



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:49 PM UTC

PDB ID : 1N5A / pdb_00001n5a
Title : Crystal structure of the Murine class I Major Histocompatibility Complex of H-2DB, B2-Microglobulin, and A 9-Residue immunodominant peptide epitope gp33 derived from LCMV
Authors : Achour, A.; Michaelsson, J.; Harris, R.A.; Odeberg, J.; Grufman, P.; Sandberg, J.K.; Levitsky, V.; Karre, K.; Sandalova, T.; Schneider, G.
Deposited on : 2002-11-05
Resolution : 2.85 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

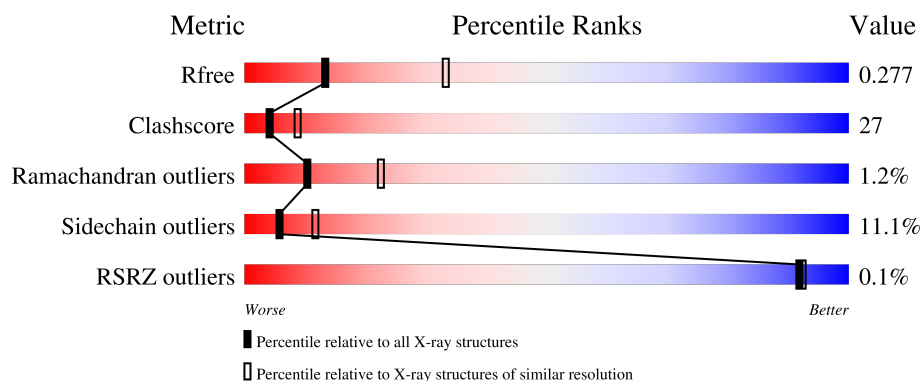
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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.



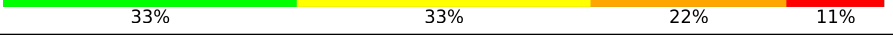
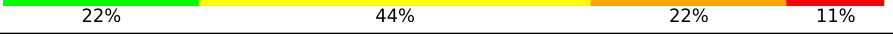
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	 49% 42% 7% •
1	D	276	 52% 36% 9% ••
1	G	276	 51% 40% 7% ••
1	J	276	 54% 38% 6% ••
2	B	99	 56% 36% 5% ••

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Mol	Chain	Length	Quality of chain
2	E	99	
2	H	99	
2	K	99	
3	C	9	
3	F	9	
3	I	9	
3	L	9	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12633 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2265	1430	400	426	9			
1	D	274	Total	C	N	O	S	0	0	0
			2248	1420	398	421	9			
1	G	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			
1	J	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			812	519	137	150	6			
2	E	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	H	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	K	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 3 is a protein called nonameric peptide, gp33 derived from lymphocytic choriomeningitis virus.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			
3	F	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			
3	I	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			
3	L	9	Total	C	N	O	S	0	0	0
			73	48	11	13	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	9	MET	CYS	engineered mutation	UNP Q9QDK7
F	9	MET	CYS	engineered mutation	UNP Q9QDK7
I	9	MET	CYS	engineered mutation	UNP Q9QDK7
L	9	MET	CYS	engineered mutation	UNP Q9QDK7

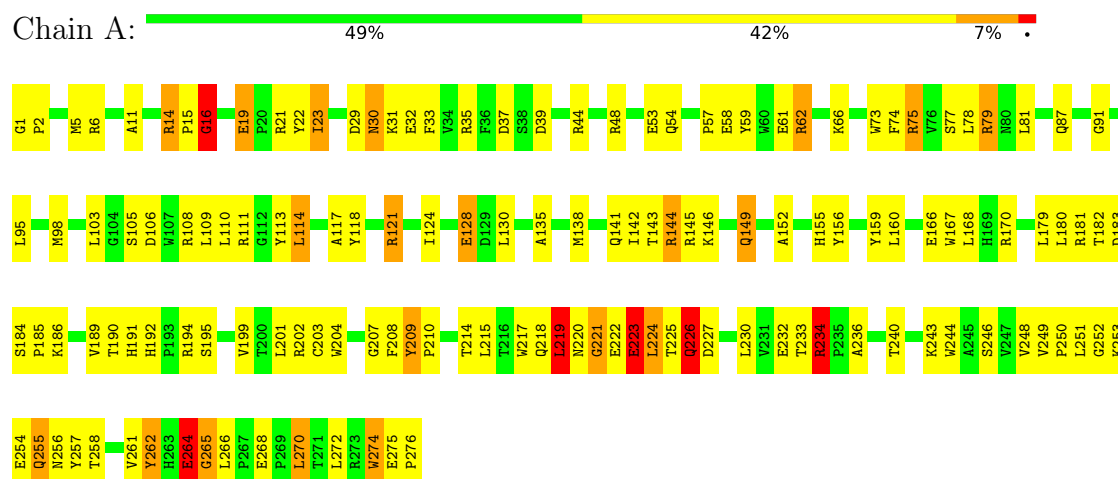
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	7	Total O 7 7	0	0
4	D	12	Total O 12 12	0	0
4	E	2	Total O 2 2	0	0
4	G	9	Total O 9 9	0	0
4	H	5	Total O 5 5	0	0
4	J	10	Total O 10 10	0	0
4	K	7	Total O 7 7	0	0
4	L	1	Total O 1 1	0	0

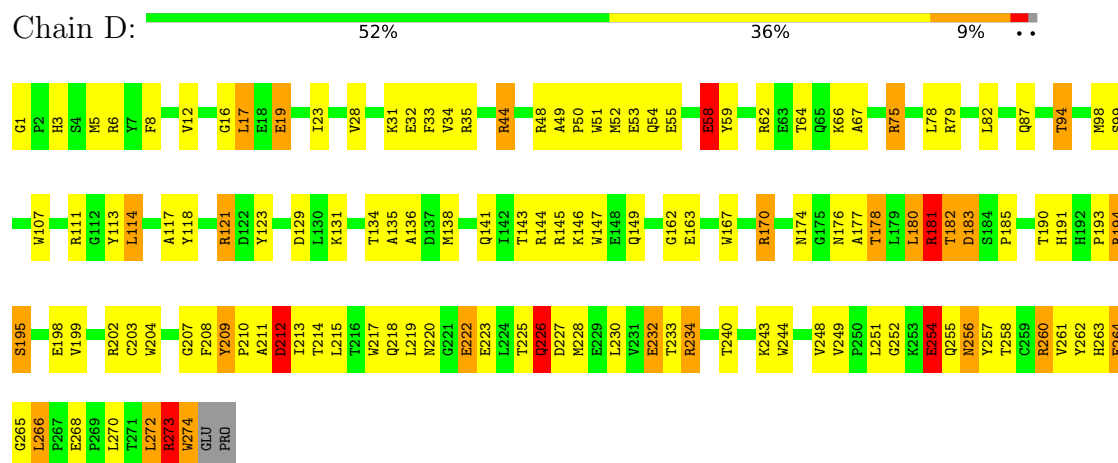
3 Residue-property plots

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

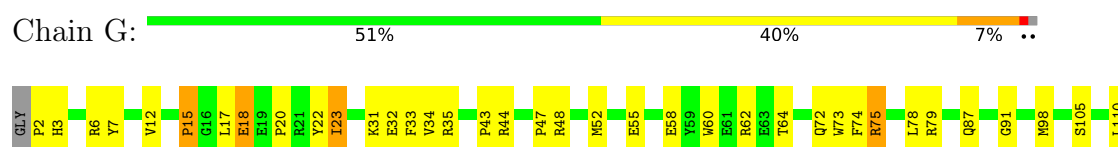
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

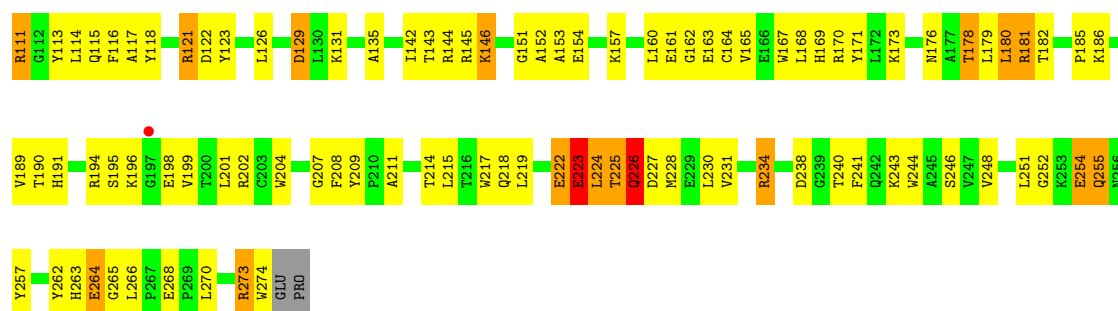


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



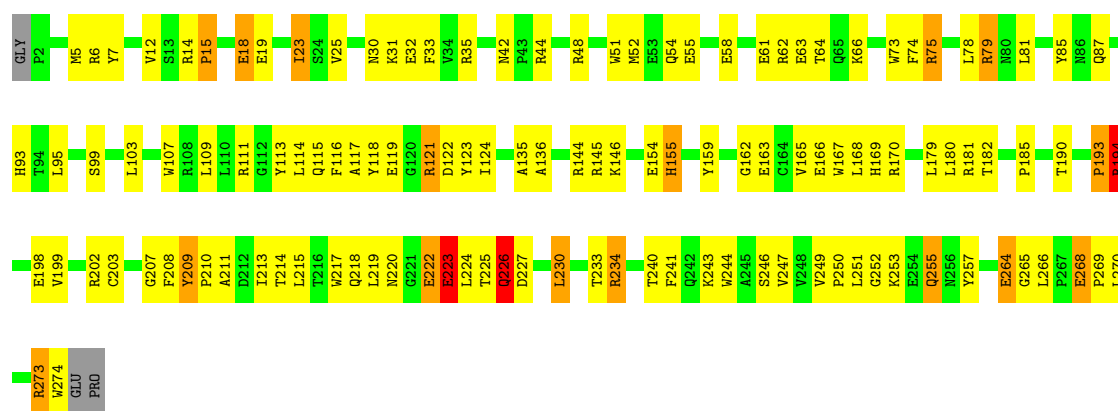
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain





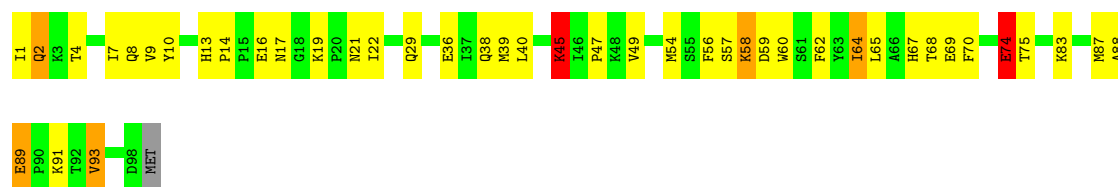
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain J: 54% 38% 6% ..



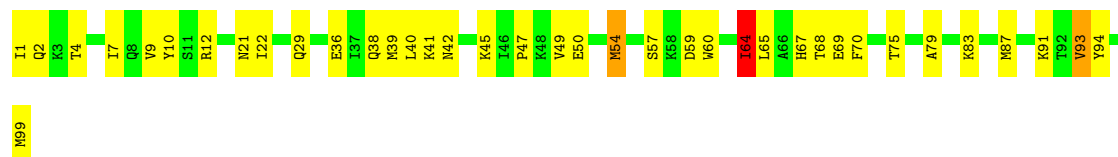
- Molecule 2: Beta-2-microglobulin

Chain B: 56% 36% 5% ..



- Molecule 2: Beta-2-microglobulin

Chain E: 62% 35% ..



- Molecule 2: Beta-2-microglobulin

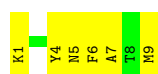
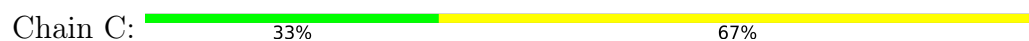
Chain H: 68% 27% 5%



- Molecule 2: Beta-2-microglobulin



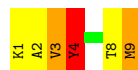
- Molecule 3: nonameric peptide, gp33 derived from lymphocytic choriomeningitis virus



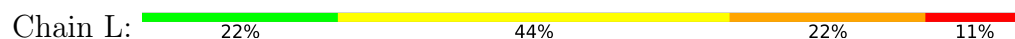
- Molecule 3: nonameric peptide, gp33 derived from lymphocytic choriomeningitis virus



- Molecule 3: nonameric peptide, gp33 derived from lymphocytic choriomeningitis virus



- Molecule 3: nonameric peptide, gp33 derived from lymphocytic choriomeningitis virus



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.00Å 122.66Å 99.18Å 90.00° 103.34° 90.00°	Depositor
Resolution (Å)	19.92 – 2.85 19.92 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.92-2.85) 91.1 (19.92-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.95 (at 2.83Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.251 , 0.279 0.252 , 0.277	Depositor DCC
R_{free} test set	2289 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 20.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12633	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.47% 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	1.16	9/2332 (0.4%)	1.43	27/3166 (0.9%)
1	D	1.19	7/2314 (0.3%)	1.47	25/3142 (0.8%)
1	G	1.14	10/2310 (0.4%)	1.28	14/3136 (0.4%)
1	J	1.14	7/2310 (0.3%)	1.34	14/3136 (0.4%)
2	B	1.11	2/838 (0.2%)	1.46	8/1138 (0.7%)
2	E	1.15	1/847 (0.1%)	1.30	0/1148
2	H	1.03	2/847 (0.2%)	1.29	0/1148
2	K	1.11	1/847 (0.1%)	1.34	3/1148 (0.3%)
3	C	1.32	0/74	1.60	2/97 (2.1%)
3	F	2.55	1/74 (1.4%)	1.69	5/97 (5.2%)
3	I	2.21	4/74 (5.4%)	1.80	2/97 (2.1%)
3	L	1.72	1/74 (1.4%)	2.25	6/97 (6.2%)
All	All	1.17	45/12941 (0.3%)	1.39	106/17550 (0.6%)

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	D	0	1
1	J	0	1
All	All	0	2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	9	MET	C-OXT	-16.86	0.89	1.23
1	A	75	ARG	NE-CZ	-10.96	1.21	1.33
3	I	4	TYR	N-CA	-8.32	1.36	1.46
3	I	3	VAL	C-N	-8.28	1.22	1.33
1	G	79	ARG	NE-CZ	-7.96	1.24	1.33
1	A	185	PRO	C-O	-7.90	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	ARG	CZ-NH1	-7.68	1.22	1.32
1	G	182	THR	CB-OG1	7.49	1.55	1.43
3	I	4	TYR	CA-CB	-7.38	1.41	1.53
1	D	62	ARG	CZ-NH2	-7.13	1.24	1.33
3	I	4	TYR	CB-CG	-6.88	1.36	1.51
2	B	2	GLN	N-CA	-6.78	1.36	1.45
1	J	155	HIS	CA-C	-6.72	1.44	1.52
1	G	74	PHE	C-N	-6.69	1.24	1.33
1	G	153	ALA	CA-CB	-6.64	1.42	1.53
1	A	79	ARG	NE-CZ	-6.54	1.25	1.33
1	J	209	TYR	C-O	-6.46	1.16	1.24
1	D	62	ARG	CZ-NH1	-6.21	1.24	1.32
1	D	58	GLU	CD-OE1	-6.07	1.13	1.25
2	K	64	ILE	CA-CB	-6.03	1.44	1.55
1	J	62	ARG	CZ-NH2	-5.90	1.25	1.33
1	G	122	ASP	C-O	-5.89	1.16	1.23
3	L	4	TYR	N-CA	-5.78	1.39	1.46
1	G	209	TYR	C-O	-5.76	1.17	1.24
1	D	58	GLU	CA-CB	-5.65	1.44	1.53
1	A	264	GLU	C-O	-5.58	1.15	1.23
1	J	58	GLU	CD-OE2	-5.57	1.14	1.25
2	B	1	ILE	C-N	-5.50	1.26	1.33
1	A	58	GLU	CD-OE2	-5.49	1.15	1.25
1	G	122	ASP	CA-C	-5.46	1.45	1.52
1	G	58	GLU	CD-OE2	-5.45	1.15	1.25
2	H	99	MET	SD-CE	5.42	1.93	1.79
1	J	136	ALA	C-O	-5.41	1.17	1.24
2	H	99	MET	CG-SD	5.35	1.94	1.80
2	E	64	ILE	CA-CB	-5.32	1.46	1.55
1	G	79	ARG	CD-NE	-5.17	1.39	1.46
1	A	79	ARG	CZ-NH2	-5.16	1.26	1.33
1	J	123	TYR	CA-C	-5.16	1.48	1.52
1	G	79	ARG	CZ-NH2	-5.14	1.26	1.33
1	A	111	ARG	CZ-NH2	-5.14	1.26	1.33
1	D	58	GLU	CD-OE2	-5.14	1.15	1.25
1	A	209	TYR	C-O	-5.12	1.18	1.24
1	D	209	TYR	C-O	-5.12	1.18	1.24
1	J	154	GLU	CG-CD	-5.11	1.39	1.52
1	D	136	ALA	C-O	-5.09	1.18	1.24

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	155	HIS	CA-CB-CG	-19.55	94.25	113.80
1	D	273	ARG	N-CA-C	-15.88	85.01	109.94
1	D	273	ARG	CA-C-N	-15.76	93.34	121.70
1	D	273	ARG	C-N-CA	-15.76	93.34	121.70
1	D	274	TRP	N-CA-C	-12.38	76.34	111.00
1	A	221	GLY	N-CA-C	-11.46	86.02	113.18
1	A	265	GLY	N-CA-C	-10.87	87.41	113.18
3	L	4	TYR	CB-CA-C	10.04	125.60	110.14
1	A	185	PRO	CB-CA-C	-9.96	99.09	111.64
1	D	58	GLU	CA-CB-CG	-9.89	94.32	114.10
1	A	186	LYS	N-CA-C	-9.85	92.35	108.41
1	A	87	GLN	OE1-CD-NE2	-9.74	112.86	122.60
2	B	2	GLN	N-CA-C	9.31	122.62	110.43
1	D	264	GLU	N-CA-C	9.25	124.38	113.18
1	G	264	GLU	N-CA-C	9.06	124.53	113.38
3	L	6	PHE	CA-CB-CG	-8.73	105.06	113.80
2	B	2	GLN	N-CA-CB	-8.70	97.81	110.26
1	A	75	ARG	NE-CZ-NH1	-8.56	112.94	121.50
1	J	264	GLU	N-CA-C	8.54	123.70	113.28
1	D	178	THR	N-CA-CB	-8.50	97.18	110.44
3	I	4	TYR	N-CA-CB	-8.10	98.52	110.84
1	D	75	ARG	CD-NE-CZ	-8.10	113.07	124.40
1	D	75	ARG	CB-CG-CD	-8.04	92.80	111.30
1	A	223	GLU	N-CA-C	7.85	122.61	108.48
1	A	255	GLN	N-CA-C	-7.79	104.26	114.31
2	B	45	LYS	CG-CD-CE	7.77	129.17	111.30
1	A	186	LYS	N-CA-CB	-7.70	98.64	110.65
1	G	223	GLU	CA-CB-CG	7.66	129.43	114.10
1	A	111	ARG	NE-CZ-NH2	7.57	126.02	119.20
1	D	181	ARG	N-CA-C	7.39	118.36	108.38
1	A	185	PRO	CA-C-O	-7.35	113.37	121.23
1	J	255	GLN	N-CA-C	-7.24	104.59	113.50
2	B	74	GLU	CB-CA-C	-7.22	97.27	110.63
1	A	66	LYS	CG-CD-CE	-7.17	94.82	111.30
2	B	74	GLU	CB-CG-CD	-7.15	100.44	112.60
1	D	182	THR	N-CA-C	7.15	120.07	110.35
1	J	75	ARG	CD-NE-CZ	-7.14	114.40	124.40
1	D	19	GLU	N-CA-C	-7.05	99.79	110.50
1	A	87	GLN	CG-CD-NE2	6.96	126.84	116.40
2	B	45	LYS	CD-CE-NZ	6.91	134.01	111.90
3	L	4	TYR	N-CA-CB	-6.74	99.78	110.77
1	D	17	LEU	CA-C-N	-6.61	110.05	122.73
1	D	17	LEU	C-N-CA	-6.61	110.05	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	GLU	N-CA-C	6.55	119.89	108.82
1	J	66	LYS	N-CA-C	-6.52	104.25	111.36
1	A	225	THR	N-CA-C	-6.47	103.38	113.02
1	D	182	THR	N-CA-CB	-6.39	100.64	110.04
1	A	264	GLU	N-CA-C	6.36	119.76	108.24
1	D	212	ASP	CA-CB-CG	-6.35	106.25	112.60
1	A	180	LEU	N-CA-C	-6.34	104.26	114.09
1	A	185	PRO	N-CA-C	6.31	120.75	111.03
2	B	89	GLU	CA-CB-CG	-6.29	101.53	114.10
1	A	254	GLU	N-CA-C	6.23	120.05	111.71
1	J	15	PRO	CA-C-O	-6.12	114.65	121.32
1	D	193	PRO	CB-CA-C	-6.09	103.96	111.64
1	G	142	ILE	N-CA-C	-6.09	104.58	110.42
1	D	16	GLY	N-CA-C	-6.08	98.76	113.18
1	A	234	ARG	CA-C-N	6.04	125.99	119.76
1	A	234	ARG	C-N-CA	6.04	125.99	119.76
1	A	236	ALA	N-CA-C	-6.02	105.77	113.23
1	G	182	THR	OG1-CB-CG2	-5.97	97.36	109.30
1	J	211	ALA	N-CA-C	5.90	117.71	111.28
1	G	255	GLN	N-CA-C	-5.85	106.28	113.41
1	G	182	THR	CA-CB-OG1	-5.84	100.84	109.60
1	D	181	ARG	CA-C-N	5.81	129.52	120.75
1	D	181	ARG	C-N-CA	5.81	129.52	120.75
1	G	223	GLU	N-CA-C	5.78	118.17	108.23
1	J	25	VAL	CA-C-N	-5.77	116.15	122.38
1	J	25	VAL	C-N-CA	-5.77	116.15	122.38
1	D	79	ARG	NE-CZ-NH2	5.76	124.39	119.20
3	C	4	TYR	CB-CA-C	5.64	119.92	109.70
3	I	4	TYR	CB-CG-CD2	-5.64	112.33	120.80
3	F	5	ASN	N-CA-C	5.62	117.95	110.53
1	G	265	GLY	N-CA-C	-5.62	99.87	113.18
1	D	185	PRO	CB-CA-C	-5.60	104.58	111.64
3	F	8	THR	CA-C-N	-5.58	111.66	121.70
3	F	8	THR	C-N-CA	-5.58	111.66	121.70
1	D	254	GLU	N-CA-C	5.58	120.20	112.90
1	J	30	ASN	N-CA-C	5.48	119.79	113.38
3	F	3	VAL	CB-CA-C	-5.46	105.59	111.59
1	J	154	GLU	CA-CB-CG	-5.43	103.23	114.10
1	A	232	GLU	CB-CA-C	-5.43	99.90	109.62
1	G	186	LYS	N-CA-C	-5.41	100.43	109.24
2	K	76	ASP	CA-C-N	-5.40	115.10	122.93
2	K	76	ASP	C-N-CA	-5.40	115.10	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	THR	N-CA-C	-5.39	99.65	108.76
1	D	274	TRP	CA-CB-CG	5.33	123.72	113.60
1	J	155	HIS	CB-CA-C	-5.31	102.78	110.96
1	G	165	VAL	CB-CA-C	-5.30	105.04	111.87
1	A	16	GLY	N-CA-C	5.29	125.71	113.18
2	B	45	LYS	CB-CA-C	-5.26	101.69	109.90
1	G	223	GLU	CB-CA-C	-5.26	102.17	111.05
3	C	5	ASN	N-CA-C	5.25	117.31	110.43
1	A	111	ARG	NH1-CZ-NH2	-5.21	112.53	119.30
2	K	70	PHE	N-CA-C	5.20	117.16	108.99
3	L	3	VAL	CA-C-N	-5.20	114.70	122.39
3	L	3	VAL	C-N-CA	-5.20	114.70	122.39
1	J	194	ARG	N-CA-C	5.17	116.77	110.41
3	F	4	TYR	CB-CA-C	5.16	118.68	109.65
1	G	58	GLU	CA-CB-CG	-5.15	103.79	114.10
1	G	129	ASP	N-CA-C	-5.10	107.03	113.20
1	J	122	ASP	CB-CA-C	-5.09	101.95	109.90
1	G	225	THR	N-CA-C	-5.08	105.77	112.94
1	D	67	ALA	N-CA-C	-5.06	105.66	111.07
3	L	4	TYR	CB-CG-CD1	-5.04	113.24	120.80
1	A	144	ARG	NE-CZ-NH2	5.03	123.72	119.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	223	GLU	Mainchain
1	J	223	GLU	Mainchain

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	2265	0	2136	155	0
1	D	2248	0	2123	143	0
1	G	2244	0	2118	127	0
1	J	2244	0	2118	141	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	812	0	787	38	0
2	E	821	0	796	40	0
2	H	821	0	796	25	0
2	K	821	0	796	32	0
3	C	73	0	74	9	0
3	F	73	0	74	15	0
3	I	73	0	74	14	0
3	L	73	0	74	18	0
4	A	12	0	0	1	0
4	B	7	0	0	0	0
4	D	12	0	0	0	0
4	E	2	0	0	0	0
4	G	9	0	0	2	0
4	H	5	0	0	0	0
4	J	10	0	0	0	0
4	K	7	0	0	0	0
4	L	1	0	0	0	0
All	All	12633	0	11966	671	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 27.

All (671) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:CG	1:A:195:SER:H	1.42	1.30
1:D:273:ARG:CG	1:D:274:TRP:O	1.77	1.30
1:A:1:GLY:O	1:A:105:SER:HA	1.38	1.21
1:G:181:ARG:HH11	1:G:181:ARG:HB2	1.07	1.18
1:J:155:HIS:HB3	3:L:6:PHE:CE1	1.79	1.16
1:D:146:LYS:HD3	3:F:9:MET:O	1.42	1.16
1:D:19:GLU:HB3	1:D:75:ARG:HH21	1.01	1.16
1:A:219:LEU:O	1:A:219:LEU:HD12	1.46	1.16
1:A:194:ARG:HG2	1:A:195:SER:N	1.54	1.15
1:A:264:GLU:O	1:A:264:GLU:CG	1.92	1.15
1:G:15:PRO:HD3	1:G:91:GLY:O	1.49	1.12
1:D:121:ARG:CZ	2:E:1:ILE:HD11	1.80	1.10
1:G:31:LYS:NZ	1:G:181:ARG:HH22	1.49	1.10
1:A:218:GLN:C	1:A:220:ASN:H	1.46	1.10
1:D:182:THR:HG21	1:D:265:GLY:HA3	1.16	1.09
1:G:273:ARG:H	1:G:273:ARG:HD3	1.18	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:255:GLN:HE22	1:G:274:TRP:HB3	1.14	1.06
1:A:14:ARG:HG2	1:A:16:GLY:H	1.20	1.05
1:D:19:GLU:HB3	1:D:75:ARG:NH2	1.72	1.05
1:A:194:ARG:HG3	1:A:195:SER:H	1.19	1.04
1:J:219:LEU:O	1:J:219:LEU:HG	1.55	1.04
1:G:181:ARG:HB2	1:G:181:ARG:NH1	1.73	1.04
1:J:155:HIS:CG	3:L:6:PHE:CZ	2.46	1.03
1:D:19:GLU:CB	1:D:75:ARG:HH21	1.73	1.02
1:D:273:ARG:HG2	1:D:274:TRP:C	1.73	1.02
1:A:218:GLN:C	1:A:220:ASN:N	2.09	1.01
1:A:194:ARG:CG	1:A:195:SER:N	2.07	0.99
1:A:218:GLN:O	1:A:220:ASN:N	1.95	0.98
1:D:258:THR:HA	1:D:273:ARG:HA	1.43	0.97
1:J:155:HIS:CB	3:L:6:PHE:CE1	2.47	0.97
1:D:273:ARG:HG2	1:D:274:TRP:O	0.81	0.97
1:A:62:ARG:NH2	3:C:1:LYS:HE3	1.78	0.97
1:A:14:ARG:HG3	1:A:14:ARG:HH11	1.25	0.96
1:A:220:ASN:C	1:A:221:GLY:O	1.97	0.96
1:D:121:ARG:CZ	2:E:1:ILE:CD1	2.44	0.94
1:G:181:ARG:HH11	1:G:181:ARG:CB	1.80	0.94
1:G:32:GLU:OE2	1:G:48:ARG:HD2	1.67	0.94
1:D:58:GLU:HG3	1:D:59:TYR:H	1.33	0.92
1:D:182:THR:HG21	1:D:265:GLY:CA	1.98	0.92
1:A:219:LEU:HD12	1:A:256:ASN:O	1.68	0.91
1:D:182:THR:CG2	1:D:265:GLY:HA3	2.01	0.91
1:J:234:ARG:NH2	2:K:99:MET:OXT	2.03	0.89
1:A:220:ASN:HD21	1:A:258:THR:HB	1.33	0.89
1:A:14:ARG:HH11	1:A:14:ARG:CG	1.87	0.87
1:J:155:HIS:CB	3:L:6:PHE:CZ	2.58	0.87
1:J:194:ARG:HG3	1:J:199:VAL:HG12	1.57	0.87
1:J:220:ASN:OD1	1:J:220:ASN:O	1.92	0.86
1:A:194:ARG:HG2	1:A:195:SER:H	1.16	0.85
1:G:31:LYS:NZ	1:G:181:ARG:NH2	2.25	0.84
1:D:146:LYS:CD	3:F:9:MET:O	2.25	0.84
1:D:82:LEU:HD12	1:D:87:GLN:HB2	1.60	0.83
1:G:31:LYS:HZ3	1:G:181:ARG:HH22	1.22	0.83
1:J:194:ARG:HB3	1:J:198:GLU:C	2.04	0.83
1:A:255:GLN:HE22	1:A:274:TRP:HB3	1.44	0.82
1:G:273:ARG:HD3	1:G:273:ARG:N	1.90	0.81
1:D:202:ARG:HG2	1:D:204:TRP:NE1	1.95	0.81
1:J:222:GLU:CD	1:J:222:GLU:H	1.88	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:GLN:OE1	1:D:226:GLN:O	1.99	0.81
1:J:155:HIS:HB3	3:L:6:PHE:CZ	2.14	0.80
2:K:87:MET:HE1	2:K:91:LYS:HB2	1.62	0.80
1:G:23:ILE:N	1:G:23:ILE:HD12	1.96	0.80
2:B:87:MET:HE1	2:B:91:LYS:HB2	1.64	0.79
1:G:20:PRO:HG3	1:G:75:ARG:HD2	1.62	0.79
1:J:194:ARG:HA	1:J:198:GLU:O	1.81	0.79
1:A:23:ILE:N	1:A:23:ILE:HD12	1.97	0.79
1:D:58:GLU:HG3	1:D:59:TYR:N	1.92	0.79
1:D:143:THR:OG1	3:F:9:MET:HB3	1.83	0.79
1:J:273:ARG:HD3	1:J:273:ARG:H	1.48	0.79
1:A:220:ASN:ND2	1:A:258:THR:HB	1.98	0.78
1:A:264:GLU:O	1:A:264:GLU:HG2	1.04	0.78
1:J:61:GLU:HA	1:J:61:GLU:OE1	1.82	0.78
1:G:226:GLN:O	1:G:226:GLN:OE1	2.01	0.78
1:A:21:ARG:HG2	1:A:23:ILE:HD11	1.64	0.77
1:G:20:PRO:HG3	1:G:75:ARG:HH11	1.48	0.77
1:D:208:PHE:CE2	1:D:213:ILE:HD12	2.19	0.77
2:B:74:GLU:CA	2:B:74:GLU:OE1	2.24	0.76
2:H:87:MET:HE1	2:H:91:LYS:HB2	1.66	0.76
1:A:14:ARG:HG2	1:A:16:GLY:N	1.97	0.76
1:J:23:ILE:HD12	1:J:23:ILE:N	2.01	0.76
1:G:273:ARG:HG2	1:G:274:TRP:O	1.86	0.76
1:J:87:GLN:OE1	1:J:93:HIS:CE1	2.38	0.76
1:D:218:GLN:OE1	1:D:260:ARG:CZ	2.33	0.76
1:D:225:THR:O	1:D:225:THR:HG22	1.83	0.76
1:J:219:LEU:O	1:J:219:LEU:CG	2.34	0.76
1:D:1:GLY:O	1:D:3:HIS:CD2	2.38	0.75
1:D:32:GLU:OE2	1:D:48:ARG:HD2	1.86	0.75
1:G:6:ARG:NH2	1:G:113:TYR:CE2	2.54	0.75
1:A:1:GLY:C	1:A:105:SER:HA	2.10	0.75
1:J:14:ARG:HB3	1:J:15:PRO:HD2	1.68	0.75
1:D:208:PHE:CE2	1:D:213:ILE:CD1	2.69	0.75
1:J:214:THR:C	1:J:215:LEU:HD12	2.12	0.75
1:G:20:PRO:CG	1:G:75:ARG:HD2	2.17	0.74
1:D:170:ARG:HG3	1:D:170:ARG:HH11	1.50	0.74
1:J:194:ARG:HB3	1:J:198:GLU:O	1.87	0.74
2:B:39:MET:CE	2:B:68:THR:HG22	2.18	0.74
1:A:219:LEU:O	1:A:219:LEU:CD1	2.33	0.74
1:G:31:LYS:HZ3	1:G:181:ARG:NH2	1.82	0.74
1:J:202:ARG:HD2	1:J:244:TRP:CD2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:GLU:OE1	2:B:74:GLU:HA	1.88	0.73
1:A:219:LEU:CD1	1:A:256:ASN:O	2.37	0.73
1:J:32:GLU:OE2	1:J:35:ARG:HD2	1.87	0.73
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.23	0.73
1:A:194:ARG:HH12	1:A:248:VAL:HG11	1.54	0.72
1:G:18:GLU:N	1:G:18:GLU:OE1	2.21	0.72
2:B:39:MET:HE1	2:B:68:THR:HG22	1.70	0.72
2:B:39:MET:HE2	2:B:49:VAL:HG13	1.72	0.72
1:A:219:LEU:HD11	1:A:256:ASN:ND2	2.05	0.72
1:J:202:ARG:HD2	1:J:244:TRP:CE3	2.23	0.72
1:A:275:GLU:HG3	1:A:275:GLU:O	1.89	0.71
1:G:194:ARG:CB	1:G:198:GLU:O	2.39	0.71
2:E:1:ILE:HG23	2:E:1:ILE:O	1.89	0.71
1:G:190:THR:OG1	1:G:202:ARG:HB3	1.91	0.71
1:G:262:TYR:HA	4:G:277:HOH:O	1.88	0.71
1:J:81:LEU:HD13	1:J:118:TYR:CD1	2.26	0.71
1:A:31:LYS:HZ2	1:A:181:ARG:HH22	1.38	0.71
1:G:194:ARG:NH2	1:G:198:GLU:OE1	2.24	0.71
1:D:19:GLU:CD	1:D:75:ARG:NH2	2.49	0.70
1:D:19:GLU:CD	1:D:75:ARG:HH21	1.99	0.70
2:B:87:MET:HE1	2:B:91:LYS:HD2	1.73	0.70
1:D:273:ARG:CG	1:D:274:TRP:C	2.50	0.69
1:A:31:LYS:HZ2	1:A:181:ARG:NH2	1.91	0.69
1:A:218:GLN:O	1:A:220:ASN:ND2	2.26	0.69
1:A:250:PRO:HB2	1:A:253:LYS:HB2	1.75	0.69
1:D:6:ARG:NH2	1:D:113:TYR:CE1	2.61	0.69
1:A:62:ARG:CZ	3:C:1:LYS:HE3	2.23	0.69
1:A:103:LEU:HD11	1:A:168:LEU:HD23	1.73	0.69
1:J:155:HIS:CD2	3:L:6:PHE:CE2	2.81	0.68
1:D:191:HIS:HB2	1:D:274:TRP:CH2	2.28	0.68
1:G:178:THR:HG22	1:G:179:LEU:HD23	1.76	0.68
1:J:208:PHE:CE1	1:J:241:PHE:HB2	2.29	0.68
1:A:183:ASP:O	1:A:208:PHE:HA	1.93	0.68
1:D:35:ARG:NH2	2:E:54:MET:O	2.24	0.68
1:J:194:ARG:CA	1:J:198:GLU:O	2.42	0.68
1:A:32:GLU:OE2	1:A:35:ARG:HD2	1.94	0.68
1:D:19:GLU:CG	1:D:75:ARG:HH21	2.07	0.68
1:J:190:THR:OG1	1:J:202:ARG:HB3	1.94	0.67
1:D:211:ALA:O	1:D:212:ASP:C	2.36	0.67
1:J:73:TRP:HH2	3:L:9:MET:HE3	1.58	0.67
1:D:263:HIS:O	1:D:266:LEU:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:TRP:H	1:D:228:MET:HE2	1.60	0.66
1:J:116:PHE:CD2	3:L:9:MET:HE1	2.30	0.66
1:G:31:LYS:HZ1	1:G:181:ARG:HH22	1.40	0.66
1:J:255:GLN:HE22	1:J:274:TRP:HB3	1.60	0.66
2:E:39:MET:HE2	2:E:49:VAL:HG13	1.77	0.66
3:I:3:VAL:HG22	3:I:4:TYR:H	1.60	0.66
1:J:35:ARG:NH2	2:K:54:MET:O	2.23	0.66
1:J:226:GLN:OE1	1:J:226:GLN:O	2.13	0.66
1:J:121:ARG:CZ	2:K:1:ILE:HD11	2.25	0.66
1:J:202:ARG:NH1	1:J:244:TRP:CH2	2.64	0.66
2:K:39:MET:HE1	2:K:67:HIS:C	2.21	0.66
1:J:170:ARG:HH11	1:J:170:ARG:HG3	1.61	0.66
1:A:194:ARG:NH1	1:A:248:VAL:HG11	2.10	0.66
1:A:218:GLN:O	1:A:219:LEU:C	2.39	0.66
1:G:18:GLU:CD	1:G:18:GLU:H	2.03	0.66
1:A:226:GLN:OE1	1:A:226:GLN:O	2.14	0.65
1:J:215:LEU:HD12	1:J:215:LEU:N	2.11	0.65
1:A:14:ARG:HG3	1:A:14:ARG:NH1	2.02	0.65
1:D:121:ARG:NE	2:E:1:ILE:HD11	2.11	0.65
1:D:31:LYS:HG3	1:D:209:TYR:OH	1.96	0.65
1:D:147:TRP:CZ2	3:F:9:MET:HG2	2.32	0.65
1:D:135:ALA:H	1:D:144:ARG:HH21	1.45	0.65
1:G:20:PRO:CD	1:G:75:ARG:HD2	2.27	0.65
1:J:116:PHE:CD2	3:L:9:MET:CE	2.80	0.65
1:A:22:TYR:C	1:A:23:ILE:HD12	2.22	0.65
1:J:103:LEU:HD11	1:J:168:LEU:HD23	1.78	0.65
1:D:87:GLN:NE2	1:D:118:TYR:OH	2.26	0.64
1:G:191:HIS:NE2	1:G:199:VAL:HG21	2.11	0.64
2:B:16:GLU:HG3	2:K:88:ALA:HB3	1.78	0.64
2:E:87:MET:HE1	2:E:91:LYS:HB2	1.79	0.64
1:G:273:ARG:N	1:G:273:ARG:CD	2.61	0.64
1:A:1:GLY:N	1:A:2:PRO:CD	2.61	0.64
1:D:66:LYS:HZ1	3:F:1:LYS:HG2	1.62	0.64
1:D:12:VAL:HG22	1:D:94:THR:HG23	1.80	0.63
1:G:230:LEU:C	1:G:230:LEU:HD12	2.24	0.63
1:D:252:GLY:N	1:D:254:GLU:OE1	2.30	0.63
1:J:87:GLN:OE1	1:J:93:HIS:HE1	1.81	0.63
1:A:194:ARG:O	1:A:195:SER:C	2.41	0.63
1:A:251:LEU:HD23	1:A:252:GLY:N	2.14	0.63
1:D:121:ARG:NH1	2:E:1:ILE:CD1	2.61	0.63
1:A:219:LEU:O	1:A:256:ASN:O	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LEU:C	1:A:114:LEU:HD22	2.24	0.63
1:A:194:ARG:NH1	1:A:248:VAL:CG1	2.63	0.62
1:G:231:VAL:O	1:G:243:LYS:NZ	2.32	0.62
1:A:29:ASP:O	1:A:30:ASN:HB2	1.98	0.61
1:G:55:GLU:CD	1:G:170:ARG:HH21	2.09	0.61
1:G:218:GLN:HG2	1:G:223:GLU:HA	1.82	0.61
1:J:32:GLU:OE2	1:J:48:ARG:HD2	2.00	0.61
1:A:44:ARG:HH22	1:A:61:GLU:HG2	1.65	0.61
1:D:203:CYS:HB2	1:D:217:TRP:CZ2	2.36	0.61
1:D:208:PHE:CD2	1:D:213:ILE:HD12	2.36	0.61
3:F:7:ALA:C	3:F:8:THR:O	2.40	0.61
1:A:31:LYS:NZ	1:A:181:ARG:HH22	1.98	0.60
1:D:51:TRP:O	1:D:54:GLN:HG3	2.00	0.60
1:J:167:TRP:CE3	1:J:170:ARG:HD3	2.36	0.60
1:G:123:TYR:HD2	3:I:9:MET:HE2	1.66	0.60
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.35	0.60
1:J:202:ARG:CD	1:J:244:TRP:CE3	2.84	0.60
1:J:222:GLU:CD	1:J:222:GLU:N	2.56	0.60
1:D:226:GLN:O	1:D:226:GLN:CD	2.44	0.60
1:J:194:ARG:CB	1:J:198:GLU:O	2.49	0.60
1:D:176:ASN:CG	1:D:177:ALA:H	2.10	0.60
1:J:7:TYR:CE2	3:L:2:ALA:HB2	2.37	0.60
3:F:5:ASN:N	3:F:5:ASN:HD22	2.00	0.60
1:J:103:LEU:CD1	1:J:168:LEU:HD23	2.32	0.59
1:A:32:GLU:OE2	1:A:48:ARG:HD2	2.01	0.59
1:J:121:ARG:CZ	2:K:1:ILE:CD1	2.81	0.59
1:G:23:ILE:N	1:G:23:ILE:CD1	2.65	0.59
1:G:194:ARG:NH1	1:G:248:VAL:HG11	2.18	0.59
2:E:39:MET:HE1	2:E:67:HIS:C	2.28	0.59
2:H:64:ILE:HG22	2:H:65:LEU:N	2.16	0.59
1:J:234:ARG:HD3	2:K:10:TYR:CE2	2.37	0.59
1:A:191:HIS:O	1:A:192:HIS:HD2	1.85	0.59
1:A:262:TYR:CD1	1:A:262:TYR:N	2.70	0.59
1:J:51:TRP:CZ3	1:J:52:MET:SD	2.96	0.59
1:A:202:ARG:HD2	1:A:244:TRP:CE3	2.37	0.59
1:D:218:GLN:HG2	1:D:222:GLU:C	2.28	0.59
1:A:79:ARG:HH11	1:A:79:ARG:HG2	1.68	0.58
1:G:20:PRO:CG	1:G:75:ARG:HH11	2.15	0.58
1:G:251:LEU:HD23	1:G:252:GLY:N	2.18	0.58
1:J:111:ARG:HD2	1:J:113:TYR:CZ	2.37	0.58
1:A:219:LEU:HD12	1:A:219:LEU:C	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:ARG:CZ	2:H:22:ILE:HD12	2.33	0.58
2:H:40:LEU:HD23	2:H:45:LYS:HA	1.84	0.58
1:D:234:ARG:HD3	2:E:10:TYR:CE2	2.39	0.58
1:G:178:THR:HG22	1:G:179:LEU:CD2	2.33	0.58
2:K:87:MET:HE1	2:K:91:LYS:CB	2.31	0.58
1:A:156:TYR:O	1:A:160:LEU:HG	2.03	0.58
2:H:21:ASN:OD1	2:H:22:ILE:N	2.33	0.58
1:A:1:GLY:H3	1:A:2:PRO:HD3	1.69	0.58
1:A:1:GLY:N	1:A:2:PRO:HD3	2.18	0.57
1:A:14:ARG:CG	1:A:14:ARG:NH1	2.57	0.57
1:J:155:HIS:CG	3:L:6:PHE:CE2	2.91	0.57
1:J:233:THR:OG1	1:J:243:LYS:HD2	2.04	0.57
1:D:121:ARG:CZ	2:E:1:ILE:HD12	2.33	0.57
3:I:3:VAL:HG22	3:I:4:TYR:N	2.19	0.57
1:J:63:GLU:OE2	3:L:1:LYS:HG2	2.05	0.57
1:D:225:THR:O	1:D:225:THR:CG2	2.52	0.57
1:A:31:LYS:HD3	1:A:179:LEU:HD22	1.86	0.57
1:A:44:ARG:NH2	4:A:288:HOH:O	2.35	0.57
1:D:19:GLU:CB	1:D:75:ARG:NH2	2.48	0.57
1:G:145:ARG:NH1	4:G:283:HOH:O	2.36	0.57
1:A:14:ARG:C	1:A:16:GLY:H	2.10	0.57
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.40	0.57
1:G:33:PHE:CD2	1:G:34:VAL:HG13	2.39	0.57
1:A:219:LEU:HD11	1:A:256:ASN:HD22	1.69	0.57
1:D:28:VAL:HG12	1:D:28:VAL:O	2.05	0.57
1:G:222:GLU:CD	1:G:222:GLU:H	2.13	0.57
1:J:250:PRO:HG2	1:J:253:LYS:HB2	1.87	0.57
1:D:44:ARG:HH11	1:D:44:ARG:CG	2.16	0.56
1:D:208:PHE:CE2	1:D:213:ILE:HD13	2.40	0.56
2:E:39:MET:HE1	2:E:68:THR:HG22	1.86	0.56
2:E:40:LEU:HD23	2:E:45:LYS:HA	1.87	0.56
2:H:39:MET:HE1	2:H:67:HIS:CA	2.35	0.56
1:D:23:ILE:N	1:D:23:ILE:HD12	2.20	0.56
1:D:170:ARG:NH1	1:D:174:ASN:HD21	2.03	0.56
1:G:111:ARG:HD2	1:G:113:TYR:CZ	2.39	0.56
1:G:33:PHE:C	1:G:48:ARG:HB2	2.30	0.56
1:G:266:LEU:HG	1:G:268:GLU:O	2.06	0.56
1:G:255:GLN:HE22	1:G:274:TRP:CB	2.04	0.56
1:D:176:ASN:O	1:D:180:LEU:HD22	2.05	0.56
1:J:42:ASN:HD21	1:J:44:ARG:HD2	1.71	0.56
1:D:121:ARG:NH2	2:E:1:ILE:CD1	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:64:ILE:HG22	2:E:65:LEU:N	2.17	0.56
1:G:6:ARG:NH2	1:G:113:TYR:CD2	2.74	0.56
1:J:207:GLY:HA2	1:J:240:THR:HB	1.88	0.56
2:K:40:LEU:HD23	2:K:45:LYS:HA	1.88	0.56
1:D:208:PHE:CZ	1:D:213:ILE:HG21	2.40	0.56
2:E:21:ASN:OD1	2:E:22:ILE:N	2.34	0.56
1:G:35:ARG:NH2	2:H:54:MET:O	2.33	0.56
1:J:33:PHE:C	1:J:48:ARG:HB2	2.31	0.56
1:A:1:GLY:HA3	1:A:105:SER:CB	2.35	0.56
1:G:194:ARG:HB3	1:G:198:GLU:O	2.04	0.56
1:J:5:MET:O	1:J:6:ARG:HG2	2.06	0.56
2:B:17:ASN:ND2	2:B:74:GLU:OE1	2.39	0.56
1:J:14:ARG:HB3	1:J:15:PRO:CD	2.33	0.56
1:A:255:GLN:C	1:A:257:TYR:H	2.14	0.55
1:A:23:ILE:N	1:A:23:ILE:CD1	2.67	0.55
2:B:88:ALA:C	2:B:89:GLU:HG2	2.31	0.55
1:D:146:LYS:HZ2	3:F:9:MET:C	2.13	0.55
1:D:6:ARG:NH2	1:D:113:TYR:CD1	2.74	0.55
1:D:207:GLY:HA2	1:D:240:THR:HB	1.89	0.55
1:J:31:LYS:HD3	1:J:179:LEU:HD21	1.88	0.55
1:A:251:LEU:HD23	1:A:251:LEU:C	2.30	0.55
1:D:167:TRP:CE3	1:D:170:ARG:HD3	2.41	0.55
1:D:176:ASN:CG	1:D:177:ALA:N	2.65	0.55
1:D:183:ASP:O	1:D:208:PHE:HA	2.06	0.55
1:D:191:HIS:HB2	1:D:274:TRP:CZ2	2.41	0.55
1:J:194:ARG:HG3	1:J:199:VAL:CG1	2.33	0.55
1:J:273:ARG:HD3	1:J:273:ARG:N	2.20	0.55
1:J:226:GLN:O	1:J:227:ASP:C	2.49	0.55
1:J:6:ARG:NH2	1:J:113:TYR:CE1	2.74	0.55
1:A:103:LEU:CD1	1:A:168:LEU:HD23	2.37	0.55
1:D:191:HIS:NE2	1:D:199:VAL:HG21	2.22	0.55
2:E:59:ASP:O	2:E:60:TRP:HB2	2.07	0.55
1:G:116:PHE:CG	3:I:9:MET:HE1	2.43	0.54
1:A:275:GLU:O	1:A:275:GLU:CG	2.53	0.54
1:D:207:GLY:HA2	1:D:240:THR:CB	2.38	0.54
1:A:202:ARG:HG2	1:A:204:TRP:NE1	2.23	0.54
2:H:12:ARG:NH1	2:H:22:ILE:HD12	2.23	0.54
1:J:155:HIS:HB3	3:L:6:PHE:HE1	1.58	0.54
1:J:107:TRP:HB3	1:J:169:HIS:HE2	1.73	0.54
1:A:219:LEU:HB2	1:A:224:LEU:HD22	1.90	0.54
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:MET:CE	2:B:68:THR:CG2	2.84	0.54
2:B:40:LEU:HD23	2:B:45:LYS:HA	1.89	0.54
1:D:218:GLN:OE1	1:D:260:ARG:NE	2.41	0.54
1:J:194:ARG:HB3	1:J:198:GLU:N	2.23	0.54
1:A:33:PHE:C	1:A:48:ARG:HB2	2.33	0.54
2:K:87:MET:CE	2:K:91:LYS:HB2	2.37	0.54
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.44	0.53
1:D:194:ARG:HB2	1:D:198:GLU:O	2.08	0.53
1:D:219:LEU:HD11	1:D:256:ASN:HD22	1.73	0.53
2:K:64:ILE:HG22	2:K:65:LEU:N	2.22	0.53
2:E:39:MET:CE	2:E:68:THR:HG22	2.39	0.53
1:G:226:GLN:O	1:G:226:GLN:CD	2.50	0.53
2:H:39:MET:HE1	2:H:67:HIS:C	2.33	0.53
1:D:55:GLU:CD	1:D:170:ARG:HH21	2.16	0.53
1:G:255:GLN:NE2	1:G:274:TRP:HB3	2.00	0.53
1:D:248:VAL:HG23	1:D:248:VAL:O	2.07	0.53
1:J:107:TRP:CE3	1:J:169:HIS:CD2	2.97	0.53
1:J:194:ARG:HE	1:J:251:LEU:HD12	1.74	0.53
1:J:167:TRP:CZ3	1:J:170:ARG:HD3	2.44	0.53
1:A:74:PHE:CD2	1:A:95:LEU:HD23	2.44	0.52
1:D:249:VAL:HG22	1:D:257:TYR:CZ	2.44	0.52
1:D:261:VAL:HB	1:D:270:LEU:HB2	1.90	0.52
1:G:194:ARG:NH1	1:G:248:VAL:CG1	2.71	0.52
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.43	0.52
2:B:21:ASN:OD1	2:B:22:ILE:N	2.40	0.52
1:G:263:HIS:O	1:G:266:LEU:HB3	2.09	0.52
3:C:6:PHE:CD2	3:C:7:ALA:N	2.77	0.52
1:G:22:TYR:C	1:G:23:ILE:HD12	2.34	0.52
1:A:98:MET:SD	2:B:58:LYS:HA	2.49	0.52
2:B:64:ILE:HG22	2:B:65:LEU:N	2.23	0.52
1:D:233:THR:OG1	1:D:243:LYS:HD2	2.09	0.52
1:J:218:GLN:HG2	1:J:223:GLU:HA	1.92	0.52
2:B:87:MET:CE	2:B:91:LYS:HB2	2.37	0.52
1:D:33:PHE:CD2	1:D:34:VAL:HG13	2.45	0.52
2:E:9:VAL:CG2	2:E:93:VAL:HG22	2.40	0.52
1:J:209:TYR:CD1	1:J:210:PRO:HA	2.45	0.52
2:B:16:GLU:HG3	2:K:88:ALA:CB	2.39	0.52
2:B:39:MET:HE3	2:B:68:THR:CG2	2.40	0.52
1:D:251:LEU:HD23	1:D:252:GLY:N	2.24	0.52
1:G:73:TRP:CE2	3:I:8:THR:HA	2.45	0.52
1:J:225:THR:O	1:J:227:ASP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:251:LEU:HD23	1:J:252:GLY:N	2.26	0.52
2:K:39:MET:CE	2:K:49:VAL:HG13	2.40	0.51
1:A:191:HIS:O	1:A:192:HIS:CD2	2.63	0.51
1:D:121:ARG:NH1	2:E:1:ILE:HD12	2.25	0.51
1:D:208:PHE:CZ	1:D:213:ILE:HD12	2.44	0.51
1:G:194:ARG:HB2	1:G:198:GLU:O	2.11	0.51
2:H:39:MET:HE1	2:H:67:HIS:HA	1.92	0.51
2:B:7:ILE:HB	2:B:93:VAL:HG11	1.93	0.51
1:G:154:GLU:CD	1:G:154:GLU:H	2.18	0.51
1:D:147:TRP:HZ2	3:F:9:MET:HG2	1.73	0.51
1:A:233:THR:OG1	1:A:243:LYS:HD2	2.11	0.51
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.46	0.51
3:F:7:ALA:O	3:F:8:THR:O	2.29	0.51
1:J:220:ASN:O	1:J:220:ASN:CG	2.54	0.51
1:A:219:LEU:HD22	1:A:257:TYR:CZ	2.47	0.50
1:D:121:ARG:NH1	2:E:1:ILE:HD11	2.20	0.50
1:J:185:PRO:CA	1:J:208:PHE:HB3	2.41	0.50
1:A:194:ARG:HH11	1:A:248:VAL:HG12	1.77	0.50
1:A:255:GLN:NE2	1:A:274:TRP:HB3	2.20	0.50
2:B:39:MET:HE1	2:B:67:HIS:C	2.36	0.50
1:G:33:PHE:HD2	1:G:52:MET:HG3	1.76	0.50
1:G:251:LEU:HD23	1:G:251:LEU:C	2.37	0.50
1:J:85:TYR:CB	1:J:87:GLN:HE21	2.24	0.50
1:G:121:ARG:CZ	2:H:1:ILE:HD11	2.41	0.50
2:H:64:ILE:CG2	2:H:65:LEU:N	2.70	0.50
1:J:180:LEU:O	1:J:180:LEU:HG	2.12	0.50
1:G:230:LEU:C	1:G:230:LEU:CD1	2.84	0.50
1:G:217:TRP:H	1:G:228:MET:HE2	1.75	0.50
1:G:234:ARG:NH2	2:H:99:MET:OXT	2.43	0.50
1:A:37:ASP:OD1	1:A:39:ASP:HB2	2.12	0.50
1:D:217:TRP:H	1:D:228:MET:CE	2.24	0.50
1:G:98:MET:HE2	2:H:60:TRP:CH2	2.47	0.50
1:G:116:PHE:CB	3:I:9:MET:HE1	2.42	0.50
1:J:145:ARG:O	1:J:146:LYS:C	2.54	0.50
1:J:194:ARG:CD	1:J:194:ARG:H	2.21	0.50
2:B:13:HIS:HB3	2:B:14:PRO:HD2	1.94	0.50
1:G:154:GLU:CD	1:G:154:GLU:N	2.69	0.50
2:K:59:ASP:O	2:K:60:TRP:HB2	2.12	0.50
2:H:10:TYR:CD1	2:H:10:TYR:N	2.80	0.50
1:D:190:THR:OG1	1:D:202:ARG:HB3	2.12	0.49
1:G:214:THR:C	1:G:215:LEU:HD12	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:PHE:HD2	3:C:7:ALA:H	1.59	0.49
1:J:182:THR:OG1	1:J:265:GLY:HA3	2.12	0.49
1:G:202:ARG:HD3	1:G:246:SER:HB3	1.94	0.49
1:J:107:TRP:HB3	1:J:169:HIS:NE2	2.27	0.49
1:J:234:ARG:HB2	2:K:10:TYR:CZ	2.47	0.49
1:A:230:LEU:C	1:A:230:LEU:HD12	2.35	0.49
2:B:36:GLU:HB2	2:B:83:LYS:HB3	1.95	0.49
1:J:266:LEU:HG	1:J:268:GLU:O	2.12	0.49
1:G:47:PRO:HG3	1:G:60:TRP:CZ2	2.47	0.49
1:J:73:TRP:CE2	3:L:8:THR:HA	2.47	0.49
2:K:39:MET:HE1	2:K:67:HIS:CA	2.42	0.49
1:A:77:SER:OG	3:C:9:MET:HG3	2.13	0.49
1:J:23:ILE:N	1:J:23:ILE:CD1	2.74	0.49
1:A:15:PRO:HD3	1:A:91:GLY:O	2.12	0.49
2:E:10:TYR:N	2:E:10:TYR:CD1	2.79	0.49
1:A:114:LEU:C	1:A:114:LEU:CD2	2.86	0.49
2:E:64:ILE:CG2	2:E:65:LEU:N	2.75	0.49
1:J:74:PHE:CD2	1:J:95:LEU:HD23	2.48	0.49
1:A:191:HIS:NE2	1:A:199:VAL:HG21	2.28	0.49
1:A:207:GLY:HA2	1:A:240:THR:HB	1.94	0.49
1:A:250:PRO:O	1:A:251:LEU:C	2.56	0.49
1:G:135:ALA:H	1:G:144:ARG:HH21	1.61	0.48
2:H:41:LYS:HG3	2:H:78:TYR:CE2	2.47	0.48
1:G:157:LYS:NZ	1:G:161:GLU:OE1	2.45	0.48
1:G:201:LEU:HD11	1:G:254:GLU:HB2	1.94	0.48
1:D:44:ARG:CG	1:D:44:ARG:NH1	2.75	0.48
1:D:226:GLN:OE1	1:D:226:GLN:C	2.57	0.48
3:I:3:VAL:CG2	3:I:4:TYR:H	2.24	0.48
1:J:55:GLU:CD	1:J:170:ARG:HH21	2.22	0.48
1:A:31:LYS:HG3	1:A:209:TYR:OH	2.13	0.48
1:D:262:TYR:N	1:D:262:TYR:CD1	2.82	0.48
2:E:7:ILE:HB	2:E:93:VAL:HG11	1.96	0.48
1:J:207:GLY:HA2	1:J:240:THR:CB	2.42	0.48
1:J:31:LYS:HZ1	1:J:181:ARG:HH22	1.62	0.47
1:J:213:ILE:HG12	1:J:214:THR:N	2.29	0.47
1:D:234:ARG:NH2	2:E:99:MET:OXT	2.45	0.47
1:G:123:TYR:CD2	3:I:9:MET:HE2	2.48	0.47
1:A:14:ARG:C	1:A:16:GLY:N	2.70	0.47
2:B:87:MET:HE1	2:B:91:LYS:CB	2.40	0.47
2:H:29:GLN:HA	2:H:61:SER:HB2	1.95	0.47
1:D:202:ARG:HG2	1:D:204:TRP:HE1	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:PHE:CZ	1:D:213:ILE:CD1	2.97	0.47
1:J:63:GLU:OE2	3:L:1:LYS:HE2	2.15	0.47
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.49	0.47
1:D:28:VAL:HG23	1:D:33:PHE:CE1	2.49	0.47
1:G:2:PRO:N	1:G:105:SER:HA	2.29	0.47
1:G:31:LYS:HZ1	1:G:181:ARG:NH2	2.02	0.47
1:G:87:GLN:NE2	1:G:118:TYR:OH	2.39	0.47
1:A:194:ARG:HG3	1:A:195:SER:N	2.00	0.47
1:A:202:ARG:CD	1:A:244:TRP:CE3	2.97	0.47
2:B:59:ASP:O	2:B:60:TRP:HB2	2.15	0.47
1:D:249:VAL:HG22	1:D:257:TYR:CE2	2.50	0.47
1:G:15:PRO:HD3	1:G:91:GLY:C	2.30	0.47
1:G:163:GLU:O	1:G:164:CYS:C	2.57	0.47
1:G:273:ARG:H	1:G:273:ARG:CD	2.05	0.47
1:J:202:ARG:HD3	1:J:246:SER:HB3	1.97	0.47
1:J:218:GLN:HG2	1:J:223:GLU:CA	2.44	0.47
1:G:17:LEU:O	1:G:18:GLU:C	2.58	0.47
1:D:258:THR:HG22	1:D:273:ARG:HB3	1.97	0.47
1:J:85:TYR:HB2	1:J:87:GLN:HE21	1.80	0.47
1:J:167:TRP:CE2	3:L:1:LYS:HD2	2.50	0.47
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.50	0.47
1:G:162:GLY:O	1:G:163:GLU:C	2.57	0.47
1:G:211:ALA:HB2	1:G:241:PHE:CE2	2.50	0.47
1:G:252:GLY:N	1:G:254:GLU:OE1	2.48	0.47
2:H:74:GLU:N	2:H:74:GLU:OE1	2.47	0.47
1:J:170:ARG:HH11	1:J:170:ARG:CG	2.26	0.47
1:J:249:VAL:HG22	1:J:257:TYR:CZ	2.50	0.47
1:D:129:ASP:O	1:D:131:LYS:HG3	2.15	0.46
1:G:20:PRO:CD	1:G:75:ARG:CD	2.92	0.46
1:G:207:GLY:HA2	1:G:240:THR:CB	2.45	0.46
1:G:225:THR:HG22	1:G:225:THR:O	2.15	0.46
1:G:123:TYR:HE2	3:I:9:MET:HG2	1.80	0.46
1:G:151:GLY:O	1:G:152:ALA:C	2.57	0.46
1:J:185:PRO:HA	1:J:208:PHE:HB3	1.96	0.46
1:J:234:ARG:HB2	2:K:10:TYR:OH	2.15	0.46
1:G:43:PRO:O	1:G:44:ARG:HG3	2.15	0.46
1:A:1:GLY:H2	1:A:2:PRO:CD	2.27	0.46
1:G:185:PRO:HB3	1:G:208:PHE:HB3	1.97	0.46
1:J:203:CYS:HB2	1:J:217:TRP:CZ2	2.49	0.46
1:J:251:LEU:HD23	1:J:251:LEU:C	2.39	0.46
2:E:36:GLU:HB2	2:E:83:LYS:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:273:ARG:H	1:J:273:ARG:CD	2.24	0.46
2:K:79:ALA:HB2	2:K:94:TYR:CD1	2.50	0.46
1:D:177:ALA:HA	1:D:180:LEU:HB2	1.98	0.46
1:A:207:GLY:HA2	1:A:240:THR:CB	2.46	0.46
1:A:226:GLN:O	1:A:227:ASP:C	2.59	0.46
1:G:238:ASP:C	1:G:238:ASP:OD1	2.58	0.46
1:A:167:TRP:CE3	1:A:170:ARG:HD3	2.51	0.46
1:A:194:ARG:O	1:A:195:SER:O	2.33	0.46
1:D:1:GLY:O	1:D:3:HIS:NE2	2.48	0.46
1:D:49:ALA:HB1	1:D:50:PRO:HD2	1.97	0.46
1:G:202:ARG:HG2	1:G:204:TRP:NE1	2.31	0.46
1:J:5:MET:C	1:J:6:ARG:HG2	2.40	0.46
1:A:275:GLU:O	1:A:276:PRO:OXT	2.34	0.46
1:D:19:GLU:CG	1:D:75:ARG:NH2	2.74	0.46
1:D:232:GLU:O	1:D:232:GLU:HG2	2.11	0.46
2:E:87:MET:HE1	2:E:91:LYS:CB	2.46	0.46
2:B:9:VAL:HG23	2:B:93:VAL:HG22	1.98	0.45
1:D:181:ARG:HG3	1:D:182:THR:N	2.31	0.45
1:J:51:TRP:O	1:J:54:GLN:HG3	2.16	0.45
1:J:135:ALA:H	1:J:144:ARG:HH21	1.65	0.45
2:K:7:ILE:HB	2:K:93:VAL:HG11	1.98	0.45
1:D:99:SER:HA	1:D:113:TYR:O	2.17	0.45
1:A:73:TRP:CH2	3:C:9:MET:HE3	2.52	0.45
1:D:162:GLY:O	1:D:163:GLU:C	2.59	0.45
1:G:224:LEU:HG	1:G:226:GLN:HB3	1.98	0.45
1:J:226:GLN:O	1:J:226:GLN:CD	2.58	0.45
1:D:98:MET:HE2	2:E:60:TRP:CH2	2.51	0.45
1:D:214:THR:C	1:D:215:LEU:HD12	2.41	0.45
1:A:214:THR:O	1:A:215:LEU:HD12	2.17	0.45
2:B:9:VAL:CG2	2:B:93:VAL:HG22	2.47	0.45
1:G:270:LEU:HD23	1:G:270:LEU:HA	1.75	0.45
1:J:51:TRP:CZ3	1:J:52:MET:HG2	2.51	0.45
1:A:106:ASP:OD1	1:A:108:ARG:HB2	2.17	0.45
2:B:16:GLU:CG	2:K:88:ALA:HB3	2.47	0.45
1:D:66:LYS:NZ	3:F:1:LYS:HG2	2.30	0.45
1:D:167:TRP:CZ3	1:D:170:ARG:HD3	2.52	0.45
1:G:121:ARG:CZ	2:H:1:ILE:CD1	2.94	0.45
1:G:160:LEU:HD23	1:G:160:LEU:HA	1.73	0.45
2:K:26:TYR:CE2	2:K:28:THR:HG21	2.52	0.45
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.99	0.45
1:J:12:VAL:HG11	2:K:33:PRO:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:31:LYS:HZ1	1:J:181:ARG:NH2	2.15	0.45
1:A:11:ALA:HA	1:A:21:ARG:O	2.17	0.45
1:D:33:PHE:C	1:D:48:ARG:HB2	2.41	0.45
1:J:213:ILE:HG12	1:J:214:THR:H	1.81	0.45
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.53	0.44
1:A:223:GLU:O	1:A:224:LEU:HD13	2.17	0.44
2:B:7:ILE:HG22	2:B:8:GLN:N	2.33	0.44
1:D:58:GLU:CG	1:D:59:TYR:N	2.67	0.44
1:J:42:ASN:ND2	1:J:44:ARG:CD	2.80	0.44
1:A:1:GLY:HA3	1:A:105:SER:HB3	1.99	0.44
1:A:21:ARG:HG2	1:A:23:ILE:CD1	2.39	0.44
1:D:209:TYR:CD1	1:D:210:PRO:HA	2.53	0.44
1:J:31:LYS:NZ	1:J:181:ARG:HH22	2.14	0.44
1:J:234:ARG:HD3	2:K:10:TYR:CZ	2.52	0.44
3:L:3:VAL:HG22	3:L:4:TYR:N	2.31	0.44
1:A:57:PRO:O	1:A:61:GLU:HG3	2.17	0.44
2:B:64:ILE:CG2	2:B:65:LEU:N	2.76	0.44
1:J:162:GLY:O	1:J:163:GLU:C	2.59	0.44
1:J:219:LEU:O	1:J:220:ASN:CG	2.60	0.44
1:A:6:ARG:NH2	1:A:113:TYR:CD1	2.86	0.44
1:A:202:ARG:HD3	1:A:246:SER:HB3	2.00	0.44
1:D:226:GLN:O	1:D:227:ASP:C	2.61	0.44
1:D:272:LEU:C	1:D:273:ARG:O	2.51	0.44
1:G:7:TYR:CE2	3:I:2:ALA:HB2	2.52	0.44
1:A:62:ARG:HE	1:A:62:ARG:HB3	1.68	0.44
1:G:181:ARG:NH1	1:G:181:ARG:CB	2.56	0.44
1:A:220:ASN:CA	1:A:221:GLY:O	2.64	0.44
2:B:87:MET:HE1	2:B:91:LYS:CD	2.43	0.44
1:D:180:LEU:HD12	1:D:180:LEU:HA	1.74	0.44
2:E:9:VAL:HG21	2:E:93:VAL:HG22	1.99	0.44
3:F:5:ASN:N	3:F:5:ASN:ND2	2.66	0.44
1:J:165:VAL:O	1:J:166:GLU:C	2.59	0.44
1:A:124:ILE:HG13	1:A:135:ALA:HB2	1.99	0.44
1:D:8:PHE:CE1	1:D:98:MET:HG2	2.53	0.44
1:D:146:LYS:NZ	3:F:9:MET:C	2.76	0.44
1:D:114:LEU:HA	1:D:114:LEU:HD23	1.78	0.44
1:A:128:GLU:C	1:A:130:LEU:H	2.26	0.44
1:A:143:THR:O	1:A:144:ARG:C	2.61	0.44
1:D:220:ASN:OD1	1:D:220:ASN:O	2.36	0.44
3:F:3:VAL:HG22	3:F:4:TYR:N	2.32	0.44
2:H:9:VAL:HG23	2:H:93:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:39:MET:CE	2:E:49:VAL:HG13	2.45	0.43
1:G:230:LEU:C	1:G:231:VAL:HG13	2.43	0.43
2:H:7:ILE:HB	2:H:93:VAL:HG11	2.00	0.43
1:J:12:VAL:HG11	2:K:33:PRO:CG	2.48	0.43
1:D:143:THR:O	1:D:144:ARG:C	2.61	0.43
1:G:73:TRP:CD1	3:I:8:THR:HG22	2.52	0.43
1:G:121:ARG:NE	2:H:1:ILE:HD11	2.34	0.43
1:A:121:ARG:HH11	1:A:121:ARG:HD2	1.70	0.43
1:J:266:LEU:HD21	1:J:270:LEU:HG	2.00	0.43
2:K:50:GLU:HG3	2:K:67:HIS:NE2	2.34	0.43
1:G:2:PRO:C	1:G:3:HIS:CG	2.96	0.43
1:G:190:THR:HG1	1:G:202:ARG:HB3	1.80	0.43
1:G:202:ARG:HD2	1:G:244:TRP:CE3	2.53	0.43
1:G:226:GLN:OE1	1:G:226:GLN:C	2.60	0.43
1:A:152:ALA:O	1:A:155:HIS:HB3	2.18	0.43
2:B:2:GLN:H	2:B:2:GLN:HG2	0.96	0.43
1:G:189:VAL:HA	1:G:202:ARG:O	2.18	0.43
1:A:138:MET:HA	1:A:138:MET:HE3	1.99	0.43
1:A:261:VAL:HB	1:A:270:LEU:HB2	1.99	0.43
1:A:272:LEU:HA	1:A:272:LEU:HD23	1.83	0.43
2:B:10:TYR:CD1	2:B:10:TYR:N	2.86	0.43
1:D:145:ARG:O	1:D:146:LYS:C	2.59	0.43
1:A:190:THR:OG1	1:A:202:ARG:HB3	2.18	0.43
1:D:5:MET:C	1:D:6:ARG:HG2	2.43	0.43
1:A:6:ARG:NH2	1:A:113:TYR:CE1	2.87	0.43
1:A:149:GLN:NE2	1:A:149:GLN:HA	2.34	0.43
1:D:52:MET:C	1:D:54:GLN:H	2.27	0.43
2:K:10:TYR:CD1	2:K:10:TYR:N	2.87	0.43
1:A:54:GLN:HE21	1:A:54:GLN:HB3	1.64	0.42
1:A:73:TRP:HH2	3:C:9:MET:HE3	1.84	0.42
1:D:214:THR:O	1:D:215:LEU:HD12	2.19	0.42
2:E:59:ASP:O	2:E:60:TRP:CB	2.67	0.42
2:E:79:ALA:HB2	2:E:94:TYR:CD1	2.54	0.42
1:G:170:ARG:O	1:G:171:TYR:C	2.57	0.42
1:G:234:ARG:HD3	2:H:10:TYR:CE2	2.54	0.42
1:J:107:TRP:HE3	1:J:169:HIS:CD2	2.37	0.42
1:J:215:LEU:N	1:J:215:LEU:CD1	2.80	0.42
1:D:58:GLU:H	1:D:58:GLU:HG2	1.25	0.42
1:J:208:PHE:CD1	1:J:208:PHE:C	2.97	0.42
1:G:207:GLY:HA2	1:G:240:THR:OG1	2.19	0.42
1:A:219:LEU:O	1:A:220:ASN:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:12:ARG:CZ	2:E:22:ILE:HD12	2.49	0.42
1:J:118:TYR:CD2	1:J:119:GLU:HG2	2.55	0.42
1:G:73:TRP:CZ2	3:I:8:THR:HA	2.54	0.42
1:J:31:LYS:NZ	1:J:181:ARG:NH2	2.68	0.42
2:E:9:VAL:HG23	2:E:93:VAL:HG22	2.01	0.42
1:A:226:GLN:O	1:A:226:GLN:CD	2.61	0.42
1:D:28:VAL:HG23	1:D:33:PHE:CD1	2.55	0.42
1:G:143:THR:OG1	3:I:9:MET:O	2.33	0.42
1:J:79:ARG:HH11	1:J:79:ARG:HD2	1.57	0.42
1:J:99:SER:HA	1:J:113:TYR:O	2.19	0.42
1:J:273:ARG:N	1:J:273:ARG:CD	2.82	0.42
1:A:194:ARG:NH1	1:A:248:VAL:HG12	2.33	0.42
2:E:12:ARG:NH1	2:E:22:ILE:HD12	2.35	0.42
1:A:141:GLN:O	1:A:142:ILE:C	2.62	0.42
1:A:167:TRP:CZ3	1:A:170:ARG:HD3	2.55	0.42
1:J:224:LEU:C	1:J:226:GLN:H	2.28	0.42
1:A:59:TYR:CD1	1:A:59:TYR:C	2.98	0.41
1:A:248:VAL:O	1:A:248:VAL:HG23	2.20	0.41
1:A:275:GLU:O	1:A:276:PRO:C	2.63	0.41
1:D:55:GLU:CD	1:D:170:ARG:NH2	2.77	0.41
1:D:182:THR:CB	1:D:265:GLY:HA3	2.50	0.41
2:E:41:LYS:O	2:E:42:ASN:C	2.62	0.41
1:J:19:GLU:OE1	1:J:75:ARG:HD2	2.19	0.41
2:K:39:MET:HE2	2:K:49:VAL:HG13	2.01	0.41
1:D:107:TRP:CE3	1:J:269:PRO:HD3	2.54	0.41
1:G:169:HIS:O	1:G:173:LYS:HG3	2.20	0.41
1:J:230:LEU:HD12	1:J:230:LEU:C	2.46	0.41
1:A:110:LEU:HD12	1:A:110:LEU:HA	1.92	0.41
2:E:57:SER:C	2:E:59:ASP:N	2.78	0.41
1:G:145:ARG:O	1:G:146:LYS:C	2.62	0.41
1:G:176:ASN:O	1:G:180:LEU:HB3	2.20	0.41
2:K:50:GLU:HB2	2:K:67:HIS:CE1	2.55	0.41
1:A:79:ARG:HG2	1:A:79:ARG:NH1	2.36	0.41
1:D:138:MET:O	1:D:141:GLN:HG2	2.21	0.41
1:A:1:GLY:HA3	1:A:105:SER:HB2	2.01	0.41
1:D:123:TYR:HE2	3:F:9:MET:SD	2.43	0.41
1:G:129:ASP:O	1:G:131:LYS:HG3	2.21	0.41
1:A:75:ARG:HH11	1:A:75:ARG:HD3	1.23	0.41
1:G:217:TRP:H	1:G:228:MET:CE	2.32	0.41
1:J:18:GLU:HG2	1:J:19:GLU:HG2	2.03	0.41
1:J:159:TYR:CE2	3:L:3:VAL:HB	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLN:OE1	1:A:226:GLN:C	2.64	0.41
1:A:230:LEU:C	1:A:230:LEU:CD1	2.94	0.41
1:A:234:ARG:HB2	2:B:10:TYR:CZ	2.56	0.41
1:G:126:LEU:HD12	1:G:126:LEU:HA	1.76	0.41
1:J:179:LEU:HD23	1:J:179:LEU:HA	1.62	0.41
1:A:35:ARG:NH2	2:B:54:MET:O	2.54	0.41
1:A:201:LEU:HD12	1:A:249:VAL:HG21	2.02	0.41
2:H:36:GLU:HB2	2:H:83:LYS:HB3	2.03	0.41
1:J:87:GLN:HE22	1:J:118:TYR:HE2	1.69	0.41
1:J:103:LEU:HD23	1:J:109:LEU:HA	2.03	0.41
1:J:124:ILE:HG13	1:J:135:ALA:HB2	2.03	0.41
1:A:167:TRP:CE2	3:C:1:LYS:HD2	2.55	0.41
1:G:55:GLU:OE2	1:G:170:ARG:NH2	2.54	0.41
1:G:167:TRP:CE2	3:I:1:LYS:HD2	2.56	0.41
1:J:31:LYS:O	1:J:32:GLU:C	2.62	0.41
1:J:121:ARG:HH11	1:J:121:ARG:HD2	1.71	0.41
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.56	0.40
1:D:202:ARG:HD3	1:D:244:TRP:CE3	2.56	0.40
2:E:50:GLU:HG3	2:E:67:HIS:NE2	2.36	0.40
2:B:56:PHE:HB3	2:B:62:PHE:CD1	2.55	0.40
2:B:57:SER:C	2:B:59:ASP:N	2.76	0.40
1:D:5:MET:O	1:D:6:ARG:HG2	2.20	0.40
1:D:255:GLN:NE2	1:D:274:TRP:HD1	2.19	0.40
1:D:263:HIS:O	1:D:266:LEU:CB	2.67	0.40
2:E:39:MET:CE	2:E:68:THR:CG2	2.99	0.40
1:G:168:LEU:O	1:G:168:LEU:HD12	2.22	0.40
1:G:219:LEU:HD13	1:G:257:TYR:CZ	2.56	0.40
2:K:29:GLN:HA	2:K:61:SER:HB2	2.03	0.40
1:A:159:TYR:OH	3:C:1:LYS:O	2.38	0.40
1:D:266:LEU:HD21	1:D:270:LEU:HG	2.03	0.40
1:G:75:ARG:O	1:G:75:ARG:HG3	2.20	0.40
1:A:145:ARG:O	1:A:146:LYS:C	2.63	0.40
1:D:52:MET:O	1:D:54:GLN:N	2.53	0.40
1:D:191:HIS:HD1	1:D:274:TRP:HZ2	1.69	0.40
1:G:218:GLN:HG2	1:G:223:GLU:CA	2.51	0.40
1:A:103:LEU:HD23	1:A:109:LEU:HA	2.04	0.40
1:A:189:VAL:HG12	1:A:190:THR:N	2.36	0.40
1:A:266:LEU:HD21	1:A:270:LEU:HD23	2.03	0.40
1:D:32:GLU:OE2	1:D:35:ARG:HD2	2.22	0.40
2:K:59:ASP:OD1	2:K:59:ASP:C	2.63	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%)	250 (91%)	20 (7%)	4 (2%)	8	18
1	D	272/276 (99%)	252 (93%)	15 (6%)	5 (2%)	6	15
1	G	271/276 (98%)	249 (92%)	19 (7%)	3 (1%)	11	24
1	J	271/276 (98%)	249 (92%)	20 (7%)	2 (1%)	18	35
2	B	96/99 (97%)	95 (99%)	0	1 (1%)	12	25
2	E	97/99 (98%)	94 (97%)	2 (2%)	1 (1%)	12	25
2	H	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	K	97/99 (98%)	95 (98%)	1 (1%)	1 (1%)	12	25
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	F	7/9 (78%)	5 (71%)	1 (14%)	1 (14%)	0	0
3	I	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	L	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1503/1536 (98%)	1401 (93%)	84 (6%)	18 (1%)	10	22

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	226	GLN
1	G	180	LEU
1	J	226	GLN
1	A	16	GLY
1	A	219	LEU
1	A	226	GLN
3	F	8	THR
1	G	226	GLN
1	A	265	GLY
1	D	17	LEU
1	D	195	SER
1	D	53	GLU

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Mol	Chain	Res	Type
1	D	212	ASP
1	G	18	GLU
2	B	47	PRO
2	E	47	PRO
2	K	47	PRO
1	J	193	PRO

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	234/234 (100%)	210 (90%)	24 (10%)	7	14
1	D	232/234 (99%)	202 (87%)	30 (13%)	4	7
1	G	232/234 (99%)	205 (88%)	27 (12%)	5	10
1	J	232/234 (99%)	213 (92%)	19 (8%)	10	23
2	B	93/94 (99%)	81 (87%)	12 (13%)	4	7
2	E	94/94 (100%)	84 (89%)	10 (11%)	6	13
2	H	94/94 (100%)	84 (89%)	10 (11%)	6	13
2	K	94/94 (100%)	82 (87%)	12 (13%)	4	7
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	6 (86%)	1 (14%)	3	6
3	I	7/7 (100%)	5 (71%)	2 (29%)	0	0
3	L	7/7 (100%)	6 (86%)	1 (14%)	3	6
All	All	1333/1340 (100%)	1185 (89%)	148 (11%)	6	12

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	19	GLU
1	A	23	ILE
1	A	30	ASN

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Mol	Chain	Res	Type
1	A	53	GLU
1	A	62	ARG
1	A	78	LEU
1	A	114	LEU
1	A	121	ARG
1	A	128	GLU
1	A	149	GLN
1	A	166	GLU
1	A	184	SER
1	A	219	LEU
1	A	222	GLU
1	A	223	GLU
1	A	224	LEU
1	A	226	GLN
1	A	234	ARG
1	A	262	TYR
1	A	264	GLU
1	A	268	GLU
1	A	270	LEU
1	A	274	TRP
2	B	4	THR
2	B	19	LYS
2	B	29	GLN
2	B	38	GLN
2	B	45	LYS
2	B	58	LYS
2	B	64	ILE
2	B	69	GLU
2	B	70	PHE
2	B	74	GLU
2	B	75	THR
2	B	93	VAL
1	D	44	ARG
1	D	58	GLU
1	D	64	THR
1	D	78	LEU
1	D	94	THR
1	D	111	ARG
1	D	114	LEU
1	D	121	ARG
1	D	134	THR
1	D	149	GLN

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Mol	Chain	Res	Type
1	D	170	ARG
1	D	178	THR
1	D	180	LEU
1	D	181	ARG
1	D	183	ASP
1	D	194	ARG
1	D	195	SER
1	D	222	GLU
1	D	226	GLN
1	D	230	LEU
1	D	232	GLU
1	D	234	ARG
1	D	254	GLU
1	D	256	ASN
1	D	260	ARG
1	D	264	GLU
1	D	266	LEU
1	D	268	GLU
1	D	272	LEU
1	D	273	ARG
2	E	2	GLN
2	E	4	THR
2	E	29	GLN
2	E	38	GLN
2	E	54	MET
2	E	64	ILE
2	E	69	GLU
2	E	70	PHE
2	E	75	THR
2	E	93	VAL
3	F	5	ASN
1	G	12	VAL
1	G	15	PRO
1	G	23	ILE
1	G	62	ARG
1	G	64	THR
1	G	72	GLN
1	G	75	ARG
1	G	78	LEU
1	G	110	LEU
1	G	111	ARG
1	G	114	LEU

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Mol	Chain	Res	Type
1	G	115	GLN
1	G	121	ARG
1	G	146	LYS
1	G	178	THR
1	G	181	ARG
1	G	195	SER
1	G	196	LYS
1	G	222	GLU
1	G	223	GLU
1	G	224	LEU
1	G	226	GLN
1	G	227	ASP
1	G	234	ARG
1	G	254	GLU
1	G	264	GLU
1	G	273	ARG
2	H	1	ILE
2	H	2	GLN
2	H	4	THR
2	H	29	GLN
2	H	38	GLN
2	H	64	ILE
2	H	69	GLU
2	H	70	PHE
2	H	75	THR
2	H	93	VAL
3	I	4	TYR
3	I	9	MET
1	J	18	GLU
1	J	23	ILE
1	J	64	THR
1	J	78	LEU
1	J	79	ARG
1	J	114	LEU
1	J	115	GLN
1	J	121	ARG
1	J	193	PRO
1	J	194	ARG
1	J	222	GLU
1	J	223	GLU
1	J	226	GLN
1	J	230	LEU

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Mol	Chain	Res	Type
1	J	234	ARG
1	J	247	VAL
1	J	264	GLU
1	J	268	GLU
1	J	273	ARG
2	K	1	ILE
2	K	2	GLN
2	K	4	THR
2	K	29	GLN
2	K	38	GLN
2	K	64	ILE
2	K	69	GLU
2	K	70	PHE
2	K	74	GLU
2	K	75	THR
2	K	93	VAL
2	K	98	ASP
3	L	4	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	97	GLN
1	A	149	GLN
1	A	192	HIS
1	A	255	GLN
2	B	29	GLN
2	B	31	HIS
3	C	5	ASN
1	D	3	HIS
1	D	54	GLN
1	D	87	GLN
1	D	97	GLN
1	D	141	GLN
1	D	174	ASN
1	D	192	HIS
1	D	220	ASN
1	D	255	GLN
1	D	256	ASN
2	E	31	HIS
2	E	34	HIS

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Mol	Chain	Res	Type
3	F	5	ASN
1	G	54	GLN
1	G	97	GLN
1	G	188	HIS
1	G	220	ASN
1	G	255	GLN
2	H	2	GLN
2	H	34	HIS
2	H	38	GLN
3	I	5	ASN
1	J	42	ASN
1	J	54	GLN
1	J	93	HIS
1	J	97	GLN
1	J	155	HIS
1	J	220	ASN
1	J	255	GLN
1	J	256	ASN
2	K	29	GLN
2	K	34	HIS
3	L	5	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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-1.58	0 100 100	2, 10, 24, 76	0
1	D	274/276 (99%)	-1.68	0 100 100	2, 9, 24, 61	0
1	G	273/276 (98%)	-1.25	1 (0%) 88 87	2, 9, 22, 65	0
1	J	273/276 (98%)	-1.50	0 100 100	2, 9, 22, 64	0
2	B	98/99 (98%)	-1.71	0 100 100	5, 8, 13, 17	0
2	E	99/99 (100%)	-1.68	0 100 100	5, 8, 13, 34	0
2	H	99/99 (100%)	-1.62	0 100 100	5, 8, 13, 40	0
2	K	99/99 (100%)	-1.69	0 100 100	5, 8, 13, 36	0
3	C	9/9 (100%)	-1.57	0 100 100	7, 9, 10, 11	0
3	F	9/9 (100%)	-1.53	0 100 100	7, 9, 10, 11	0
3	I	9/9 (100%)	-1.29	0 100 100	7, 9, 10, 11	0
3	L	9/9 (100%)	-1.41	0 100 100	7, 9, 10, 11	0
All	All	1527/1536 (99%)	-1.55	1 (0%) 92 92	2, 9, 22, 76	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	197	GLY	4.6

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.