



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:08 AM UTC

PDB ID : 5X8L / pdb_00005x8l
Title : PD-L1 in complex with atezolizumab
Authors : Heo, Y.S.; Lee, H.T.
Deposited on : 2017-03-03
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

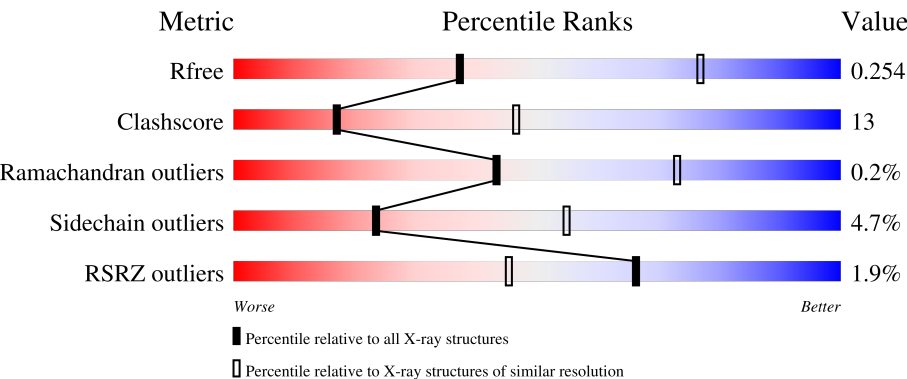
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 <=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	123	62%25%5%8%
1	B	123	71%22%6%
1	C	123	70%23%6%
1	D	123	68%24%6%
1	E	123	76%17%7%

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Mol	Chain	Length	Quality of chain
2	K	214	82%17%
2	L	214	4% 59%29%5% 6%
2	M	214	2% 71%25%
2	N	214	5% 63%23%7% 5%
2	O	214	5% 56%38%5%
3	F	230	76%16%8%
3	G	230	3% 72%19%8%
3	H	230	2% 68%20% 8%
3	J	230	2% 66%24%10%
3	S	230	% 67%23% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20566 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 Programmed cell death 1 ligand 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	113	Total	C	N	O	S	0	0	0
			903	577	151	170	5			
1	B	116	Total	C	N	O	S	0	0	0
			928	593	155	175	5			
1	C	116	Total	C	N	O	S	0	0	0
			928	593	155	175	5			
1	D	116	Total	C	N	O	S	0	0	0
			928	593	155	175	5			
1	E	114	Total	C	N	O	S	0	0	0
			910	582	152	171	5			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	GLU	GLN	engineered mutation	UNP Q9NZQ7
A	135	HIS	-	expression tag	UNP Q9NZQ7
A	136	HIS	-	expression tag	UNP Q9NZQ7
A	137	HIS	-	expression tag	UNP Q9NZQ7
A	138	HIS	-	expression tag	UNP Q9NZQ7
A	139	HIS	-	expression tag	UNP Q9NZQ7
A	140	HIS	-	expression tag	UNP Q9NZQ7
B	47	GLU	GLN	engineered mutation	UNP Q9NZQ7
B	135	HIS	-	expression tag	UNP Q9NZQ7
B	136	HIS	-	expression tag	UNP Q9NZQ7
B	137	HIS	-	expression tag	UNP Q9NZQ7
B	138	HIS	-	expression tag	UNP Q9NZQ7
B	139	HIS	-	expression tag	UNP Q9NZQ7
B	140	HIS	-	expression tag	UNP Q9NZQ7
C	47	GLU	GLN	engineered mutation	UNP Q9NZQ7
C	135	HIS	-	expression tag	UNP Q9NZQ7
C	136	HIS	-	expression tag	UNP Q9NZQ7
C	137	HIS	-	expression tag	UNP Q9NZQ7
C	138	HIS	-	expression tag	UNP Q9NZQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	139	HIS	-	expression tag	UNP Q9NZQ7
C	140	HIS	-	expression tag	UNP Q9NZQ7
D	47	GLU	GLN	engineered mutation	UNP Q9NZQ7
D	135	HIS	-	expression tag	UNP Q9NZQ7
D	136	HIS	-	expression tag	UNP Q9NZQ7
D	137	HIS	-	expression tag	UNP Q9NZQ7
D	138	HIS	-	expression tag	UNP Q9NZQ7
D	139	HIS	-	expression tag	UNP Q9NZQ7
D	140	HIS	-	expression tag	UNP Q9NZQ7
E	47	GLU	GLN	engineered mutation	UNP Q9NZQ7
E	135	HIS	-	expression tag	UNP Q9NZQ7
E	136	HIS	-	expression tag	UNP Q9NZQ7
E	137	HIS	-	expression tag	UNP Q9NZQ7
E	138	HIS	-	expression tag	UNP Q9NZQ7
E	139	HIS	-	expression tag	UNP Q9NZQ7
E	140	HIS	-	expression tag	UNP Q9NZQ7

- Molecule 2 is a protein called atezolizumab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	213	Total	C	N	O	S	0	0	0
			1638	1029	272	332	5			
2	L	202	Total	C	N	O	S	0	0	0
			1561	984	258	314	5			
2	M	213	Total	C	N	O	S	0	0	0
			1638	1029	272	332	5			
2	N	204	Total	C	N	O	S	0	0	0
			1574	991	260	318	5			
2	O	213	Total	C	N	O	S	0	0	0
			1638	1029	272	332	5			

- Molecule 3 is a protein called atezolizumab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	212	Total	C	N	O	S	0	0	0
			1594	1015	267	307	5			
3	G	211	Total	C	N	O	S	0	0	0
			1588	1012	266	305	5			
3	H	212	Total	C	N	O	S	0	0	0
			1592	1014	267	306	5			
3	S	211	Total	C	N	O	S	0	0	0
			1585	1007	266	307	5			

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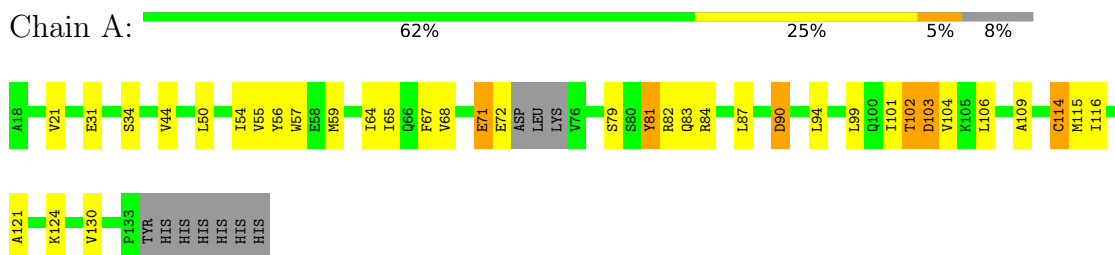
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	208	Total	C	N	O	S	0	0	0
			1561	992	262	302	5			

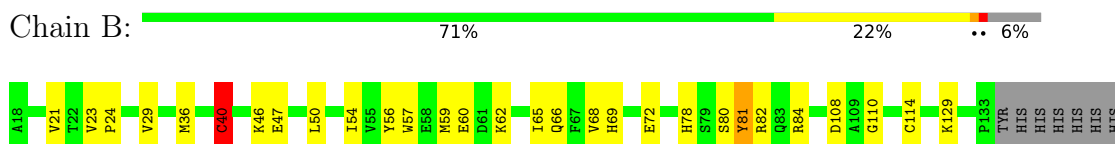
3 Residue-property plots

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 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.

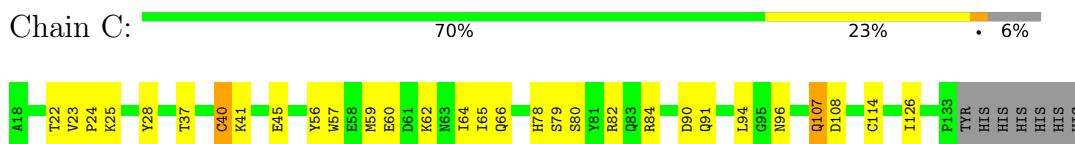
- Molecule 1: Programmed cell death 1 ligand 1



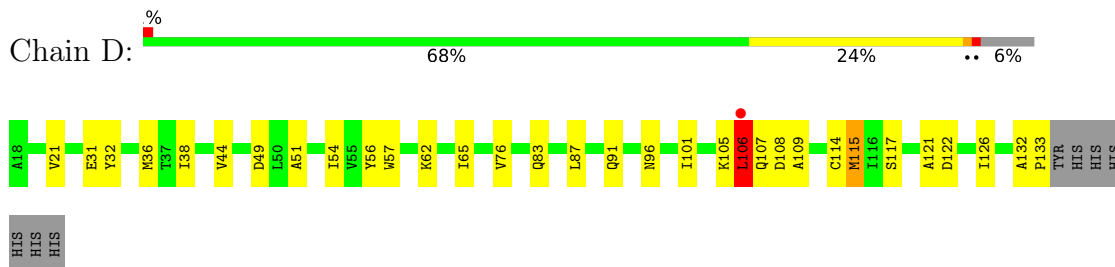
- Molecule 1: Programmed cell death 1 ligand 1



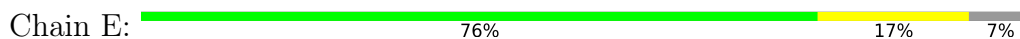
- Molecule 1: Programmed cell death 1 ligand 1



- Molecule 1: Programmed cell death 1 ligand 1



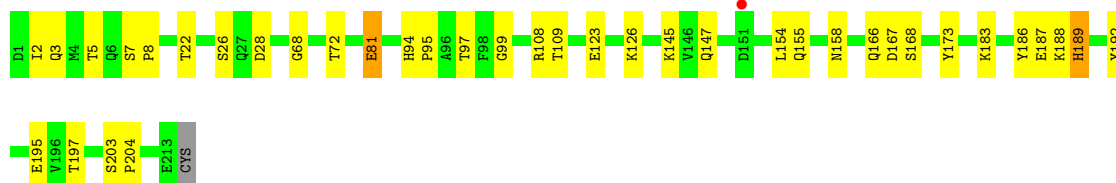
- Molecule 1: Programmed cell death 1 ligand 1





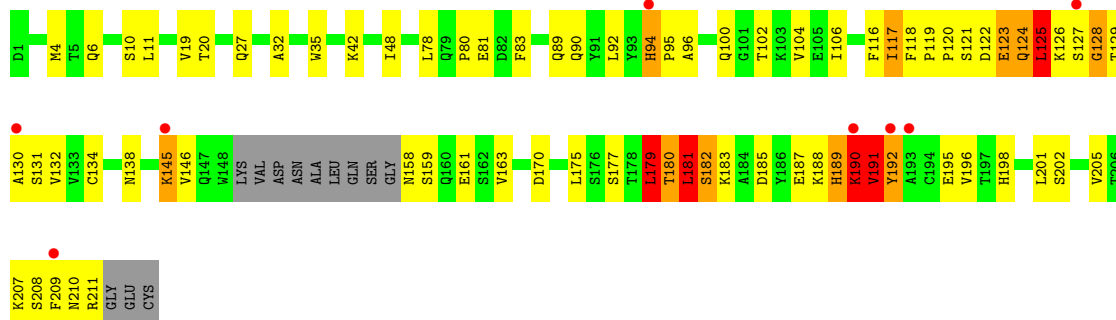
- Molecule 2: atezolizumab light chain

Chain K: 82% 17%



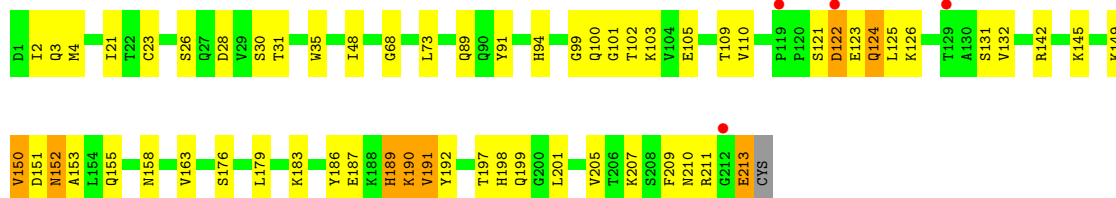
- Molecule 2: atezolizumab light chain

Chain L: 4% 59% 29% 5% 6%



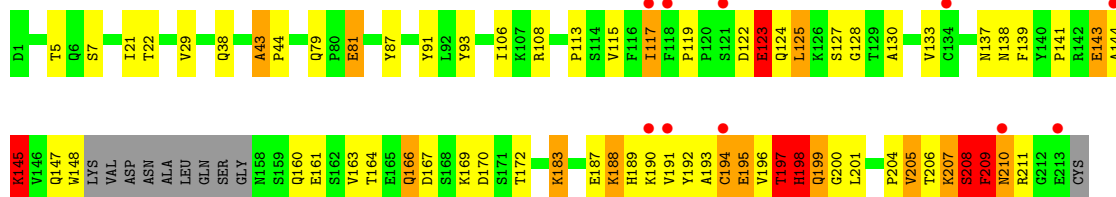
- Molecule 2: atezolizumab light chain

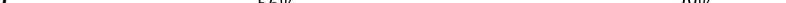
Chain M: 2% 71% 25%



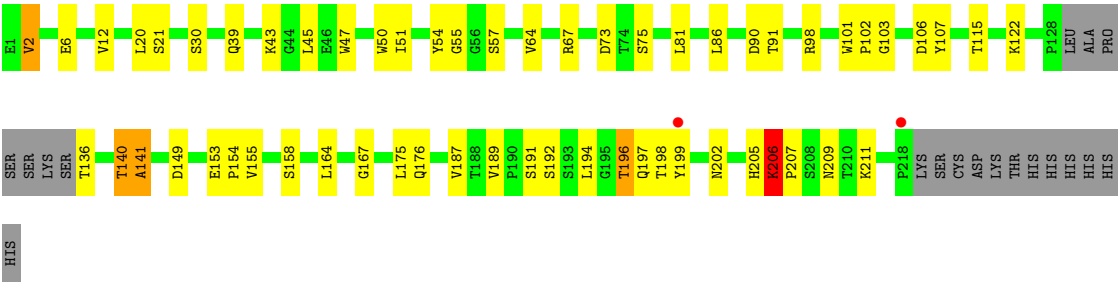
- Molecule 2: atezolizumab light chain

Chain N: 5% 63% 23% 7% 5%

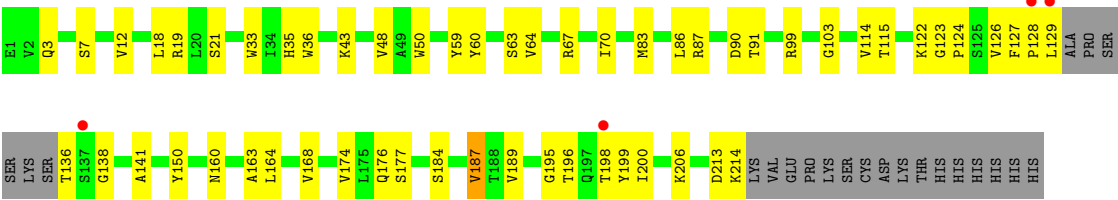


- Chain O:  5% 56% 38% 5%





• Molecule 3: atezolizumab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.20Å 169.79Å 206.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 3.10 29.92 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.92-3.10) 96.8 (29.92-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.11Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.208 , 0.256 0.211 , 0.254	Depositor DCC
R_{free} test set	2896 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 20.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	20566	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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 [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	0.48	0/918	0.90	1/1240 (0.1%)
1	B	0.46	0/944	0.89	1/1276 (0.1%)
1	C	0.52	0/944	0.78	0/1276
1	D	0.63	1/944 (0.1%)	0.96	5/1276 (0.4%)
1	E	0.45	0/925	0.81	0/1250
2	K	0.48	0/1675	0.86	4/2276 (0.2%)
2	L	0.53	0/1597	1.03	14/2170 (0.6%)
2	M	0.50	0/1675	0.90	4/2276 (0.2%)
2	N	0.63	0/1610	1.14	16/2187 (0.7%)
2	O	0.52	0/1675	1.04	5/2276 (0.2%)
3	F	0.48	0/1640	0.80	0/2241
3	G	0.47	0/1634	0.84	3/2233 (0.1%)
3	H	0.51	0/1638	0.90	3/2238 (0.1%)
3	J	0.45	0/1605	0.85	2/2192 (0.1%)
3	S	0.43	0/1630	0.89	3/2226 (0.1%)
All	All	0.50	1/21054 (0.0%)	0.92	61/28633 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
2	K	0	1
2	L	0	4
2	M	0	2
2	N	0	6
2	O	0	5
3	G	0	1
3	H	0	5
3	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	S	0	2
All	All	0	29

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	106	LEU	CA-C	7.54	1.62	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	208	SER	N-CA-C	11.58	123.53	108.24
1	D	106	LEU	N-CA-C	-11.44	98.89	111.36
1	A	81	TYR	N-CA-C	8.64	124.06	113.17
3	G	43	LYS	CD-CE-NZ	-8.58	84.46	111.90
2	L	123	GLU	N-CA-C	-8.48	102.03	111.28
2	M	150	VAL	N-CA-C	-8.44	100.85	110.05
2	O	154	LEU	N-CA-C	7.93	120.19	110.91
3	S	206	LYS	CA-C-N	7.83	127.49	119.19
3	S	206	LYS	C-N-CA	7.83	127.49	119.19
2	O	127	SER	N-CA-C	7.79	127.39	110.80
2	M	152	ASN	N-CA-C	-7.26	103.72	112.58
3	H	191	SER	N-CA-C	7.18	122.07	113.16
2	K	99	GLY	N-CA-C	-7.17	101.78	111.54
2	N	197	THR	N-CA-C	-7.13	98.89	109.81
2	N	197	THR	CA-C-O	-6.98	113.45	121.68
2	L	119	PRO	CA-C-N	-6.93	113.55	120.21
2	L	119	PRO	C-N-CA	-6.93	113.55	120.21
1	B	40	CYS	N-CA-C	6.82	122.44	113.30
2	N	145	LYS	N-CA-C	6.81	119.57	108.26
2	N	199	GLN	N-CA-C	6.68	119.42	111.33
2	L	124	GLN	N-CA-C	6.66	119.53	111.40
2	L	125	LEU	CA-CB-CG	6.65	139.57	116.30
2	N	210	ASN	CA-C-N	6.62	130.55	120.82
2	N	210	ASN	C-N-CA	6.62	130.55	120.82
2	N	194	CYS	N-CA-C	6.58	119.42	108.96
3	S	141	ALA	N-CA-C	6.57	120.25	109.94
2	M	189	HIS	N-CA-C	6.45	118.92	108.34
2	O	130	ALA	N-CA-C	6.39	117.00	108.38
2	L	190	LYS	CA-C-N	6.32	133.34	121.97
2	L	190	LYS	C-N-CA	6.32	133.34	121.97
2	N	211	ARG	N-CA-C	6.28	118.40	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	40	ALA	CA-C-N	-6.22	112.07	119.84
3	G	40	ALA	C-N-CA	-6.22	112.07	119.84
2	K	189	HIS	N-CA-C	6.16	118.99	108.02
2	O	153	ALA	N-CA-C	5.90	118.83	108.75
2	L	191	VAL	N-CA-C	-5.82	97.23	109.34
2	N	43	ALA	CA-C-N	5.82	125.84	119.90
2	N	43	ALA	C-N-CA	5.82	125.84	119.90
2	L	189	HIS	N-CA-C	5.73	118.94	109.94
3	H	210	THR	N-CA-C	5.71	118.18	108.02
1	D	108	ASP	N-CA-C	5.65	119.79	113.01
2	O	184	ALA	N-CA-C	-5.61	105.26	111.71
2	N	144	ALA	N-CA-C	5.60	117.53	108.41
1	D	105	LYS	N-CA-C	-5.56	102.25	110.48
1	D	106	LEU	CA-C-O	-5.46	114.63	120.42
2	N	117	ILE	N-CA-C	5.41	116.46	108.45
1	D	107	GLN	CB-CG-CD	-5.31	103.57	112.60
3	J	195	GLY	N-CA-C	-5.27	108.81	115.08
2	L	182	SER	N-CA-C	5.24	121.96	110.80
2	L	122	ASP	N-CA-C	-5.21	106.76	113.02
2	L	128	GLY	N-CA-C	5.18	122.98	115.32
2	N	195	GLU	N-CA-C	5.13	117.19	109.23
3	H	197	GLN	N-CA-C	5.10	121.67	110.80
2	L	94	HIS	CB-CA-C	-5.09	101.48	109.52
2	N	198	HIS	CA-C-N	5.07	127.32	120.38
2	N	198	HIS	C-N-CA	5.07	127.32	120.38
3	J	176	GLN	N-CA-C	5.06	117.33	110.35
2	M	101	GLY	N-CA-C	-5.06	106.36	112.48
2	K	99	GLY	CA-C-N	-5.05	115.67	123.14
2	K	99	GLY	C-N-CA	-5.05	115.67	123.14
2	L	192	TYR	N-CA-C	5.04	117.83	109.46

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	THR	Peptide
1	D	132	ALA	Peptide
3	G	41	PRO	Peptide
3	H	190	PRO	Peptide
3	H	194	LEU	Peptide
3	H	196	THR	Peptide
3	H	208	SER	Peptide

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Mol	Chain	Res	Type	Group
3	H	209	ASN	Peptide
3	J	198	THR	Peptide
2	K	189	HIS	Peptide
2	L	179	LEU	Peptide
2	L	181	LEU	Peptide
2	L	190	LYS	Peptide
2	L	191	VAL	Peptide
2	M	122	ASP	Peptide
2	M	189	HIS	Peptide
2	N	122	ASP	Peptide
2	N	143	GLU	Peptide
2	N	207	LYS	Peptide
2	N	208	SER	Peptide
2	N	209	PHE	Peptide
2	N	210	ASN	Peptide
2	O	129	THR	Peptide
2	O	183	LYS	Peptide
2	O	201	LEU	Peptide
2	O	203	SER	Peptide
2	O	211	ARG	Peptide
3	S	196	THR	Peptide
3	S	206	LYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	903	0	903	26	0
1	B	928	0	932	20	0
1	C	928	0	932	28	0
1	D	928	0	932	18	0
1	E	910	0	912	14	0
2	K	1638	0	1588	20	0
2	L	1561	0	1514	60	0
2	M	1638	0	1588	50	0
2	N	1574	0	1523	67	0
2	O	1638	0	1588	75	0
3	F	1594	0	1538	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1588	0	1533	35	0
3	H	1592	0	1536	41	0
3	J	1561	0	1501	37	0
3	S	1585	0	1525	40	0
All	All	20566	0	20045	517	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (517) 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)
3:S:140:THR:HA	3:S:191:SER:HB2	1.46	0.96
2:O:130:ALA:HB3	2:O:183:LYS:HD3	1.54	0.90
3:J:136:THR:HG22	3:J:138:GLY:H	1.39	0.86
1:A:82:ARG:HD2	1:A:83:GLN:H	1.41	0.85
3:G:67:ARG:NH2	3:G:90:ASP:OD2	2.11	0.84
3:H:193:SER:HG	3:H:199:TYR:HH	1.25	0.81
2:N:143:GLU:OE2	2:N:145:LYS:NZ	2.14	0.81
3:H:211:LYS:NZ	3:H:213:ASP:OD1	2.15	0.80
2:N:148:TRP:CZ3	2:N:194:CYS:HB2	2.17	0.79
2:M:190:LYS:HE2	2:M:191:VAL:H	1.48	0.79
2:O:124:GLN:O	2:O:127:SER:HB3	1.83	0.78
2:O:188:LYS:HG2	2:O:189:HIS:ND1	1.98	0.78
1:A:82:ARG:HD2	1:A:83:GLN:N	1.98	0.78
2:L:6:GLN:O	2:L:100:GLN:NE2	2.17	0.77
3:F:47:TRP:HZ2	3:F:50:TRP:HD1	1.32	0.77
2:O:125:LEU:HD21	2:O:183:LYS:HE2	1.65	0.76
2:O:121:SER:OG	3:J:128:PRO:O	2.03	0.76
2:L:27:GLN:HE21	1:C:37:THR:HG21	1.49	0.76
2:N:117:ILE:HD13	2:N:209:PHE:CE1	2.22	0.75
2:N:125:LEU:HD21	2:N:183:LYS:HD2	1.68	0.74
1:A:84:ARG:NH2	1:A:103:ASP:O	2.21	0.74
3:J:67:ARG:NH2	3:J:90:ASP:OD2	2.21	0.74
3:F:47:TRP:CZ2	3:F:50:TRP:HD1	2.06	0.73
2:N:123:GLU:HG3	2:N:124:GLN:H	1.52	0.73
3:S:136:THR:HG21	3:S:141:ALA:HA	1.69	0.73
2:O:108:ARG:NH2	2:O:109:THR:O	2.20	0.72
1:B:84:ARG:NH2	1:B:108:ASP:OD2	2.21	0.72
2:N:115:VAL:O	2:N:207:LYS:NZ	2.21	0.71
2:L:190:LYS:O	2:L:191:VAL:HG23	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:206:LYS:HA	3:S:209:ASN:H	1.55	0.71
2:O:127:SER:HB2	2:O:129:THR:H	1.56	0.71
2:N:115:VAL:HG21	2:N:196:VAL:HG21	1.72	0.70
3:S:155:VAL:HG12	3:S:205:HIS:HB2	1.73	0.70
2:K:147:GLN:HB3	2:K:154:LEU:HD11	1.73	0.70
3:H:67:ARG:NH2	3:H:90:ASP:OD2	2.25	0.70
2:N:123:GLU:HG3	2:N:124:GLN:N	2.05	0.70
2:K:22:THR:HG22	2:K:72:THR:HG22	1.73	0.70
3:H:197:GLN:NE2	3:H:217:GLU:OE1	2.25	0.70
2:O:125:LEU:CD2	2:O:183:LYS:HE2	2.22	0.69
1:A:21:VAL:O	1:A:124:LYS:NZ	2.26	0.69
2:N:137:ASN:OD1	2:N:138:ASN:ND2	2.24	0.69
2:N:190:LYS:HG3	2:N:191:VAL:N	2.07	0.69
2:L:190:LYS:HG3	2:L:191:VAL:H	1.56	0.69
2:N:198:HIS:ND1	2:N:201:LEU:HG	2.07	0.69
1:C:80:SER:HB2	1:C:107:GLN:HE22	1.57	0.68
1:E:84:ARG:NH2	1:E:108:ASP:OD2	2.25	0.68
1:A:55:VAL:HG22	1:A:116:ILE:HG13	1.76	0.68
3:J:122:LYS:NZ	3:J:123:GLY:O	2.26	0.68
3:F:126:VAL:O	3:F:214:LYS:NZ	2.27	0.67
3:S:158:SER:HB2	3:S:202:ASN:HB2	1.75	0.67
1:A:109:ALA:HB2	1:A:130:VAL:HG22	1.76	0.66
1:D:115:MET:HE1	1:D:121:ALA:HB1	1.75	0.66
3:S:73:ASP:OD1	3:S:75:SER:OG	2.12	0.66
3:J:160:ASN:HB3	3:J:163:ALA:HB3	1.78	0.66
3:F:33:TRP:CE3	3:F:99:ARG:HG2	2.30	0.66
2:N:123:GLU:HB3	2:N:125:LEU:HB2	1.77	0.66
3:G:33:TRP:HB3	3:G:99:ARG:HB3	1.78	0.66
3:H:33:TRP:HB3	3:H:99:ARG:HB3	1.77	0.66
2:O:127:SER:CB	2:O:129:THR:H	2.09	0.65
2:O:94:HIS:HD2	2:O:95:PRO:CA	2.10	0.65
3:F:153:GLU:HG2	3:F:154:PRO:HA	1.79	0.65
2:N:197:THR:O	2:N:198:HIS:HB3	1.96	0.65
3:G:11:LEU:HD22	3:G:152:PRO:HG3	1.78	0.65
2:N:117:ILE:HD13	2:N:209:PHE:HE1	1.61	0.65
2:L:89:GLN:HE21	2:L:96:ALA:HB1	1.61	0.65
1:C:79:SER:HA	1:C:82:ARG:HE	1.62	0.65
2:N:117:ILE:HG21	2:N:209:PHE:CE1	2.32	0.65
3:J:141:ALA:N	3:J:189:VAL:O	2.23	0.64
3:S:67:ARG:NH2	3:S:90:ASP:OD2	2.30	0.64
2:O:22:THR:HG22	2:O:72:THR:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:124:GLN:O	2:N:128:GLY:N	2.24	0.64
2:M:187:GLU:O	2:M:211:ARG:NH1	2.30	0.64
2:L:35:TRP:HD1	2:L:48:ILE:HD11	1.61	0.64
3:J:33:TRP:HB3	3:J:99:ARG:HB3	1.79	0.63
2:O:153:ALA:HB1	2:O:154:LEU:HD13	1.79	0.63
2:M:121:SER:O	2:M:124:GLN:HB2	1.97	0.63
3:F:47:TRP:HZ2	3:F:50:TRP:CD1	2.16	0.63
2:O:48:ILE:HG22	2:O:54:LEU:HA	1.79	0.63
2:O:131:SER:HA	2:O:179:LEU:O	1.98	0.63
2:L:192:TYR:O	2:L:208:SER:HB3	1.99	0.63
2:O:108:ARG:HH22	2:O:111:ALA:CB	2.12	0.63
3:J:160:ASN:OD1	3:J:199:TYR:HB3	1.99	0.62
2:L:94:HIS:CD2	2:L:95:PRO:HA	2.35	0.62
3:H:217:GLU:OE1	3:H:218:PRO:HD2	1.99	0.62
3:S:153:GLU:HG2	3:S:154:PRO:HA	1.81	0.62
1:A:54:ILE:HG12	1:A:68:VAL:HG13	1.81	0.62
3:J:164:LEU:HD21	3:J:187:VAL:HG21	1.80	0.62
3:F:83:MET:HE1	3:F:114:VAL:HG11	1.82	0.61
1:D:56:TYR:CZ	1:D:115:MET:HG2	2.35	0.61
2:K:94:HIS:CD2	3:F:59:TYR:HE2	2.19	0.61
3:G:124:PRO:HB3	3:G:150:TYR:HB3	1.82	0.61
3:G:42:GLY:HA2	3:G:43:LYS:HB3	1.82	0.61
1:E:57:TRP:HB2	1:E:65:ILE:HB	1.83	0.61
2:N:188:LYS:HG2	2:N:189:HIS:CD2	2.35	0.61
1:A:79:SER:OG	2:O:157:GLY:O	2.18	0.61
3:S:12:VAL:HG21	3:S:86:LEU:HD13	1.83	0.60
2:O:187:GLU:HA	2:O:190:LYS:HG3	1.83	0.60
2:O:137:ASN:OD1	2:O:138:ASN:ND2	2.34	0.60
1:A:71:GLU:HG3	1:A:72:GLU:H	1.65	0.60
2:N:145:LYS:HD3	2:N:197:THR:OG1	2.02	0.60
3:G:197:GLN:OE1	3:G:198:THR:N	2.35	0.60
3:H:157:VAL:HG22	3:H:203:VAL:HG13	1.82	0.60
2:N:148:TRP:CE3	2:N:194:CYS:HB2	2.35	0.60
2:L:158:ASN:N	2:L:158:ASN:OD1	2.35	0.60
2:L:198:HIS:H	2:L:201:LEU:HD12	1.67	0.60
1:C:80:SER:CB	1:C:107:GLN:HE22	2.15	0.60
1:B:47:GLU:OE1	1:C:22:THR:OG1	2.18	0.59
2:L:4:MET:HE3	2:L:90:GLN:HB3	1.84	0.59
2:N:170:ASP:OD2	2:N:172:THR:OG1	2.21	0.59
1:C:84:ARG:NH2	1:C:108:ASP:OD2	2.36	0.59
3:G:40:ALA:HB3	3:G:42:GLY:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:163:VAL:HG22	2:O:175:LEU:HD13	1.85	0.59
1:A:56:TYR:CZ	1:A:115:MET:HG2	2.38	0.59
1:A:59:MET:HG3	1:A:64:ILE:HD11	1.83	0.58
2:M:125:LEU:HD13	2:M:183:LYS:HD2	1.85	0.58
3:S:205:HIS:CD2	3:S:207:PRO:HD2	2.38	0.58
2:L:145:LYS:HE3	2:L:161:GLU:OE1	2.03	0.58
2:M:186:TYR:O	2:M:192:TYR:OH	2.21	0.58
3:H:204:ASN:HB2	3:H:211:LYS:HD3	1.86	0.58
2:L:190:LYS:HG3	2:L:191:VAL:N	2.18	0.58
2:M:150:VAL:HG22	2:M:192:TYR:CD1	2.37	0.58
2:L:131:SER:HA	2:L:180:THR:OG1	2.03	0.58
2:O:202:SER:OG	2:O:203:SER:N	2.37	0.58
1:A:65:ILE:HD13	1:A:87:LEU:HB2	1.84	0.57
2:M:190:LYS:HE2	2:M:191:VAL:N	2.19	0.57
2:N:113:PRO:HD2	2:N:198:HIS:CE1	2.39	0.57
2:N:183:LYS:HE2	2:N:187:GLU:HG3	1.86	0.57
3:F:33:TRP:HB3	3:F:99:ARG:HB3	1.86	0.57
1:B:57:TRP:HB2	1:B:65:ILE:HB	1.84	0.57
2:O:160:GLN:NE2	2:O:178:THR:O	2.37	0.57
3:J:83:MET:HE1	3:J:114:VAL:HG21	1.86	0.57
2:L:125:LEU:HD13	2:L:183:LYS:HG3	1.85	0.57
2:O:125:LEU:HD21	2:O:183:LYS:CE	2.35	0.57
2:L:124:GLN:HG2	2:L:129:THR:O	2.05	0.56
2:M:155:GLN:HB3	2:M:158:ASN:HD21	1.70	0.56
2:O:167:ASP:OD1	2:O:168:SER:N	2.37	0.56
1:D:91:GLN:HG3	1:D:96:ASN:HB3	1.87	0.56
2:N:145:LYS:HD2	2:N:197:THR:C	2.30	0.56
2:L:6:GLN:NE2	2:L:102:THR:HG22	2.21	0.56
2:L:161:GLU:HG2	2:L:177:SER:HA	1.87	0.56
2:M:94:HIS:CE1	3:H:59:TYR:HE2	2.23	0.56
2:O:130:ALA:CB	2:O:183:LYS:HD3	2.33	0.56
2:M:150:VAL:O	2:M:153:ALA:N	2.35	0.56
2:O:187:GLU:HA	2:O:190:LYS:CG	2.36	0.56
2:N:117:ILE:HG13	2:N:133:VAL:O	2.05	0.55
2:N:201:LEU:HD22	2:N:205:VAL:HG13	1.87	0.55
2:O:169:LYS:HG3	2:O:170:ASP:H	1.71	0.55
2:L:120:PRO:HG3	2:L:130:ALA:HB1	1.88	0.55
2:M:151:ASP:HA	2:M:190:LYS:HD3	1.88	0.55
2:O:115:VAL:HG21	2:O:196:VAL:HG21	1.87	0.55
1:D:65:ILE:HG21	1:D:87:LEU:HB2	1.87	0.55
2:N:167:ASP:OD2	2:N:170:ASP:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:VAL:HG23	1:E:122:ASP:HB3	1.89	0.55
3:H:194:LEU:HA	3:H:197:GLN:CG	2.37	0.55
2:O:108:ARG:HH22	2:O:111:ALA:HB2	1.71	0.55
2:L:121:SER:O	2:L:124:GLN:HB3	2.07	0.54
3:G:173:ALA:HA	3:G:183:LEU:HB3	1.89	0.54
2:L:123:GLU:OE1	3:G:214:LYS:HE3	2.07	0.54
1:A:59:MET:SD	1:A:81:TYR:OH	2.62	0.54
1:E:79:SER:HA	1:E:82:ARG:HG3	1.90	0.54
2:O:132:VAL:O	2:O:179:LEU:N	2.37	0.54
1:B:81:TYR:O	1:B:82:ARG:HG3	2.07	0.54
3:H:208:SER:O	3:H:210:THR:N	2.41	0.54
1:D:54:ILE:HB	1:D:117:SER:HB3	1.90	0.54
2:O:94:HIS:CE1	3:J:59:TYR:CE2	2.96	0.54
1:B:59:MET:HE3	1:B:110:GLY:HA3	1.90	0.54
3:G:173:ALA:HB2	3:G:183:LEU:HD23	1.90	0.54
2:M:121:SER:HB3	2:M:123:GLU:HB2	1.90	0.54
2:M:125:LEU:HD22	2:M:183:LYS:HD2	1.89	0.54
2:M:183:LYS:HA	2:M:186:TYR:HB3	1.90	0.54
2:O:121:SER:O	2:O:125:LEU:HG	2.08	0.54
3:J:136:THR:HG22	3:J:138:GLY:N	2.16	0.54
2:L:161:GLU:OE1	2:L:175:LEU:HD21	2.08	0.54
2:O:80:PRO:O	2:O:83:PHE:HD2	1.91	0.54
3:J:168:VAL:HG22	3:J:187:VAL:HB	1.89	0.53
2:L:125:LEU:C	2:L:128:GLY:H	2.16	0.53
3:H:140:THR:HA	3:H:190:PRO:HA	1.90	0.53
2:M:21:ILE:HG21	2:M:102:THR:HG21	1.90	0.53
3:G:43:LYS:HD3	1:D:106:LEU:C	2.34	0.53
2:L:120:PRO:HD3	2:L:132:VAL:HG12	1.90	0.53
2:K:145:LYS:HB3	2:K:197:THR:HB	1.89	0.53
2:K:167:ASP:OD1	2:K:168:SER:N	2.42	0.53
3:G:98:ARG:NH2	3:G:106:ASP:OD2	2.27	0.53
1:C:23:VAL:HG11	1:C:126:ILE:HD11	1.90	0.53
1:C:91:GLN:HB3	1:C:96:ASN:HB3	1.91	0.53
1:D:21:VAL:HG23	1:D:122:ASP:HB3	1.91	0.53
2:K:28:ASP:OD1	2:K:68:GLY:HA2	2.09	0.52
2:M:142:ARG:HD3	2:M:163:VAL:HG11	1.91	0.52
3:J:18:LEU:HD12	3:J:19:ARG:H	1.74	0.52
2:N:160:GLN:HE22	3:S:176:GLN:HA	1.74	0.52
2:M:142:ARG:HE	2:M:163:VAL:HG21	1.75	0.52
2:N:163:VAL:HG12	2:N:164:THR:O	2.10	0.52
1:A:82:ARG:O	1:A:83:GLN:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:124:GLN:HG3	3:G:127:PHE:CE2	2.45	0.52
2:N:145:LYS:HD2	2:N:197:THR:O	2.10	0.52
1:A:115:MET:HE1	1:A:121:ALA:HB1	1.90	0.51
3:H:155:VAL:HG12	3:H:205:HIS:HB2	1.91	0.51
2:L:10:SER:HB2	1:D:133:PRO:HB2	1.92	0.51
1:C:56:TYR:OH	1:C:66:GLN:NE2	2.42	0.51
2:K:166:GLN:HG3	2:K:173:TYR:CZ	2.46	0.51
3:S:194:LEU:HD23	3:S:197:GLN:NE2	2.25	0.51
2:O:94:HIS:HD2	2:O:95:PRO:HA	1.75	0.51
1:C:23:VAL:HG12	1:C:40:CYS:HA	1.92	0.51
3:J:91:THR:HG23	3:J:115:THR:HA	1.91	0.51
1:A:106:LEU:HA	1:A:130:VAL:HG21	1.92	0.51
2:N:148:TRP:HA	2:N:193:ALA:O	2.11	0.51
3:J:33:TRP:HE3	3:J:99:ARG:HG2	1.75	0.51
3:S:30:SER:O	3:S:54:TYR:HB2	2.11	0.51
3:S:206:LYS:HA	3:S:209:ASN:N	2.22	0.51
2:L:201:LEU:HD21	2:L:205:VAL:HG23	1.93	0.51
1:D:49:ASP:OD2	2:N:93:TYR:OH	2.20	0.51
2:L:19:VAL:HG21	2:L:78:LEU:HD22	1.93	0.51
2:M:210:ASN:O	2:M:213:GLU:HG3	2.11	0.51
2:O:123:GLU:OE1	3:J:214:LYS:HD3	2.11	0.51
2:N:169:LYS:HD3	2:N:169:LYS:N	2.26	0.50
1:A:57:TRP:CH2	1:A:114:CYS:HB2	2.46	0.50
2:O:124:GLN:HG3	3:J:127:PHE:CE2	2.46	0.50
2:N:124:GLN:O	2:N:127:SER:HB2	2.11	0.50
2:N:167:ASP:HB3	2:N:170:ASP:HB3	1.94	0.50
3:S:20:LEU:HD12	3:S:81:LEU:HD23	1.92	0.50
2:L:145:LYS:HE3	2:L:161:GLU:CD	2.37	0.50
1:C:62:LYS:NZ	1:C:107:GLN:HE21	2.09	0.50
2:L:179:LEU:HD23	2:L:180:THR:HA	1.94	0.50
3:H:127:PHE:HE2	3:H:148:LYS:HD3	1.76	0.50
3:J:67:ARG:NH2	3:J:87:ARG:HG3	2.27	0.50
2:K:147:GLN:HB2	2:K:195:GLU:HB3	1.93	0.50
3:S:164:LEU:HD21	3:S:187:VAL:HG21	1.92	0.50
3:F:170:THR:HG23	3:F:185:SER:HB2	1.93	0.50
3:J:200:ILE:HD13	3:J:213:ASP:HB3	1.94	0.50
2:L:159:SER:HB3	2:L:179:LEU:HD12	1.93	0.50
3:H:106:ASP:OD1	3:H:106:ASP:N	2.43	0.49
2:O:187:GLU:C	2:O:189:HIS:H	2.19	0.49
2:L:130:ALA:O	2:L:180:THR:HG21	2.12	0.49
3:G:42:GLY:HA2	3:G:43:LYS:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:198:HIS:N	2:L:201:LEU:HD12	2.27	0.49
2:M:145:LYS:HB2	2:M:197:THR:HB	1.95	0.49
3:H:98:ARG:NH2	3:H:106:ASP:OD2	2.45	0.49
2:O:35:TRP:CD1	2:O:48:ILE:HD11	2.47	0.49
1:D:62:LYS:N	3:S:55:GLY:HA2	2.28	0.49
2:M:3:GLN:OE1	3:J:19:ARG:NH2	2.46	0.49
3:F:173:ALA:HA	3:F:183:LEU:HB3	1.93	0.49
1:B:54:ILE:HG23	1:B:68:VAL:HG22	1.95	0.49
3:J:67:ARG:HH21	3:J:87:ARG:HG3	1.77	0.49
2:L:27:GLN:HE22	1:C:91:GLN:NE2	2.11	0.49
2:M:191:VAL:HG23	2:M:210:ASN:HD22	1.77	0.49
2:K:158:ASN:OD1	2:K:158:ASN:N	2.38	0.48
2:L:4:MET:HE3	2:L:90:GLN:HG2	1.95	0.48
2:N:79:GLN:HB3	2:N:81:GLU:HG3	1.95	0.48
2:O:125:LEU:HA	2:O:125:LEU:HD23	1.36	0.48
2:K:155:GLN:OE1	2:K:158:ASN:ND2	2.42	0.48
2:O:127:SER:HB2	2:O:129:THR:N	2.24	0.48
3:F:60:TYR:CE1	3:F:70:ILE:HG22	2.49	0.48
2:N:190:LYS:NZ	2:N:191:VAL:O	2.47	0.48
3:S:98:ARG:NH2	3:S:106:ASP:OD2	2.34	0.48
2:O:35:TRP:HB2	2:O:48:ILE:HG12	1.95	0.48
2:L:117:ILE:HG23	2:L:209:PHE:CE2	2.48	0.48
2:N:139:PHE:O	2:N:172:THR:HB	2.14	0.48
3:H:195:GLY:O	3:H:197:GLN:HB2	2.14	0.48
3:J:126:VAL:O	3:J:214:LYS:HD2	2.14	0.48
2:L:116:PHE:CD2	3:G:142:ALA:HB3	2.49	0.47
2:L:182:SER:HB3	2:L:185:ASP:H	1.78	0.47
1:E:67:PHE:CE2	1:E:71:GLU:HA	2.48	0.47
3:F:124:PRO:HB3	3:F:150:TYR:HB3	1.97	0.47
2:K:2:ILE:HG23	2:K:26:SER:HB3	1.96	0.47
2:M:125:LEU:HA	2:M:125:LEU:HD23	1.53	0.47
2:N:195:GLU:OE1	2:N:206:THR:HA	2.14	0.47
3:S:211:LYS:HE2	3:S:211:LYS:HB2	1.64	0.47
1:E:84:ARG:HH22	1:E:108:ASP:CG	2.21	0.47
3:F:156:THR:HG22	3:F:204:ASN:HB2	1.96	0.47
3:H:145:CYS:HB2	3:H:159:TRP:CZ2	2.49	0.47
3:G:43:LYS:HZ2	1:D:109:ALA:HB3	1.80	0.47
3:H:194:LEU:HA	3:H:197:GLN:HG3	1.97	0.47
2:N:38:GLN:HE21	2:N:87:TYR:HE2	1.62	0.47
3:S:198:THR:O	3:S:199:TYR:HD1	1.97	0.47
1:E:107:GLN:HG3	1:E:108:ASP:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:145:LYS:O	2:O:145:LYS:HG3	2.13	0.47
3:H:205:HIS:CD2	3:H:207:PRO:HD2	2.50	0.47
2:N:108:ARG:HE	2:N:172:THR:CG2	2.28	0.47
2:O:49:TYR:O	2:O:53:PHE:HB2	2.15	0.47
2:M:89:GLN:HE21	2:M:91:TYR:HB3	1.80	0.46
2:N:117:ILE:HG21	2:N:209:PHE:HE1	1.76	0.46
2:O:124:GLN:O	2:O:124:GLN:HG2	2.14	0.46
3:H:83:MET:HE1	3:H:114:VAL:HG21	1.98	0.46
2:O:140:TYR:CD2	2:O:141:PRO:HA	2.50	0.46
1:A:56:TYR:CE1	1:A:115:MET:HG2	2.50	0.46
2:L:32:ALA:HB3	2:L:92:LEU:HB2	1.98	0.46
2:N:201:LEU:HD22	2:N:205:VAL:CG1	2.45	0.46
3:J:12:VAL:HG11	3:J:86:LEU:HD13	1.98	0.46
2:L:6:GLN:HE21	2:L:102:THR:HG22	1.80	0.46
2:M:103:LYS:HG2	2:M:105:GLU:HG3	1.98	0.46
3:S:122:LYS:NZ	3:S:149:ASP:O	2.49	0.46
3:J:48:VAL:HG13	3:J:64:VAL:HG21	1.98	0.46
2:M:2:ILE:HG23	2:M:26:SER:HB3	1.98	0.46
2:M:28:ASP:OD1	2:M:68:GLY:HA2	2.15	0.46
3:H:173:ALA:HB2	3:H:183:LEU:HD23	1.98	0.46
2:L:11:LEU:HD22	2:L:104:VAL:HG22	1.98	0.46
3:G:42:GLY:HA3	3:G:43:LYS:HE3	1.98	0.46
2:N:21:ILE:HG22	2:N:22:THR:H	1.81	0.46
2:L:35:TRP:HB2	2:L:48:ILE:HG13	1.98	0.46
2:M:150:VAL:O	2:M:152:ASN:N	2.49	0.46
2:O:125:LEU:C	2:O:127:SER:H	2.21	0.46
2:L:179:LEU:O	2:L:180:THR:OG1	2.30	0.46
3:S:194:LEU:HA	3:S:197:GLN:HE21	1.81	0.46
2:O:118:PHE:HB3	3:J:129:LEU:HB3	1.99	0.45
3:G:44:GLY:C	3:G:45:LEU:HG	2.41	0.45
1:C:90:ASP:OD2	1:D:83:GLN:NE2	2.50	0.45
2:M:94:HIS:NE2	3:H:59:TYR:HE2	2.12	0.45
2:M:149:LYS:HB3	2:M:152:ASN:HA	1.98	0.45
3:S:6:GLU:HA	3:S:21:SER:O	2.16	0.45
1:E:64:ILE:O	1:E:77:GLN:HG3	2.16	0.45
3:J:33:TRP:CE3	3:J:99:ARG:HG2	2.52	0.45
1:B:69:HIS:CE1	1:C:94:LEU:HD11	2.51	0.45
2:M:176:SER:HB3	3:H:171:PHE:CZ	2.51	0.45
2:O:37:GLN:HB2	2:O:47:LEU:HD11	1.98	0.45
3:F:50:TRP:CE2	3:F:59:TYR:HB3	2.50	0.45
1:C:57:TRP:CZ3	1:C:114:CYS:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:106:ILE:HG13	2:N:166:GLN:NE2	2.31	0.45
1:E:80:SER:HB2	1:E:107:GLN:HE22	1.81	0.45
2:K:186:TYR:O	2:K:192:TYR:OH	2.35	0.45
1:C:64:ILE:HG22	1:C:65:ILE:HG12	1.98	0.45
1:A:94:LEU:HD13	1:D:51:ALA:HA	1.98	0.45
3:G:30:SER:O	3:G:54:TYR:HB2	2.17	0.45
1:C:57:TRP:HB2	1:C:65:ILE:HB	1.98	0.45
3:S:2:VAL:HG11	3:S:107:TYR:CZ	2.52	0.45
2:N:119:PRO:HB3	2:N:192:TYR:OH	2.17	0.45
2:O:113:PRO:HD3	2:O:198:HIS:CD2	2.52	0.45
3:F:83:MET:HE3	3:F:86:LEU:HD21	1.99	0.45
2:L:198:HIS:O	2:L:201:LEU:HB2	2.17	0.45
2:O:134:CYS:HB2	2:O:148:TRP:CZ2	2.52	0.45
3:G:200:ILE:HG13	3:G:214:LYS:O	2.16	0.44
2:M:142:ARG:HD2	2:M:142:ARG:O	2.16	0.44
3:S:187:VAL:HG22	3:S:189:VAL:HG13	1.99	0.44
1:E:79:SER:HA	1:E:82:ARG:HE	1.82	0.44
2:O:6:GLN:HB2	2:O:100:GLN:HG2	1.98	0.44
1:A:90:ASP:OD1	1:A:90:ASP:N	2.48	0.44
3:F:48:VAL:HG13	3:F:64:VAL:HG21	1.99	0.44
2:O:160:GLN:HE21	2:O:178:THR:HG22	1.81	0.44
3:J:127:PHE:HA	3:J:128:PRO:HD2	1.92	0.44
1:B:21:VAL:HG13	1:B:40:CYS:O	2.16	0.44
2:L:180:THR:HG22	2:L:181:LEU:N	2.32	0.44
1:C:107:GLN:HG2	1:C:108:ASP:N	2.29	0.44
1:D:57:TRP:CZ3	1:D:114:CYS:HB3	2.52	0.44
3:G:35:HIS:CE1	3:G:50:TRP:CD1	3.05	0.44
3:G:142:ALA:HB2	3:G:188:THR:HA	2.00	0.44
2:N:117:ILE:HG21	2:N:209:PHE:CD1	2.53	0.44
3:J:35:HIS:CE1	3:J:50:TRP:CD1	3.05	0.44
3:F:36:TRP:CE2	3:F:81:LEU:HB2	2.52	0.44
3:G:42:GLY:CA	3:G:43:LYS:HE3	2.47	0.44
2:N:123:GLU:OE2	2:N:130:ALA:HB2	2.18	0.44
2:L:188:LYS:HE2	2:L:189:HIS:CE1	2.52	0.44
2:M:91:TYR:CZ	3:H:103:GLY:HA3	2.53	0.44
2:M:187:GLU:HG3	2:M:211:ARG:NH1	2.32	0.44
2:O:190:LYS:HE3	2:O:211:ARG:HG2	1.99	0.44
2:O:213:GLU:OE1	2:O:213:GLU:N	2.50	0.44
2:L:124:GLN:OE1	2:L:131:SER:N	2.50	0.44
2:M:30:SER:OG	2:M:31:THR:N	2.51	0.44
2:M:198:HIS:CD2	2:M:199:GLN:H	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:105:GLU:OE1	2:O:173:TYR:OH	2.36	0.44
2:O:126:LYS:HD2	2:O:126:LYS:HA	1.33	0.44
3:J:83:MET:HB3	3:J:86:LEU:HD21	2.00	0.44
3:J:124:PRO:HB3	3:J:150:TYR:HB3	2.00	0.44
2:M:201:LEU:HD13	2:M:205:VAL:HG23	2.00	0.44
3:H:67:ARG:HH22	3:H:90:ASP:CG	2.26	0.44
3:F:36:TRP:HD1	3:F:70:ILE:HD12	1.84	0.43
1:C:23:VAL:HA	1:C:24:PRO:HD3	1.88	0.43
2:M:192:TYR:HD2	2:M:209:PHE:CZ	2.36	0.43
3:H:48:VAL:HG13	3:H:64:VAL:HG11	2.00	0.43
3:H:83:MET:HE1	3:H:114:VAL:HG11	2.00	0.43
1:E:77:GLN:NE2	1:E:85:ALA:HB3	2.33	0.43
1:A:34:SER:O	1:A:104:VAL:HG23	2.18	0.43
3:G:126:VAL:O	3:G:214:LYS:HE2	2.18	0.43
3:S:47:TRP:HZ2	3:S:50:TRP:CD1	2.36	0.43
3:S:101:TRP:HB2	3:S:102:PRO:HD3	2.00	0.43
1:E:55:VAL:HB	1:E:67:PHE:HB3	1.99	0.43
1:B:62:LYS:HE2	1:B:78:HIS:CE1	2.53	0.43
3:G:129:LEU:HD12	3:G:144:GLY:HA3	2.01	0.43
2:O:94:HIS:CD2	2:O:95:PRO:N	2.86	0.43
3:J:60:TYR:CZ	3:J:70:ILE:HG22	2.53	0.43
2:M:122:ASP:CG	2:M:125:LEU:HD12	2.44	0.43
1:D:38:ILE:HG22	1:D:126:ILE:HD13	2.00	0.43
2:N:43:ALA:HA	2:N:44:PRO:HD3	1.92	0.43
2:N:160:GLN:NE2	3:S:175:LEU:O	2.50	0.43
1:A:67:PHE:CE2	1:A:71:GLU:HA	2.53	0.43
1:C:25:LYS:HB2	1:C:28:TYR:CE1	2.54	0.43
3:S:64:VAL:HA	3:S:67:ARG:NH1	2.34	0.43
2:O:89:GLN:HE21	2:O:96:ALA:HB1	1.84	0.43
2:K:3:GLN:HG3	3:H:69:THR:HG21	2.01	0.43
3:G:121:THR:HG22	3:G:208:SER:HB3	2.00	0.43
1:C:22:THR:O	1:C:41:LYS:HB2	2.19	0.43
2:M:176:SER:HB3	3:H:171:PHE:CE2	2.54	0.43
2:N:141:PRO:C	2:N:143:GLU:H	2.26	0.43
3:G:67:ARG:HH22	3:G:90:ASP:CG	2.20	0.43
2:M:4:MET:HE3	2:M:23:CYS:SG	2.58	0.43
2:N:125:LEU:C	2:N:127:SER:N	2.75	0.43
2:L:187:GLU:HG3	2:L:211:ARG:NH1	2.34	0.43
3:H:215:LYS:HE3	3:H:215:LYS:HB2	1.89	0.43
2:K:108:ARG:HG2	2:K:109:THR:H	1.84	0.43
3:F:87:ARG:HA	3:F:87:ARG:HD3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:MET:HG2	1:C:60:GLU:H	1.84	0.43
1:C:80:SER:HB2	1:C:107:GLN:NE2	2.31	0.43
2:M:132:VAL:CG2	2:M:179:LEU:HB3	2.49	0.43
3:S:194:LEU:HD23	3:S:197:GLN:HE21	1.83	0.43
2:O:188:LYS:HE3	2:O:189:HIS:CE1	2.54	0.43
1:C:80:SER:O	1:C:84:ARG:NH1	2.52	0.42
2:M:4:MET:O	2:M:99:GLY:HA2	2.19	0.42
2:N:113:PRO:CD	2:N:198:HIS:CE1	3.01	0.42
3:S:47:TRP:CZ2	3:S:50:TRP:CD1	3.06	0.42
1:A:102:THR:O	1:A:103:ASP:C	2.62	0.42
2:L:146:VAL:HG12	2:L:196:VAL:HA	2.01	0.42
3:G:51:ILE:HD12	3:G:58:THR:HG22	2.01	0.42
1:A:64:ILE:HG21	1:A:99:LEU:HD21	2.02	0.42
3:F:89:GLU:H	3:F:89:GLU:HG3	1.66	0.42
1:B:78:HIS:ND1	1:B:80:SER:HB3	2.33	0.42
2:L:138:ASN:ND2	2:L:170:ASP:OD2	2.52	0.42
2:N:190:LYS:HZ1	2:N:192:TYR:C	2.26	0.42
1:E:54:ILE:HG23	1:E:68:VAL:HG22	2.01	0.42
2:O:159:SER:OG	2:O:161:GLU:OE1	2.37	0.42
3:G:91:THR:HG23	3:G:115:THR:HA	2.02	0.42
2:M:213:GLU:CD	2:M:213:GLU:H	2.27	0.42
2:O:169:LYS:HG3	2:O:170:ASP:N	2.33	0.42
3:J:35:HIS:CG	3:J:50:TRP:HB3	2.54	0.42
2:K:7:SER:HA	2:K:8:PRO:C	2.43	0.42
3:H:47:TRP:CZ2	3:H:50:TRP:CD1	3.07	0.42
2:O:169:LYS:HE3	2:O:169:LYS:HB2	1.75	0.42
1:C:56:TYR:HE1	3:H:50:TRP:CH2	2.37	0.42
2:N:198:HIS:CE1	2:N:200:GLY:C	2.98	0.42
2:K:81:GLU:H	2:K:81:GLU:HG3	1.58	0.42
1:B:46:LYS:O	1:B:47:GLU:C	2.62	0.42
3:G:47:TRP:CZ2	3:G:50:TRP:CD1	3.08	0.42
3:S:43:LYS:HD3	3:S:43:LYS:HA	1.79	0.42
2:M:124:GLN:OE1	2:M:131:SER:N	2.36	0.42
1:D:36:MET:HE3	1:D:36:MET:HB2	1.80	0.42
2:K:95:PRO:O	2:K:97:THR:HG23	2.20	0.42
2:K:183:LYS:HE3	2:K:187:GLU:OE2	2.19	0.42
2:L:117:ILE:HD12	2:L:134:CYS:SG	2.60	0.42
3:H:60:TYR:CE1	3:H:70:ILE:HG22	2.55	0.42
3:S:51:ILE:HA	3:S:57:SER:O	2.20	0.42
3:F:99:ARG:HD2	3:F:104:GLY:O	2.20	0.41
2:N:198:HIS:CE1	2:N:200:GLY:CA	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:203:SER:HB2	2:K:204:PRO:HD2	2.02	0.41
3:F:56:GLY:O	3:F:58:THR:HG23	2.19	0.41
2:M:150:VAL:HG22	2:M:192:TYR:CE1	2.54	0.41
2:O:35:TRP:CD2	2:O:73:LEU:HB2	2.55	0.41
2:O:105:GLU:OE1	2:O:142:ARG:NH2	2.53	0.41
2:O:190:LYS:HA	2:O:192:TYR:HE2	1.85	0.41
2:L:118:PHE:CD1	3:G:129:LEU:HB3	2.55	0.41
1:C:62:LYS:HG2	1:C:78:HIS:CD2	2.55	0.41
2:N:208:SER:HB3	2:N:209:PHE:H	1.54	0.41
2:K:123:GLU:OE1	2:K:123:GLU:N	2.40	0.41
1:B:56:TYR:O	1:B:114:CYS:HA	2.20	0.41
2:L:180:THR:HG22	2:L:181:LEU:H	1.85	0.41
2:L:188:LYS:HG3	2:L:189:HIS:ND1	2.35	0.41
2:M:207:LYS:HB3	2:M:207:LYS:HE2	1.71	0.41
3:H:191:SER:O	3:H:194:LEU:HG	2.20	0.41
2:N:123:GLU:CG	2:N:124:GLN:N	2.78	0.41
2:N:125:LEU:HD21	2:N:183:LYS:CD	2.45	0.41
2:L:180:THR:HG22	2:L:181:LEU:O	2.21	0.41
2:O:89:GLN:HB2	2:O:98:PHE:CD2	2.56	0.41
2:O:147:GLN:O	2:O:195:GLU:HB3	2.21	0.41
2:O:171:SER:O	2:O:171:SER:OG	2.37	0.41
2:M:123:GLU:O	2:M:126:LYS:HG2	2.20	0.41
3:H:173:ALA:HA	3:H:183:LEU:HB3	2.01	0.41
3:J:7:SER:HB3	3:J:21:SER:HB3	2.03	0.41
1:A:31:GLU:H	1:A:31:GLU:HG2	1.66	0.41
1:A:65:ILE:HD11	1:A:72:GLU:OE1	2.21	0.41
1:B:29:VAL:HG12	1:B:129:LYS:HB2	2.02	0.41
3:H:131:PRO:HG3	3:H:143:LEU:HB3	2.02	0.41
1:B:65:ILE:HD13	1:B:65:ILE:HA	1.82	0.41
1:B:66:GLN:O	1:B:72:GLU:HA	2.21	0.41
2:N:193:ALA:HA	2:N:209:PHE:HE2	1.86	0.41
2:O:130:ALA:HB3	2:O:183:LYS:CD	2.39	0.41
3:F:153:GLU:CG	3:F:154:PRO:HA	2.50	0.41
2:L:94:HIS:CE1	3:G:59:TYR:CE2	3.08	0.41
3:G:33:TRP:HE3	3:G:99:ARG:HG2	1.86	0.41
2:M:35:TRP:CD2	2:M:73:LEU:HB2	2.56	0.41
2:M:191:VAL:HG22	2:M:209:PHE:O	2.21	0.41
3:H:211:LYS:HD2	3:H:212:VAL:N	2.36	0.41
2:N:91:TYR:CZ	3:S:103:GLY:HA3	2.55	0.41
2:N:145:LYS:CE	2:N:198:HIS:HA	2.51	0.41
3:S:39:GLN:HB2	3:S:45:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:106:ASP:OD1	3:S:106:ASP:N	2.49	0.41
1:E:38:ILE:HD11	1:E:99:LEU:HD23	2.03	0.41
2:O:183:LYS:HA	2:O:186:TYR:H	1.86	0.41
2:L:80:PRO:HA	2:L:83:PHE:CE1	2.56	0.41
2:L:210:ASN:CG	2:L:211:ARG:N	2.79	0.41
3:G:2:VAL:HG11	3:G:107:TYR:CD2	2.56	0.41
3:S:140:THR:OG1	3:S:189:VAL:O	2.39	0.41
3:S:167:GLY:O	3:S:187:VAL:HA	2.21	0.41
2:O:91:TYR:CZ	3:J:103:GLY:HA3	2.55	0.41
1:B:59:MET:HG2	1:B:60:GLU:H	1.86	0.40
3:G:43:LYS:HD3	1:D:106:LEU:HB3	2.03	0.40
1:C:79:SER:HA	1:C:82:ARG:NE	2.34	0.40
2:N:197:THR:HB	2:N:204:PRO:HB3	2.02	0.40
2:L:4:MET:O	1:D:32:TYR:OH	2.39	0.40
2:N:145:LYS:HE2	2:N:198:HIS:HA	2.03	0.40
2:N:192:TYR:HB2	2:N:209:PHE:CD2	2.56	0.40
2:O:21:ILE:HG21	2:O:102:THR:HG21	2.04	0.40
3:J:64:VAL:HA	3:J:67:ARG:HH11	1.87	0.40
3:F:6:GLU:HA	3:F:21:SER:O	2.21	0.40
1:B:36:MET:HE3	1:B:36:MET:HB2	1.93	0.40
3:H:194:LEU:HD22	3:H:197:GLN:HE21	1.86	0.40
2:N:38:GLN:O	2:N:38:GLN:HG3	2.20	0.40
2:N:106:ILE:HG13	2:N:166:GLN:CD	2.47	0.40
2:O:187:GLU:C	2:O:189:HIS:N	2.76	0.40
3:J:36:TRP:HD1	3:J:70:ILE:HD12	1.86	0.40
1:B:23:VAL:HA	1:B:24:PRO:HD3	1.95	0.40
1:B:69:HIS:C	1:C:94:LEU:HD21	2.46	0.40
2:N:197:THR:O	2:N:198:HIS:CB	2.69	0.40
3:S:91:THR:HG23	3:S:115:THR:HA	2.03	0.40
2:O:152:ASN:O	2:O:152:ASN:OD1	2.40	0.40
1:B:50:LEU:HD12	1:B:50:LEU:HA	1.89	0.40
2:L:124:GLN:CD	2:L:131:SER:H	2.30	0.40
2:M:94:HIS:CE1	3:H:59:TYR:CE2	3.08	0.40
3:H:127:PHE:CE2	3:H:148:LYS:HD3	2.54	0.40
3:S:155:VAL:HG12	3:S:205:HIS:CB	2.47	0.40
2:O:94:HIS:HD2	2:O:95:PRO:N	2.20	0.40
2:O:170:ASP:N	2:O:170:ASP:OD1	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	109/123 (89%)	103 (94%)	6 (6%)	0	100	100
1	B	114/123 (93%)	109 (96%)	5 (4%)	0	100	100
1	C	114/123 (93%)	106 (93%)	7 (6%)	1 (1%)	14	44
1	D	114/123 (93%)	110 (96%)	4 (4%)	0	100	100
1	E	110/123 (89%)	109 (99%)	1 (1%)	0	100	100
2	K	211/214 (99%)	198 (94%)	13 (6%)	0	100	100
2	L	198/214 (92%)	180 (91%)	17 (9%)	1 (0%)	24	57
2	M	211/214 (99%)	199 (94%)	12 (6%)	0	100	100
2	N	200/214 (94%)	183 (92%)	16 (8%)	1 (0%)	24	57
2	O	211/214 (99%)	199 (94%)	12 (6%)	0	100	100
3	F	208/230 (90%)	199 (96%)	9 (4%)	0	100	100
3	G	207/230 (90%)	202 (98%)	5 (2%)	0	100	100
3	H	208/230 (90%)	203 (98%)	4 (2%)	1 (0%)	24	57
3	J	204/230 (89%)	200 (98%)	4 (2%)	0	100	100
3	S	207/230 (90%)	201 (97%)	6 (3%)	0	100	100
All	All	2626/2835 (93%)	2501 (95%)	121 (5%)	4 (0%)	43	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	45	GLU
2	N	123	GLU
3	H	209	ASN
2	L	191	VAL

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	98/108 (91%)	91 (93%)	7 (7%)	13	41
1	B	101/108 (94%)	99 (98%)	2 (2%)	48	72
1	C	101/108 (94%)	99 (98%)	2 (2%)	48	72
1	D	101/108 (94%)	95 (94%)	6 (6%)	18	48
1	E	99/108 (92%)	98 (99%)	1 (1%)	68	79
2	K	186/187 (100%)	182 (98%)	4 (2%)	45	71
2	L	178/187 (95%)	162 (91%)	16 (9%)	9	33
2	M	186/187 (100%)	178 (96%)	8 (4%)	26	57
2	N	179/187 (96%)	162 (90%)	17 (10%)	8	30
2	O	186/187 (100%)	170 (91%)	16 (9%)	10	34
3	F	174/191 (91%)	170 (98%)	4 (2%)	44	70
3	G	173/191 (91%)	169 (98%)	4 (2%)	44	70
3	H	173/191 (91%)	165 (95%)	8 (5%)	24	55
3	J	170/191 (89%)	161 (95%)	9 (5%)	20	51
3	S	173/191 (91%)	169 (98%)	4 (2%)	44	70
All	All	2278/2430 (94%)	2170 (95%)	108 (5%)	23	55

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	VAL
1	A	50	LEU
1	A	71	GLU
1	A	90	ASP
1	A	101	ILE
1	A	103	ASP
1	A	114	CYS
2	K	5	THR
2	K	81	GLU
2	K	126	LYS

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Mol	Chain	Res	Type
2	K	188	LYS
3	F	5	VAL
3	F	30	SER
3	F	45	LEU
3	F	192	SER
1	B	40	CYS
1	B	81	TYR
2	L	20	THR
2	L	42	LYS
2	L	81	GLU
2	L	106	ILE
2	L	117	ILE
2	L	125	LEU
2	L	126	LYS
2	L	127	SER
2	L	145	LYS
2	L	163	VAL
2	L	179	LEU
2	L	180	THR
2	L	181	LEU
2	L	195	GLU
2	L	202	SER
2	L	207	LYS
3	G	7	SER
3	G	43	LYS
3	G	174	VAL
3	G	194	LEU
1	C	40	CYS
1	C	107	GLN
2	M	48	ILE
2	M	100	GLN
2	M	109	THR
2	M	110	VAL
2	M	124	GLN
2	M	190	LYS
2	M	191	VAL
2	M	213	GLU
3	H	5	VAL
3	H	7	SER
3	H	76	LYS
3	H	189	VAL
3	H	190	PRO

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Mol	Chain	Res	Type
3	H	203	VAL
3	H	214	LYS
3	H	215	LYS
1	D	31	GLU
1	D	44	VAL
1	D	76	VAL
1	D	101	ILE
1	D	106	LEU
1	D	115	MET
2	N	5	THR
2	N	7	SER
2	N	29	VAL
2	N	81	GLU
2	N	123	GLU
2	N	125	LEU
2	N	145	LYS
2	N	147	GLN
2	N	161	GLU
2	N	166	GLN
2	N	183	LYS
2	N	188	LYS
2	N	197	THR
2	N	198	HIS
2	N	199	GLN
2	N	205	VAL
2	N	209	PHE
3	S	2	VAL
3	S	140	THR
3	S	192	SER
3	S	196	THR
1	E	86	ARG
2	O	11	LEU
2	O	33	VAL
2	O	45	LYS
2	O	81	GLU
2	O	110	VAL
2	O	126	LYS
2	O	132	VAL
2	O	136	LEU
2	O	147	GLN
2	O	150	VAL
2	O	156	SER

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Mol	Chain	Res	Type
2	O	176	SER
2	O	181	LEU
2	O	183	LYS
2	O	199	GLN
2	O	205	VAL
3	J	3	GLN
3	J	43	LYS
3	J	63	SER
3	J	174	VAL
3	J	177	SER
3	J	184	SER
3	J	187	VAL
3	J	196	THR
3	J	206	LYS

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	77	GLN
2	K	152	ASN
3	F	82	GLN
3	F	204	ASN
1	B	63	ASN
1	B	69	HIS
1	B	96	ASN
1	B	100	GLN
2	L	27	GLN
2	L	79	GLN
2	L	138	ASN
3	G	82	GLN
3	G	84	ASN
3	G	176	GLN
1	C	66	GLN
1	C	96	ASN
1	C	100	GLN
1	C	107	GLN
2	M	79	GLN
2	M	89	GLN
2	M	189	HIS
2	M	198	HIS
2	M	210	ASN
3	H	13	GLN

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Mol	Chain	Res	Type
3	H	82	GLN
3	H	84	ASN
3	H	197	GLN
3	H	202	ASN
1	D	69	HIS
2	N	189	HIS
2	N	199	GLN
3	S	209	ASN
2	O	94	HIS
2	O	124	GLN
2	O	138	ASN
2	O	160	GLN
3	J	82	GLN
3	J	84	ASN
3	J	209	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	113/123 (91%)	-0.04	0 100 100	22, 34, 72, 83	0
1	B	116/123 (94%)	-0.17	0 100 100	20, 36, 57, 66	0
1	C	116/123 (94%)	-0.26	0 100 100	20, 28, 40, 51	0
1	D	116/123 (94%)	-0.12	1 (0%) 81 63	21, 34, 48, 61	0
1	E	114/123 (92%)	-0.11	0 100 100	26, 36, 48, 70	0
2	K	213/214 (99%)	-0.22	1 (0%) 87 73	14, 32, 57, 75	0
2	L	202/214 (94%)	0.23	8 (3%) 42 23	22, 44, 111, 122	0
2	M	213/214 (99%)	0.01	4 (1%) 66 45	14, 33, 90, 109	0
2	N	204/214 (95%)	0.30	10 (4%) 35 18	19, 51, 113, 120	0
2	O	213/214 (99%)	0.35	11 (5%) 33 17	20, 48, 106, 119	0
3	F	212/230 (92%)	-0.22	0 100 100	17, 31, 51, 65	0
3	G	211/230 (91%)	-0.16	6 (2%) 55 34	24, 33, 85, 112	0
3	H	212/230 (92%)	0.02	4 (1%) 66 45	14, 32, 90, 136	0
3	J	208/230 (90%)	-0.08	4 (1%) 66 45	14, 32, 83, 121	0
3	S	211/230 (91%)	0.04	2 (0%) 81 63	24, 43, 108, 136	0
All	All	2674/2835 (94%)	-0.01	51 (1%) 66 45	14, 35, 97, 136	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	119	PRO	5.4
2	O	181	LEU	4.3
2	M	122	ASP	3.9
2	O	154	LEU	3.9
3	J	198	THR	3.4
2	O	158	ASN	3.2
3	H	199	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
3	J	128	PRO	3.0
1	D	106	LEU	2.9
2	O	183	LYS	2.9
2	L	192	TYR	2.9
3	G	42	GLY	2.9
2	N	190	LYS	2.8
2	O	182	SER	2.8
2	L	209	PHE	2.7
2	N	194	CYS	2.6
2	O	204	PRO	2.6
3	H	130	ALA	2.6
2	O	155	GLN	2.5
3	H	198	THR	2.5
3	S	199	TYR	2.5
2	N	121	SER	2.5
2	O	184	ALA	2.5
2	N	117	ILE	2.5
3	G	192	SER	2.4
2	O	180	THR	2.4
3	S	218	PRO	2.4
2	L	94	HIS	2.4
2	K	151	ASP	2.3
3	G	131	PRO	2.3
2	N	144	ALA	2.3
3	G	143	LEU	2.3
3	H	131	PRO	2.3
3	G	139	GLY	2.3
2	M	129	THR	2.3
3	J	129	LEU	2.3
2	O	119	PRO	2.3
2	L	190	LYS	2.3
2	N	134	CYS	2.3
2	N	118	PHE	2.2
2	O	83	PHE	2.2
3	J	137	SER	2.2
2	N	213	GLU	2.2
2	L	130	ALA	2.2
2	L	145	LYS	2.2
3	G	43	LYS	2.2
2	M	212	GLY	2.1
2	N	210	ASN	2.1
2	L	193	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	191	VAL	2.0
2	L	127	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.