



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:03 PM UTC

PDB ID : 3HAE / pdb_00003hae
Title : Rational development of high-affinity T-cell receptor-like antibodies
Authors : Stewart-Jones, G.; Wadle, A.; Hombach, A.; Shenderov, E.; Held, G.; Fischer, E.
Deposited on : 2009-05-01
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

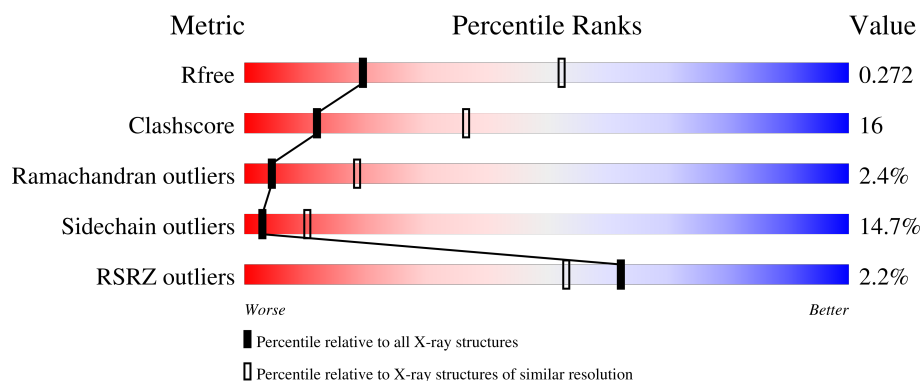
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	 69% 25% 6%
1	D	276	 11% 64% 30% 5%
1	J	276	 70% 26% 4%
1	P	276	 67% 28% 5%
2	B	100	 11% 55% 40% 4%

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Mol	Chain	Length	Quality of chain
2	E	100	% 61% 34% . .
2	K	100	% 56% 39% 5%
2	Q	100	58% 36% 5% .
3	C	9	44% 44% 33% 11% 11%
3	F	9	11% 33% 44% 11% 11%
3	M	9	11% 67% 22% 11%
3	R	9	44% 44% 11%
4	G	212	% 56% 35% 7% .
4	L	212	4% 65% 28% 6% .
4	N	212	9% 57% 33% 9%
4	S	212	58% 34% 6% .
5	H	220	3% 65% 23% 9% .
5	I	220	3% 61% 30% 7% .
5	O	220	3% 59% 34% 7% .
5	T	220	% 59% 30% 9% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25472 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			
1	D	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			
1	J	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			
1	P	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	E	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	K	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	Q	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	expression tag	UNP P61769
E	0	MET	-	expression tag	UNP P61769
K	0	MET	-	expression tag	UNP P61769
Q	0	MET	-	expression tag	UNP P61769

- Molecule 3 is a protein called NYESO-1 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			
3	F	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			
3	M	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			
3	R	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			

- Molecule 4 is a protein called Antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	211	Total	C	N	O	S	0	0	0
			1595	1002	270	319	4			
4	G	211	Total	C	N	O	S	0	0	0
			1595	1002	270	319	4			
4	N	211	Total	C	N	O	S	0	0	0
			1595	1002	270	319	4			
4	S	211	Total	C	N	O	S	0	0	0
			1595	1002	270	319	4			

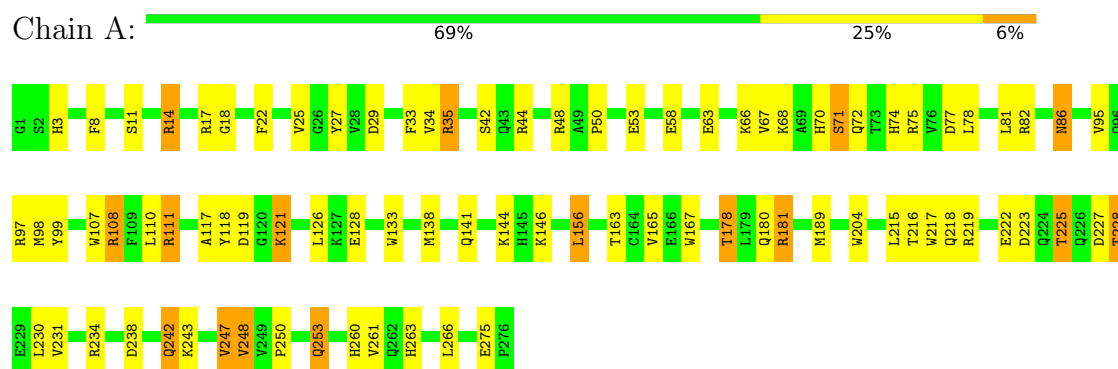
- Molecule 5 is a protein called Antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	220	Total	C	N	O	S	0	0	0
			1609	1012	268	322	7			
5	I	220	Total	C	N	O	S	0	0	0
			1609	1012	268	322	7			
5	O	220	Total	C	N	O	S	0	0	0
			1609	1012	268	322	7			
5	T	220	Total	C	N	O	S	0	0	0
			1609	1012	268	322	7			

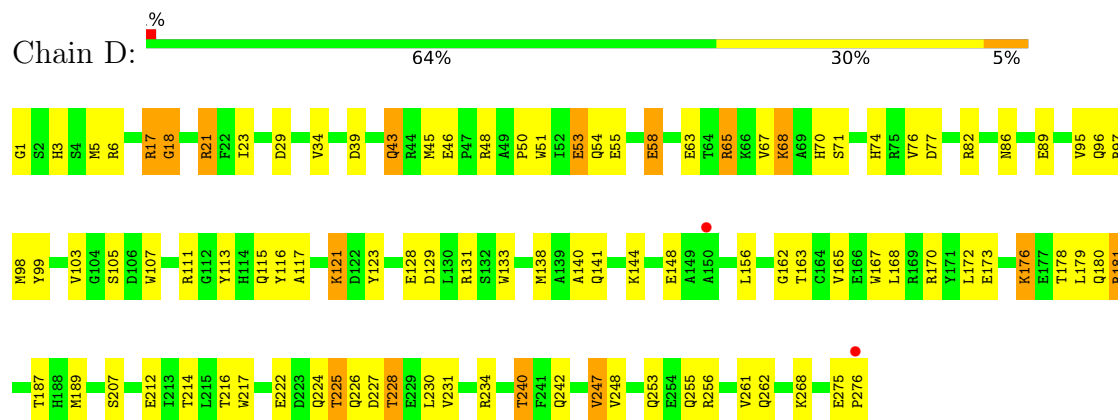
3 Residue-property plots

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.

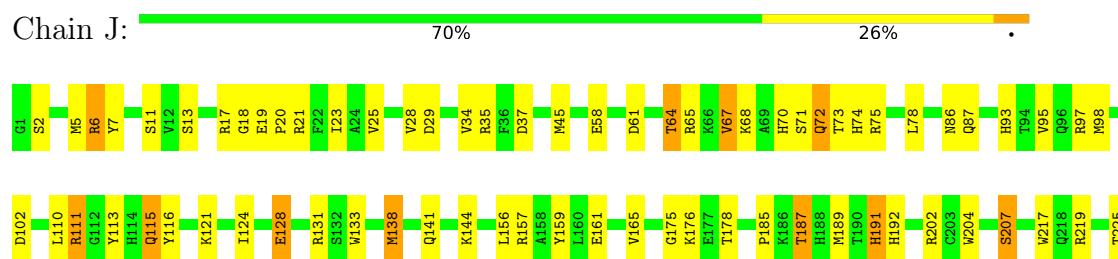
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



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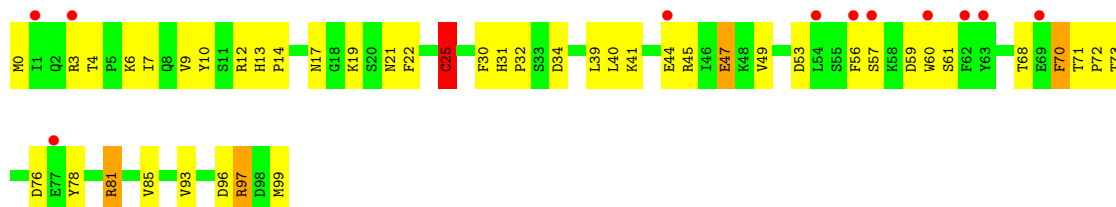




- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



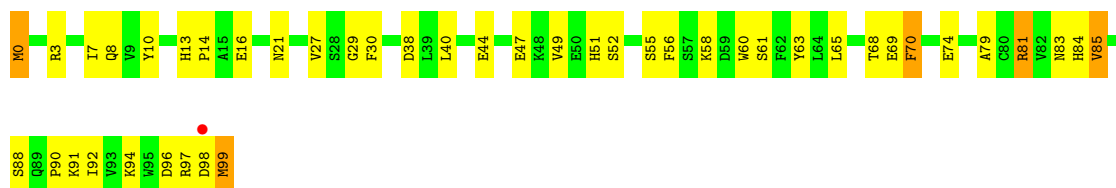
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

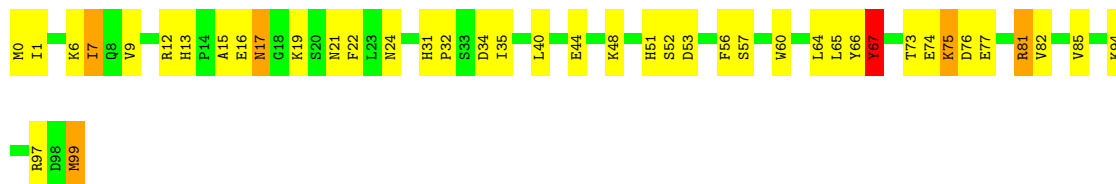


- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

Chain Q:  58% 36% 5%



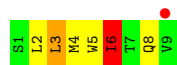
- Molecule 3: NYESO-1 peptide

Chain C:  44% 44% 33% 11% 11%



- Molecule 3: NYESO-1 peptide

Chain F:  11% 33% 44% 11% 11%

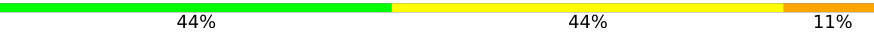


- Molecule 3: NYESO-1 peptide

Chain M:  11% 67% 22% 11%



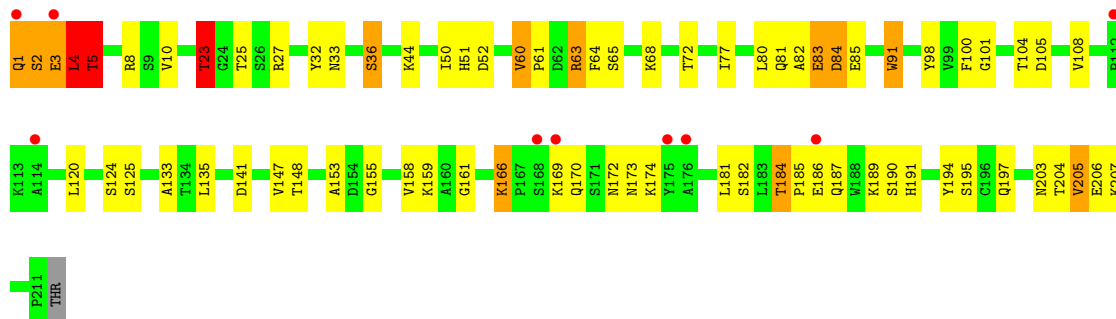
- Molecule 3: NYESO-1 peptide

Chain R:  44% 44% 11%

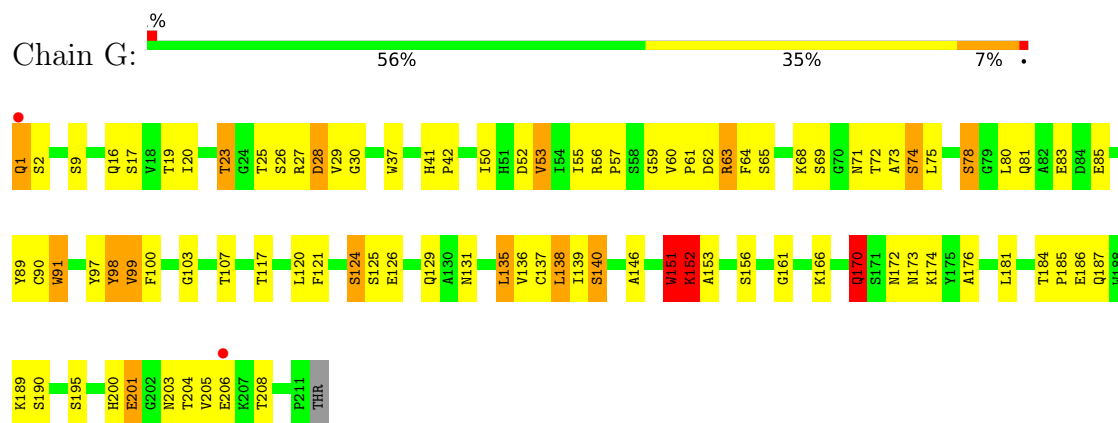


- Molecule 4: Antibody light chain

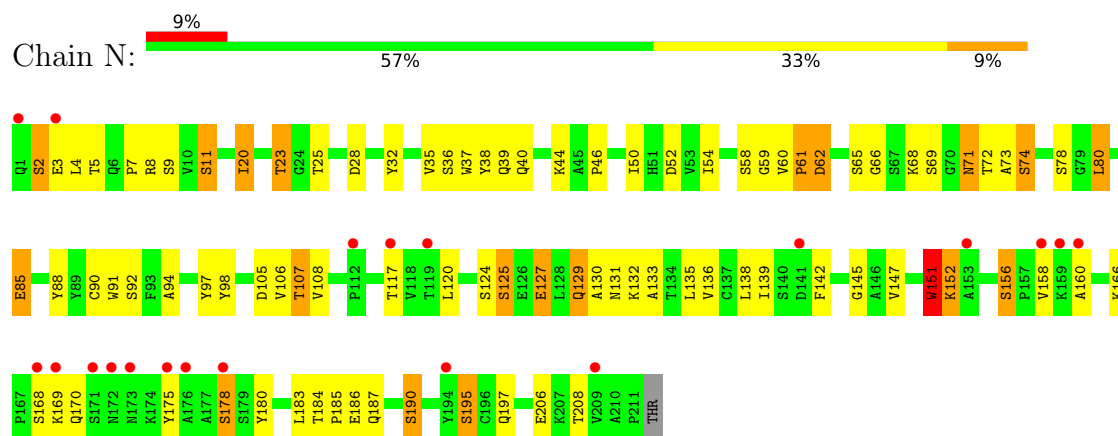
Chain L:  4% 65% 28% 6%



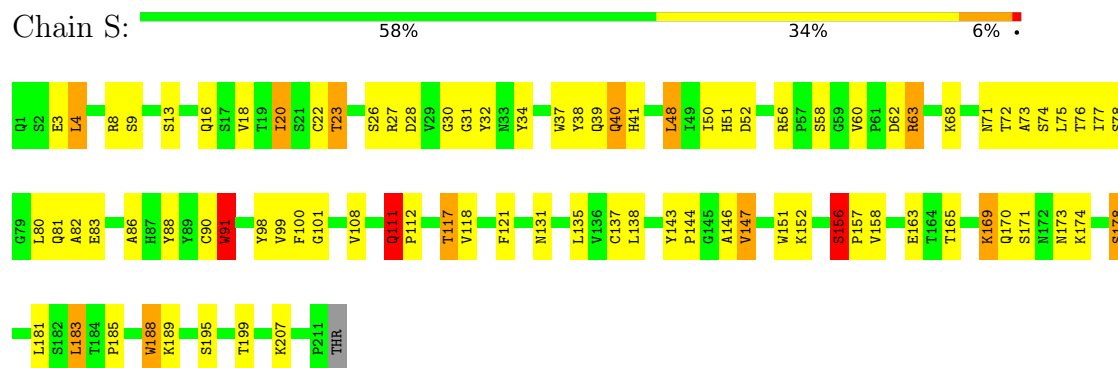
- Molecule 4: Antibody light chain



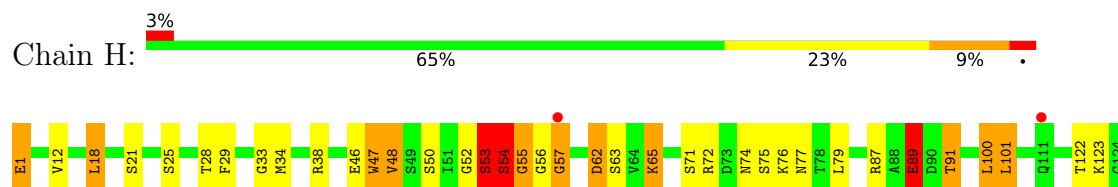
- Molecule 4: Antibody light chain



- Molecule 4: Antibody light chain

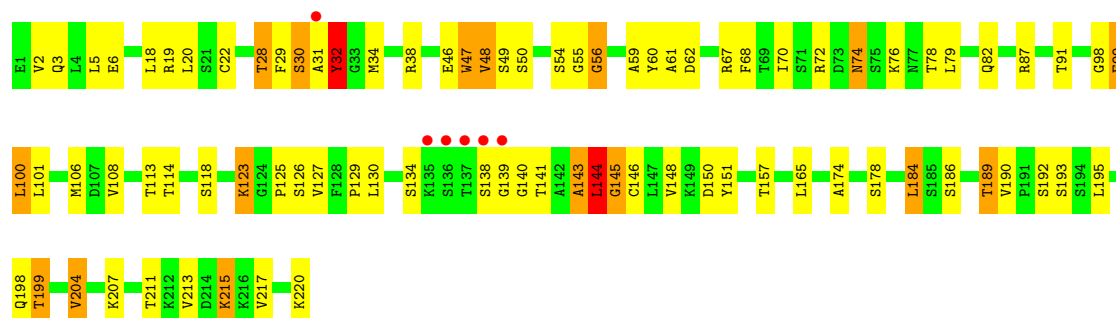


- Molecule 5: Antibody heavy chain

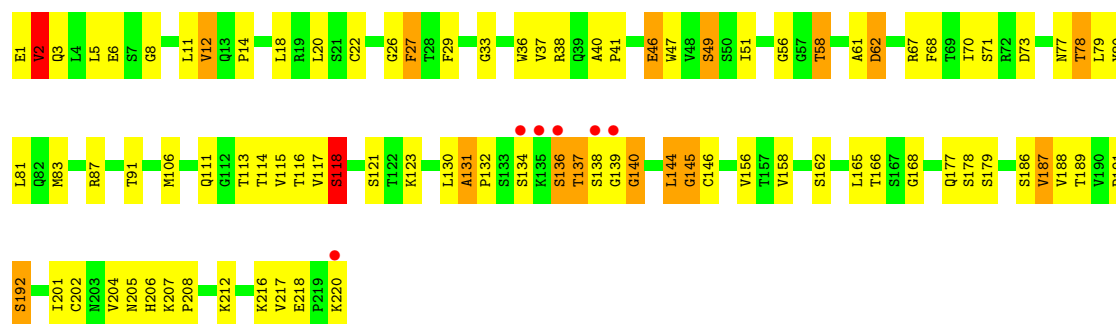




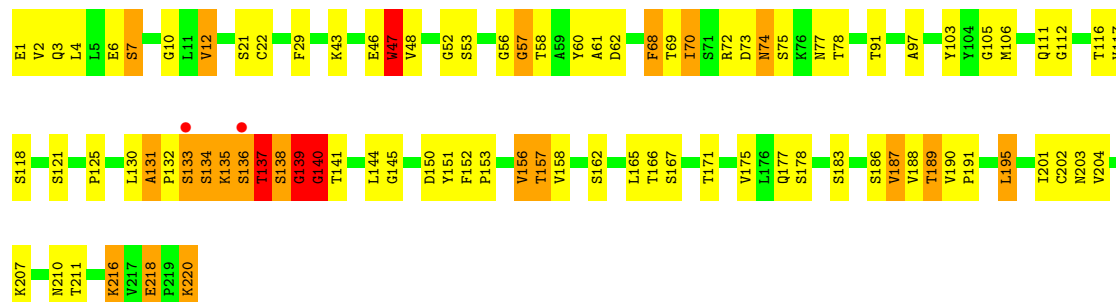
• Molecule 5: Antibody heavy chain



• Molecule 5: Antibody heavy chain



• Molecule 5: Antibody heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.79Å 105.60Å 256.45Å 90.00° 92.26° 90.00°	Depositor
Resolution (Å)	25.00 – 2.90 25.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (25.00-2.90) 98.2 (25.00-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.283 0.195 , 0.272	Depositor DCC
R_{free} test set	4225 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 16.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	25472	wwPDB-VP
Average B, all atoms (Å ²)	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.02	0/2319	1.11	1/3149 (0.0%)
1	D	1.04	0/2319	1.11	7/3149 (0.2%)
1	J	0.90	0/2319	1.01	1/3149 (0.0%)
1	P	1.00	0/2319	1.04	3/3149 (0.1%)
2	B	1.02	0/859	1.36	7/1162 (0.6%)
2	E	0.99	0/859	1.12	2/1162 (0.2%)
2	K	0.99	0/859	1.18	4/1162 (0.3%)
2	Q	1.08	0/859	1.20	7/1162 (0.6%)
3	C	1.10	0/76	1.18	1/103 (1.0%)
3	F	1.15	0/76	1.26	1/103 (1.0%)
3	M	0.87	0/76	1.08	0/103
3	R	1.11	0/76	1.07	1/103 (1.0%)
4	G	0.99	1/1638 (0.1%)	1.25	9/2237 (0.4%)
4	L	1.02	2/1638 (0.1%)	1.26	7/2237 (0.3%)
4	N	0.97	0/1638	1.17	4/2237 (0.2%)
4	S	1.03	1/1638 (0.1%)	1.19	7/2237 (0.3%)
5	H	1.05	4/1646 (0.2%)	1.36	12/2239 (0.5%)
5	I	1.15	2/1646 (0.1%)	1.31	14/2239 (0.6%)
5	O	0.92	0/1646	1.17	7/2239 (0.3%)
5	T	1.06	1/1646 (0.1%)	1.23	10/2239 (0.4%)
All	All	1.01	11/26152 (0.0%)	1.18	105/35560 (0.3%)

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
4	G	0	1
4	L	0	2
4	N	0	2
5	H	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	T	0	1
All	All	0	10

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	137	THR	CA-CB	6.72	1.64	1.53
5	H	137	THR	CA-CB	6.17	1.63	1.53
5	I	38	ARG	CA-C	-5.62	1.46	1.52
5	H	47	TRP	CA-C	-5.44	1.45	1.52
4	G	98	TYR	CA-C	-5.42	1.45	1.52
4	S	117	THR	CA-CB	5.41	1.61	1.53
5	I	48	VAL	CA-CB	-5.36	1.48	1.54
4	L	5	THR	CA-CB	5.31	1.62	1.53
5	H	47	TRP	N-CA	5.27	1.52	1.46
5	H	217	VAL	CA-CB	-5.16	1.48	1.54
4	L	4	LEU	CA-C	5.13	1.59	1.52

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	152	PHE	CA-C-N	15.65	139.41	119.84
5	H	152	PHE	C-N-CA	15.65	139.41	119.84
2	B	4	THR	CA-C-N	10.21	130.85	119.83
2	B	4	THR	C-N-CA	10.21	130.85	119.83
5	I	146	CYS	N-CA-C	10.01	124.97	109.96
4	L	60	VAL	CA-C-N	9.95	130.04	119.89
4	L	60	VAL	C-N-CA	9.95	130.04	119.89
4	S	60	VAL	CA-C-N	9.85	129.95	119.90
4	S	60	VAL	C-N-CA	9.85	129.95	119.90
5	H	48	VAL	N-CA-C	-9.20	104.35	111.62
5	H	53	SER	N-CA-C	8.81	129.57	110.80
5	I	46	GLU	N-CA-C	8.65	123.98	112.13
5	H	53	SER	CA-C-N	8.60	137.18	121.70
5	H	53	SER	C-N-CA	8.60	137.18	121.70
5	T	131	ALA	CA-C-N	8.47	128.98	119.83
5	T	131	ALA	C-N-CA	8.47	128.98	119.83
4	S	156	SER	N-CA-C	8.33	120.14	109.65
5	O	131	ALA	CA-C-N	8.03	128.09	119.90
5	O	131	ALA	C-N-CA	8.03	128.09	119.90
4	L	60	VAL	N-CA-C	7.94	117.69	108.96
2	Q	67	TYR	N-CA-C	7.58	119.67	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	55	ILE	N-CA-C	7.51	118.95	107.99
5	T	145	GLY	N-CA-C	7.44	122.75	110.55
5	T	166	THR	N-CA-C	-7.38	105.45	114.75
5	O	12	VAL	N-CA-C	7.27	117.95	108.35
4	G	98	TYR	N-CA-C	-7.12	97.35	109.24
1	P	247	VAL	CB-CA-C	-7.07	99.93	110.82
4	G	59	GLY	CA-C-N	-7.02	117.54	122.59
4	G	59	GLY	C-N-CA	-7.02	117.54	122.59
4	S	111	GLN	N-CA-C	6.76	124.75	109.81
5	T	48	VAL	N-CA-C	-6.69	106.48	111.90
1	D	76	VAL	CB-CA-C	-6.66	103.03	112.22
4	N	92	SER	N-CA-C	6.66	120.35	109.24
5	H	47	TRP	N-CA-CB	6.65	121.73	110.49
4	G	91	TRP	CA-CB-CG	6.57	126.08	113.60
5	I	143	ALA	CA-C-N	6.48	133.37	121.70
5	I	143	ALA	C-N-CA	6.48	133.37	121.70
2	K	56	PHE	N-CA-C	6.44	118.87	109.07
2	B	7	ILE	CB-CA-C	-6.37	101.82	110.42
3	F	6	ILE	CB-CA-C	-6.35	102.73	110.99
5	H	33	GLY	N-CA-C	-6.17	104.14	111.36
4	N	151	TRP	CA-C-N	6.16	132.79	121.70
4	N	151	TRP	C-N-CA	6.16	132.79	121.70
5	I	32	TYR	N-CA-C	6.16	123.91	110.80
1	A	108	ARG	CB-CA-C	6.12	120.72	109.46
2	Q	56	PHE	N-CA-C	6.12	118.59	108.99
4	N	156	SER	N-CA-C	6.09	118.52	110.36
5	H	101	LEU	N-CA-C	-6.00	102.73	108.13
1	D	247	VAL	CB-CA-C	-5.96	101.64	110.82
5	T	70	ILE	N-CA-C	5.95	116.43	107.80
5	T	140	GLY	N-CA-C	5.95	127.27	113.18
4	G	151	TRP	CA-C-N	5.94	132.39	121.70
4	G	151	TRP	C-N-CA	5.94	132.39	121.70
5	I	204	VAL	CB-CA-C	-5.78	102.83	110.98
4	S	188	TRP	N-CA-C	-5.76	104.63	111.03
2	K	8	GLN	CA-C-N	-5.75	115.61	123.14
2	K	8	GLN	C-N-CA	-5.75	115.61	123.14
1	D	18	GLY	N-CA-C	5.73	126.77	113.18
2	Q	19	LYS	N-CA-C	5.72	117.63	108.41
5	T	10	GLY	N-CA-C	5.71	118.14	110.43
5	I	118	SER	CA-C-N	-5.69	113.73	122.60
5	I	118	SER	C-N-CA	-5.69	113.73	122.60
1	D	255	GLN	N-CA-C	5.63	118.19	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	74	ASN	N-CA-C	5.62	117.41	111.28
5	H	139	GLY	N-CA-C	-5.59	99.92	113.18
2	E	47	GLU	CA-C-N	-5.59	115.57	122.84
2	E	47	GLU	C-N-CA	-5.59	115.57	122.84
2	B	25	CYS	N-CA-C	5.56	117.46	108.34
5	I	91	THR	CB-CA-C	-5.55	102.16	110.16
3	C	6	ILE	CB-CA-C	-5.55	102.89	110.77
1	D	63	GLU	N-CA-C	-5.54	105.32	111.36
3	R	6	ILE	CB-CA-C	-5.46	103.02	110.77
5	O	33	GLY	N-CA-C	-5.45	103.08	111.64
4	L	84	ASP	N-CA-C	-5.44	106.56	114.12
5	H	187	VAL	N-CA-C	5.40	116.51	108.46
4	S	91	TRP	CA-CB-CG	5.40	123.86	113.60
2	B	70	PHE	N-CA-C	5.39	115.24	108.45
5	T	3	GLN	N-CA-C	5.38	117.15	108.32
4	L	133	ALA	N-CA-C	5.37	116.80	107.93
4	L	23	THR	N-CA-C	5.36	118.14	109.40
5	O	118	SER	N-CA-C	5.35	117.22	108.76
4	S	40	GLN	N-CA-C	5.35	117.11	108.34
4	L	5	THR	N-CA-CB	5.34	119.51	110.49
5	H	141	THR	N-CA-C	5.33	117.18	108.76
5	O	46	GLU	N-CA-C	5.32	119.46	111.96
5	T	47	TRP	N-CA-CB	5.29	119.42	110.49
5	I	126	SER	N-CA-C	-5.28	101.93	110.32
5	I	99	GLU	N-CA-C	5.24	117.95	109.40
2	Q	9	VAL	N-CA-C	5.20	115.39	108.11
5	I	47	TRP	N-CA-CB	5.19	119.27	110.49
5	I	190	VAL	N-CA-C	5.17	114.65	108.45
2	Q	0	MET	CA-C-N	5.16	131.26	121.97
2	Q	0	MET	C-N-CA	5.16	131.26	121.97
2	B	7	ILE	N-CA-C	5.15	115.39	107.77
1	D	54	GLN	CB-CA-C	-5.15	100.47	110.46
4	G	140	SER	N-CA-C	5.12	118.08	109.95
2	K	85	VAL	CB-CA-C	-5.10	105.36	112.04
1	P	238	ASP	N-CA-C	-5.10	105.37	112.30
4	G	170	GLN	N-CA-C	5.08	117.57	109.65
5	O	114	THR	N-CA-C	5.03	116.96	108.96
2	Q	77	GLU	N-CA-C	5.03	118.01	109.76
1	D	231	VAL	N-CA-C	5.02	116.48	109.55
1	P	72	GLN	CB-CG-CD	5.01	121.11	112.60
2	B	93	VAL	N-CA-C	5.00	114.68	106.72
1	J	207	SER	CB-CA-C	-5.00	105.16	111.86

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	GLU	Peptide
4	G	9	SER	Peptide
5	H	140	GLY	Peptide
5	H	152	PHE	Peptide
5	H	153	PRO	Peptide
4	L	1	GLN	Peptide
4	L	2	SER	Peptide
4	N	2	SER	Peptide
4	N	61	PRO	Peptide
5	T	139	GLY	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	2253	0	2103	61	0
1	D	2253	0	2103	74	0
1	J	2253	0	2103	62	0
1	P	2253	0	2103	67	0
2	B	836	0	803	29	0
2	E	836	0	803	28	0
2	K	836	0	803	29	0
2	Q	836	0	803	26	0
3	C	75	0	83	15	0
3	F	75	0	83	12	0
3	M	75	0	83	4	0
3	R	75	0	83	3	0
4	G	1595	0	1537	67	0
4	L	1595	0	1537	58	0
4	N	1595	0	1537	55	0
4	S	1595	0	1537	55	0
5	H	1609	0	1577	59	0
5	I	1609	0	1577	52	0
5	O	1609	0	1577	58	0
5	T	1609	0	1577	59	0
All	All	25472	0	24412	783	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 16.

All (783) 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)
4:N:11:SER:HB3	4:N:107:THR:HG22	1.31	1.11
1:P:256:ARG:HG3	1:P:256:ARG:HH11	1.17	1.06
1:J:138:MET:HE2	1:J:138:MET:HA	1.35	1.04
1:J:6:ARG:HH22	1:J:113:TYR:HE1	1.08	1.00
1:P:111:ARG:HH12	1:P:128:GLU:HB3	1.26	0.99
4:S:63:ARG:HH21	4:S:63:ARG:HG3	1.29	0.97
5:H:53:SER:HB3	5:H:54:SER:CB	1.98	0.94
4:S:63:ARG:HB2	4:S:78:SER:O	1.67	0.94
1:P:72:GLN:NE2	1:P:75:ARG:HH21	1.67	0.92
2:E:0:MET:SD	2:E:32:PRO:HG3	2.10	0.91
4:S:13:SER:O	4:S:16:GLN:HB2	1.71	0.91
4:G:187:GLN:HA	4:G:190:SER:OG	1.71	0.90
5:I:139:GLY:O	5:I:141:THR:HG22	1.70	0.90
5:I:49:SER:HB2	5:I:59:ALA:O	1.72	0.89
5:T:136:SER:C	5:T:138:SER:H	1.81	0.89
1:P:6:ARG:NH2	1:P:113:TYR:CD1	2.40	0.89
5:T:97:ALA:HB1	5:T:106:MET:HG3	1.55	0.88
1:P:215:LEU:HD22	1:P:261:VAL:HG22	1.55	0.87
1:A:178:THR:O	1:A:181:ARG:HG2	1.75	0.85
1:P:72:GLN:HE22	1:P:75:ARG:HH21	1.19	0.85
4:G:1:GLN:N	4:G:2:SER:HA	1.90	0.85
4:N:54:ILE:HG22	4:N:66:GLY:O	1.76	0.85
5:O:130:LEU:HB2	5:O:145:GLY:CA	2.07	0.85
1:J:6:ARG:NH2	1:J:113:TYR:CE1	2.45	0.85
1:D:65:ARG:HG2	1:D:65:ARG:HH11	1.40	0.84
1:D:253:GLN:NE2	1:D:256:ARG:HH11	1.74	0.84
1:J:111:ARG:HG2	1:J:111:ARG:HH11	1.42	0.84
2:Q:81:ARG:HH11	2:Q:81:ARG:HG2	1.40	0.84
1:P:215:LEU:CD2	1:P:261:VAL:HG22	2.08	0.84
1:J:204:TRP:HZ2	2:K:99:MET:C	1.87	0.83
3:C:8:GLN:NE2	4:L:27:ARG:HD2	1.94	0.82
1:J:138:MET:HA	1:J:138:MET:CE	2.10	0.82
4:N:151:TRP:HA	4:N:152:LYS:HB2	1.61	0.82
3:C:8:GLN:NE2	4:L:27:ARG:CD	2.43	0.82
2:E:89:GLN:HE21	2:E:90:PRO:HD2	1.44	0.82
1:P:256:ARG:HG3	1:P:256:ARG:NH1	1.93	0.81
5:H:53:SER:HB3	5:H:54:SER:HB3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:62:ASP:HB2	5:H:178:SER:HB2	1.62	0.80
4:N:32:TYR:O	4:N:68:LYS:NZ	2.14	0.80
1:D:58:GLU:CD	1:D:58:GLU:H	1.89	0.80
4:S:63:ARG:HG3	4:S:63:ARG:NH2	1.94	0.80
4:L:3:GLU:HG2	4:L:4:LEU:N	1.96	0.80
1:P:6:ARG:NH2	1:P:113:TYR:CE1	2.48	0.80
4:G:170:GLN:NE2	4:G:172:ASN:OD1	2.14	0.80
1:P:165:VAL:O	1:P:169:ARG:HG3	1.81	0.78
5:O:130:LEU:HB2	5:O:145:GLY:C	2.07	0.77
4:L:63:ARG:NH2	4:L:84:ASP:OD2	2.16	0.77
5:T:132:PRO:O	5:T:220:LYS:NZ	2.16	0.77
5:O:37:VAL:HG22	5:O:47:TRP:HA	1.67	0.77
1:A:181:ARG:HG2	1:A:181:ARG:HH11	1.51	0.76
1:A:74:HIS:HE1	1:A:97:ARG:HE	1.30	0.76
3:C:4:MET:HB2	5:H:56:GLY:HA3	1.69	0.75
2:B:81:ARG:HG2	2:B:81:ARG:HH11	1.51	0.75
1:D:163:THR:CG2	5:I:55:GLY:HA3	2.17	0.75
1:D:111:ARG:HD3	1:D:113:TYR:CZ	2.21	0.74
4:L:91:TRP:CH2	4:L:98:TYR:CD1	2.75	0.74
4:N:184:THR:C	4:N:186:GLU:H	1.95	0.74
4:S:63:ARG:CB	4:S:78:SER:O	2.35	0.73
5:H:152:PHE:CD2	5:H:153:PRO:HD3	2.24	0.73
5:H:53:SER:HB3	5:H:54:SER:OG	1.89	0.72
5:I:100:LEU:HD12	5:I:101:LEU:HG	1.70	0.72
3:C:8:GLN:HE22	4:L:27:ARG:CD	2.03	0.72
1:D:163:THR:HG21	5:I:55:GLY:CA	2.19	0.72
1:J:235:PRO:HG2	2:K:65:LEU:HD13	1.72	0.72
4:N:129:GLN:C	4:N:131:ASN:H	1.98	0.72
4:N:25:THR:HA	4:N:71:ASN:OD1	1.89	0.71
1:A:231:VAL:O	1:A:243:LYS:HE3	1.91	0.71
1:J:6:ARG:NH2	1:J:113:TYR:HE1	1.85	0.71
1:P:17:ARG:HH11	1:P:17:ARG:HG3	1.56	0.71
1:P:51:TRP:CZ2	1:P:179:LEU:HD11	2.26	0.70
1:A:250:PRO:HB2	1:A:253:GLN:HG3	1.73	0.70
4:G:65:SER:O	4:G:75:LEU:HD12	1.92	0.70
1:J:234:ARG:HE	1:J:242:GLN:HE21	1.37	0.70
1:P:51:TRP:CE2	1:P:179:LEU:HD11	2.25	0.70
1:J:115:GLN:HB2	2:K:60:TRP:HH2	1.56	0.70
4:G:1:GLN:HG3	5:I:62:ASP:HB2	1.74	0.69
4:G:151:TRP:HA	4:G:152:LYS:HB2	1.74	0.69
5:H:171:THR:HA	5:H:186:SER:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:189:MET:HE2	1:J:217:TRP:HH2	1.55	0.69
1:D:111:ARG:HD3	1:D:113:TYR:OH	1.91	0.69
1:D:225:THR:O	1:D:228:THR:HB	1.92	0.69
5:O:130:LEU:HB2	5:O:145:GLY:HA2	1.73	0.69
5:H:53:SER:CB	5:H:54:SER:OG	2.40	0.69
4:G:1:GLN:H2	4:G:2:SER:HA	1.54	0.69
4:L:91:TRP:CH2	4:L:98:TYR:CE1	2.80	0.69
4:L:63:ARG:HH22	4:L:84:ASP:CG	2.01	0.69
1:J:189:MET:HE2	1:J:217:TRP:CH2	2.28	0.68
5:H:125:PRO:HD2	5:H:211:THR:HG21	1.74	0.68
2:E:41:LYS:HG3	2:E:78:TYR:CE1	2.27	0.68
1:D:68:LYS:O	1:D:71:SER:HB3	1.93	0.68
3:F:4:MET:HB2	5:I:56:GLY:HA3	1.75	0.68
4:S:81:GLN:O	4:S:108:VAL:HG21	1.93	0.67
2:E:24:ASN:HB3	2:E:65:LEU:HD11	1.77	0.67
2:K:29:GLY:HA2	2:K:61:SER:HB2	1.75	0.67
4:G:135:LEU:CD2	4:G:181:LEU:HB3	2.25	0.67
1:D:163:THR:HG21	5:I:55:GLY:HA3	1.77	0.67
1:D:21:ARG:NH1	1:D:23:ILE:HD11	2.10	0.67
1:D:178:THR:O	1:D:181:ARG:HD3	1.94	0.67
1:J:204:TRP:CZ2	2:K:99:MET:C	2.73	0.67
4:N:184:THR:O	4:N:186:GLU:N	2.27	0.67
5:O:26:GLY:O	5:O:27:PHE:HB3	1.95	0.66
1:D:45:MET:HE1	3:F:2:LEU:HD11	1.77	0.66
4:N:85:GLU:HG2	4:N:107:THR:HA	1.78	0.66
4:G:57:PRO:HD2	4:G:60:VAL:HG21	1.78	0.66
5:H:160:TRP:CZ3	5:H:202:CYS:HB3	2.31	0.66
4:L:4:LEU:O	4:L:23:THR:O	2.12	0.65
4:S:23:THR:HB	4:S:72:THR:HG23	1.78	0.65
3:C:5:TRP:HE1	5:H:57:GLY:HA2	1.61	0.65
4:L:91:TRP:HD1	4:L:100:PHE:CD1	2.15	0.65
4:N:184:THR:C	4:N:186:GLU:N	2.54	0.64
2:E:89:GLN:HE21	2:E:89:GLN:HA	1.62	0.64
2:E:89:GLN:NE2	2:E:90:PRO:HD2	2.11	0.64
4:G:187:GLN:HA	4:G:190:SER:HG	1.60	0.64
5:I:67:ARG:C	5:I:68:PHE:HD1	2.06	0.64
1:A:72:GLN:HE21	4:L:32:TYR:HA	1.63	0.64
5:H:74:ASN:C	5:H:76:LYS:H	2.05	0.63
2:E:1:ILE:HG22	2:E:1:ILE:O	1.98	0.63
5:H:125:PRO:HG3	5:H:151:TYR:HB3	1.80	0.63
1:D:144:LYS:O	1:D:148:GLU:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:139:GLY:O	5:H:140:GLY:C	2.41	0.63
1:D:58:GLU:CD	1:D:58:GLU:N	2.57	0.63
1:A:72:GLN:NE2	4:L:32:TYR:HA	2.13	0.63
5:H:100:LEU:HD13	5:H:101:LEU:HG	1.80	0.63
5:H:89:GLU:H	5:H:89:GLU:CD	2.07	0.63
5:O:11:LEU:HD12	5:O:116:THR:HB	1.81	0.63
4:N:187:GLN:HA	4:N:190:SER:OG	1.99	0.62
2:K:96:ASP:C	2:K:96:ASP:OD1	2.43	0.62
4:S:165:THR:HG22	5:T:175:VAL:HB	1.80	0.62
4:L:172:ASN:O	4:L:173:ASN:HB2	1.98	0.62
4:N:124:SER:HB3	4:N:127:GLU:HB2	1.81	0.62
1:J:219:ARG:HD3	1:J:256:ARG:NH2	2.15	0.62
5:H:56:GLY:C	5:H:57:GLY:O	2.40	0.61
1:A:181:ARG:HH11	1:A:181:ARG:CG	2.13	0.61
2:K:29:GLY:HA2	2:K:61:SER:CB	2.31	0.61
1:P:227:ASP:HB3	1:P:248:VAL:HG22	1.82	0.61
2:Q:31:HIS:CD2	2:Q:32:PRO:HA	2.34	0.61
1:A:163:THR:HG21	5:H:55:GLY:HA2	1.82	0.61
2:Q:64:LEU:HD13	2:Q:66:TYR:HE1	1.65	0.61
5:O:140:GLY:O	5:O:192:SER:HB2	2.00	0.61
2:E:89:GLN:HA	2:E:89:GLN:NE2	2.15	0.61
1:J:19:GLU:CG	1:J:75:ARG:HH21	2.14	0.61
5:T:136:SER:C	5:T:138:SER:N	2.52	0.61
1:D:55:GLU:OE1	1:D:170:ARG:NH2	2.33	0.61
5:T:188:VAL:HG22	5:T:190:VAL:HG13	1.82	0.61
5:H:152:PHE:CD2	5:H:153:PRO:CD	2.84	0.61
5:I:198:GLN:HE21	5:I:199:THR:H	1.47	0.61
1:P:33:PHE:CE2	1:P:34:VAL:HG22	2.36	0.60
3:C:8:GLN:HE22	4:L:27:ARG:HD3	1.67	0.60
4:L:170:GLN:HB2	4:L:172:ASN:OD1	2.01	0.60
1:D:45:MET:CE	3:F:2:LEU:HD11	2.31	0.60
1:D:50:PRO:O	1:D:53:GLU:HB2	2.01	0.60
5:I:130:LEU:O	5:I:145:GLY:HA2	2.00	0.60
2:B:13:HIS:O	2:B:14:PRO:C	2.42	0.60
4:L:85:GLU:HG2	4:L:108:VAL:HG23	1.82	0.60
1:A:163:THR:CG2	5:H:55:GLY:HA2	2.31	0.60
2:Q:81:ARG:HG2	2:Q:81:ARG:NH1	2.10	0.60
3:F:8:GLN:HE22	4:G:27:ARG:HB3	1.67	0.60
1:A:133:TRP:HB2	1:A:144:LYS:HG3	1.84	0.60
1:J:115:GLN:HB2	2:K:60:TRP:CH2	2.37	0.60
2:Q:15:ALA:HB3	2:Q:97:ARG:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:124:SER:OG	5:I:129:PRO:O	2.20	0.60
2:Q:7:ILE:HD12	2:Q:82:VAL:HG21	1.82	0.59
1:J:138:MET:HE2	1:J:138:MET:CA	2.22	0.59
5:I:148:VAL:HB	5:I:184:LEU:HD12	1.83	0.59
1:D:253:GLN:NE2	1:D:256:ARG:NH1	2.46	0.59
4:L:1:GLN:NE2	5:H:62:ASP:H	2.00	0.59
4:G:68:LYS:HA	4:G:73:ALA:HA	1.85	0.59
4:N:11:SER:CB	4:N:107:THR:HG22	2.21	0.59
1:A:50:PRO:O	1:A:53:GLU:HB2	2.03	0.59
1:P:14:ARG:HG3	1:P:17:ARG:HB2	1.83	0.59
1:P:54:GLN:OE1	1:P:174:ASN:ND2	2.36	0.59
5:I:130:LEU:HB2	5:I:145:GLY:O	2.03	0.59
1:A:3:HIS:HD2	1:A:29:ASP:OD2	1.85	0.59
2:B:10:TYR:CD1	2:B:10:TYR:N	2.71	0.59
1:A:63:GLU:OE2	1:A:66:LYS:NZ	2.24	0.59
4:L:80:LEU:HD21	4:L:108:VAL:HG22	1.84	0.59
4:S:39:GLN:HG3	4:S:88:TYR:CE1	2.38	0.59
1:J:5:MET:HE3	1:J:7:TYR:CE2	2.38	0.59
1:J:61:ASP:O	1:J:65:ARG:HG3	2.03	0.59
5:I:127:VAL:HG21	5:I:204:VAL:HG21	1.83	0.59
1:D:167:TRP:CZ2	5:I:54:SER:HB2	2.38	0.58
1:J:133:TRP:HB2	1:J:144:LYS:HG3	1.84	0.58
4:G:30:GLY:HA3	4:G:71:ASN:HD22	1.66	0.58
1:D:189:MET:HE2	1:D:217:TRP:CH2	2.37	0.58
4:N:35:VAL:HA	4:N:91:TRP:O	2.04	0.58
1:A:70:HIS:CE1	3:C:6:ILE:HD12	2.39	0.58
1:A:189:MET:HE2	1:A:217:TRP:CH2	2.39	0.58
1:J:202:ARG:HD2	2:K:99:MET:C	2.29	0.58
5:O:36:TRP:NE1	5:O:81:LEU:HB2	2.19	0.58
4:L:100:PHE:HD2	5:H:46:GLU:O	1.87	0.58
1:J:138:MET:CE	1:J:138:MET:CA	2.77	0.58
4:G:52:ASP:C	4:G:53:VAL:HG23	2.29	0.58
4:G:61:PRO:HG2	4:G:64:PHE:HE2	1.69	0.58
4:S:83:GLU:O	4:S:83:GLU:HG2	2.03	0.58
5:I:125:PRO:HD2	5:I:211:THR:HG21	1.84	0.58
2:Q:17:ASN:OD1	2:Q:73:THR:C	2.47	0.57
4:N:59:GLY:HA2	5:H:181:LEU:HD11	1.86	0.57
1:A:178:THR:O	1:A:181:ARG:NH1	2.36	0.57
1:J:70:HIS:CE1	3:M:6:ILE:HD12	2.38	0.57
5:H:12:VAL:HB	5:H:18:LEU:HD13	1.86	0.57
1:D:234:ARG:HE	1:D:242:GLN:HE21	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:176:LEU:HD13	5:H:182:TYR:CZ	2.39	0.57
5:O:29:PHE:CB	5:O:77:ASN:HD22	2.17	0.57
5:H:144:LEU:HG	5:H:188:VAL:HG12	1.85	0.57
4:N:138:LEU:HD13	5:O:187:VAL:HG11	1.86	0.57
5:H:29:PHE:CB	5:H:77:ASN:HD22	2.18	0.57
1:J:5:MET:HE3	1:J:7:TYR:HE2	1.69	0.57
1:A:22:PHE:CG	1:A:71:SER:HB2	2.40	0.57
5:O:29:PHE:HB3	5:O:77:ASN:ND2	2.20	0.57
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.53	0.57
1:P:227:ASP:HB3	1:P:248:VAL:CG2	2.35	0.57
2:Q:16:GLU:O	2:Q:17:ASN:C	2.47	0.57
1:A:215:LEU:HD22	1:A:261:VAL:HG22	1.86	0.56
5:I:47:TRP:CZ2	5:I:49:SER:HA	2.39	0.56
5:T:188:VAL:HG22	5:T:190:VAL:CG1	2.35	0.56
4:L:91:TRP:HH2	4:L:98:TYR:CE1	2.24	0.56
4:G:30:GLY:HA3	4:G:71:ASN:ND2	2.20	0.56
4:N:120:LEU:HD12	4:N:136:VAL:O	2.04	0.56
5:I:72:ARG:HE	5:I:74:ASN:HD21	1.54	0.56
1:D:65:ARG:HG2	1:D:65:ARG:NH1	2.08	0.56
5:O:91:THR:HG23	5:O:116:THR:HA	1.87	0.56
1:P:218:GLN:HB2	1:P:260:HIS:NE2	2.20	0.56
4:L:23:THR:HB	4:L:72:THR:OG1	2.06	0.56
4:L:4:LEU:O	4:L:5:THR:CB	2.52	0.56
4:G:151:TRP:HA	4:G:152:LYS:CB	2.36	0.56
4:G:17:SER:HB2	4:G:78:SER:HB3	1.86	0.56
4:S:4:LEU:HB2	4:S:101:GLY:HA2	1.88	0.56
1:A:111:ARG:CZ	1:A:128:GLU:HG3	2.36	0.55
1:J:234:ARG:HE	1:J:242:GLN:NE2	2.02	0.55
2:K:40:LEU:HD11	2:K:81:ARG:HB3	1.87	0.55
5:H:52:GLY:H	5:H:57:GLY:HA3	1.71	0.55
5:O:29:PHE:HB3	5:O:77:ASN:HD22	1.70	0.55
1:A:74:HIS:CE1	1:A:97:ARG:HE	2.18	0.55
1:J:111:ARG:HG2	1:J:111:ARG:NH1	2.12	0.55
5:I:48:VAL:O	5:I:49:SER:HB3	2.06	0.55
2:Q:13:HIS:O	2:Q:21:ASN:ND2	2.33	0.55
1:D:74:HIS:CE1	1:D:97:ARG:HE	2.24	0.55
5:T:132:PRO:HG3	5:T:144:LEU:CB	2.36	0.55
1:A:74:HIS:HE1	1:A:97:ARG:NE	2.02	0.55
4:S:20:ILE:HD12	4:S:75:LEU:HD23	1.88	0.55
4:N:23:THR:HG22	4:N:72:THR:HG23	1.89	0.55
1:D:172:LEU:O	1:D:180:GLN:NE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:67:TYR:HD2	2:Q:67:TYR:N	2.05	0.55
1:J:19:GLU:HG2	1:J:75:ARG:HH21	1.71	0.55
1:P:106:ASP:O	1:P:107:TRP:HB2	2.06	0.55
4:N:142:PHE:CE2	4:N:145:GLY:HA2	2.42	0.55
1:A:238:ASP:HB3	2:B:12:ARG:HH11	1.71	0.55
1:D:96:GLN:OE1	2:E:31:HIS:HE1	1.89	0.55
4:L:91:TRP:HD1	4:L:100:PHE:CE1	2.25	0.55
5:H:74:ASN:C	5:H:76:LYS:N	2.64	0.55
2:B:40:LEU:HD23	2:B:45:ARG:HA	1.88	0.54
2:E:16:GLU:O	2:E:72:PRO:HG2	2.07	0.54
4:S:100:PHE:HD2	5:T:46:GLU:O	1.89	0.54
5:T:60:TYR:CZ	5:T:70:ILE:HG22	2.42	0.54
1:J:13:SER:HB3	1:J:78:LEU:HD13	1.89	0.54
1:P:35:ARG:HH11	1:P:48:ARG:NE	2.05	0.54
5:O:6:GLU:CB	5:O:113:THR:HG22	2.38	0.54
1:D:162:GLY:O	1:D:165:VAL:HG22	2.06	0.54
2:Q:67:TYR:N	2:Q:67:TYR:CD2	2.76	0.54
5:T:187:VAL:HG23	5:T:187:VAL:O	2.06	0.54
4:G:1:GLN:N	4:G:2:SER:CA	2.67	0.54
4:N:151:TRP:N	4:N:151:TRP:CD1	2.76	0.54
2:B:59:ASP:O	2:B:60:TRP:HB2	2.08	0.54
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.43	0.54
5:O:205:ASN:HD21	5:O:207:LYS:HE2	1.73	0.54
5:T:72:ARG:NE	5:T:74:ASN:OD1	2.38	0.54
5:T:220:LYS:H	5:T:220:LYS:HZ3	1.55	0.54
2:B:39:LEU:HD12	2:B:49:VAL:HG22	1.88	0.54
5:H:205:ASN:HD21	5:H:212:LYS:HE2	1.73	0.54
4:N:62:ASP:CB	5:H:178:SER:HB2	2.35	0.53
5:O:56:GLY:O	5:O:58:THR:HG23	2.09	0.53
5:T:7:SER:OG	5:T:21:SER:HB2	2.08	0.53
1:A:238:ASP:HB3	2:B:12:ARG:NH1	2.24	0.53
3:R:8:GLN:NE2	4:S:27:ARG:HE	2.06	0.53
1:J:45:MET:HE2	1:J:67:VAL:HB	1.89	0.53
1:J:111:ARG:HH12	1:J:128:GLU:HA	1.73	0.53
1:J:189:MET:CE	1:J:217:TRP:CH2	2.91	0.53
1:A:14:ARG:HD2	1:A:17:ARG:HE	1.74	0.53
2:E:4:THR:OG1	2:E:5:PRO:HD2	2.09	0.53
4:G:85:GLU:OE2	4:G:107:THR:HA	2.08	0.53
5:T:132:PRO:HG3	5:T:144:LEU:HB3	1.89	0.53
4:S:30:GLY:HA3	4:S:71:ASN:HD22	1.72	0.53
5:H:53:SER:HB2	5:H:54:SER:OG	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:111:ARG:NH1	1:P:128:GLU:HB3	2.10	0.53
5:T:56:GLY:O	5:T:57:GLY:C	2.51	0.53
1:D:107:TRP:CD1	1:D:107:TRP:N	2.76	0.53
1:D:253:GLN:HE21	1:D:256:ARG:HH11	1.51	0.53
4:S:111:GLN:CB	4:S:112:PRO:HD2	2.39	0.53
2:B:3:ARG:O	2:B:30:PHE:HA	2.09	0.53
4:S:63:ARG:NH2	4:S:63:ARG:CG	2.70	0.53
2:K:29:GLY:CA	2:K:61:SER:HB2	2.39	0.52
5:I:47:TRP:O	5:I:61:ALA:HB2	2.08	0.52
1:A:70:HIS:ND1	3:C:6:ILE:HD12	2.23	0.52
1:P:1:GLY:HA3	1:P:264:GLU:OE1	2.09	0.52
4:L:25:THR:C	4:L:27:ARG:H	2.15	0.52
4:S:169:LYS:HZ2	4:S:173:ASN:HA	1.74	0.52
5:H:125:PRO:HG3	5:H:151:TYR:CB	2.39	0.52
1:P:60:TRP:O	1:P:64:THR:OG1	2.20	0.52
4:G:37:TRP:CZ3	4:G:90:CYS:HB3	2.44	0.52
5:O:11:LEU:HG	5:O:12:VAL:N	2.23	0.52
5:O:136:SER:C	5:O:138:SER:H	2.16	0.52
1:A:25:VAL:HG21	1:A:27:TYR:HE1	1.75	0.52
5:T:46:GLU:O	5:T:47:TRP:CB	2.56	0.52
5:T:216:LYS:HE3	5:T:218:GLU:OE2	2.10	0.52
1:P:17:ARG:HG3	1:P:17:ARG:NH1	2.25	0.52
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.44	0.52
1:P:129:ASP:OD2	1:P:131:ARG:HB2	2.10	0.52
2:K:21:ASN:HB3	2:K:70:PHE:CE1	2.45	0.52
5:O:14:PRO:HG3	5:O:117:VAL:CG1	2.40	0.52
1:J:253:GLN:NE2	1:J:256:ARG:NH1	2.58	0.52
4:G:56:ARG:HB3	4:G:60:VAL:HB	1.91	0.52
4:G:135:LEU:HD22	4:G:181:LEU:HB3	1.92	0.52
1:D:17:ARG:HB2	1:D:17:ARG:CZ	2.40	0.52
1:J:131:ARG:HG3	1:J:157:ARG:NH1	2.25	0.52
3:C:4:MET:H	5:H:56:GLY:HA2	1.76	0.51
1:D:163:THR:CG2	5:I:55:GLY:CA	2.83	0.51
2:E:55:SER:HB3	2:E:63:TYR:CZ	2.46	0.51
4:G:91:TRP:CH2	4:G:98:TYR:CE1	2.98	0.51
4:S:91:TRP:CH2	4:S:98:TYR:CE1	2.98	0.51
5:I:143:ALA:HB2	5:I:189:THR:HA	1.92	0.51
4:L:60:VAL:HG13	4:L:61:PRO:HD2	1.92	0.51
1:A:35:ARG:HH12	1:A:48:ARG:NH1	2.08	0.51
5:I:141:THR:HG23	5:I:141:THR:O	2.10	0.51
4:N:129:GLN:C	4:N:131:ASN:N	2.67	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:236:ALA:O	2:Q:12:ARG:HG3	2.11	0.51
5:O:206:HIS:CD2	5:O:208:PRO:HD2	2.45	0.51
2:B:81:ARG:HG2	2:B:81:ARG:NH1	2.21	0.51
2:E:51:HIS:HB3	2:E:66:TYR:CD2	2.46	0.51
1:P:202:ARG:HD3	1:P:244:TRP:CD2	2.45	0.51
4:N:36:SER:HA	4:N:50:ILE:O	2.10	0.51
4:S:37:TRP:HB2	4:S:50:ILE:HB	1.92	0.51
1:D:45:MET:HE2	1:D:67:VAL:HB	1.93	0.51
1:P:111:ARG:HH12	1:P:128:GLU:CB	2.13	0.51
4:N:20:ILE:HD11	4:N:106:VAL:CG2	2.41	0.51
5:O:14:PRO:HG3	5:O:117:VAL:HG12	1.92	0.51
1:A:8:PHE:HD2	2:B:56:PHE:CE1	2.28	0.51
1:D:98:MET:C	1:D:98:MET:SD	2.94	0.51
4:L:104:THR:HG22	4:L:105:ASP:N	2.25	0.51
5:H:1:GLU:HA	5:H:1:GLU:OE2	2.11	0.51
5:I:184:LEU:HD12	5:I:184:LEU:C	2.36	0.51
1:D:214:THR:HB	1:D:262:GLN:HB2	1.93	0.50
1:P:117:ALA:HB2	2:Q:60:TRP:CE2	2.46	0.50
4:S:165:THR:HG22	5:T:175:VAL:CB	2.41	0.50
2:E:81:ARG:HH11	2:E:81:ARG:HG2	1.77	0.50
4:L:104:THR:CG2	4:L:105:ASP:N	2.75	0.50
5:T:187:VAL:O	5:T:187:VAL:CG2	2.59	0.50
1:A:126:LEU:HD13	1:A:133:TRP:CH2	2.46	0.50
1:A:128:GLU:O	1:A:128:GLU:HG2	2.10	0.50
1:D:123:TYR:CZ	1:D:140:ALA:HA	2.47	0.50
5:H:91:THR:HG22	5:H:91:THR:O	2.11	0.50
5:T:133:SER:OG	5:T:134:SER:N	2.45	0.50
1:P:3:HIS:HD2	1:P:29:ASP:OD2	1.94	0.50
5:O:2:VAL:O	5:O:2:VAL:HG12	2.11	0.50
5:H:52:GLY:O	5:H:72:ARG:NH1	2.44	0.50
5:I:19:ARG:HD2	5:I:82:GLN:OE1	2.12	0.50
5:I:22:CYS:O	5:I:78:THR:HG23	2.11	0.50
1:D:212:GLU:OE1	1:D:212:GLU:HA	2.11	0.50
4:S:146:ALA:O	4:S:147:VAL:HG13	2.11	0.50
1:J:65:ARG:NH2	4:N:52:ASP:OD1	2.44	0.50
1:J:74:HIS:CD2	1:J:97:ARG:HH21	2.30	0.50
2:K:7:ILE:HD12	2:K:91:LYS:HD3	1.94	0.50
1:D:5:MET:HB2	1:D:168:LEU:HD13	1.94	0.49
5:O:138:SER:O	5:O:140:GLY:N	2.46	0.49
1:D:253:GLN:HE22	1:D:256:ARG:NH1	2.09	0.49
2:E:74:GLU:HG3	2:E:75:LYS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:72:GLN:HG2	4:S:32:TYR:HA	1.93	0.49
4:L:166:LYS:HD3	4:L:166:LYS:N	2.28	0.49
5:I:34:MET:HB3	5:I:79:LEU:HD22	1.94	0.49
5:I:130:LEU:CB	5:I:145:GLY:O	2.59	0.49
1:A:204:TRP:HZ2	2:B:99:MET:C	2.20	0.49
2:Q:40:LEU:HA	2:Q:44:GLU:O	2.12	0.49
4:N:142:PHE:HE2	4:N:145:GLY:HA2	1.76	0.49
1:D:133:TRP:HB2	1:D:144:LYS:HG3	1.94	0.49
3:C:4:MET:HB2	5:H:56:GLY:CA	2.42	0.49
4:L:91:TRP:CD1	4:L:100:PHE:CE1	3.00	0.49
4:G:121:PHE:CD1	5:I:130:LEU:HB3	2.47	0.49
4:S:41:HIS:CD2	4:S:86:ALA:HB2	2.47	0.49
1:D:65:ARG:HH11	1:D:65:ARG:CG	2.19	0.49
1:J:21:ARG:NH2	1:J:37:ASP:OD2	2.44	0.49
4:S:37:TRP:CZ3	4:S:90:CYS:HB3	2.48	0.49
4:S:138:LEU:HD23	4:S:178:SER:HB3	1.95	0.49
2:K:47:GLU:OE2	2:K:47:GLU:N	2.46	0.49
1:P:176:LYS:HB3	1:P:180:GLN:NE2	2.28	0.49
4:G:37:TRP:HB2	4:G:50:ILE:HB	1.94	0.49
1:A:35:ARG:NH1	1:A:48:ARG:NH1	2.61	0.49
2:K:40:LEU:HD12	2:K:79:ALA:HB3	1.95	0.49
4:G:184:THR:OG1	4:G:187:GLN:HG2	2.12	0.49
4:N:4:LEU:HD23	4:N:90:CYS:SG	2.53	0.49
1:D:70:HIS:CE1	3:F:6:ILE:HD12	2.48	0.49
4:G:200:HIS:O	4:G:201:GLU:C	2.55	0.49
4:G:126:GLU:O	4:G:129:GLN:HB2	2.13	0.49
5:H:175:VAL:HG22	5:H:176:LEU:N	2.28	0.49
4:G:1:GLN:CG	5:I:62:ASP:HB2	2.42	0.48
5:I:32:TYR:HA	5:I:99:GLU:O	2.13	0.48
1:D:253:GLN:O	1:D:256:ARG:HG2	2.13	0.48
2:E:23:LEU:HD21	2:E:39:LEU:HD22	1.94	0.48
5:I:198:GLN:NE2	5:I:199:THR:H	2.11	0.48
5:T:138:SER:O	5:T:139:GLY:C	2.55	0.48
1:D:275:GLU:O	1:D:276:PRO:C	2.56	0.48
1:J:58:GLU:H	1:J:58:GLU:CD	2.22	0.48
2:Q:24:ASN:HB3	2:Q:65:LEU:HD11	1.95	0.48
4:N:133:ALA:HB3	4:N:183:LEU:O	2.13	0.48
4:S:121:PHE:CD1	5:T:130:LEU:HB3	2.48	0.48
5:T:210:ASN:HD22	5:T:210:ASN:C	2.20	0.48
1:A:225:THR:O	1:A:228:THR:HB	2.13	0.48
2:Q:7:ILE:HD13	2:Q:7:ILE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:137:CYS:C	4:G:138:LEU:HG	2.38	0.48
5:H:38:ARG:HG2	5:H:48:VAL:HG22	1.95	0.48
2:E:41:LYS:HG3	2:E:78:TYR:CZ	2.48	0.48
4:G:135:LEU:HD21	4:G:181:LEU:HD23	1.94	0.48
5:T:132:PRO:O	5:T:220:LYS:CE	2.62	0.48
1:J:191:HIS:CD2	1:J:191:HIS:C	2.91	0.48
5:I:125:PRO:HB3	5:I:151:TYR:HB3	1.94	0.48
2:E:89:GLN:HE21	2:E:89:GLN:CA	2.26	0.48
1:J:6:ARG:NH2	1:J:113:TYR:CD1	2.82	0.48
5:H:135:LYS:C	5:H:137:THR:N	2.71	0.48
5:T:29:PHE:CD2	5:T:77:ASN:HA	2.48	0.48
5:T:144:LEU:HD12	5:T:144:LEU:C	2.39	0.48
1:D:187:THR:HG21	1:D:261:VAL:HG21	1.96	0.48
4:N:85:GLU:OE1	4:N:169:LYS:HE3	2.14	0.48
5:I:127:VAL:HB	5:I:213:VAL:HG11	1.96	0.48
5:O:61:ALA:O	5:O:62:ASP:C	2.55	0.48
2:Q:51:HIS:HD2	2:Q:52:SER:O	1.97	0.47
2:Q:73:THR:OG1	2:Q:76:ASP:HB2	2.13	0.47
4:L:4:LEU:HB2	4:L:101:GLY:HA2	1.96	0.47
2:Q:17:ASN:OD1	2:Q:73:THR:O	2.32	0.47
4:N:178:SER:HB2	4:N:180:TYR:CE1	2.49	0.47
4:S:80:LEU:HG	4:S:108:VAL:HG22	1.95	0.47
5:H:62:ASP:HA	5:H:65:LYS:HD3	1.96	0.47
5:H:135:LYS:O	5:H:136:SER:C	2.56	0.47
1:J:110:LEU:HD12	1:J:110:LEU:HA	1.77	0.47
4:G:60:VAL:HA	4:G:61:PRO:HD2	1.72	0.47
4:S:135:LEU:HD11	4:S:183:LEU:HD11	1.95	0.47
1:D:77:ASP:OD2	1:D:116:TYR:OH	2.28	0.47
2:E:96:ASP:O	2:E:97:ARG:C	2.57	0.47
4:N:91:TRP:CH2	4:N:98:TYR:CE1	3.02	0.47
5:O:11:LEU:HD11	5:O:118:SER:HB2	1.96	0.47
5:T:189:THR:C	5:T:190:VAL:HG13	2.40	0.47
1:A:234:ARG:HE	1:A:242:GLN:NE2	2.12	0.47
1:D:167:TRP:CH2	5:I:54:SER:HB2	2.50	0.47
1:P:108:ARG:HB2	4:G:17:SER:CB	2.45	0.47
3:F:4:MET:HB2	5:I:56:GLY:CA	2.42	0.47
1:A:217:TRP:CE2	1:A:247:VAL:HG22	2.50	0.47
2:B:31:HIS:CD2	2:B:32:PRO:HA	2.49	0.47
1:J:19:GLU:HB3	1:J:20:PRO:HD2	1.96	0.47
1:P:33:PHE:CD2	1:P:34:VAL:HG22	2.50	0.47
1:P:234:ARG:HE	1:P:242:GLN:HE21	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:9:SER:HB3	4:N:105:ASP:HB3	1.97	0.47
5:I:184:LEU:C	5:I:184:LEU:CD1	2.87	0.47
5:O:6:GLU:HB3	5:O:113:THR:CG2	2.45	0.47
5:O:6:GLU:HB3	5:O:113:THR:HG22	1.97	0.47
2:K:58:LYS:O	2:K:58:LYS:HG2	2.15	0.47
4:L:64:PHE:CE1	4:L:77:ILE:HG12	2.49	0.47
4:L:189:LYS:HE3	5:O:166:THR:HG23	1.97	0.47
5:O:20:LEU:HG	5:O:83:MET:HE2	1.96	0.47
1:A:138:MET:HG3	1:D:138:MET:HG3	1.97	0.47
2:B:39:LEU:HD13	2:B:68:THR:HG22	1.96	0.47
1:J:45:MET:CE	1:J:67:VAL:HB	2.45	0.47
1:P:42:SER:O	1:P:44:ARG:HG2	2.15	0.47
1:P:72:GLN:HG2	4:S:31:GLY:O	2.14	0.47
1:P:234:ARG:HE	1:P:242:GLN:NE2	2.13	0.47
5:O:73:ASP:C	5:O:73:ASP:OD2	2.58	0.47
5:O:144:LEU:O	5:O:188:VAL:N	2.39	0.47
5:T:46:GLU:O	5:T:47:TRP:HB3	2.15	0.47
2:B:39:LEU:HD12	2:B:49:VAL:CG2	2.44	0.47
1:A:42:SER:O	1:A:44:ARG:HG2	2.16	0.46
1:A:77:ASP:OD1	3:C:9:VAL:HG22	2.15	0.46
4:N:152:LYS:HB2	4:N:195:SER:O	2.15	0.46
4:N:139:ILE:HG22	4:N:142:PHE:CE1	2.51	0.46
5:O:37:VAL:HG13	5:O:47:TRP:H	1.79	0.46
5:T:12:VAL:O	5:T:117:VAL:HA	2.15	0.46
1:D:212:GLU:OE1	1:D:212:GLU:CA	2.63	0.46
1:J:6:ARG:HE	1:J:6:ARG:HB3	1.56	0.46
2:K:3:ARG:O	2:K:30:PHE:HA	2.15	0.46
1:P:238:ASP:HB3	2:Q:12:ARG:HD3	1.98	0.46
4:G:63:ARG:H	4:G:63:ARG:HG2	1.38	0.46
2:B:70:PHE:CZ	2:B:72:PRO:HG3	2.50	0.46
1:J:64:THR:O	1:J:68:LYS:HG2	2.16	0.46
1:J:68:LYS:O	1:J:72:GLN:OE1	2.34	0.46
5:I:28:THR:O	5:I:29:PHE:C	2.57	0.46
5:T:97:ALA:HB1	5:T:106:MET:CG	2.38	0.46
1:D:48:ARG:HD2	1:D:48:ARG:HA	1.63	0.46
1:J:98:MET:SD	1:J:98:MET:C	2.99	0.46
4:L:36:SER:HB3	4:L:50:ILE:O	2.15	0.46
4:N:39:GLN:HG3	4:N:88:TYR:CE1	2.51	0.46
5:I:19:ARG:HH11	5:I:19:ARG:HG3	1.81	0.46
1:A:263:HIS:HB3	1:A:266:LEU:HD12	1.98	0.46
1:J:187:THR:HG21	1:J:261:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:3:GLU:HG2	4:L:4:LEU:C	2.41	0.46
4:L:81:GLN:O	4:L:84:ASP:HB2	2.16	0.46
4:L:185:PRO:O	4:L:189:LYS:HG3	2.15	0.46
4:S:91:TRP:CZ2	4:S:98:TYR:CD1	3.03	0.46
5:H:146:CYS:O	5:H:185:SER:HA	2.15	0.46
5:O:137:THR:HG22	5:O:137:THR:O	2.16	0.46
1:J:192:HIS:NE2	2:K:98:ASP:O	2.49	0.46
2:K:38:ASP:OD2	2:K:81:ARG:NH1	2.49	0.46
1:P:66:LYS:HD2	3:R:4:MET:HA	1.97	0.46
1:P:238:ASP:OD1	1:P:240:THR:OG1	2.33	0.46
4:N:40:GLN:HB2	4:N:46:PRO:HA	1.97	0.46
4:S:181:LEU:HG	4:S:183:LEU:HD21	1.98	0.46
2:B:40:LEU:HA	2:B:44:GLU:O	2.16	0.46
5:H:144:LEU:HG	5:H:188:VAL:CG1	2.45	0.46
2:E:23:LEU:HB2	2:E:70:PHE:CE1	2.51	0.45
2:K:49:VAL:HG22	2:K:68:THR:HB	1.96	0.45
1:P:118:TYR:O	1:P:121:LYS:HD2	2.15	0.45
4:N:60:VAL:HG13	4:N:61:PRO:HD2	1.98	0.45
5:H:53:SER:CB	5:H:54:SER:CB	2.82	0.45
1:D:55:GLU:CD	1:D:170:ARG:HH21	2.23	0.45
1:J:68:LYS:O	1:J:71:SER:HB3	2.16	0.45
1:P:72:GLN:CD	1:P:75:ARG:HH21	2.23	0.45
4:L:124:SER:O	4:L:125:SER:C	2.60	0.45
4:L:141:ASP:O	4:L:174:LYS:HD3	2.16	0.45
4:G:91:TRP:HA	4:G:99:VAL:O	2.17	0.45
5:O:40:ALA:O	5:O:41:PRO:C	2.58	0.45
1:P:176:LYS:HB3	1:P:180:GLN:HE21	1.82	0.45
4:N:94:ALA:HB3	4:N:97:TYR:CE1	2.52	0.45
4:S:38:TYR:CE1	4:S:48:LEU:HD12	2.52	0.45
1:A:98:MET:SD	1:A:98:MET:C	2.99	0.45
1:P:133:TRP:HB2	1:P:144:LYS:HG3	1.98	0.45
1:P:218:GLN:HB2	1:P:260:HIS:CD2	2.52	0.45
4:N:142:PHE:CE2	4:N:175:TYR:HB2	2.52	0.45
4:N:151:TRP:HA	4:N:152:LYS:CB	2.41	0.45
4:S:91:TRP:HD1	4:S:100:PHE:CZ	2.34	0.45
5:I:144:LEU:HD13	5:I:217:VAL:CG1	2.46	0.45
5:I:144:LEU:HD13	5:I:217:VAL:HG11	1.99	0.45
5:T:73:ASP:C	5:T:75:SER:H	2.24	0.45
4:L:4:LEU:CB	4:L:101:GLY:HA2	2.46	0.45
4:N:80:LEU:HD21	4:N:108:VAL:HG22	1.99	0.45
4:S:40:GLN:O	4:S:86:ALA:HB1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:132:PRO:HG3	5:O:144:LEU:HD22	1.96	0.45
1:D:121:LYS:HE3	1:D:121:LYS:HB2	1.59	0.45
4:G:146:ALA:O	4:G:200:HIS:HD2	1.98	0.45
2:B:41:LYS:HD3	2:B:78:TYR:OH	2.16	0.45
1:J:95:VAL:HG13	1:J:116:TYR:CE1	2.52	0.45
3:R:5:TRP:NE1	5:T:57:GLY:O	2.50	0.45
4:N:131:ASN:O	4:N:132:LYS:HG2	2.17	0.45
1:D:96:GLN:NE2	2:E:56:PHE:CD2	2.84	0.45
1:J:185:PRO:HD3	1:J:263:HIS:ND1	2.32	0.45
1:P:5:MET:HB2	1:P:168:LEU:HD13	1.98	0.45
1:P:196:ASP:N	1:P:196:ASP:OD1	2.49	0.45
5:I:6:GLU:HB3	5:I:113:THR:CG2	2.46	0.45
5:O:51:ILE:HG23	5:O:51:ILE:O	2.17	0.45
1:A:118:TYR:O	1:A:121:LYS:HG3	2.17	0.45
2:E:13:HIS:O	2:E:14:PRO:C	2.60	0.45
1:J:17:ARG:HE	1:J:17:ARG:HB2	1.59	0.45
1:J:189:MET:CE	1:J:217:TRP:HH2	2.23	0.45
1:P:233:THR:OG1	1:P:243:LYS:HD2	2.17	0.45
3:F:3:LEU:HG	3:F:5:TRP:O	2.17	0.45
4:N:7:PRO:O	4:N:8:ARG:C	2.59	0.45
1:P:275:GLU:HA	1:P:276:PRO:HD2	1.59	0.44
4:L:3:GLU:HG2	4:L:4:LEU:CA	2.46	0.44
2:B:13:HIS:HB2	2:B:21:ASN:ND2	2.31	0.44
4:G:91:TRP:CH2	4:G:98:TYR:CD1	3.05	0.44
4:G:120:LEU:HD12	4:G:136:VAL:O	2.17	0.44
5:O:205:ASN:ND2	5:O:207:LYS:HE2	2.32	0.44
5:T:61:ALA:O	5:T:62:ASP:C	2.60	0.44
2:B:25:CYS:HB3	2:B:39:LEU:HD21	1.99	0.44
1:P:6:ARG:HE	1:P:6:ARG:HB3	1.64	0.44
1:P:47:PRO:O	1:P:48:ARG:HG2	2.18	0.44
1:P:176:LYS:CB	1:P:180:GLN:HE21	2.30	0.44
4:L:191:HIS:HB2	4:L:194:TYR:CE1	2.52	0.44
4:G:20:ILE:O	4:G:74:SER:HA	2.17	0.44
4:N:68:LYS:HB2	4:N:73:ALA:HA	1.99	0.44
4:S:170:GLN:NE2	4:S:174:LYS:HB2	2.32	0.44
5:H:152:PHE:CE2	5:H:153:PRO:HD3	2.51	0.44
5:I:143:ALA:HA	5:I:144:LEU:HB3	1.99	0.44
5:T:135:LYS:C	5:T:137:THR:N	2.75	0.44
1:A:70:HIS:CE1	3:C:6:ILE:CD1	3.01	0.44
1:A:99:TYR:CD1	1:A:99:TYR:C	2.96	0.44
1:D:70:HIS:CG	3:F:6:ILE:HD12	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:MET:HE2	1:D:217:TRP:HH2	1.80	0.44
1:P:176:LYS:HA	1:P:180:GLN:HE21	1.82	0.44
2:Q:15:ALA:CB	2:Q:97:ARG:HG3	2.47	0.44
4:L:184:THR:OG1	4:L:187:GLN:OE1	2.27	0.44
1:A:35:ARG:NH1	1:A:48:ARG:CZ	2.80	0.44
1:A:215:LEU:CD2	1:A:261:VAL:HG22	2.47	0.44
2:B:96:ASP:O	2:B:97:ARG:C	2.61	0.44
2:Q:21:ASN:OD1	2:Q:22:PHE:N	2.43	0.44
5:T:131:ALA:HA	5:T:132:PRO:HD3	1.69	0.44
5:T:136:SER:O	5:T:138:SER:N	2.49	0.44
1:J:6:ARG:NH2	1:J:102:ASP:OD1	2.51	0.44
4:L:135:LEU:HB2	4:L:181:LEU:HB3	1.99	0.44
1:D:43:GLN:O	1:D:68:LYS:HE3	2.18	0.44
5:T:195:LEU:HD12	5:T:195:LEU:HA	1.78	0.44
4:L:153:ALA:HB2	4:L:194:TYR:CE2	2.53	0.44
4:G:17:SER:CB	4:G:78:SER:HB3	2.48	0.44
4:S:152:LYS:HD3	4:S:157:PRO:HA	2.00	0.44
5:T:138:SER:O	5:T:140:GLY:HA2	2.17	0.44
1:P:81:LEU:HD13	1:P:118:TYR:CD1	2.53	0.44
1:P:256:ARG:NH1	1:P:256:ARG:CG	2.69	0.44
4:S:48:LEU:HD21	4:S:51:HIS:HB3	1.99	0.44
5:O:106:MET:HE2	5:O:106:MET:HB2	1.84	0.44
5:O:136:SER:C	5:O:138:SER:N	2.75	0.44
1:A:167:TRP:HZ2	5:H:54:SER:HA	1.82	0.43
5:O:87:ARG:O	5:O:117:VAL:HG21	2.18	0.43
5:O:191:PRO:O	5:O:192:SER:C	2.59	0.43
5:T:150:ASP:H	5:T:183:SER:HB3	1.83	0.43
1:D:82:ARG:HH11	1:D:82:ARG:HG2	1.83	0.43
1:J:70:HIS:ND1	3:M:6:ILE:HD12	2.34	0.43
3:C:8:GLN:HE21	4:L:27:ARG:HD2	1.80	0.43
1:J:21:ARG:CZ	1:J:23:ILE:HD11	2.48	0.43
5:I:184:LEU:HD12	5:I:184:LEU:O	2.18	0.43
5:T:6:GLU:CD	5:T:112:GLY:H	2.27	0.43
5:T:68:PHE:CD1	5:T:68:PHE:N	2.86	0.43
1:D:6:ARG:HG3	1:D:6:ARG:HH11	1.83	0.43
2:K:13:HIS:O	2:K:14:PRO:C	2.61	0.43
4:G:1:GLN:H3	4:G:2:SER:CA	2.30	0.43
4:N:91:TRP:CH2	4:N:98:TYR:CD1	3.07	0.43
5:H:29:PHE:HB3	5:H:77:ASN:ND2	2.33	0.43
1:P:44:ARG:HA	1:P:64:THR:HG23	2.00	0.43
5:O:158:VAL:HG21	5:O:186:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:204:VAL:HG12	5:O:205:ASN:N	2.33	0.43
1:D:207:SER:HA	1:D:240:THR:HB	2.00	0.43
2:K:40:LEU:HA	2:K:44:GLU:O	2.18	0.43
5:H:176:LEU:HD13	5:H:182:TYR:CE1	2.53	0.43
5:O:70:ILE:HD11	5:O:79:LEU:HD11	2.01	0.43
5:T:52:GLY:N	5:T:57:GLY:HA3	2.32	0.43
5:T:150:ASP:OD1	5:T:177:GLN:OE1	2.35	0.43
5:T:156:VAL:HG13	5:T:157:THR:N	2.33	0.43
2:E:12:ARG:HG2	2:E:13:HIS:CD2	2.54	0.43
1:J:78:LEU:HA	1:J:78:LEU:HD23	1.82	0.43
4:G:151:TRP:CD1	4:G:151:TRP:N	2.87	0.43
5:I:174:ALA:HA	5:I:184:LEU:HB3	1.99	0.43
5:O:22:CYS:O	5:O:78:THR:HG22	2.19	0.43
1:D:21:ARG:NE	1:D:39:ASP:HB2	2.34	0.43
1:D:99:TYR:OH	3:F:3:LEU:HB2	2.19	0.43
1:D:163:THR:HG21	5:I:55:GLY:HA2	1.97	0.43
2:K:51:HIS:HD2	2:K:52:SER:O	2.01	0.43
4:S:163:GLU:OE1	4:S:163:GLU:HA	2.18	0.43
5:T:125:PRO:HB3	5:T:151:TYR:HB3	2.00	0.43
5:T:135:LYS:C	5:T:137:THR:H	2.27	0.43
4:L:191:HIS:HB2	4:L:194:TYR:HE1	1.84	0.43
4:S:68:LYS:HA	4:S:73:ALA:HA	2.00	0.43
4:S:91:TRP:CH2	5:T:105:GLY:HA2	2.54	0.43
1:A:227:ASP:HB3	1:A:248:VAL:HG13	2.01	0.43
1:P:202:ARG:NH1	2:Q:99:MET:O	2.50	0.43
3:C:8:GLN:NE2	4:L:27:ARG:HD3	2.24	0.43
4:L:91:TRP:CZ2	4:L:98:TYR:CD1	3.07	0.43
4:G:23:THR:HG22	4:G:72:THR:HG23	2.01	0.43
4:G:151:TRP:HB3	4:G:195:SER:O	2.19	0.43
4:N:37:TRP:CZ3	4:N:90:CYS:HB3	2.53	0.43
4:S:23:THR:CB	4:S:72:THR:HG23	2.48	0.43
5:T:4:LEU:HD22	5:T:22:CYS:SG	2.59	0.43
1:D:129:ASP:OD1	1:D:131:ARG:N	2.52	0.42
4:N:197:GLN:HB3	4:N:206:GLU:HG3	2.00	0.42
4:S:81:GLN:HB3	4:S:82:ALA:H	1.64	0.42
4:S:156:SER:HA	4:S:157:PRO:HD2	1.80	0.42
5:H:152:PHE:CG	5:H:153:PRO:CD	3.02	0.42
5:T:68:PHE:N	5:T:68:PHE:HD1	2.16	0.42
5:T:73:ASP:O	5:T:75:SER:N	2.51	0.42
1:D:103:VAL:CG2	1:D:107:TRP:HA	2.49	0.42
4:L:83:GLU:O	4:L:83:GLU:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:168:GLY:O	5:O:188:VAL:HA	2.19	0.42
5:T:171:THR:HA	5:T:186:SER:HA	2.01	0.42
1:A:72:GLN:HE22	4:L:33:ASN:H	1.67	0.42
2:B:39:LEU:CD1	2:B:68:THR:HG22	2.48	0.42
1:D:70:HIS:CE1	3:F:6:ILE:CD1	3.02	0.42
1:D:111:ARG:HD3	1:D:113:TYR:CE2	2.55	0.42
1:P:17:ARG:NH1	1:P:17:ARG:CG	2.82	0.42
4:L:189:LYS:HB2	4:L:189:LYS:HE2	1.90	0.42
4:S:34:TYR:CD1	5:T:103:TYR:HB2	2.54	0.42
1:D:70:HIS:HE1	3:F:3:LEU:O	2.03	0.42
1:D:227:ASP:HB3	1:D:248:VAL:HG12	2.02	0.42
4:N:195:SER:OG	4:N:208:THR:HA	2.20	0.42
5:O:71:SER:OG	5:O:80:TYR:HB2	2.19	0.42
1:J:87:GLN:NE2	1:J:93:HIS:CE1	2.88	0.42
2:K:55:SER:HB3	2:K:63:TYR:CZ	2.55	0.42
5:H:87:ARG:HH11	5:H:87:ARG:HD2	1.66	0.42
5:T:132:PRO:HG3	5:T:144:LEU:HB2	2.00	0.42
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.55	0.42
1:A:107:TRP:CD1	1:A:107:TRP:N	2.86	0.42
2:K:83:ASN:ND2	2:K:84:HIS:H	2.18	0.42
4:G:28:ASP:O	4:G:29:VAL:C	2.63	0.42
4:S:91:TRP:HA	4:S:99:VAL:O	2.19	0.42
4:S:118:VAL:O	4:S:207:LYS:HE2	2.20	0.42
5:H:144:LEU:HD12	5:H:144:LEU:C	2.45	0.42
1:A:81:LEU:O	1:A:82:ARG:C	2.62	0.42
1:A:218:GLN:HG3	1:A:260:HIS:CD2	2.55	0.42
4:G:41:HIS:O	4:G:42:PRO:C	2.63	0.42
4:G:125:SER:O	4:G:126:GLU:C	2.61	0.42
1:J:45:MET:HE1	3:M:2:LEU:HD11	2.01	0.42
4:N:152:LYS:HD3	4:N:152:LYS:HA	1.75	0.42
4:N:170:GLN:HE21	4:N:170:GLN:HB2	1.72	0.42
5:H:29:PHE:CB	5:H:77:ASN:ND2	2.83	0.42
5:H:100:LEU:O	5:H:100:LEU:HD22	2.19	0.42
5:I:98:GLY:O	5:I:106:MET:HA	2.19	0.42
2:E:23:LEU:HB2	2:E:70:PHE:CZ	2.55	0.42
2:K:0:MET:HE2	2:K:0:MET:HB3	2.01	0.42
1:P:25:VAL:HG21	1:P:27:TYR:HE1	1.85	0.42
4:L:195:SER:HA	4:L:207:LYS:O	2.20	0.42
4:S:185:PRO:O	4:S:188:TRP:HB3	2.20	0.42
2:Q:97:ARG:HE	2:Q:97:ARG:HB3	1.75	0.41
4:G:1:GLN:H3	4:G:2:SER:HA	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:57:PRO:HG2	4:G:60:VAL:CG2	2.49	0.41
5:O:46:GLU:O	5:O:47:TRP:HB3	2.20	0.41
1:D:51:TRP:CZ2	1:D:179:LEU:HD11	2.55	0.41
4:N:124:SER:OG	4:N:125:SER:N	2.52	0.41
4:S:39:GLN:HG3	4:S:88:TYR:CZ	2.55	0.41
5:H:134:SER:O	5:H:137:THR:HB	2.20	0.41
5:T:70:ILE:HG23	5:T:70:ILE:O	2.20	0.41
2:K:83:ASN:HB2	2:K:90:PRO:HB3	2.02	0.41
4:G:161:GLY:O	4:G:181:LEU:HA	2.20	0.41
5:O:132:PRO:HG3	5:O:144:LEU:HB3	2.02	0.41
5:T:137:THR:HG22	5:T:137:THR:O	2.20	0.41
1:D:21:ARG:HE	1:D:39:ASP:HB2	1.85	0.41
1:D:173:GLU:O	1:D:176:LYS:HD2	2.20	0.41
1:P:103:VAL:HG12	1:P:109:PHE:HA	2.02	0.41
4:G:16:GLN:O	4:G:80:LEU:HB2	2.20	0.41
4:N:94:ALA:CB	4:N:97:TYR:CE1	3.04	0.41
5:T:152:PHE:HA	5:T:153:PRO:HA	1.70	0.41
1:A:77:ASP:O	1:A:78:LEU:C	2.63	0.41
2:B:61:SER:H	2:B:61:SER:HG	1.57	0.41
1:D:1:GLY:O	1:D:3:HIS:CE1	2.73	0.41
1:D:129:ASP:OD1	1:D:129:ASP:C	2.63	0.41
1:D:226:GLN:HE21	1:D:226:GLN:HB3	1.51	0.41
4:G:26:SER:HA	4:G:71:ASN:HD21	1.84	0.41
4:G:56:ARG:CZ	4:G:62:ASP:HB2	2.50	0.41
4:G:89:TYR:CE1	4:G:103:GLY:HA3	2.56	0.41
4:G:151:TRP:CA	4:G:152:LYS:HB2	2.48	0.41
4:N:38:TYR:OH	5:O:106:MET:N	2.53	0.41
4:S:4:LEU:HB2	4:S:101:GLY:CA	2.50	0.41
4:S:51:HIS:O	4:S:52:ASP:HB2	2.21	0.41
5:O:177:GLN:C	5:O:179:SER:H	2.28	0.41
1:A:111:ARG:NH1	1:A:128:GLU:HG3	2.36	0.41
2:E:74:GLU:HG3	2:E:75:LYS:HB2	2.01	0.41
2:Q:75:LYS:HB2	2:Q:75:LYS:NZ	2.34	0.41
4:L:204:THR:CG2	4:L:205:VAL:N	2.83	0.41
4:N:20:ILE:O	4:N:74:SER:HA	2.20	0.41
4:S:18:VAL:O	4:S:76:THR:HA	2.21	0.41
4:S:143:TYR:HA	4:S:144:PRO:C	2.44	0.41
1:A:219:ARG:O	1:A:222:GLU:HG2	2.21	0.41
2:B:73:THR:OG1	2:B:76:ASP:OD2	2.39	0.41
3:C:6:ILE:H	3:C:6:ILE:HG12	1.71	0.41
3:F:8:GLN:NE2	4:G:27:ARG:HE	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:34:MET:CB	5:H:79:LEU:HD13	2.51	0.41
5:H:160:TRP:CE3	5:H:202:CYS:HB3	2.54	0.41
5:O:131:ALA:HA	5:O:132:PRO:HD3	1.93	0.41
1:J:159:TYR:CG	3:M:3:LEU:HD13	2.56	0.41
2:K:97:ARG:HE	2:K:97:ARG:HB2	1.58	0.41
4:G:37:TRP:CE3	4:G:90:CYS:HB3	2.56	0.41
4:G:61:PRO:HG2	4:G:64:PHE:CE2	2.53	0.41
4:G:99:VAL:CG2	4:G:100:PHE:N	2.83	0.41
4:G:152:LYS:CG	4:G:195:SER:HB2	2.50	0.41
5:O:49:SER:HB3	5:O:70:ILE:HD12	2.03	0.41
2:B:47:GLU:N	2:B:47:GLU:OE2	2.53	0.41
4:L:51:HIS:O	4:L:52:ASP:HB2	2.21	0.41
4:L:82:ALA:C	4:L:84:ASP:H	2.29	0.41
4:G:1:GLN:HB2	4:G:97:TYR:CE1	2.56	0.41
4:G:131:ASN:ND2	4:G:185:PRO:HG2	2.35	0.41
4:G:152:LYS:HA	4:G:152:LYS:HD3	1.77	0.41
5:I:123:LYS:HE2	5:I:150:ASP:O	2.21	0.41
5:I:215:LYS:HE3	5:I:215:LYS:HA	2.03	0.41
5:O:37:VAL:CG1	5:O:38:ARG:N	2.84	0.41
5:O:83:MET:HE1	5:O:115:VAL:HG21	2.02	0.41
5:O:207:LYS:N	5:O:208:PRO:CD	2.84	0.41
1:A:156:LEU:HD13	1:A:156:LEU:HA	1.89	0.41
2:K:10:TYR:CD1	2:K:10:TYR:N	2.88	0.41
1:P:49:ALA:O	1:P:52:ILE:HG22	2.21	0.41
4:L:80:LEU:CD2	4:L:108:VAL:HG22	2.50	0.41
4:G:57:PRO:HG2	4:G:60:VAL:HG23	2.03	0.41
4:S:111:GLN:HB2	4:S:112:PRO:HD2	2.02	0.41
5:O:8:GLY:O	5:O:20:LEU:HD23	2.21	0.41
5:O:67:ARG:C	5:O:68:PHE:HD1	2.29	0.41
5:T:158:VAL:HG22	5:T:204:VAL:HG22	2.02	0.41
2:E:41:LYS:HE3	2:E:78:TYR:OH	2.21	0.40
4:G:1:GLN:CD	5:I:62:ASP:HB2	2.46	0.40
2:B:12:ARG:O	2:B:12:ARG:HG2	2.18	0.40
1:J:28:VAL:O	1:J:29:ASP:C	2.64	0.40
1:P:129:ASP:CG	1:P:131:ARG:HB2	2.46	0.40
1:P:213:ILE:HG13	1:P:262:GLN:O	2.21	0.40
4:S:137:CYS:HB2	4:S:151:TRP:CH2	2.56	0.40
5:T:220:LYS:NZ	5:T:220:LYS:H	2.18	0.40
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.86	0.40
2:E:1:ILE:HD12	2:E:1:ILE:HA	1.93	0.40
1:J:175:GLY:O	1:J:176:LYS:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:161:GLY:O	4:L:181:LEU:HA	2.22	0.40
1:A:35:ARG:HD3	2:B:53:ASP:OD2	2.22	0.40
2:B:21:ASN:OD1	2:B:22:PHE:N	2.51	0.40
1:P:257:TYR:CD1	1:P:257:TYR:N	2.88	0.40
4:L:141:ASP:C	4:L:174:LYS:HD3	2.46	0.40
5:H:34:MET:HB3	5:H:79:LEU:HD13	2.04	0.40
5:I:60:TYR:OH	5:I:70:ILE:HG22	2.22	0.40
1:P:35:ARG:HD3	2:Q:53:ASP:OD2	2.22	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	274/276 (99%)	261 (95%)	10 (4%)	3 (1%)	11	36
1	D	274/276 (99%)	258 (94%)	15 (6%)	1 (0%)	30	59
1	J	274/276 (99%)	260 (95%)	12 (4%)	2 (1%)	18	48
1	P	274/276 (99%)	260 (95%)	11 (4%)	3 (1%)	11	36
2	B	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	12	39
2	E	98/100 (98%)	86 (88%)	10 (10%)	2 (2%)	6	22
2	K	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
2	Q	98/100 (98%)	86 (88%)	9 (9%)	3 (3%)	3	14
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
3	M	7/9 (78%)	7 (100%)	0	0	100	100
3	R	7/9 (78%)	7 (100%)	0	0	100	100
4	G	209/212 (99%)	182 (87%)	23 (11%)	4 (2%)	6	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	209/212 (99%)	186 (89%)	17 (8%)	6 (3%)	3	15
4	N	209/212 (99%)	183 (88%)	19 (9%)	7 (3%)	3	13
4	S	209/212 (99%)	186 (89%)	20 (10%)	3 (1%)	9	30
5	H	218/220 (99%)	197 (90%)	10 (5%)	11 (5%)	1	6
5	I	218/220 (99%)	189 (87%)	21 (10%)	8 (4%)	2	11
5	O	218/220 (99%)	189 (87%)	19 (9%)	10 (5%)	2	7
5	T	218/220 (99%)	188 (86%)	18 (8%)	12 (6%)	1	4
All	All	3224/3268 (99%)	2917 (90%)	231 (7%)	76 (2%)	4	18

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLY
1	D	18	GLY
1	J	18	GLY
1	P	18	GLY
4	L	2	SER
4	L	3	GLU
4	G	152	LYS
4	N	62	ASP
4	N	152	LYS
4	S	111	GLN
5	H	136	SER
5	H	153	PRO
5	I	31	ALA
5	O	27	PHE
5	T	53	SER
5	T	133	SER
5	T	136	SER
5	T	137	THR
5	T	162	SER
1	J	86	ASN
4	L	5	THR
4	N	80	LEU
4	N	130	ALA
4	N	160	ALA
5	H	47	TRP
5	H	53	SER
5	H	57	GLY
5	H	65	LYS

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Mol	Chain	Res	Type
5	I	30	SER
5	I	56	GLY
5	I	140	GLY
5	O	137	THR
5	O	139	GLY
5	O	140	GLY
5	O	145	GLY
5	O	192	SER
5	T	47	TRP
5	T	58	THR
5	T	74	ASN
5	T	140	GLY
1	A	86	ASN
2	B	17	ASN
2	E	74	GLU
2	Q	17	ASN
2	Q	74	GLU
4	G	153	ALA
4	G	201	GLU
4	N	185	PRO
5	H	54	SER
5	I	32	TYR
5	I	145	GLY
5	I	178	SER
5	O	178	SER
5	T	139	GLY
2	E	1	ILE
1	P	220	ASP
4	L	4	LEU
4	L	91	TRP
4	L	155	GLY
4	G	176	ALA
4	N	2	SER
4	S	3	GLU
5	H	89	GLU
5	T	57	GLY
1	P	86	ASN
4	S	26	SER
5	H	75	SER
5	H	150	ASP
5	O	2	VAL
5	O	62	ASP

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Mol	Chain	Res	Type
5	O	162	SER
1	A	119	ASP
5	I	144	LEU
5	T	191	PRO
2	Q	35	ILE
5	H	55	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	232/232 (100%)	202 (87%)	30 (13%)	4	13
1	D	232/232 (100%)	202 (87%)	30 (13%)	4	13
1	J	232/232 (100%)	202 (87%)	30 (13%)	4	13
1	P	232/232 (100%)	205 (88%)	27 (12%)	5	18
2	B	95/95 (100%)	83 (87%)	12 (13%)	4	14
2	E	95/95 (100%)	83 (87%)	12 (13%)	4	14
2	K	95/95 (100%)	83 (87%)	12 (13%)	4	14
2	Q	95/95 (100%)	83 (87%)	12 (13%)	4	14
3	C	9/9 (100%)	7 (78%)	2 (22%)	1	3
3	F	9/9 (100%)	7 (78%)	2 (22%)	1	3
3	M	9/9 (100%)	8 (89%)	1 (11%)	6	20
3	R	9/9 (100%)	7 (78%)	2 (22%)	1	3
4	G	178/179 (99%)	145 (82%)	33 (18%)	1	5
4	L	178/179 (99%)	154 (86%)	24 (14%)	4	12
4	N	178/179 (99%)	149 (84%)	29 (16%)	2	8
4	S	178/179 (99%)	151 (85%)	27 (15%)	3	9
5	H	178/178 (100%)	146 (82%)	32 (18%)	2	6
5	I	178/178 (100%)	149 (84%)	29 (16%)	2	8
5	O	178/178 (100%)	151 (85%)	27 (15%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	T	178/178 (100%)	145 (82%)	33 (18%)	1 5
All	All	2768/2772 (100%)	2362 (85%)	406 (15%)	3 10

All (406) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	14	ARG
1	A	35	ARG
1	A	58	GLU
1	A	67	VAL
1	A	68	LYS
1	A	71	SER
1	A	75	ARG
1	A	86	ASN
1	A	95	VAL
1	A	108	ARG
1	A	110	LEU
1	A	111	ARG
1	A	121	LYS
1	A	141	GLN
1	A	146	LYS
1	A	156	LEU
1	A	165	VAL
1	A	178	THR
1	A	180	GLN
1	A	181	ARG
1	A	216	THR
1	A	223	ASP
1	A	225	THR
1	A	228	THR
1	A	230	LEU
1	A	242	GLN
1	A	247	VAL
1	A	248	VAL
1	A	253	GLN
2	B	0	MET
2	B	6	LYS
2	B	9	VAL
2	B	19	LYS
2	B	25	CYS
2	B	34	ASP

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Mol	Chain	Res	Type
2	B	47	GLU
2	B	57	SER
2	B	71	THR
2	B	81	ARG
2	B	85	VAL
2	B	97	ARG
1	D	17	ARG
1	D	21	ARG
1	D	29	ASP
1	D	34	VAL
1	D	43	GLN
1	D	46	GLU
1	D	53	GLU
1	D	58	GLU
1	D	65	ARG
1	D	68	LYS
1	D	86	ASN
1	D	89	GLU
1	D	95	VAL
1	D	105	SER
1	D	115	GLN
1	D	121	LYS
1	D	128	GLU
1	D	141	GLN
1	D	156	LEU
1	D	176	LYS
1	D	181	ARG
1	D	216	THR
1	D	222	GLU
1	D	224	GLN
1	D	225	THR
1	D	228	THR
1	D	230	LEU
1	D	240	THR
1	D	247	VAL
1	D	268	LYS
2	E	0	MET
2	E	1	ILE
2	E	9	VAL
2	E	23	LEU
2	E	34	ASP
2	E	46	ILE

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Mol	Chain	Res	Type
2	E	50	GLU
2	E	57	SER
2	E	74	GLU
2	E	75	LYS
2	E	88	SER
2	E	94	LYS
1	J	2	SER
1	J	6	ARG
1	J	11	SER
1	J	25	VAL
1	J	34	VAL
1	J	35	ARG
1	J	64	THR
1	J	67	VAL
1	J	72	GLN
1	J	73	THR
1	J	111	ARG
1	J	115	GLN
1	J	121	LYS
1	J	124	ILE
1	J	128	GLU
1	J	138	MET
1	J	141	GLN
1	J	156	LEU
1	J	161	GLU
1	J	165	VAL
1	J	178	THR
1	J	187	THR
1	J	191	HIS
1	J	207	SER
1	J	225	THR
1	J	228	THR
1	J	230	LEU
1	J	247	VAL
1	J	248	VAL
1	J	272	LEU
2	K	0	MET
2	K	16	GLU
2	K	27	VAL
2	K	69	GLU
2	K	70	PHE
2	K	74	GLU

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Mol	Chain	Res	Type
2	K	81	ARG
2	K	85	VAL
2	K	88	SER
2	K	92	ILE
2	K	94	LYS
2	K	99	MET
1	P	6	ARG
1	P	23	ILE
1	P	34	VAL
1	P	67	VAL
1	P	86	ASN
1	P	108	ARG
1	P	111	ARG
1	P	115	GLN
1	P	121	LYS
1	P	124	ILE
1	P	131	ARG
1	P	138	MET
1	P	154	GLU
1	P	178	THR
1	P	196	ASP
1	P	200	THR
1	P	218	GLN
1	P	222	GLU
1	P	226	GLN
1	P	228	THR
1	P	232	GLU
1	P	240	THR
1	P	247	VAL
1	P	251	SER
1	P	253	GLN
1	P	256	ARG
1	P	268	LYS
2	Q	1	ILE
2	Q	6	LYS
2	Q	7	ILE
2	Q	34	ASP
2	Q	48	LYS
2	Q	57	SER
2	Q	67	TYR
2	Q	75	LYS
2	Q	81	ARG

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Mol	Chain	Res	Type
2	Q	85	VAL
2	Q	94	LYS
2	Q	99	MET
3	C	6	ILE
3	C	8	GLN
3	F	3	LEU
3	F	6	ILE
3	M	6	ILE
3	R	3	LEU
3	R	6	ILE
4	L	8	ARG
4	L	10	VAL
4	L	23	THR
4	L	36	SER
4	L	44	LYS
4	L	63	ARG
4	L	65	SER
4	L	68	LYS
4	L	83	GLU
4	L	120	LEU
4	L	147	VAL
4	L	148	THR
4	L	158	VAL
4	L	159	LYS
4	L	166	LYS
4	L	169	LYS
4	L	182	SER
4	L	184	THR
4	L	186	GLU
4	L	190	SER
4	L	197	GLN
4	L	203	ASN
4	L	205	VAL
4	L	206	GLU
4	G	1	GLN
4	G	19	THR
4	G	23	THR
4	G	25	THR
4	G	28	ASP
4	G	53	VAL
4	G	63	ARG
4	G	69	SER

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Mol	Chain	Res	Type
4	G	74	SER
4	G	78	SER
4	G	81	GLN
4	G	83	GLU
4	G	99	VAL
4	G	117	THR
4	G	124	SER
4	G	135	LEU
4	G	138	LEU
4	G	139	ILE
4	G	140	SER
4	G	151	TRP
4	G	152	LYS
4	G	156	SER
4	G	166	LYS
4	G	170	GLN
4	G	173	ASN
4	G	174	LYS
4	G	186	GLU
4	G	189	LYS
4	G	203	ASN
4	G	204	THR
4	G	205	VAL
4	G	206	GLU
4	G	208	THR
4	N	3	GLU
4	N	5	THR
4	N	11	SER
4	N	20	ILE
4	N	23	THR
4	N	28	ASP
4	N	44	LYS
4	N	58	SER
4	N	65	SER
4	N	69	SER
4	N	71	ASN
4	N	74	SER
4	N	78	SER
4	N	85	GLU
4	N	107	THR
4	N	117	THR
4	N	125	SER

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Mol	Chain	Res	Type
4	N	127	GLU
4	N	129	GLN
4	N	135	LEU
4	N	147	VAL
4	N	151	TRP
4	N	156	SER
4	N	158	VAL
4	N	166	LYS
4	N	168	SER
4	N	178	SER
4	N	190	SER
4	N	195	SER
4	S	4	LEU
4	S	8	ARG
4	S	9	SER
4	S	20	ILE
4	S	22	CYS
4	S	23	THR
4	S	28	ASP
4	S	48	LEU
4	S	56	ARG
4	S	58	SER
4	S	62	ASP
4	S	63	ARG
4	S	74	SER
4	S	77	ILE
4	S	91	TRP
4	S	117	THR
4	S	131	ASN
4	S	147	VAL
4	S	156	SER
4	S	158	VAL
4	S	169	LYS
4	S	171	SER
4	S	178	SER
4	S	183	LEU
4	S	189	LYS
4	S	195	SER
4	S	199	THR
5	H	1	GLU
5	H	18	LEU
5	H	21	SER

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Mol	Chain	Res	Type
5	H	25	SER
5	H	28	THR
5	H	50	SER
5	H	54	SER
5	H	62	ASP
5	H	63	SER
5	H	71	SER
5	H	89	GLU
5	H	91	THR
5	H	100	LEU
5	H	122	THR
5	H	123	LYS
5	H	134	SER
5	H	136	SER
5	H	138	SER
5	H	141	THR
5	H	156	VAL
5	H	165	LEU
5	H	166	THR
5	H	177	GLN
5	H	181	LEU
5	H	185	SER
5	H	187	VAL
5	H	189	THR
5	H	192	SER
5	H	195	LEU
5	H	199	THR
5	H	205	ASN
5	H	220	LYS
5	I	2	VAL
5	I	3	GLN
5	I	5	LEU
5	I	18	LEU
5	I	20	LEU
5	I	28	THR
5	I	30	SER
5	I	50	SER
5	I	76	LYS
5	I	87	ARG
5	I	100	LEU
5	I	108	VAL
5	I	114	THR

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Mol	Chain	Res	Type
5	I	123	LYS
5	I	134	SER
5	I	138	SER
5	I	144	LEU
5	I	157	THR
5	I	165	LEU
5	I	184	LEU
5	I	186	SER
5	I	189	THR
5	I	192	SER
5	I	193	SER
5	I	195	LEU
5	I	199	THR
5	I	207	LYS
5	I	215	LYS
5	I	220	LYS
5	O	1	GLU
5	O	2	VAL
5	O	3	GLN
5	O	5	LEU
5	O	18	LEU
5	O	49	SER
5	O	58	THR
5	O	78	THR
5	O	111	GLN
5	O	118	SER
5	O	121	SER
5	O	123	LYS
5	O	134	SER
5	O	136	SER
5	O	144	LEU
5	O	146	CYS
5	O	156	VAL
5	O	165	LEU
5	O	187	VAL
5	O	189	THR
5	O	201	ILE
5	O	202	CYS
5	O	212	LYS
5	O	216	LYS
5	O	217	VAL
5	O	218	GLU

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Mol	Chain	Res	Type
5	O	220	LYS
5	T	1	GLU
5	T	2	VAL
5	T	7	SER
5	T	12	VAL
5	T	43	LYS
5	T	68	PHE
5	T	69	THR
5	T	78	THR
5	T	91	THR
5	T	111	GLN
5	T	116	THR
5	T	118	SER
5	T	121	SER
5	T	134	SER
5	T	135	LYS
5	T	138	SER
5	T	141	THR
5	T	156	VAL
5	T	157	THR
5	T	165	LEU
5	T	167	SER
5	T	178	SER
5	T	187	VAL
5	T	189	THR
5	T	195	LEU
5	T	201	ILE
5	T	202	CYS
5	T	203	ASN
5	T	207	LYS
5	T	211	THR
5	T	216	LYS
5	T	218	GLU
5	T	220	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	43	GLN
1	A	72	GLN
1	A	74	HIS

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Mol	Chain	Res	Type
1	A	141	GLN
1	A	174	ASN
1	A	188	HIS
1	A	224	GLN
1	A	242	GLN
1	A	253	GLN
1	A	255	GLN
2	B	2	GLN
2	B	31	HIS
2	B	83	ASN
1	D	43	GLN
1	D	74	HIS
1	D	141	GLN
1	D	174	ASN
1	D	226	GLN
1	D	242	GLN
1	D	253	GLN
1	D	255	GLN
1	D	262	GLN
2	E	2	GLN
2	E	31	HIS
2	E	83	ASN
2	E	89	GLN
1	J	3	HIS
1	J	43	GLN
1	J	72	GLN
1	J	87	GLN
1	J	115	GLN
1	J	141	GLN
1	J	155	GLN
1	J	174	ASN
1	J	191	HIS
1	J	242	GLN
1	J	253	GLN
2	K	42	ASN
2	K	51	HIS
2	K	83	ASN
1	P	3	HIS
1	P	43	GLN
1	P	54	GLN
1	P	72	GLN
1	P	115	GLN

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Mol	Chain	Res	Type
1	P	151	HIS
1	P	155	GLN
1	P	174	ASN
1	P	180	GLN
1	P	191	HIS
1	P	226	GLN
1	P	242	GLN
1	P	262	GLN
2	Q	13	HIS
2	Q	31	HIS
2	Q	51	HIS
2	Q	84	HIS
2	Q	89	GLN
3	C	8	GLN
3	F	8	GLN
3	M	8	GLN
3	R	8	GLN
4	L	1	GLN
4	L	51	HIS
4	L	71	ASN
4	L	111	GLN
4	L	129	GLN
4	L	173	ASN
4	G	1	GLN
4	G	40	GLN
4	G	71	ASN
4	G	81	GLN
4	G	111	GLN
4	G	115	ASN
4	G	131	ASN
4	G	173	ASN
4	G	187	GLN
4	N	81	GLN
4	N	115	ASN
4	N	129	GLN
4	N	173	ASN
4	N	187	GLN
4	N	200	HIS
4	N	203	ASN
4	S	71	ASN
4	S	81	GLN
4	S	111	GLN

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Mol	Chain	Res	Type
4	S	129	GLN
4	S	170	GLN
4	S	172	ASN
4	S	191	HIS
5	H	13	GLN
5	H	77	ASN
5	H	84	ASN
5	H	198	GLN
5	H	205	ASN
5	I	3	GLN
5	I	39	GLN
5	I	74	ASN
5	I	77	ASN
5	I	170	HIS
5	I	198	GLN
5	O	3	GLN
5	O	77	ASN
5	T	77	ASN
5	T	177	GLN
5	T	198	GLN
5	T	210	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/276 (100%)	-0.18	0 100 100	2, 2, 2, 2	0
1	D	276/276 (100%)	-0.08	2 (0%) 84 79	2, 2, 2, 2	0
1	J	276/276 (100%)	-0.00	1 (0%) 88 85	2, 2, 2, 2	0
1	P	276/276 (100%)	-0.25	0 100 100	2, 2, 2, 2	0
2	B	100/100 (100%)	0.76	11 (11%) 10 9	2, 2, 2, 2	0
2	E	100/100 (100%)	0.02	1 (1%) 79 73	2, 2, 2, 2	0
2	K	100/100 (100%)	-0.08	1 (1%) 79 73	2, 2, 2, 2	0
2	Q	100/100 (100%)	-0.32	0 100 100	2, 2, 2, 2	0
3	C	9/9 (100%)	1.55	4 (44%) 0 0	2, 2, 2, 2	0
3	F	9/9 (100%)	0.83	1 (11%) 10 9	2, 2, 2, 2	0
3	M	9/9 (100%)	1.04	1 (11%) 10 9	2, 2, 2, 2	0
3	R	9/9 (100%)	-0.32	0 100 100	2, 2, 2, 2	0
4	G	211/212 (99%)	0.17	2 (0%) 81 75	2, 2, 2, 2	0
4	L	211/212 (99%)	0.21	9 (4%) 40 31	2, 2, 2, 2	0
4	N	211/212 (99%)	0.41	20 (9%) 14 11	2, 2, 2, 2	0
4	S	211/212 (99%)	-0.38	0 100 100	2, 2, 2, 2	0
5	H	220/220 (100%)	-0.06	6 (2%) 56 47	2, 2, 2, 2	0
5	I	220/220 (100%)	0.20	6 (2%) 56 47	2, 2, 2, 2	0
5	O	220/220 (100%)	0.10	6 (2%) 56 47	2, 2, 2, 2	0
5	T	220/220 (100%)	-0.38	2 (0%) 81 75	2, 2, 2, 2	0
All	All	3264/3268 (99%)	-0.01	73 (2%) 62 53	2, 2, 2, 2	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	136	SER	6.9
4	N	171	SER	5.5
5	O	136	SER	5.2
2	B	60	TRP	3.8
4	N	117	THR	3.8
5	O	134	SER	3.7
1	J	276	PRO	3.6
5	I	139	GLY	3.3
4	N	112	PRO	3.3
5	H	57	GLY	3.2
4	N	194	TYR	3.1
2	B	56	PHE	3.1
5	I	135	LYS	2.9
5	O	220	LYS	2.9
2	B	44	GLU	2.8
4	N	159	LYS	2.8
2	B	54	LEU	2.8
5	H	137	THR	2.8
5	T	136	SER	2.8
4	N	173	ASN	2.7
4	N	169	LYS	2.6
5	H	139	GLY	2.6
4	N	1	GLN	2.6
4	L	112	PRO	2.6
5	O	135	LYS	2.6
2	B	69	GLU	2.6
5	I	138	SER	2.6
4	L	169	LYS	2.6
4	N	209	VAL	2.6
4	L	3	GLU	2.6
4	L	114	ALA	2.5
3	C	1	SER	2.5
5	H	220	LYS	2.5
5	H	111	GLN	2.5
4	N	153	ALA	2.5
5	O	138	SER	2.5
4	N	160	ALA	2.5
4	L	1	GLN	2.4
2	B	3	ARG	2.4
4	N	168	SER	2.4
4	L	176	ALA	2.4
4	L	175	TYR	2.3
4	N	141	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	276	PRO	2.3
4	N	3	GLU	2.3
2	B	63	TYR	2.3
2	B	77	GLU	2.3
2	B	57	SER	2.3
5	I	137	THR	2.3
4	N	119	THR	2.2
1	D	150	ALA	2.2
4	L	186	GLU	2.2
2	K	98	ASP	2.2
3	C	9	VAL	2.2
4	L	168	SER	2.2
4	N	178	SER	2.2
5	O	139	GLY	2.2
4	G	1	GLN	2.2
3	F	9	VAL	2.2
4	N	158	VAL	2.1
3	M	1	SER	2.1
5	I	31	ALA	2.1
2	B	1	ILE	2.1
3	C	2	LEU	2.1
5	H	136	SER	2.1
4	N	175	TYR	2.1
5	T	133	SER	2.1
2	B	62	PHE	2.1
4	N	172	ASN	2.0
3	C	5	TRP	2.0
2	E	0	MET	2.0
4	N	176	ALA	2.0
4	G	206	GLU	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.