83	LEU
2	M	91	LEU
2	M	103	LEU
2	M	124	ASP
2	M	144	LEU

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Mol	Chain	Res	Type
2	M	150	LEU
2	N	7	THR
2	N	12	VAL
2	N	39	GLU
2	N	45	ILE
2	N	83	LEU
2	N	91	LEU
2	N	103	LEU
2	N	124	ASP
2	N	144	LEU
2	N	150	LEU
2	N	191	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	105	GLN
1	B	11	GLN
1	B	105	GLN
1	C	11	GLN
1	C	105	GLN
1	D	11	GLN
1	D	105	GLN
1	E	11	GLN
1	E	105	GLN
1	F	11	GLN
1	F	105	GLN
1	G	11	GLN
1	G	105	GLN
2	H	65	HIS
2	H	137	HIS
2	H	204	HIS
2	H	224	GLN
2	I	65	HIS
2	I	137	HIS
2	I	199	GLN
2	I	204	HIS
2	I	224	GLN
2	J	65	HIS
2	J	224	GLN
2	K	65	HIS

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Mol	Chain	Res	Type
2	K	137	HIS
2	K	204	HIS
2	K	224	GLN
2	L	65	HIS
2	L	204	HIS
2	L	224	GLN
2	M	65	HIS
2	M	224	GLN
2	N	65	HIS
2	N	90	ASN
2	N	199	GLN
2	N	204	HIS
2	N	224	GLN

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.