



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:57 AM UTC

PDB ID : 3TBW / pdb_00003tbw
Title : CRYSTAL STRUCTURE OF THE MURINE CLASS I MAJOR HISTO-COMPATIBILITY COMPLEX H-2DB IN COMPLEX WITH THE LCMV-DERIVED GP33 ALTERED PEPTIDE ligand (A2G, V3P, Y4S)
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Deposited on : 2011-08-08
Resolution : 2.15 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

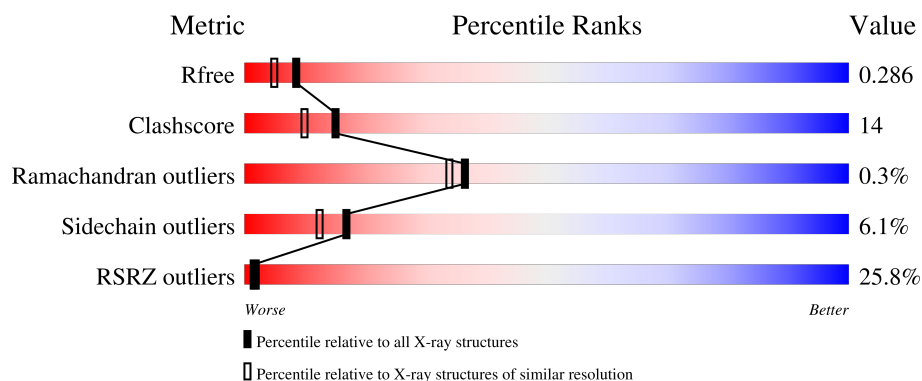
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	25% 67% 27% ...
1	C	276	29% 67% 28% ...
1	E	276	30% 72% 24% ...
1	G	276	29% 66% 28% ...
2	B	99	17% 73% 26% ...

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Mol	Chain	Length	Quality of chain
2	D	99	13%76%22%
2	F	99	30%72%25%
2	H	99	17%74%23%
3	I	9	67%33%
3	J	9	22%78%
3	K	9	11%33%67%
3	L	9	44%56%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13054 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	274	Total	C	N	O	S	14	0	0
			2248	1420	398	421	9			
1	C	274	Total	C	N	O	S	14	0	0
			2248	1420	398	421	9			
1	E	274	Total	C	N	O	S	30	0	0
			2248	1418	398	423	9			
1	G	267	Total	C	N	O	S	30	0	0
			2196	1387	390	410	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			
2	D	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			
2	F	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			
2	H	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			

- Molecule 3 is a protein called GLYCOPROTEIN GPC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	9	Total	C	N	O	S	0	0	0
			65	41	11	12	1			
3	J	9	Total	C	N	O	S	0	0	0
			65	41	11	12	1			
3	K	9	Total	C	N	O	S	0	0	0
			65	41	11	12	1			
3	L	9	Total	C	N	O	S	0	0	0
			65	41	11	12	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	2	GLY	ALA	engineered mutation	UNP P07399
I	3	PRO	VAL	engineered mutation	UNP P07399
I	4	SER	TYR	engineered mutation	UNP P07399
I	9	MET	CYS	engineered mutation	UNP P07399
J	2	GLY	ALA	engineered mutation	UNP P07399
J	3	PRO	VAL	engineered mutation	UNP P07399
J	4	SER	TYR	engineered mutation	UNP P07399
J	9	MET	CYS	engineered mutation	UNP P07399
K	2	GLY	ALA	engineered mutation	UNP P07399
K	3	PRO	VAL	engineered mutation	UNP P07399
K	4	SER	TYR	engineered mutation	UNP P07399
K	9	MET	CYS	engineered mutation	UNP P07399
L	2	GLY	ALA	engineered mutation	UNP P07399
L	3	PRO	VAL	engineered mutation	UNP P07399
L	4	SER	TYR	engineered mutation	UNP P07399
L	9	MET	CYS	engineered mutation	UNP P07399

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	124	Total O 124 124	0	0
4	B	51	Total O 51 51	0	0
4	C	87	Total O 87 87	0	0
4	D	52	Total O 52 52	0	0
4	E	84	Total O 84 84	0	0
4	F	31	Total O 31 31	0	0
4	G	83	Total O 83 83	0	0
4	H	45	Total O 45 45	0	0
4	I	8	Total O 8 8	0	0
4	J	2	Total O 2 2	0	0
4	K	2	Total O 2 2	0	0

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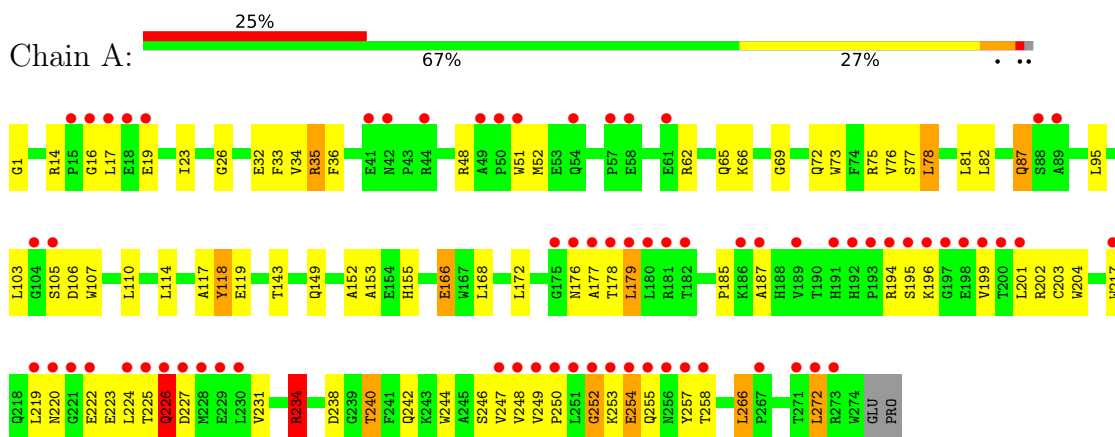
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	5	Total	O	0	0
			5	5		

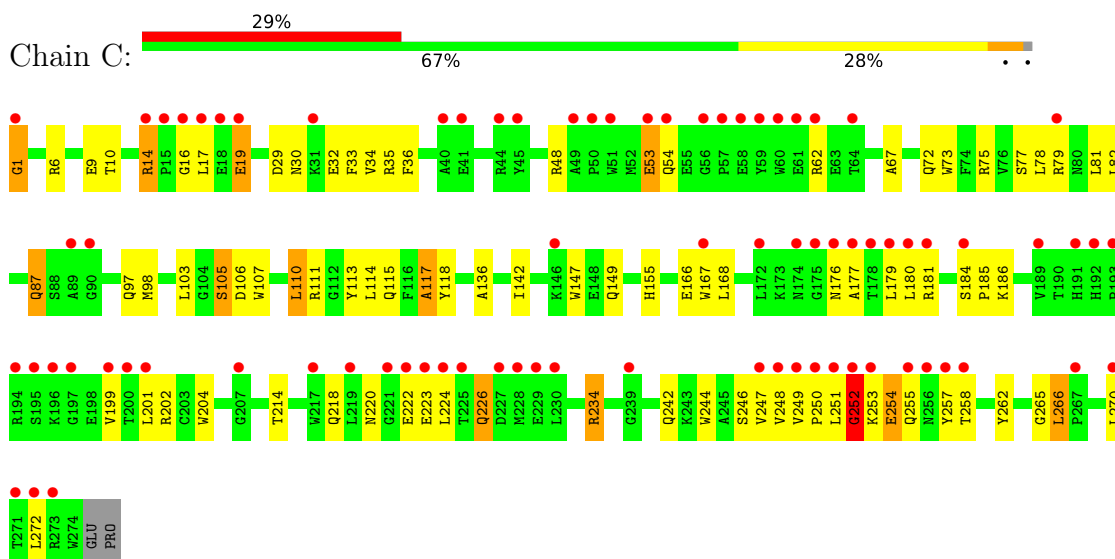
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

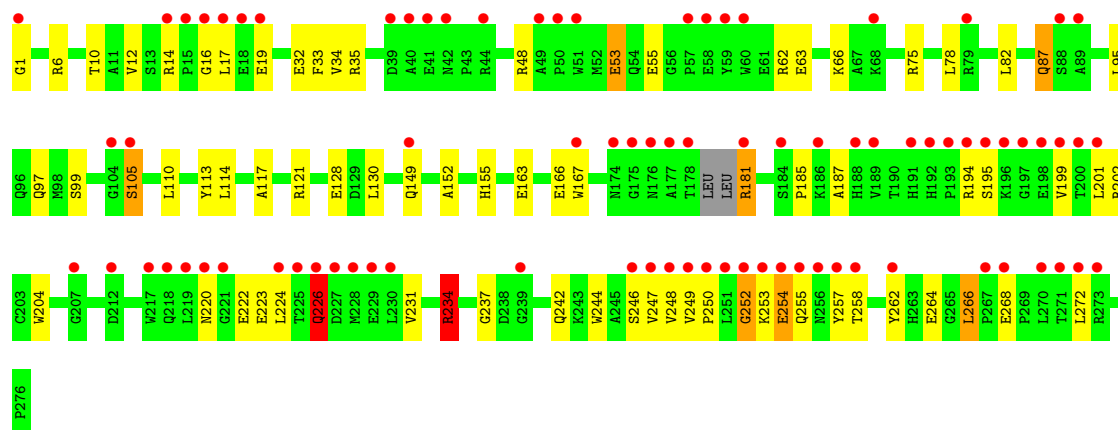


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

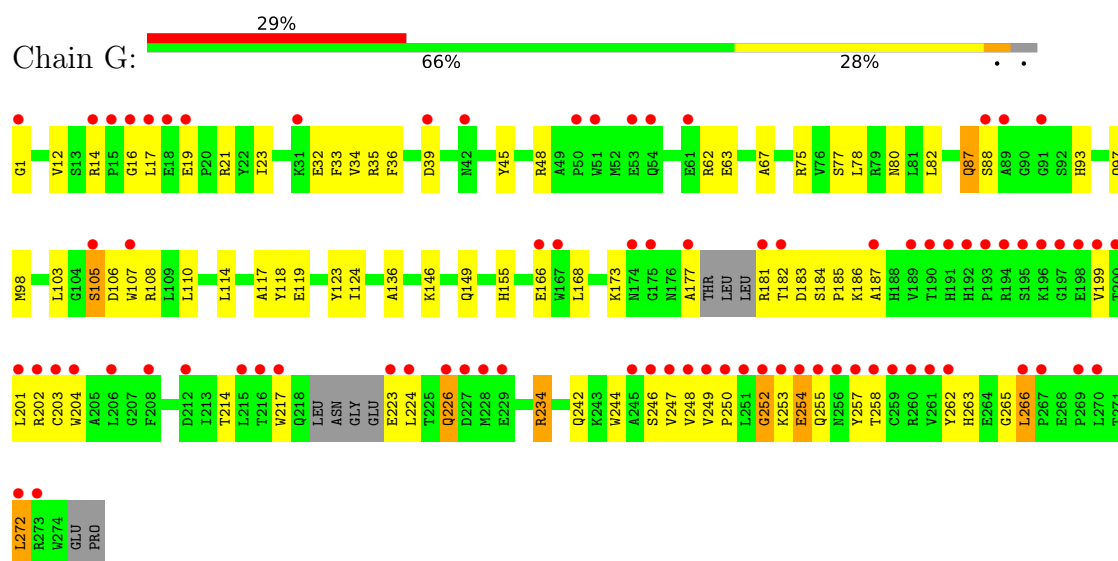


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

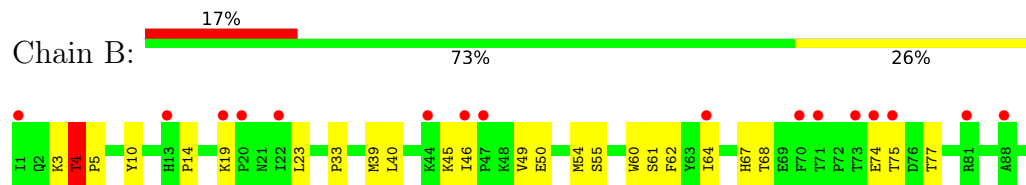




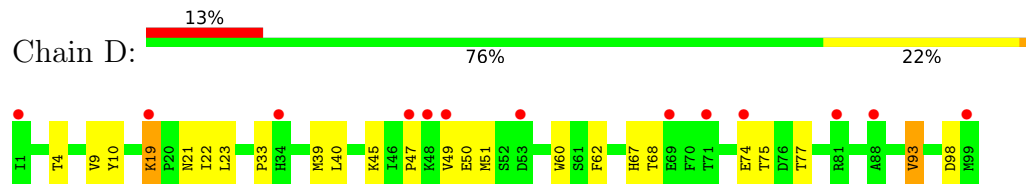
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



- Molecule 2: Beta-2-microglobulin

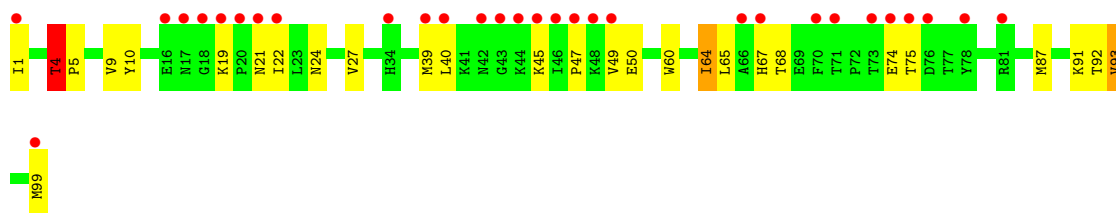


- Molecule 2: Beta-2-microglobulin

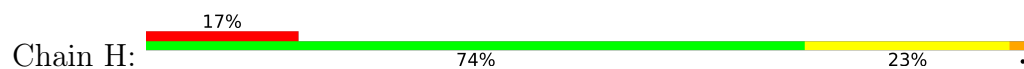


- Molecule 2: Beta-2-microglobulin





● Molecule 2: Beta-2-microglobulin



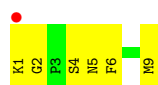
● Molecule 3: GLYCOPROTEIN GPC



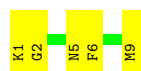
● Molecule 3: GLYCOPROTEIN GPC



● Molecule 3: GLYCOPROTEIN GPC



● Molecule 3: GLYCOPROTEIN GPC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.40Å 124.28Å 99.89Å 90.00° 103.23° 90.00°	Depositor
Resolution (Å)	47.48 – 2.15 47.48 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.6 (47.48-2.15) 98.4 (47.48-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.16Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.232 , 0.283 0.241 , 0.286	Depositor DCC
R_{free} test set	5819 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.4	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	0.93	EDS
Total number of atoms	13054	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0489e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	8/2314 (0.3%)	1.13	15/3142 (0.5%)
1	C	1.12	6/2314 (0.3%)	1.13	16/3142 (0.5%)
1	E	1.09	1/2314 (0.0%)	1.08	11/3141 (0.4%)
1	G	1.10	8/2260 (0.4%)	1.07	6/3065 (0.2%)
2	B	1.25	3/846 (0.4%)	1.16	2/1148 (0.2%)
2	D	1.20	1/846 (0.1%)	1.15	0/1148
2	F	1.11	1/846 (0.1%)	1.13	5/1148 (0.4%)
2	H	1.14	1/846 (0.1%)	1.16	0/1148
3	I	2.11	1/66 (1.5%)	1.59	0/87
3	J	1.51	0/66	1.70	1/87 (1.1%)
3	K	1.60	0/66	1.73	3/87 (3.4%)
3	L	1.53	0/66	2.09	2/87 (2.3%)
All	All	1.15	30/12850 (0.2%)	1.13	61/17430 (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
1	C	0	1
1	E	0	2
1	G	0	1
All	All	0	5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	4	SER	CA-CB	9.78	1.66	1.53
1	E	152	ALA	CA-CB	9.19	1.68	1.53
1	C	9	GLU	CA-C	-8.09	1.42	1.52
1	A	77	SER	CA-C	7.20	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	136	ALA	C-O	-6.88	1.15	1.23
1	G	93	HIS	C-O	-6.64	1.15	1.23
1	C	72	GLN	CA-CB	6.43	1.63	1.53
2	B	46	ILE	CA-C	6.29	1.58	1.53
1	C	117	ALA	CA-CB	6.20	1.66	1.53
1	G	80	ASN	CA-C	6.20	1.60	1.52
1	A	69	GLY	CA-C	6.03	1.58	1.52
2	H	74	GLU	CA-CB	5.96	1.62	1.53
1	G	118	TYR	CA-C	5.93	1.59	1.52
1	C	67	ALA	CA-CB	5.82	1.62	1.53
1	G	124	ILE	CA-CB	5.77	1.63	1.55
2	B	77	THR	CA-CB	5.71	1.61	1.53
1	A	66	LYS	CA-C	5.65	1.59	1.52
1	A	118	TYR	CA-C	5.62	1.59	1.52
1	C	115	GLN	C-O	-5.54	1.17	1.23
2	B	61	SER	C-O	-5.49	1.17	1.23
1	A	76	VAL	CA-C	5.39	1.59	1.52
1	A	73	TRP	CA-C	5.36	1.59	1.52
1	G	123	TYR	CA-C	5.36	1.57	1.52
1	C	136	ALA	CA-CB	5.22	1.61	1.53
1	G	93	HIS	CA-C	-5.17	1.46	1.52
1	A	26	GLY	CA-C	-5.16	1.48	1.52
2	F	27	VAL	CA-CB	-5.14	1.48	1.54
1	A	152	ALA	CA-CB	5.13	1.62	1.53
1	G	119	GLU	C-O	-5.11	1.16	1.23
2	D	51	MET	CA-C	5.10	1.58	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ASN	N-CA-C	12.56	128.75	111.92
3	L	2	GLY	CA-C-N	-10.36	110.26	120.52
3	L	2	GLY	C-N-CA	-10.36	110.26	120.52
1	C	220	ASN	N-CA-C	9.80	124.51	111.28
1	E	220	ASN	N-CA-C	9.40	124.68	111.52
1	A	234	ARG	NE-CZ-NH1	8.32	129.82	121.50
1	C	252	GLY	N-CA-C	8.32	126.42	115.36
1	E	252	GLY	N-CA-C	7.79	125.69	115.40
1	G	252	GLY	N-CA-C	7.68	125.57	115.36
1	A	252	GLY	N-CA-C	7.65	125.16	115.21
1	A	234	ARG	NE-CZ-NH2	-7.59	112.36	119.20
1	A	35	ARG	NE-CZ-NH2	-7.37	112.56	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	THR	CA-C-N	7.03	127.45	119.93
2	B	4	THR	C-N-CA	7.03	127.45	119.93
1	E	53	GLU	CB-CA-C	-6.70	97.38	110.11
1	A	176	ASN	N-CA-C	6.64	119.53	111.82
2	F	4	THR	CA-C-N	6.61	126.97	119.83
2	F	4	THR	C-N-CA	6.61	126.97	119.83
1	E	53	GLU	CA-C-N	6.56	129.40	120.54
1	E	53	GLU	C-N-CA	6.56	129.40	120.54
1	C	252	GLY	CA-C-N	6.14	133.26	121.54
1	C	252	GLY	C-N-CA	6.14	133.26	121.54
1	G	252	GLY	CA-C-N	5.99	132.98	121.54
1	G	252	GLY	C-N-CA	5.99	132.98	121.54
1	C	19	GLU	CB-CA-C	5.83	118.00	109.08
1	A	119	GLU	N-CA-C	-5.81	104.80	112.24
1	C	1	GLY	CA-C-N	5.78	125.97	120.31
1	C	1	GLY	C-N-CA	5.78	125.97	120.31
1	E	87	GLN	CA-C-N	-5.68	111.28	122.02
1	E	87	GLN	C-N-CA	-5.68	111.28	122.02
1	C	87	GLN	CA-C-N	-5.66	112.61	122.64
1	C	87	GLN	C-N-CA	-5.66	112.61	122.64
1	E	234	ARG	NE-CZ-NH2	-5.60	114.16	119.20
2	F	92	THR	CA-C-N	-5.59	115.17	122.94
2	F	92	THR	C-N-CA	-5.59	115.17	122.94
1	A	78	LEU	N-CA-C	-5.58	105.09	111.07
1	G	39	ASP	CB-CA-C	-5.56	98.25	109.55
1	E	252	GLY	CA-C-N	5.47	131.99	121.54
1	E	252	GLY	C-N-CA	5.47	131.99	121.54
3	K	2	GLY	CA-C-N	-5.45	114.97	120.31
3	K	2	GLY	C-N-CA	-5.45	114.97	120.31
1	E	226	GLN	N-CA-C	5.42	122.35	110.80
2	F	24	ASN	N-CA-C	5.41	118.64	109.76
1	C	54	GLN	CB-CA-C	-5.38	101.53	110.68
1	C	14	ARG	CA-C-N	5.38	126.56	119.84
1	C	14	ARG	C-N-CA	5.38	126.56	119.84
1	C	53	GLU	CA-C-N	5.28	127.62	120.38
1	C	53	GLU	C-N-CA	5.28	127.62	120.38
1	C	10	THR	CA-C-N	-5.21	115.13	122.94
1	C	10	THR	C-N-CA	-5.21	115.13	122.94
1	A	35	ARG	NE-CZ-NH1	5.20	126.70	121.50
3	J	2	GLY	CA-C-O	-5.11	117.51	122.46
1	A	143	THR	N-CA-C	5.07	116.50	111.07
3	K	4	SER	N-CA-C	-5.05	100.94	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	GLY	CA-C-N	5.04	131.17	121.54
1	A	252	GLY	C-N-CA	5.04	131.17	121.54
1	A	172	LEU	N-CA-C	-5.04	105.97	111.82
1	G	87	GLN	CA-C-N	-5.03	113.27	122.12
1	G	87	GLN	C-N-CA	-5.03	113.27	122.12
1	A	87	GLN	CA-C-N	-5.01	113.59	121.86
1	A	87	GLN	C-N-CA	-5.01	113.59	121.86

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	GLY	Peptide
1	C	252	GLY	Peptide
1	E	252	GLY	Peptide
1	E	53	GLU	Peptide
1	G	252	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	2248	0	2123	62	0
1	C	2248	0	2123	68	0
1	E	2248	0	2113	61	0
1	G	2196	0	2066	78	0
2	B	820	0	796	19	0
2	D	820	0	796	25	0
2	F	820	0	796	24	0
2	H	820	0	796	31	0
3	I	65	0	66	2	0
3	J	65	0	66	10	0
3	K	65	0	66	9	0
3	L	65	0	66	7	0
4	A	124	0	0	11	0
4	B	51	0	0	2	0
4	C	87	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	52	0	0	4	0
4	E	84	0	0	4	0
4	F	31	0	0	3	0
4	G	83	0	0	9	0
4	H	45	0	0	3	0
4	I	8	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	5	0	0	0	0
All	All	13054	0	11873	331	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 14.

All (331) 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)
2:D:39:MET:SD	4:D:190:HOH:O	2.18	1.01
2:H:39:MET:HE2	2:H:49:VAL:HG13	1.42	0.98
2:F:39:MET:HE2	2:F:49:VAL:HG13	1.43	0.96
2:D:39:MET:HE2	2:D:49:VAL:HG13	1.55	0.89
1:G:184:SER:HA	4:G:389:HOH:O	1.73	0.89
1:C:167:TRP:CE2	3:J:1:LYS:HD2	2.10	0.86
2:B:39:MET:HE2	2:B:49:VAL:HG13	1.57	0.86
1:C:186:LYS:HE3	1:G:177:ALA:HB2	1.64	0.80
1:C:97:GLN:HE22	3:J:5:ASN:HD21	1.33	0.76
1:G:185:PRO:HD2	1:G:266:LEU:HD13	1.68	0.76
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.22	0.74
2:D:39:MET:CE	2:D:68:THR:HB	2.18	0.73
1:G:234:ARG:HD3	2:H:10:TYR:CE2	2.24	0.73
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.24	0.72
1:E:226:GLN:CG	1:E:226:GLN:O	2.38	0.72
1:C:185:PRO:HD2	1:C:266:LEU:HD13	1.72	0.71
1:C:202:ARG:HD2	1:C:244:TRP:CD2	2.26	0.71
2:H:39:MET:HE2	2:H:49:VAL:CG1	2.18	0.70
1:A:19:GLU:OE2	1:A:75:ARG:HD2	1.93	0.69
1:G:185:PRO:HD3	4:G:389:HOH:O	1.91	0.69
1:C:155:HIS:HB3	3:J:6:PHE:CZ	2.28	0.69
1:G:155:HIS:HB3	3:L:6:PHE:CZ	2.28	0.69
1:A:185:PRO:HD2	1:A:266:LEU:HD13	1.74	0.68
1:E:55:GLU:OE2	4:E:364:HOH:O	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLU:HB3	4:A:556:HOH:O	1.94	0.67
1:C:234:ARG:HD3	2:D:10:TYR:CE2	2.29	0.67
1:C:186:LYS:HE3	1:G:177:ALA:CB	2.25	0.67
1:C:19:GLU:OE2	1:C:75:ARG:HD2	1.94	0.66
1:A:32:GLU:OE2	1:A:48:ARG:HD2	1.95	0.66
2:H:39:MET:CE	2:H:68:THR:HB	2.26	0.66
1:G:32:GLU:OE2	1:G:48:ARG:HD2	1.96	0.66
1:E:202:ARG:HD2	1:E:244:TRP:CD2	2.31	0.66
2:D:39:MET:HE1	2:D:67:HIS:C	2.21	0.66
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.31	0.65
1:G:19:GLU:OE2	1:G:75:ARG:HD2	1.96	0.65
1:G:201:LEU:O	1:G:246:SER:HA	1.96	0.65
1:E:97:GLN:HE22	3:K:5:ASN:HD21	1.44	0.65
1:E:234:ARG:HD3	2:F:10:TYR:CE2	2.31	0.65
1:G:146:LYS:CD	4:G:450:HOH:O	2.45	0.64
2:H:91:LYS:HD3	4:H:522:HOH:O	1.97	0.64
2:H:9:VAL:CG2	2:H:93:VAL:HG22	2.28	0.64
1:C:53:GLU:O	2:H:19:LYS:CE	2.46	0.63
1:A:226:GLN:CG	1:A:226:GLN:O	2.41	0.63
1:C:201:LEU:O	1:C:246:SER:HA	1.99	0.63
1:A:155:HIS:HB3	3:I:6:PHE:CZ	2.34	0.62
1:C:53:GLU:O	2:H:19:LYS:HD3	2.00	0.62
1:C:167:TRP:CZ2	3:J:1:LYS:HD2	2.35	0.62
1:E:226:GLN:O	1:E:226:GLN:CD	2.42	0.61
2:H:9:VAL:HG21	2:H:93:VAL:HG22	1.82	0.61
1:C:53:GLU:O	2:H:19:LYS:CD	2.47	0.61
1:A:234:ARG:HD2	1:A:242:GLN:HB2	1.82	0.61
1:G:146:LYS:HD2	4:G:450:HOH:O	2.01	0.61
1:E:185:PRO:HD2	1:E:266:LEU:HD13	1.83	0.61
1:C:62:ARG:HG2	4:C:401:HOH:O	2.01	0.60
2:F:40:LEU:HD23	2:F:45:LYS:HA	1.83	0.60
1:A:194:ARG:HG2	4:A:508:HOH:O	2.02	0.60
1:C:167:TRP:CE2	3:J:1:LYS:CD	2.82	0.59
1:C:77:SER:HB3	3:J:9:MET:HG2	1.84	0.59
1:E:223:GLU:C	1:E:224:LEU:HD22	2.27	0.59
1:G:103:LEU:HD11	1:G:168:LEU:HD23	1.84	0.59
2:F:1:ILE:N	4:F:311:HOH:O	2.32	0.59
1:C:79:ARG:NH1	4:C:570:HOH:O	2.36	0.58
1:E:19:GLU:OE2	1:E:75:ARG:HD2	2.03	0.58
1:G:12:VAL:HG21	2:H:33:PRO:HG2	1.86	0.58
1:A:226:GLN:O	1:A:226:GLN:CD	2.47	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:MET:HE2	2:D:49:VAL:CG1	2.31	0.58
1:G:263:HIS:CE1	4:G:389:HOH:O	2.57	0.58
2:F:39:MET:HE2	2:F:49:VAL:CG1	2.25	0.58
2:H:39:MET:HE1	2:H:67:HIS:C	2.29	0.58
1:C:177:ALA:N	1:G:186:LYS:HZ1	2.03	0.57
1:C:222:GLU:OE2	1:C:222:GLU:HA	2.04	0.57
1:G:88:SER:O	4:G:374:HOH:O	2.17	0.57
1:E:163:GLU:OE1	3:K:1:LYS:HD3	2.05	0.57
1:A:201:LEU:O	1:A:246:SER:HA	2.04	0.56
1:C:53:GLU:O	2:H:19:LYS:NZ	2.38	0.56
2:F:39:MET:CE	2:F:68:THR:HG22	2.35	0.56
1:G:223:GLU:C	1:G:224:LEU:HD22	2.30	0.56
2:F:39:MET:CE	2:F:68:THR:CG2	2.84	0.56
2:H:39:MET:HE1	2:H:68:THR:HB	1.86	0.56
1:E:32:GLU:OE2	1:E:48:ARG:HD2	2.06	0.56
2:F:39:MET:HE3	2:F:68:THR:CG2	2.36	0.56
2:B:3:LYS:HE3	4:B:118:HOH:O	2.06	0.56
1:G:32:GLU:OE2	1:G:35:ARG:HD2	2.05	0.56
1:A:95:LEU:HD11	3:I:9:MET:HE1	1.88	0.55
1:A:223:GLU:C	1:A:224:LEU:HD22	2.31	0.55
1:E:201:LEU:O	1:E:246:SER:HA	2.07	0.55
2:B:40:LEU:HD23	2:B:45:LYS:HA	1.89	0.55
1:C:110:LEU:HD13	4:C:575:HOH:O	2.06	0.55
1:E:262:TYR:CG	1:G:108:ARG:HD3	2.42	0.55
1:A:222:GLU:OE2	1:A:222:GLU:HA	2.07	0.55
1:E:97:GLN:NE2	3:K:5:ASN:HD21	2.04	0.55
1:E:155:HIS:HB3	3:K:6:PHE:CZ	2.41	0.55
2:F:39:MET:CE	2:F:68:THR:HB	2.37	0.55
1:A:227:ASP:O	4:A:381:HOH:O	2.18	0.54
2:B:39:MET:HE1	2:B:67:HIS:C	2.32	0.54
1:C:223:GLU:C	1:C:224:LEU:HD22	2.32	0.54
1:E:234:ARG:HD3	2:F:10:TYR:CZ	2.42	0.54
2:B:39:MET:HE2	2:B:49:VAL:CG1	2.33	0.54
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.42	0.54
2:B:39:MET:CE	2:B:68:THR:HB	2.38	0.54
1:C:176:ASN:HB3	1:G:186:LYS:HE2	1.88	0.54
1:C:249:VAL:HG22	1:C:257:TYR:CZ	2.42	0.54
2:H:40:LEU:HD23	2:H:45:LYS:HA	1.90	0.54
2:D:19:LYS:HE3	4:D:309:HOH:O	2.08	0.54
1:E:222:GLU:HA	1:E:222:GLU:OE2	2.07	0.54
1:C:33:PHE:CD2	1:C:34:VAL:HG13	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:TYR:CD2	1:G:108:ARG:HG2	2.43	0.53
1:E:95:LEU:HD11	3:K:9:MET:HE1	1.90	0.53
1:E:66:LYS:NZ	3:K:1:LYS:HG2	2.23	0.53
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.43	0.53
2:D:39:MET:HE1	2:D:68:THR:HB	1.88	0.53
1:E:226:GLN:O	1:E:226:GLN:HG2	2.09	0.53
2:F:39:MET:HE1	2:F:68:THR:HG22	1.91	0.53
2:F:39:MET:HE1	2:F:67:HIS:C	2.33	0.53
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.43	0.52
2:B:39:MET:HE3	2:B:68:THR:CG2	2.39	0.52
1:E:1:GLY:N	1:E:105:SER:HB3	2.24	0.52
1:G:1:GLY:N	1:G:105:SER:HB3	2.24	0.52
2:D:39:MET:HE3	2:D:68:THR:CG2	2.39	0.52
1:A:202:ARG:HG2	1:A:204:TRP:NE1	2.25	0.52
1:C:234:ARG:HD2	1:C:242:GLN:HB2	1.91	0.52
1:G:201:LEU:HD12	1:G:249:VAL:HG21	1.90	0.52
1:E:234:ARG:HD2	1:E:242:GLN:HB2	1.91	0.52
1:A:272:LEU:HD22	4:A:383:HOH:O	2.10	0.52
1:G:234:ARG:HD3	2:H:10:TYR:CZ	2.45	0.52
1:C:1:GLY:N	1:C:105:SER:HB3	2.25	0.51
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.45	0.51
1:G:249:VAL:HG22	1:G:257:TYR:CZ	2.46	0.51
1:C:14:ARG:HB3	1:C:14:ARG:NH1	2.25	0.51
1:E:264:GLU:HG2	4:E:351:HOH:O	2.10	0.51
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.46	0.51
2:D:33:PRO:HG3	2:D:62:PHE:CZ	2.46	0.51
1:A:195:SER:N	4:A:508:HOH:O	2.43	0.50
1:E:201:LEU:HD12	1:E:249:VAL:HG21	1.94	0.50
1:E:163:GLU:OE1	3:K:1:LYS:CD	2.58	0.50
1:G:1:GLY:H2	1:G:105:SER:HB3	1.76	0.50
2:H:39:MET:CE	2:H:68:THR:CG2	2.89	0.50
2:H:39:MET:HE3	2:H:68:THR:CG2	2.41	0.50
1:C:32:GLU:OE2	1:C:35:ARG:HD2	2.11	0.50
1:C:218:GLN:NE2	4:C:355:HOH:O	2.45	0.50
1:G:247:VAL:HG22	1:G:248:VAL:N	2.25	0.50
1:A:72:GLN:HG2	4:A:389:HOH:O	2.12	0.50
2:B:39:MET:CE	2:B:68:THR:CG2	2.90	0.50
2:H:39:MET:HE1	2:H:68:THR:CB	2.42	0.50
1:E:262:TYR:CD2	1:G:108:ARG:HD3	2.46	0.49
1:E:244:TRP:HZ2	2:F:99:MET:HE2	1.76	0.49
1:C:226:GLN:O	1:C:226:GLN:CG	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:77:SER:HB3	3:L:9:MET:HG2	1.95	0.49
1:C:97:GLN:NE2	3:J:5:ASN:HD21	2.04	0.49
1:G:14:ARG:NH1	1:G:14:ARG:HB3	2.26	0.49
1:G:146:LYS:NZ	4:G:450:HOH:O	2.15	0.49
2:D:39:MET:CE	2:D:68:THR:CB	2.90	0.49
1:C:32:GLU:OE2	1:C:48:ARG:HD2	2.12	0.49
2:H:40:LEU:CD1	4:H:446:HOH:O	2.59	0.49
1:E:82:LEU:HD12	1:E:87:GLN:HB2	1.95	0.49
1:C:106:ASP:O	1:C:107:TRP:HB2	2.11	0.48
1:A:14:ARG:HB3	1:A:14:ARG:NH1	2.28	0.48
2:F:21:ASN:OD1	2:F:22:ILE:N	2.44	0.48
1:C:81:LEU:HD13	1:C:118:TYR:CD1	2.48	0.48
2:H:51:MET:HB3	4:H:405:HOH:O	2.13	0.48
1:A:36:PHE:CD1	1:A:36:PHE:C	2.92	0.48
2:B:39:MET:CE	2:B:68:THR:HG22	2.43	0.48
1:E:99:SER:HB2	4:E:354:HOH:O	2.14	0.48
2:F:91:LYS:NZ	4:F:552:HOH:O	2.47	0.48
1:G:183:ASP:O	4:G:389:HOH:O	2.20	0.48
1:E:16:GLY:O	1:E:17:LEU:C	2.57	0.48
1:G:202:ARG:HD3	1:G:244:TRP:CE3	2.49	0.48
2:D:39:MET:HE3	2:D:68:THR:HB	1.94	0.48
1:C:250:PRO:HB2	1:C:253:LYS:HB2	1.96	0.47
1:G:199:VAL:HG21	1:G:254:GLU:OE1	2.13	0.47
1:G:234:ARG:HD2	1:G:242:GLN:HB2	1.95	0.47
1:C:98:MET:HG3	2:D:60:TRP:CZ3	2.49	0.47
1:C:255:GLN:OE1	1:C:255:GLN:HA	2.14	0.47
2:D:23:LEU:O	2:D:67:HIS:HA	2.15	0.47
1:A:223:GLU:CG	4:A:556:HOH:O	2.62	0.47
1:C:82:LEU:HD12	1:C:87:GLN:HB2	1.96	0.47
1:E:249:VAL:HG22	1:E:257:TYR:CZ	2.50	0.47
1:G:82:LEU:HD12	1:G:87:GLN:HB2	1.97	0.47
1:G:249:VAL:HG13	1:G:257:TYR:CE2	2.49	0.47
1:A:166:GLU:OE2	4:A:404:HOH:O	2.20	0.47
1:A:231:VAL:HG13	1:A:244:TRP:CZ2	2.50	0.47
1:C:234:ARG:HD3	2:D:10:TYR:CZ	2.49	0.46
1:E:14:ARG:HB3	1:E:14:ARG:NH1	2.30	0.46
1:C:33:PHE:C	1:C:48:ARG:HB2	2.40	0.46
2:D:21:ASN:OD1	2:D:22:ILE:N	2.43	0.46
1:E:202:ARG:HG2	1:E:204:TRP:NE1	2.30	0.46
1:A:247:VAL:HG22	1:A:248:VAL:N	2.31	0.46
2:B:23:LEU:O	2:B:67:HIS:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:226:GLN:O	1:G:226:GLN:CG	2.62	0.46
2:H:79:ALA:HB2	2:H:94:TYR:CD1	2.50	0.46
1:C:177:ALA:HB2	1:G:186:LYS:HE3	1.97	0.46
1:C:184:SER:OG	1:C:265:GLY:O	2.30	0.46
2:H:39:MET:CE	2:H:68:THR:HG22	2.45	0.46
1:A:187:ALA:HA	1:A:204:TRP:O	2.16	0.46
1:G:33:PHE:C	1:G:48:ARG:HB2	2.41	0.46
1:G:249:VAL:CG1	1:G:254:GLU:HA	2.45	0.46
2:D:40:LEU:HD23	2:D:45:LYS:HA	1.96	0.46
1:G:202:ARG:CD	1:G:244:TRP:CD2	2.98	0.46
1:C:201:LEU:HD12	1:C:249:VAL:HG21	1.97	0.46
1:G:202:ARG:HG2	1:G:204:TRP:NE1	2.30	0.46
2:B:4:THR:HA	2:B:5:PRO:HD3	1.84	0.45
2:B:33:PRO:HG3	2:B:62:PHE:CZ	2.51	0.45
2:D:39:MET:CE	2:D:68:THR:CG2	2.94	0.45
1:E:250:PRO:HB2	1:E:253:LYS:HB2	1.98	0.45
2:H:64:ILE:CG2	2:H:65:LEU:N	2.78	0.45
1:E:117:ALA:HB2	2:F:60:TRP:CE2	2.52	0.45
1:A:103:LEU:HD11	1:A:168:LEU:HD23	1.97	0.45
2:B:14:PRO:HD3	4:B:157:HOH:O	2.17	0.45
1:G:185:PRO:HD2	1:G:266:LEU:CD1	2.43	0.45
1:C:176:ASN:HB3	1:G:186:LYS:CE	2.46	0.45
1:A:1:GLY:N	1:A:105:SER:HB3	2.30	0.45
1:C:16:GLY:O	1:C:17:LEU:C	2.60	0.45
1:C:247:VAL:HG22	1:C:248:VAL:N	2.32	0.45
1:E:199:VAL:HG21	1:E:254:GLU:OE1	2.17	0.45
1:E:231:VAL:HG13	1:E:244:TRP:CZ2	2.52	0.45
2:F:9:VAL:CG2	2:F:93:VAL:HG22	2.46	0.45
1:A:195:SER:O	1:A:196:LYS:C	2.59	0.45
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.52	0.45
1:G:106:ASP:O	1:G:107:TRP:HB2	2.16	0.45
1:A:82:LEU:HD12	1:A:87:GLN:HB2	1.99	0.45
1:A:155:HIS:CD2	4:A:466:HOH:O	2.69	0.45
2:D:39:MET:HE1	2:D:68:THR:CB	2.46	0.45
1:G:36:PHE:CD1	1:G:36:PHE:C	2.94	0.45
1:E:1:GLY:H2	1:E:105:SER:HB3	1.82	0.44
1:G:63:GLU:OE2	3:L:1:LYS:HD3	2.17	0.44
1:A:51:TRP:CZ3	1:A:52:MET:SD	3.10	0.44
1:C:214:THR:HB	1:C:262:TYR:HB2	1.99	0.44
1:E:234:ARG:HD2	1:E:242:GLN:OE1	2.17	0.44
2:H:9:VAL:HG23	2:H:93:VAL:HG22	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:PHE:C	1:A:48:ARG:HB2	2.42	0.44
1:A:178:THR:C	1:A:179:LEU:HD22	2.42	0.44
1:C:103:LEU:HD11	1:C:168:LEU:HD23	1.99	0.44
1:E:10:THR:HG22	1:E:12:VAL:HG23	1.99	0.44
1:G:103:LEU:CD1	1:G:168:LEU:HD23	2.48	0.44
1:A:201:LEU:HD12	1:A:249:VAL:HG21	1.99	0.44
1:C:251:LEU:HD23	1:C:252:GLY:N	2.33	0.44
2:D:33:PRO:HG3	2:D:62:PHE:CE2	2.53	0.44
1:E:247:VAL:HG22	1:E:248:VAL:N	2.31	0.44
1:G:16:GLY:O	1:G:17:LEU:C	2.60	0.44
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.52	0.44
4:C:401:HOH:O	3:J:1:LYS:CE	2.66	0.44
1:G:181:ARG:HG2	1:G:182:THR:N	2.32	0.44
1:C:36:PHE:CD1	1:C:36:PHE:C	2.95	0.44
1:E:63:GLU:OE2	3:K:1:LYS:HG3	2.17	0.44
1:E:167:TRP:CZ2	3:K:1:LYS:HE3	2.53	0.44
1:E:268:GLU:OE1	1:G:173:LYS:HE2	2.18	0.44
1:E:255:GLN:OE1	1:E:255:GLN:HA	2.17	0.44
1:G:250:PRO:HB2	1:G:253:LYS:HB2	2.00	0.44
1:E:6:ARG:NH2	1:E:113:TYR:CE1	2.86	0.43
1:G:184:SER:OG	1:G:265:GLY:O	2.30	0.43
1:G:255:GLN:HA	1:G:255:GLN:OE1	2.18	0.43
2:B:39:MET:HE1	2:B:68:THR:HG22	2.00	0.43
1:C:73:TRP:CD1	3:J:8:THR:HG22	2.53	0.43
1:E:262:TYR:CD1	1:G:108:ARG:HD3	2.53	0.43
2:F:4:THR:HA	2:F:5:PRO:HD3	1.83	0.43
1:G:23:ILE:HD12	2:H:54:MET:SD	2.58	0.43
1:A:65:GLN:NE2	4:A:421:HOH:O	2.51	0.43
1:G:214:THR:HB	1:G:262:TYR:HB2	2.00	0.43
1:A:250:PRO:HB2	1:A:253:LYS:HB2	2.00	0.43
1:C:177:ALA:H	1:G:186:LYS:HZ1	1.64	0.43
1:G:155:HIS:HB3	3:L:6:PHE:CE1	2.53	0.43
1:C:199:VAL:HG21	1:C:254:GLU:OE1	2.18	0.43
1:G:77:SER:HB3	3:L:9:MET:CG	2.48	0.43
1:G:249:VAL:HG11	1:G:254:GLU:HA	2.00	0.43
1:C:202:ARG:HG2	1:C:204:TRP:NE1	2.33	0.43
1:E:32:GLU:OE2	1:E:35:ARG:HD2	2.18	0.43
1:G:97:GLN:NE2	3:L:5:ASN:HD21	2.16	0.43
2:H:21:ASN:OD1	2:H:22:ILE:N	2.47	0.43
2:H:39:MET:CE	2:H:68:THR:CB	2.94	0.43
1:A:199:VAL:HG21	1:A:254:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:64:ILE:CG2	2:F:65:LEU:N	2.82	0.43
1:A:225:THR:O	1:A:225:THR:HG22	2.19	0.43
1:A:249:VAL:HG13	1:A:257:TYR:CE2	2.54	0.43
1:C:29:ASP:O	1:C:30:ASN:HB2	2.19	0.43
1:E:121:ARG:NH1	2:F:1:ILE:HB	2.34	0.42
1:A:244:TRP:CZ2	2:B:99:MET:HE3	2.54	0.42
1:A:249:VAL:HG22	1:A:257:TYR:CE2	2.54	0.42
1:G:203:CYS:HB2	1:G:217:TRP:CZ2	2.54	0.42
1:A:177:ALA:HB3	1:E:181:ARG:HD3	2.00	0.42
1:E:244:TRP:CZ2	2:F:99:MET:CE	3.02	0.42
1:C:249:VAL:HG13	1:C:257:TYR:CE2	2.54	0.42
1:G:187:ALA:O	1:G:272:LEU:HD11	2.19	0.42
1:E:33:PHE:CD2	1:E:34:VAL:HG13	2.55	0.42
1:G:33:PHE:CD2	1:G:34:VAL:HG13	2.54	0.42
1:G:97:GLN:HE22	3:L:5:ASN:HD21	1.67	0.42
1:A:16:GLY:O	1:A:17:LEU:C	2.62	0.42
1:C:176:ASN:OD1	1:C:180:LEU:HD13	2.19	0.42
2:D:77:THR:HG22	4:D:558:HOH:O	2.19	0.42
1:E:33:PHE:C	1:E:48:ARG:HB2	2.44	0.42
1:G:98:MET:HG3	2:H:60:TRP:CZ3	2.54	0.42
1:G:181:ARG:HG2	1:G:182:THR:H	1.83	0.42
1:A:23:ILE:HD12	2:B:54:MET:SD	2.60	0.42
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.55	0.42
1:A:255:GLN:OE1	1:A:255:GLN:HA	2.18	0.42
1:C:249:VAL:CG1	1:C:254:GLU:HA	2.50	0.42
1:E:128:GLU:C	1:E:130:LEU:H	2.27	0.42
1:A:219:LEU:HG	1:A:219:LEU:O	2.19	0.42
2:D:39:MET:HE1	2:D:68:THR:N	2.35	0.42
1:C:1:GLY:H2	1:C:105:SER:HB3	1.84	0.42
1:A:153:ALA:HB3	4:A:509:HOH:O	2.19	0.42
1:C:266:LEU:HD21	1:C:270:LEU:HG	2.02	0.42
2:H:64:ILE:HG22	2:H:65:LEU:N	2.34	0.42
1:E:99:SER:CB	4:E:354:HOH:O	2.67	0.41
1:E:194:ARG:HG2	1:E:195:SER:H	1.84	0.41
1:A:106:ASP:O	1:A:107:TRP:HB2	2.20	0.41
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.55	0.41
1:G:263:HIS:O	1:G:266:LEU:HB2	2.20	0.41
1:G:21:ARG:NE	1:G:23:ILE:HD11	2.36	0.41
2:D:9:VAL:CG2	2:D:93:VAL:HG22	2.50	0.41
2:F:87:MET:HE1	2:F:91:LYS:HD2	2.03	0.41
1:G:45:TYR:CE2	1:G:67:ALA:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HD12	1:A:266:LEU:HA	1.96	0.41
1:A:254:GLU:H	1:A:254:GLU:HG2	1.76	0.41
2:D:98:ASP:HA	4:D:553:HOH:O	2.21	0.41
1:C:6:ARG:NH2	1:C:113:TYR:CE1	2.89	0.41
1:A:226:GLN:O	1:A:226:GLN:HG2	2.11	0.41
1:A:238:ASP:OD1	1:A:240:THR:OG1	2.37	0.41
1:E:187:ALA:HA	1:E:204:TRP:O	2.20	0.41
1:E:244:TRP:HZ2	2:F:99:MET:CE	2.33	0.41
1:E:266:LEU:HD12	1:E:266:LEU:HA	1.92	0.41
2:F:39:MET:HE1	2:F:68:THR:CG2	2.49	0.41
1:A:32:GLU:OE2	1:A:35:ARG:HD2	2.21	0.40
1:C:147:TRP:N	1:C:147:TRP:CD1	2.86	0.40
1:C:226:GLN:O	1:C:226:GLN:CD	2.64	0.40
1:G:62:ARG:HG3	4:G:358:HOH:O	2.20	0.40
1:G:247:VAL:CG2	1:G:248:VAL:N	2.84	0.40
1:C:142:ILE:H	1:C:142:ILE:HG13	1.70	0.40
1:G:202:ARG:CD	1:G:244:TRP:CE3	3.04	0.40
3:J:6:PHE:O	3:J:7:ALA:C	2.63	0.40
1:C:111:ARG:HD3	1:C:113:TYR:OH	2.22	0.40
1:E:237:GLY:HA3	4:F:207:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	272/276 (99%)	254 (93%)	17 (6%)	1 (0%)	30 26
1	C	272/276 (99%)	254 (93%)	18 (7%)	0	100 100
1	E	270/276 (98%)	253 (94%)	16 (6%)	1 (0%)	30 26
1	G	261/276 (95%)	246 (94%)	15 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
2	D	97/99 (98%)	94 (97%)	2 (2%)	1 (1%)	12	8
2	F	97/99 (98%)	93 (96%)	3 (3%)	1 (1%)	12	8
2	H	97/99 (98%)	93 (96%)	3 (3%)	1 (1%)	12	8
3	I	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	J	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	K	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	L	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1491/1536 (97%)	1403 (94%)	83 (6%)	5 (0%)	36	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
1	E	226	GLN
2	H	47	PRO
2	D	47	PRO
2	F	47	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	232/234 (99%)	218 (94%)	14 (6%)	17	13
1	C	232/234 (99%)	218 (94%)	14 (6%)	17	13
1	E	232/234 (99%)	218 (94%)	14 (6%)	17	13
1	G	226/234 (97%)	214 (95%)	12 (5%)	20	17
2	B	94/94 (100%)	86 (92%)	8 (8%)	10	6
2	D	94/94 (100%)	88 (94%)	6 (6%)	16	11
2	F	94/94 (100%)	87 (93%)	7 (7%)	13	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	94/94 (100%)	88 (94%)	6 (6%)	16	11
3	I	7/7 (100%)	7 (100%)	0	100	100
3	J	7/7 (100%)	7 (100%)	0	100	100
3	K	7/7 (100%)	7 (100%)	0	100	100
3	L	7/7 (100%)	7 (100%)	0	100	100
All	All	1326/1340 (99%)	1245 (94%)	81 (6%)	17	12

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ARG
1	A	78	LEU
1	A	110	LEU
1	A	114	LEU
1	A	149	GLN
1	A	166	GLU
1	A	179	LEU
1	A	226	GLN
1	A	234	ARG
1	A	240	THR
1	A	254	GLU
1	A	258	THR
1	A	266	LEU
1	A	272	LEU
2	B	4	THR
2	B	19	LYS
2	B	50	GLU
2	B	55	SER
2	B	64	ILE
2	B	74	GLU
2	B	75	THR
2	B	93	VAL
1	C	78	LEU
1	C	105	SER
1	C	110	LEU
1	C	114	LEU
1	C	149	GLN
1	C	166	GLU
1	C	179	LEU
1	C	181	ARG

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Mol	Chain	Res	Type
1	C	226	GLN
1	C	234	ARG
1	C	254	GLU
1	C	258	THR
1	C	266	LEU
1	C	272	LEU
2	D	4	THR
2	D	19	LYS
2	D	50	GLU
2	D	74	GLU
2	D	75	THR
2	D	93	VAL
1	E	62	ARG
1	E	78	LEU
1	E	105	SER
1	E	110	LEU
1	E	114	LEU
1	E	149	GLN
1	E	166	GLU
1	E	181	ARG
1	E	226	GLN
1	E	234	ARG
1	E	254	GLU
1	E	258	THR
1	E	266	LEU
1	E	272	LEU
2	F	4	THR
2	F	19	LYS
2	F	50	GLU
2	F	64	ILE
2	F	74	GLU
2	F	75	THR
2	F	93	VAL
1	G	78	LEU
1	G	105	SER
1	G	110	LEU
1	G	114	LEU
1	G	149	GLN
1	G	166	GLU
1	G	226	GLN
1	G	234	ARG
1	G	254	GLU

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Mol	Chain	Res	Type
1	G	258	THR
1	G	266	LEU
1	G	272	LEU
2	H	4	THR
2	H	19	LYS
2	H	50	GLU
2	H	74	GLU
2	H	75	THR
2	H	93	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	97	GLN
1	A	176	ASN
1	A	220	ASN
1	A	256	ASN
2	B	34	HIS
2	B	38	GLN
1	C	30	ASN
1	C	97	GLN
1	C	220	ASN
1	C	256	ASN
1	E	97	GLN
1	E	176	ASN
1	E	220	ASN
1	E	256	ASN
2	F	38	GLN
1	G	30	ASN
1	G	80	ASN
1	G	97	GLN
1	G	256	ASN
2	H	38	GLN

5.3.3 RNA ⓘ

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	273/276 (98%)	1.15	69 (25%) 1 2	20, 49, 123, 195	0
1	C	273/276 (98%)	1.48	80 (29%) 1 1	22, 51, 130, 169	0
1	E	271/276 (98%)	1.44	83 (30%) 1 1	25, 52, 125, 160	0
1	G	264/276 (95%)	1.38	80 (30%) 1 1	22, 51, 123, 159	0
2	B	99/99 (100%)	1.12	17 (17%) 4 4	26, 46, 74, 100	0
2	D	99/99 (100%)	0.93	13 (13%) 7 8	27, 43, 76, 102	0
2	F	99/99 (100%)	1.56	30 (30%) 1 1	30, 51, 78, 103	0
2	H	99/99 (100%)	1.20	17 (17%) 4 4	28, 48, 79, 102	0
3	I	9/9 (100%)	-0.26	0 100 100	21, 27, 36, 37	0
3	J	9/9 (100%)	0.43	0 100 100	25, 33, 44, 61	0
3	K	9/9 (100%)	0.50	1 (11%) 10 11	31, 37, 42, 74	0
3	L	9/9 (100%)	0.03	0 100 100	27, 32, 40, 48	0
All	All	1513/1536 (98%)	1.29	390 (25%) 1 2	20, 49, 118, 195	0

All (390) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	LEU	8.5
1	C	16	GLY	7.8
1	C	17	LEU	7.4
1	E	17	LEU	7.0
1	A	193	PRO	6.6
1	E	258	THR	6.6
1	E	256	ASN	6.3
2	F	1	ILE	6.3
1	C	219	LEU	6.2
1	C	15	PRO	6.2
1	G	199	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	E	199	VAL	5.9
2	B	1	ILE	5.8
1	G	17	LEU	5.7
1	C	193	PRO	5.5
1	G	177	ALA	5.5
2	H	74	GLU	5.3
1	G	217	TRP	5.3
1	A	179	LEU	5.3
1	E	201	LEU	5.3
1	G	258	THR	5.2
1	A	252	GLY	5.1
1	E	40	ALA	5.1
1	C	19	GLU	5.1
1	G	193	PRO	5.0
2	B	47	PRO	5.0
1	A	16	GLY	4.9
1	A	177	ALA	4.8
2	D	1	ILE	4.8
1	A	195	SER	4.8
1	A	178	THR	4.8
1	C	199	VAL	4.8
1	G	201	LEU	4.7
1	E	197	GLY	4.7
1	G	267	PRO	4.7
1	A	194	ARG	4.6
1	E	252	GLY	4.6
1	A	249	VAL	4.6
1	G	257	TYR	4.6
1	A	199	VAL	4.5
1	E	251	LEU	4.5
1	C	41	GLU	4.5
1	A	256	ASN	4.5
1	E	178	THR	4.5
1	E	228	MET	4.4
1	G	248	VAL	4.4
1	G	224	LEU	4.4
2	F	47	PRO	4.4
1	G	272	LEU	4.4
1	C	195	SER	4.3
1	E	272	LEU	4.3
2	F	19	LYS	4.3
1	E	193	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	175	GLY	4.3
1	A	175	GLY	4.2
1	C	180	LEU	4.2
1	A	196	LYS	4.2
1	G	15	PRO	4.2
2	F	74	GLU	4.2
1	A	272	LEU	4.1
2	H	1	ILE	4.1
1	E	219	LEU	4.1
1	G	249	VAL	4.1
1	E	15	PRO	4.1
1	C	251	LEU	4.0
1	A	50	PRO	4.0
1	G	256	ASN	4.0
1	C	228	MET	4.0
1	G	189	VAL	4.0
1	G	216	THR	4.0
2	F	44	LYS	4.0
1	G	19	GLU	4.0
2	F	17	ASN	3.9
1	E	189	VAL	3.9
1	C	221	GLY	3.9
1	C	179	LEU	3.9
1	C	176	ASN	3.9
1	C	253	LYS	3.9
1	G	253	LYS	3.9
1	G	228	MET	3.8
1	E	247	VAL	3.8
1	A	253	LYS	3.8
1	G	191	HIS	3.8
1	C	267	PRO	3.8
2	F	20	PRO	3.7
1	A	258	THR	3.7
2	B	71	THR	3.7
1	G	18	GLU	3.7
1	E	257	TYR	3.7
1	G	251	LEU	3.7
1	G	250	PRO	3.7
1	A	248	VAL	3.7
1	E	177	ALA	3.7
1	C	224	LEU	3.6
1	C	60	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	189	VAL	3.6
2	F	49	VAL	3.6
1	C	225	THR	3.6
1	E	50	PRO	3.6
1	G	270	LEU	3.6
1	C	175	GLY	3.6
2	F	18	GLY	3.6
1	G	227	ASP	3.6
1	E	267	PRO	3.6
1	E	42	ASN	3.6
2	H	47	PRO	3.6
1	A	180	LEU	3.6
1	G	260	ARG	3.6
1	C	197	GLY	3.6
1	C	257	TYR	3.6
1	G	252	GLY	3.6
1	C	249	VAL	3.5
2	H	71	THR	3.5
1	C	248	VAL	3.5
2	D	74	GLU	3.5
1	G	197	GLY	3.5
1	E	249	VAL	3.5
2	B	75	THR	3.5
1	C	1	GLY	3.5
1	C	201	LEU	3.5
1	E	41	GLU	3.5
1	G	196	LYS	3.5
2	D	48	LYS	3.5
1	E	230	LEU	3.4
1	G	195	SER	3.4
1	A	273	ARG	3.4
1	G	190	THR	3.4
1	E	195	SER	3.4
1	C	272	LEU	3.4
1	A	257	TYR	3.4
1	A	197	GLY	3.4
1	E	255	GLN	3.4
1	C	178	THR	3.4
1	E	225	THR	3.4
1	G	202	ARG	3.4
2	H	18	GLY	3.4
1	A	201	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	255	GLN	3.4
1	A	42	ASN	3.3
2	F	75	THR	3.3
2	H	19	LYS	3.3
1	A	15	PRO	3.3
1	E	250	PRO	3.3
1	A	49	ALA	3.3
1	E	51	TRP	3.3
1	C	59	TYR	3.3
1	G	54	GLN	3.3
2	D	47	PRO	3.3
2	D	49	VAL	3.3
1	A	224	LEU	3.3
2	H	48	LYS	3.3
2	F	73	THR	3.3
1	E	184	SER	3.3
1	C	250	PRO	3.3
2	B	19	LYS	3.3
1	C	56	GLY	3.2
1	G	89	ALA	3.2
1	E	186	LYS	3.2
1	C	54	GLN	3.2
1	E	254	GLU	3.2
1	C	247	VAL	3.2
1	C	89	ALA	3.2
1	A	227	ASP	3.2
1	G	203	CYS	3.2
1	E	217	TRP	3.2
1	C	196	LYS	3.2
1	C	51	TRP	3.1
2	F	76	ASP	3.1
1	C	53	GLU	3.1
1	C	222	GLU	3.1
1	G	53	GLU	3.1
1	C	31	LYS	3.1
2	F	71	THR	3.1
1	A	228	MET	3.1
1	A	251	LEU	3.1
1	C	191	HIS	3.1
1	C	146	LYS	3.1
1	C	258	THR	3.1
1	G	200	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	194	ARG	3.1
1	C	49	ALA	3.1
1	C	58	GLU	3.1
1	G	229	GLU	3.1
2	H	16	GLU	3.1
1	C	167	TRP	3.0
1	C	252	GLY	3.0
2	F	43	GLY	3.0
1	E	220	ASN	3.0
1	C	230	LEU	3.0
1	G	247	VAL	3.0
1	C	90	GLY	3.0
1	A	219	LEU	3.0
1	G	181	ARG	3.0
1	E	1	GLY	3.0
1	A	217	TRP	3.0
1	E	88	SER	3.0
1	G	261	VAL	3.0
1	C	256	ASN	3.0
1	A	181	ARG	2.9
1	G	16	GLY	2.9
1	A	250	PRO	2.9
1	A	44	ARG	2.9
1	E	181	ARG	2.9
1	G	204	TRP	2.9
1	E	176	ASN	2.9
1	G	174	ASN	2.9
1	A	191	HIS	2.9
1	E	192	HIS	2.9
2	D	34	HIS	2.9
2	F	78	TYR	2.9
1	E	246	SER	2.9
1	A	247	VAL	2.9
1	E	226	GLN	2.8
1	A	271	THR	2.8
1	A	254	GLU	2.8
1	C	184	SER	2.8
1	G	255	GLN	2.8
1	E	227	ASP	2.8
1	E	224	LEU	2.8
1	A	225	THR	2.8
1	A	267	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	50	PRO	2.8
1	A	58	GLU	2.8
1	C	177	ALA	2.8
1	E	89	ALA	2.8
1	A	200	THR	2.8
1	G	31	LYS	2.8
1	C	273	ARG	2.8
1	C	61	GLU	2.7
1	G	166	GLU	2.7
1	C	200	THR	2.7
1	C	44	ARG	2.7
1	C	217	TRP	2.7
1	A	104	GLY	2.7
1	E	253	LYS	2.7
2	B	88	ALA	2.7
1	G	273	ARG	2.7
1	A	226	GLN	2.7
1	G	269	PRO	2.7
1	G	42	ASN	2.7
1	E	196	LYS	2.7
1	E	16	GLY	2.7
1	E	200	THR	2.7
2	H	20	PRO	2.7
2	B	22	ILE	2.7
2	D	19	LYS	2.7
1	C	18	GLU	2.6
1	G	223	GLU	2.6
1	A	230	LEU	2.6
1	C	62	ARG	2.6
1	A	57	PRO	2.6
1	C	50	PRO	2.6
1	C	40	ALA	2.6
2	H	73	THR	2.6
2	F	81	ARG	2.6
1	C	239	GLY	2.6
1	G	175	GLY	2.6
1	C	64	THR	2.6
1	C	172	LEU	2.6
1	G	88	SER	2.6
1	G	105	SER	2.6
1	G	226	GLN	2.5
2	B	74	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	221	GLY	2.5
1	A	176	ASN	2.5
2	D	88	ALA	2.5
1	E	207	GLY	2.5
1	E	248	VAL	2.5
3	K	1	LYS	2.5
1	C	79	ARG	2.5
2	F	46	ILE	2.5
1	G	262	TYR	2.5
1	A	41	GLU	2.5
1	C	255	GLN	2.5
1	A	61	GLU	2.4
1	G	198	GLU	2.4
2	H	75	THR	2.4
2	H	88	ALA	2.4
1	G	206	LEU	2.4
1	C	14	ARG	2.4
2	D	81	ARG	2.4
2	F	70	PHE	2.4
1	A	54	GLN	2.4
1	A	222	GLU	2.4
1	E	104	GLY	2.4
1	C	174	ASN	2.4
1	E	58	GLU	2.4
1	G	208	PHE	2.4
2	D	99	MET	2.4
1	E	262	TYR	2.4
1	E	191	HIS	2.4
1	E	270	LEU	2.4
1	A	220	ASN	2.4
1	E	167	TRP	2.4
1	G	192	HIS	2.4
2	F	34	HIS	2.4
1	E	19	GLU	2.3
2	F	40	LEU	2.3
2	F	42	ASN	2.3
1	A	186	LYS	2.3
1	E	79	ARG	2.3
1	A	18	GLU	2.3
1	A	198	GLU	2.3
2	H	69	GLU	2.3
1	A	51	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	218	GLN	2.3
1	C	227	ASP	2.3
2	F	39	MET	2.3
1	G	246	SER	2.3
2	H	77	THR	2.3
1	E	49	ALA	2.3
2	F	66	ALA	2.3
1	E	212	ASP	2.3
2	H	81	ARG	2.3
2	F	16	GLU	2.3
1	C	57	PRO	2.3
1	E	271	THR	2.3
2	B	20	PRO	2.3
1	C	194	ARG	2.3
2	H	99	MET	2.3
2	D	69	GLU	2.2
2	H	34	HIS	2.2
1	A	88	SER	2.2
2	B	46	ILE	2.2
2	D	71	THR	2.2
1	E	44	ARG	2.2
1	E	273	ARG	2.2
1	E	239	GLY	2.2
1	G	91	GLY	2.2
2	F	99	MET	2.2
1	C	223	GLU	2.2
1	G	254	GLU	2.2
1	G	51	TRP	2.2
1	A	105	SER	2.2
1	E	105	SER	2.2
2	B	70	PHE	2.2
1	C	271	THR	2.2
1	G	182	THR	2.2
2	B	64	ILE	2.2
2	D	53	ASP	2.2
1	A	89	ALA	2.2
2	B	13	HIS	2.2
1	E	60	TRP	2.2
1	G	14	ARG	2.2
1	G	107	TRP	2.2
1	E	268	GLU	2.2
1	E	149	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	245	ALA	2.2
1	G	266	LEU	2.2
1	E	14	ARG	2.2
1	E	68	LYS	2.2
2	F	48	LYS	2.2
1	E	229	GLU	2.1
2	F	22	ILE	2.1
1	C	207	GLY	2.1
1	C	192	HIS	2.1
1	G	187	ALA	2.1
1	G	215	LEU	2.1
1	E	59	TYR	2.1
1	A	229	GLU	2.1
1	C	229	GLU	2.1
1	E	39	ASP	2.1
1	G	212	ASP	2.1
1	A	192	HIS	2.1
1	G	1	GLY	2.1
1	C	181	ARG	2.1
2	B	81	ARG	2.1
1	A	187	ALA	2.1
1	G	259	CYS	2.1
1	E	174	ASN	2.1
2	B	99	MET	2.1
1	G	61	GLU	2.1
1	A	189	VAL	2.1
2	F	45	LYS	2.1
1	G	39	ASP	2.1
1	E	221	GLY	2.1
1	A	19	GLU	2.0
1	C	270	LEU	2.0
2	F	21	ASN	2.0
2	F	67	HIS	2.0
1	A	182	THR	2.0
2	B	73	THR	2.0
2	B	44	LYS	2.0
1	E	18	GLU	2.0
1	E	198	GLU	2.0
1	G	167	TRP	2.0
1	G	194	ARG	2.0
1	E	188	HIS	2.0
1	E	57	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	45	TYR	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.