



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:16 PM GMT

PDB ID : 3TBW
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)
Authors : Duru, A.D.; Allerbring, E.B.; Uchtenhagen, H.; Mazumdar, P.A.; Badia-Martinez, D.; Madhurantakam, C.; Sandalova, T.; Nygren, P.; Achour, A.
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

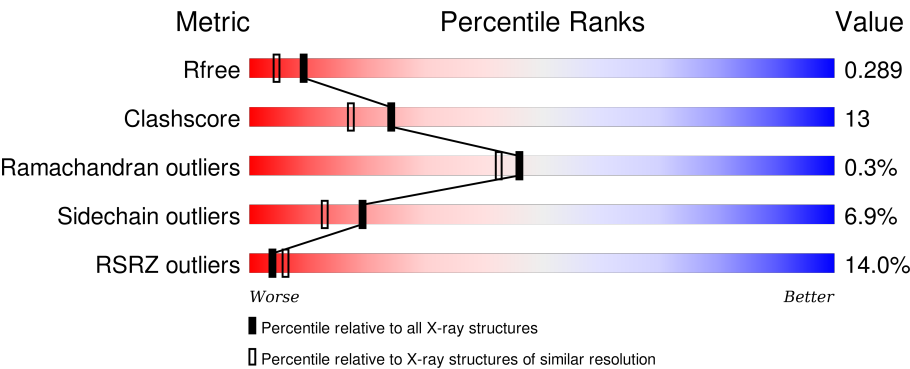
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	338	<div><div>12%</div><div>58%</div><div>20%</div><div>• •</div><div>19%</div></div>
1	C	338	<div><div>15%</div><div>56%</div><div>22%</div><div>• •</div><div>19%</div></div>
1	E	338	<div><div>16%</div><div>59%</div><div>18%</div><div>• •</div><div>19%</div></div>
1	G	338	<div><div>13%</div><div>55%</div><div>22%</div><div>•</div><div>21%</div></div>
2	B	99	<div><div>5%</div><div>75%</div><div>24%</div><div>•</div></div>

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Mol	Chain	Length	Quality of chain
2	D	99	<div><div></div><div>5%</div><div>75%</div><div>22%</div><div></div></div>
2	F	99	<div><div></div><div>9%</div><div>74%</div><div>24%</div><div></div></div>
2	H	99	<div><div></div><div>4%</div><div>72%</div><div>27%</div><div></div></div>
3	I	9	<div><div></div><div></div><div>78%</div><div>11%</div><div>11%</div></div>
3	J	9	<div><div></div><div></div><div>44%</div><div>56%</div><div></div></div>
3	K	9	<div><div></div><div></div><div>67%</div><div>22%</div><div>11%</div></div>
3	L	9	<div><div></div><div></div><div>56%</div><div>33%</div><div>11%</div></div>

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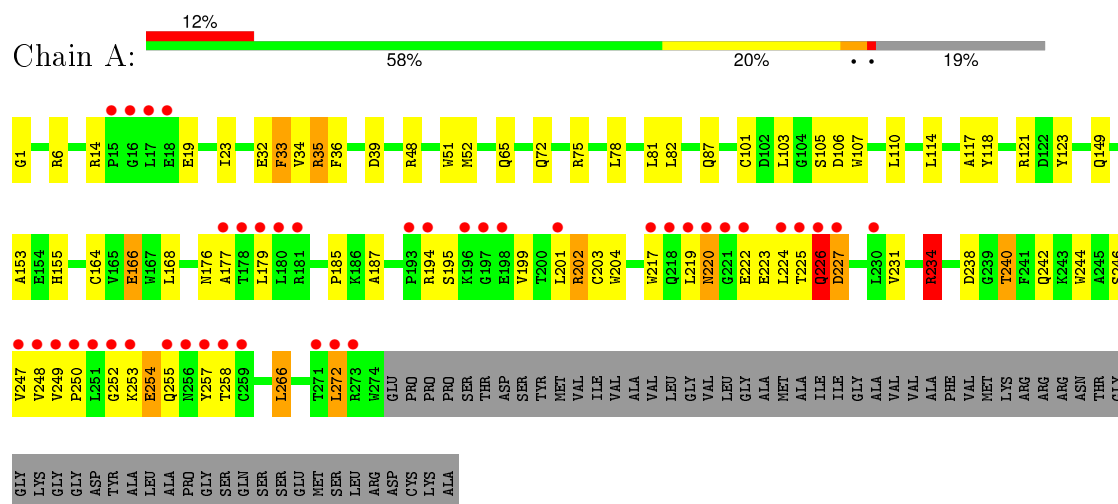
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	5	Total	O	0	0
			5	5		

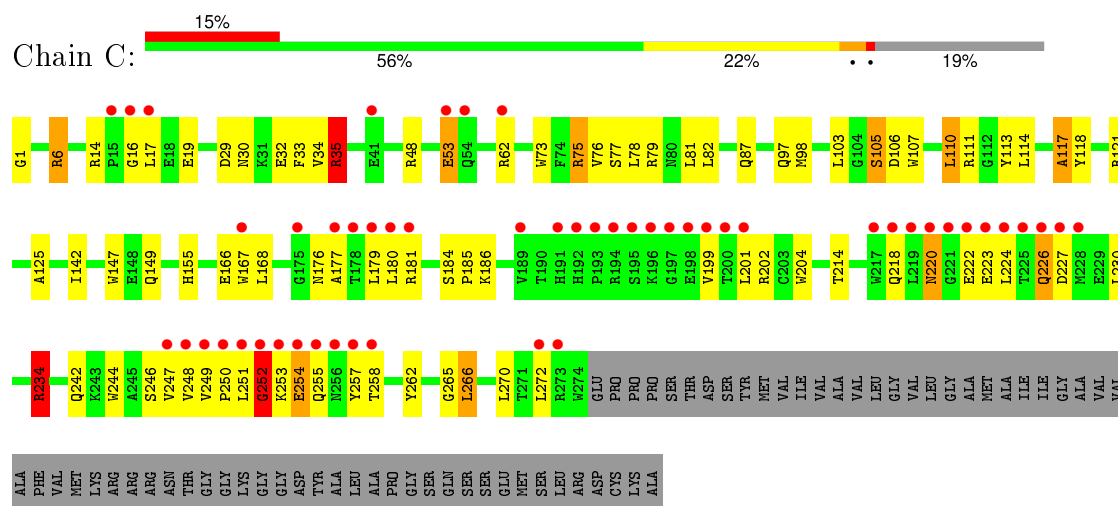
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

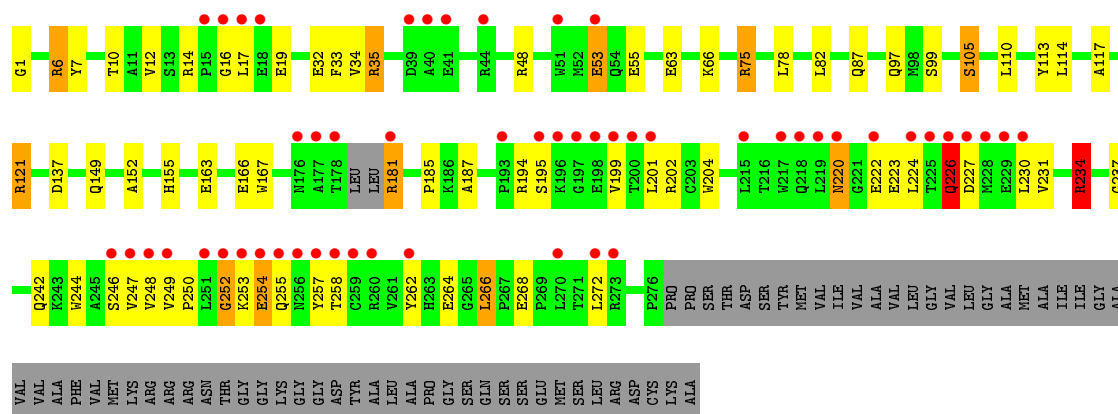


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

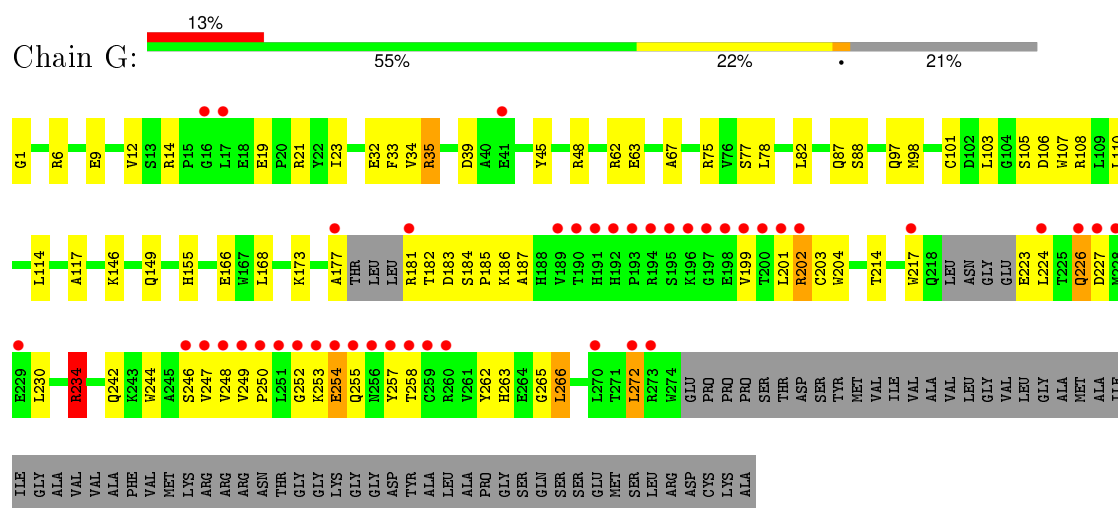


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

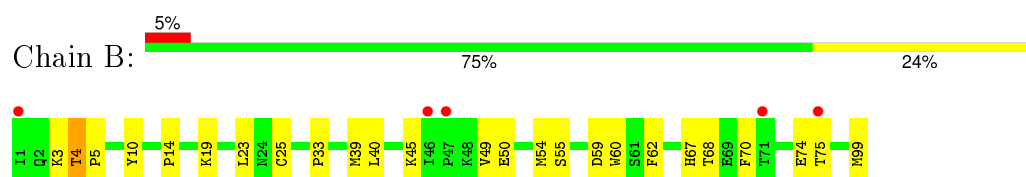




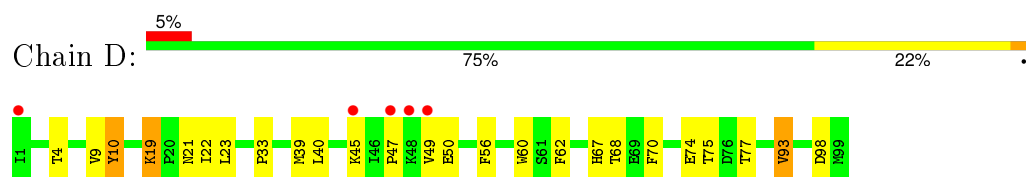
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



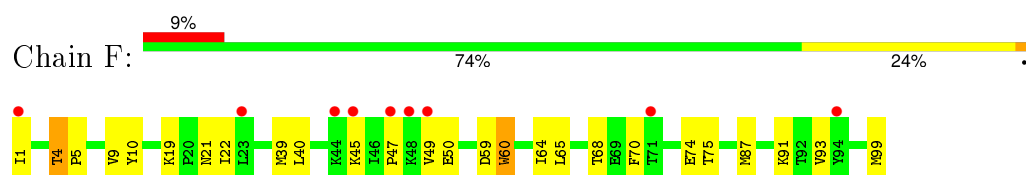
- Molecule 2: Beta-2-microglobulin



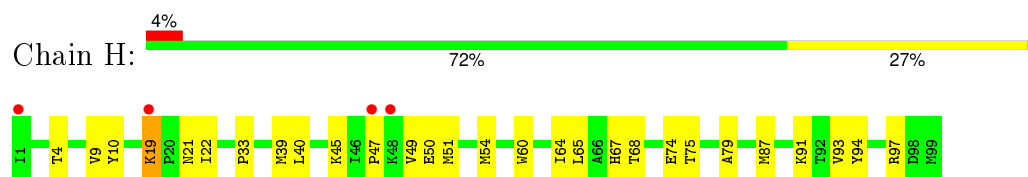
- Molecule 2: Beta-2-microglobulin



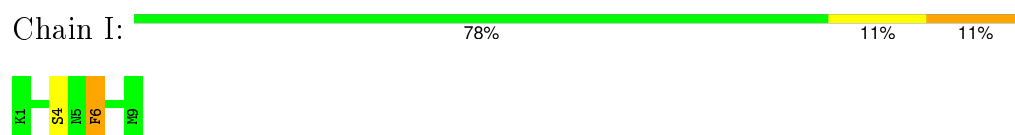
- Molecule 2: Beta-2-microglobulin



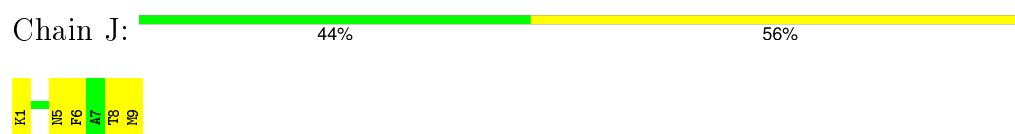
● Molecule 2: Beta-2-microglobulin



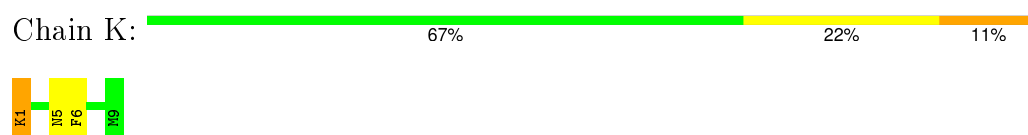
● Molecule 3: GLYCOPROTEIN GPC



● 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	91.40 Å 124.28 Å 99.89 Å 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 2.16 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.232 , 0.283 0.244 , 0.289	Depositor DCC
R_{free} test set	5819 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	3 of 116037 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.00	4/2314 (0.2%)	1.05	10/3142 (0.3%)
1	C	0.92	3/2314 (0.1%)	0.90	10/3142 (0.3%)
1	E	0.93	2/2314 (0.1%)	0.93	12/3141 (0.4%)
1	G	0.91	2/2260 (0.1%)	0.89	6/3065 (0.2%)
2	B	1.01	1/846 (0.1%)	0.89	1/1148 (0.1%)
2	D	1.02	3/846 (0.4%)	0.89	0/1148
2	F	0.93	1/846 (0.1%)	0.87	1/1148 (0.1%)
2	H	0.91	0/846	0.89	1/1148 (0.1%)
3	I	1.96	2/66 (3.0%)	1.16	0/87
3	J	1.34	0/66	1.17	0/87
3	K	1.37	0/66	1.20	0/87
3	L	1.35	0/66	1.27	1/87 (1.1%)
All	All	0.96	18/12850 (0.1%)	0.94	42/17430 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	2
1	G	0	1
All	All	0	5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	4	SER	CA-CB	9.23	1.66	1.52
2	B	25	CYS	CB-SG	-7.80	1.69	1.82
1	E	152	ALA	CA-CB	7.47	1.68	1.52
1	A	164	CYS	CB-SG	7.12	1.94	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	7	TYR	CD2-CE2	6.79	1.49	1.39
1	C	117	ALA	CA-CB	6.67	1.66	1.52
2	D	10	TYR	CD1-CE1	6.33	1.48	1.39
1	G	101	CYS	CB-SG	6.07	1.92	1.82
1	A	33	PHE	CE1-CZ	5.84	1.48	1.37
1	C	76	VAL	CB-CG2	5.70	1.64	1.52
2	D	93	VAL	CB-CG1	-5.65	1.41	1.52
2	F	60	TRP	CE3-CZ3	5.47	1.47	1.38
1	A	123	TYR	CE1-CZ	5.45	1.45	1.38
1	A	101	CYS	CB-SG	5.40	1.91	1.82
1	G	9	GLU	CG-CD	5.25	1.59	1.51
1	C	125	ALA	CA-CB	5.05	1.63	1.52
3	I	6	PHE	CB-CG	5.02	1.59	1.51
2	D	56	PHE	CD1-CE1	5.01	1.49	1.39

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	NE-CZ-NH1	19.05	129.82	120.30
1	A	234	ARG	NE-CZ-NH2	-15.87	112.36	120.30
1	A	35	ARG	NE-CZ-NH2	-15.47	112.56	120.30
1	A	35	ARG	NE-CZ-NH1	12.80	126.70	120.30
1	E	234	ARG	NE-CZ-NH2	-12.28	114.16	120.30
1	E	234	ARG	NE-CZ-NH1	11.26	125.93	120.30
1	G	35	ARG	NE-CZ-NH2	-10.81	114.90	120.30
1	A	6	ARG	NE-CZ-NH2	-10.49	115.06	120.30
1	E	121	ARG	NE-CZ-NH2	-9.75	115.42	120.30
1	C	35	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	C	234	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	C	35	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	G	234	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	E	121	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	G	234	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	A	121	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	E	35	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	A	220	ASN	N-CA-C	6.58	128.75	111.00
1	E	53	GLU	CB-CA-C	-6.51	97.38	110.40
1	A	121	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	G	39	ASP	CB-CA-C	-6.07	98.25	110.40
2	H	97	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	E	6	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	C	75	ARG	NE-CZ-NH1	5.82	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	35	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	C	6	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	C	234	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	C	121	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	E	137	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	G	6	ARG	NE-CZ-NH2	-5.55	117.52	120.30
3	L	9	MET	CG-SD-CE	5.49	108.99	100.20
2	B	59	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	39	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	252	GLY	N-CA-C	5.33	126.42	113.10
1	E	35	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	6	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	53	GLU	CB-CA-C	-5.21	99.99	110.40
2	F	59	ASP	CB-CG-OD1	5.17	122.95	118.30
1	E	220	ASN	N-CA-C	5.07	124.68	111.00
1	E	252	GLY	N-CA-C	5.03	125.69	113.10
1	C	220	ASN	N-CA-C	5.00	124.51	111.00
1	E	75	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	57	0
1	C	2248	0	2123	65	0
1	E	2248	0	2113	57	0
1	G	2196	0	2066	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	820	0	796	20	0
2	D	820	0	796	23	0
2	F	820	0	796	23	0
2	H	820	0	796	33	0
3	I	65	0	66	1	0
3	J	65	0	66	9	0
3	K	65	0	66	8	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
4	D	52	0	0	5	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	315	0

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

All (315) 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:H:39:MET:HE2	2:H:49:VAL:HG13	1.41	1.02
2:D:39:MET:SD	4:D:190:HOH:O	2.18	1.01
2:F:39:MET:HE2	2:F:49:VAL:HG13	1.46	0.97
1:G:184:SER:HA	4:G:389:HOH:O	1.73	0.89
2:D:39:MET:HE2	2:D:49:VAL:HG13	1.56	0.87
1:C:167:TRP:CE2	3:J:1:LYS:HD2	2.10	0.86
2:B:39:MET:HE2	2:B:49:VAL:HG13	1.59	0.83
1:C:186:LYS:HE3	1:G:177:ALA:HB2	1.64	0.80
1:G:146:LYS:NZ	4:G:450:HOH:O	2.15	0.79
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:39:MET:HE1	2:F:68:THR:HG22	1.73	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	2.19	0.70
1:G:185:PRO:HD3	4:G:389:HOH:O	1.91	0.69
1:A:19:GLU:OE2	1:A:75:ARG:HD2	1.93	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
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
2:H:39:MET:CE	2:H:68:THR:HB	2.26	0.66
1:A:32:GLU:OE2	1:A:48:ARG:HD2	1.95	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
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
2:D:39:MET:HE1	2:D:68:THR:HB	1.79	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
2:B:39:MET:HE1	2:B:68:THR:HG22	1.80	0.64
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
2:F:1:ILE:N	4:F:311:HOH:O	2.32	0.62
1:A:155:HIS:HB3	3:I:6:PHE:CZ	2.34	0.62
2:D:39:MET:HE1	2:D:68:THR:CB	2.30	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:39:MET:HE1	2:F:68:THR:CG2	2.31	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:G:103:LEU:HD11	1:G:168:LEU:HD23	1.84	0.59
2:H:39:MET:HE1	2:H:68:THR:HB	1.83	0.59
1:E:19:GLU:OE2	1:E:75:ARG:HD2	2.03	0.58
1:C:79:ARG:NH1	4:C:570:HOH:O	2.36	0.58
1:G:12:VAL:HG21	2:H:33:PRO:HG2	1.86	0.58
1:G:263:HIS:CE1	4:G:389:HOH:O	2.57	0.58
1:E:226:GLN:CD	1:E:226:GLN:O	2.42	0.58
1:G:88:SER:O	4:G:374:HOH:O	2.17	0.57
1:C:222:GLU:OE2	1:C:222:GLU:HA	2.04	0.57
1:E:163:GLU:OE1	3:K:1:LYS:HD3	2.05	0.57
1:C:53:GLU:O	2:H:19:LYS:NZ	2.38	0.56
1:A:201:LEU:O	1:A:246:SER:HA	2.04	0.56
2:F:39:MET:CE	2:F:68:THR:CG2	2.84	0.56
1:C:177:ALA:N	1:G:186:LYS:HZ1	2.04	0.56
2:F:39:MET:CE	2:F:68:THR:HG22	2.35	0.56
1:E:32:GLU:OE2	1:E:48:ARG:HD2	2.06	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: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
2:B:39:MET:HE1	2:B:68:THR:CG2	2.36	0.55
1:C:110:LEU:HD13	4:C:575:HOH:O	2.06	0.55
2:D:39:MET:HE1	2:D:68:THR:HG22	1.88	0.55
1:E:262:TYR:CG	1:G:108:ARG:HD3	2.42	0.55
1:E:97:GLN:NE2	3:K:5:ASN:HD21	2.04	0.55
1:A:222:GLU:HA	1:A:222:GLU:OE2	2.07	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:E:223:GLU:C	1:E:224:LEU:HD22	2.27	0.55
2:H:39:MET:HE1	2:H:68:THR:CB	2.37	0.55
2:D:39:MET:HE1	2:D:68:THR:CG2	2.36	0.55
1:E:234:ARG:HD3	2:F:10:TYR:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASP:O	4:A:381:HOH:O	2.18	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:249:VAL:HG22	1:C:257:TYR:CZ	2.42	0.54
1:C:176:ASN:HB3	1:G:186:LYS:HE2	1.88	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
1:E:262:TYR:CD2	1:G:108:ARG:HG2	2.43	0.53
1:A:226:GLN:CD	1:A:226:GLN:O	2.47	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
1:E:226:GLN:HG2	1:E:226:GLN:O	2.09	0.53
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.43	0.52
1:G:1:GLY:N	1:G:105:SER:HB3	2.24	0.52
1:E:1:GLY:N	1:E:105:SER:HB3	2.24	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:G:223:GLU:C	1:G:224:LEU:HD22	2.30	0.52
1:G:234:ARG:HD3	2:H:10:TYR:CZ	2.45	0.52
1:A:272:LEU:HD22	4:A:383:HOH:O	2.10	0.52
1:C:1:GLY:N	1:C:105:SER:HB3	2.25	0.51
1:G:247:VAL:HG22	1:G:248:VAL:N	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:A:223:GLU:C	1:A:224:LEU:HD22	2.31	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:226:GLN:HG2	1:A:226:GLN:O	2.11	0.50
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
2:H:39:MET:CE	2:H:68:THR:CG2	2.89	0.50
1:E:163:GLU:OE1	3:K:1:LYS:CD	2.58	0.50
1:C:32:GLU:OE2	1:C:35:ARG:HD2	2.11	0.50
1:A:244:TRP:HZ2	2:B:99:MET:HE2	1.77	0.50
1:C:218:GLN:NE2	4:C:355:HOH:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:223:GLU:C	1:C:224:LEU:HD22	2.32	0.49
1:C:226:GLN:CG	1:C:226:GLN:O	2.60	0.49
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:HB3	1:G:14:ARG:NH1	2.26	0.49
2:H:40:LEU:CD1	4:H:446:HOH:O	2.59	0.49
1:C:32:GLU:OE2	1:C:48:ARG:HD2	2.12	0.49
2:F:39:MET:HE1	2:F:68:THR:CB	2.42	0.49
1:E:82:LEU:HD12	1:E:87:GLN:HB2	1.95	0.49
2:H:39:MET:HE1	2:H:67:HIS:C	2.33	0.49
1:C:106:ASP:O	1:C:107:TRP:HB2	2.11	0.48
1:A:14:ARG:NH1	1:A:14:ARG:HB3	2.28	0.48
2:F:21:ASN:OD1	2:F:22:ILE:N	2.44	0.48
2:H:51:MET:HB3	4:H:405:HOH:O	2.13	0.48
1:C:81:LEU:HD13	1:C:118:TYR:CD1	2.48	0.48
1:G:183:ASP:O	4:G:389:HOH:O	2.20	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:202:ARG:HD3	1:G:244:TRP:CE3	2.49	0.48
1:G:199:VAL:HG21	1:G:254:GLU:OE1	2.13	0.47
1:C:250:PRO:HB2	1:C:253:LYS:HB2	1.96	0.47
1:G:234:ARG:HD2	1:G:242:GLN:HB2	1.95	0.47
1:C:255:GLN:HA	1:C:255:GLN:OE1	2.14	0.47
1:C:98:MET:HG3	2:D:60:TRP:CZ3	2.49	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:G:249:VAL:HG13	1:G:257:TYR:CE2	2.49	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:A:166:GLU:OE2	4:A:404:HOH:O	2.20	0.47
2:B:39:MET:CE	2:B:68:THR:HG22	2.43	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:NH1	1:E:14:ARG:HB3	2.30	0.46
1:E:202:ARG:HG2	1:E:204:TRP:NE1	2.30	0.46
2:D:21:ASN:OD1	2:D:22:ILE:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:226:GLN:CG	1:G:226:GLN:O	2.62	0.46
2:H:79:ALA:HB2	2:H:94:TYR:CD1	2.50	0.46
2:H:39:MET:CE	2:H:68:THR:HG22	2.45	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
1:A:187:ALA:HA	1:A:204:TRP:O	2.16	0.46
1:G:249:VAL:CG1	1:G:254:GLU:HA	2.45	0.46
1:G:202:ARG:CD	1:G:244:TRP:CD2	2.98	0.46
2:D:40:LEU:HD23	2:D:45:LYS:HA	1.96	0.46
1:G:202:ARG:HG2	1:G:204:TRP:NE1	2.30	0.46
1:C:201:LEU:HD12	1:C:249:VAL:HG21	1.97	0.46
2:D:39:MET:CE	2:D:68:THR:CB	2.90	0.46
2:B:39:MET:HE1	2:B:68:THR:CB	2.45	0.46
2:D:39:MET:CE	2:D:68:THR:CG2	2.94	0.45
2:B:4:THR:HA	2:B:5:PRO:HD3	1.84	0.45
1:E:250:PRO:HB2	1:E:253:LYS:HB2	1.98	0.45
2:B:33:PRO:HG3	2:B:62:PHE:CZ	2.51	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:247:VAL:HG22	1:C:248:VAL:N	2.32	0.45
1:C:176:ASN:HB3	1:G:186:LYS:CE	2.46	0.45
1:E:231:VAL:HG13	1:E:244:TRP:CZ2	2.52	0.45
1:A:1:GLY:N	1:A:105:SER:HB3	2.30	0.45
1:E:199:VAL:HG21	1:E:254:GLU:OE1	2.17	0.45
2:F:9:VAL:CG2	2:F:93:VAL:HG22	2.46	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:155:HIS:CD2	4:A:466:HOH:O	2.69	0.45
1:A:82:LEU:HD12	1:A:87:GLN:HB2	1.99	0.45
1:G:63:GLU:OE2	3:L:1:LYS:HD3	2.17	0.44
1:E:234:ARG:HD2	1:E:242:GLN:OE1	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
2:H:9:VAL:HG23	2:H:93:VAL:HG22	1.97	0.44
1:G:103:LEU:CD1	1:G:168:LEU:HD23	2.48	0.44
1:E:10:THR:HG22	1:E:12:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:LEU:HD11	1:C:168:LEU:HD23	1.99	0.44
1:A:201:LEU:HD12	1:A:249:VAL:HG21	1.99	0.44
2:D:33:PRO:HG3	2:D:62:PHE:CE2	2.53	0.44
1:C:251:LEU:HD23	1:C:252:GLY:N	2.33	0.44
1:E:247:VAL:HG22	1:E:248:VAL:N	2.31	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:E:167:TRP:CZ2	3:K:1:LYS:HE3	2.53	0.44
1:E:63:GLU:OE2	3:K:1:LYS:HG3	2.17	0.44
1:E:268:GLU:OE1	1:G:173:LYS:HE2	2.18	0.44
1:E:255:GLN:HA	1:E:255:GLN:OE1	2.17	0.44
1:G:250:PRO:HB2	1:G:253:LYS:HB2	2.00	0.44
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
1:E:6:ARG:NH2	1:E:113:TYR:CE1	2.86	0.43
1:E:262:TYR:CD1	1:G:108:ARG:HD3	2.53	0.43
1:C:73:TRP:CD1	3:J:8:THR:HG22	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
2:H:39:MET:HE1	2:H:68:THR:HG22	2.01	0.43
1:G:155:HIS:HB3	3:L:6:PHE:CE1	2.53	0.43
1:A:36:PHE:C	1:A:36:PHE:CD1	2.92	0.43
1:A:250:PRO:HB2	1:A:253:LYS:HB2	2.00	0.43
2:H:39:MET:HE3	2:H:68:THR:CG2	2.49	0.43
1:G:249:VAL:HG11	1:G:254:GLU:HA	2.00	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:E:16:GLY:O	1:E:17:LEU:C	2.57	0.43
2:B:39:MET:HE1	2:B:68:THR:HB	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:F:64:ILE:CG2	2:F:65:LEU:N	2.82	0.43
1:A:199:VAL:HG21	1:A:254:GLU:OE1	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:A:225:THR:HG22	1:A:225:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:ARG:NH1	2:F:1:ILE:HB	2.34	0.42
2:H:39:MET:CE	2:H:68:THR:CB	2.94	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:E:244:TRP:CZ2	2:F:99:MET:CE	3.02	0.42
2:D:45:LYS:NZ	4:D:318:HOH:O	2.52	0.42
1:A:177:ALA:HB3	1:E:181:ARG:HD3	2.00	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: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:E:33:PHE:CD2	1:E:34:VAL:HG13	2.55	0.42
1:C:176:ASN:OD1	1:C:180:LEU:HD13	2.19	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
2:D:77:THR:HG22	4:D:558:HOH:O	2.19	0.42
1:C:249:VAL:CG1	1:C:254:GLU:HA	2.50	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:A:23:ILE:HD12	2:B:54:MET:SD	2.60	0.42
1:A:219:LEU:HG	1:A:219:LEU:O	2.19	0.42
1:C:33:PHE:C	1:C:48:ARG:HB2	2.40	0.42
1:C:1:GLY:H2	1:C:105:SER:HB3	1.84	0.42
2:H:39:MET:HE1	2:H:68:THR:CG2	2.50	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:A:153:ALA:HB3	4:A:509:HOH:O	2.19	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:G:263:HIS:O	1:G:266:LEU:HB2	2.20	0.41
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.55	0.41
1:A:106:ASP:O	1:A:107:TRP:HB2	2.20	0.41
2:F:39:MET:HE1	2:F:68:THR:HB	2.00	0.41
1:G:33:PHE:C	1:G:48:ARG:HB2	2.41	0.41
1:G:21:ARG:NE	1:G:23:ILE:HD11	2.36	0.41
1:G:45:TYR:CE2	1:G:67:ALA:HB2	2.56	0.41
2:D:9:VAL:CG2	2:D:93:VAL:HG22	2.50	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:238:ASP:OD1	1:A:240:THR:OG1	2.37	0.41
1:A:32:GLU:OE2	1:A:35:ARG:HD2	2.21	0.40
1:G:62:ARG:HG3	4:G:358:HOH:O	2.20	0.40
1:C:147:TRP:N	1:C:147:TRP:CD1	2.86	0.40
1:G:247:VAL:CG2	1:G:248:VAL:N	2.84	0.40
1:G:202:ARG:CD	1:G:244:TRP:CE3	3.04	0.40
1:C:142:ILE:H	1:C:142:ILE:HG13	1.70	0.40
2:F:39:MET:HE2	2:F:49:VAL:CG1	2.33	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
2:B:39:MET:HE2	2:B:49:VAL:CG1	2.41	0.40
1:C:16:GLY:O	1:C:17:LEU:C	2.60	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	272/338 (80%)	254 (93%)	17 (6%)	1 (0%)	39	34
1	C	272/338 (80%)	254 (93%)	18 (7%)	0	100	100
1	E	270/338 (80%)	253 (94%)	16 (6%)	1 (0%)	39	34
1	G	261/338 (77%)	246 (94%)	15 (6%)	0	100	100
2	B	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
2	D	97/99 (98%)	94 (97%)	2 (2%)	1 (1%)	19	11
2	F	97/99 (98%)	93 (96%)	3 (3%)	1 (1%)	19	11
2	H	97/99 (98%)	93 (96%)	3 (3%)	1 (1%)	19	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	1491/1784 (84%)	1403 (94%)	83 (6%)	5 (0%)	46	42

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	232/280 (83%)	215 (93%)	17 (7%)	17	11
1	C	232/280 (83%)	214 (92%)	18 (8%)	16	9
1	E	232/280 (83%)	216 (93%)	16 (7%)	19	13
1	G	226/280 (81%)	212 (94%)	14 (6%)	23	17
2	B	94/94 (100%)	87 (93%)	7 (7%)	17	11
2	D	94/94 (100%)	88 (94%)	6 (6%)	22	15
2	F	94/94 (100%)	87 (93%)	7 (7%)	17	11
2	H	94/94 (100%)	88 (94%)	6 (6%)	22	15
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%)	6 (86%)	1 (14%)	4	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	7/7 (100%)	7 (100%)	0	100	100
All	All	1326/1524 (87%)	1234 (93%)	92 (7%)	19	13

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	110	LEU
1	A	114	LEU
1	A	149	GLN
1	A	166	GLU
1	A	176	ASN
1	A	179	LEU
1	A	202	ARG
1	A	220	ASN
1	A	226	GLN
1	A	227	ASP
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	70	PHE
2	B	74	GLU
2	B	75	THR
1	C	35	ARG
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
1	C	220	ASN
1	C	226	GLN
1	C	227	ASP

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Mol	Chain	Res	Type
1	C	230	LEU
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	70	PHE
2	D	74	GLU
2	D	75	THR
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	220	ASN
1	E	226	GLN
1	E	227	ASP
1	E	230	LEU
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	70	PHE
2	F	74	GLU
2	F	75	THR
2	F	87	MET
1	G	78	LEU
1	G	110	LEU
1	G	114	LEU
1	G	149	GLN
1	G	166	GLU
1	G	202	ARG
1	G	226	GLN

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Mol	Chain	Res	Type
1	G	227	ASP
1	G	230	LEU
1	G	234	ARG
1	G	254	GLU
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	87	MET
3	K	1	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	220	ASN
2	B	38	GLN
1	C	97	GLN
1	C	220	ASN
1	E	30	ASN
1	E	97	GLN
1	E	220	ASN
2	F	38	GLN
1	G	30	ASN
1	G	97	GLN
1	G	192	HIS
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 ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	273/338 (80%)	1.02	41 (15%) 3 5	20, 49, 123, 195	0
1	C	273/338 (80%)	1.34	52 (19%) 2 2	22, 51, 130, 169	0
1	E	271/338 (80%)	1.15	53 (19%) 1 2	25, 52, 125, 160	0
1	G	264/338 (78%)	1.32	43 (16%) 2 4	22, 51, 123, 159	0
2	B	99/99 (100%)	0.65	5 (5%) 32 42	26, 46, 74, 100	0
2	D	99/99 (100%)	0.58	5 (5%) 32 42	27, 43, 76, 102	0
2	F	99/99 (100%)	0.99	9 (9%) 11 17	30, 51, 78, 103	0
2	H	99/99 (100%)	0.69	4 (4%) 42 52	28, 48, 79, 102	0
3	I	9/9 (100%)	0.28	0 100 100	21, 27, 36, 37	0
3	J	9/9 (100%)	0.17	0 100 100	25, 33, 44, 61	0
3	K	9/9 (100%)	0.26	0 100 100	31, 37, 42, 74	0
3	L	9/9 (100%)	0.29	0 100 100	27, 32, 40, 48	0
All	All	1513/1784 (84%)	1.06	212 (14%) 4 6	20, 49, 118, 195	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	ALA	12.6
1	A	17	LEU	12.6
1	E	178	THR	12.0
1	G	177	ALA	11.1
1	G	199	VAL	10.7
1	A	178	THR	10.6
1	G	193	PRO	10.5
1	C	225	THR	9.6
1	E	219	LEU	9.2
1	G	257	TYR	9.1
1	G	201	LEU	8.9

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Mol	Chain	Res	Type	RSRZ
1	C	179	LEU	8.5
1	A	179	LEU	8.3
1	A	252	GLY	8.2
1	C	195	SER	8.2
1	C	178	THR	8.2
1	E	17	LEU	8.0
1	G	197	GLY	7.8
1	C	257	TYR	7.8
1	G	249	VAL	7.6
1	C	224	LEU	7.5
1	G	195	SER	7.5
1	A	220	ASN	7.5
1	E	257	TYR	7.4
1	A	226	GLN	7.4
1	C	249	VAL	7.3
1	E	227	ASP	7.3
1	E	224	LEU	7.2
1	C	219	LEU	7.1
1	C	253	LYS	7.0
1	E	226	GLN	6.9
1	G	256	ASN	6.7
1	G	251	LEU	6.6
1	C	53	GLU	6.6
1	E	177	ALA	6.6
1	E	197	GLY	6.6
1	G	247	VAL	6.5
1	C	251	LEU	6.4
1	C	199	VAL	6.3
1	G	228	MET	6.2
1	A	227	ASP	6.2
1	C	256	ASN	6.2
1	G	224	LEU	6.2
1	G	258	THR	6.1
1	C	252	GLY	6.0
1	C	194	ARG	6.0
1	C	41	GLU	5.9
2	F	47	PRO	5.9
1	G	255	GLN	5.9
1	G	252	GLY	5.7
1	G	194	ARG	5.6
1	A	197	GLY	5.6
1	G	196	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	G	227	ASP	5.5
1	A	253	LYS	5.4
1	A	256	ASN	5.3
1	G	250	PRO	5.3
1	E	195	SER	5.2
1	C	221	GLY	5.1
1	E	218	GLN	5.1
1	E	41	GLU	5.1
1	C	220	ASN	5.1
1	G	189	VAL	5.0
1	C	250	PRO	4.9
1	E	253	LYS	4.9
1	A	180	LEU	4.9
1	A	249	VAL	4.8
1	E	220	ASN	4.8
1	C	196	LYS	4.8
1	C	248	VAL	4.8
1	G	253	LYS	4.8
1	C	197	GLY	4.8
1	E	247	VAL	4.7
2	F	1	ILE	4.7
1	A	273	ARG	4.7
1	E	196	LYS	4.7
1	E	255	GLN	4.6
1	E	249	VAL	4.6
1	A	193	PRO	4.6
1	E	256	ASN	4.5
1	G	190	THR	4.4
1	C	177	ALA	4.4
1	C	200	THR	4.3
2	D	49	VAL	4.3
1	A	201	LEU	4.2
1	C	255	GLN	4.2
1	C	222	GLU	4.2
1	A	258	THR	4.2
2	B	47	PRO	4.1
1	G	272	LEU	4.1
1	C	16	GLY	4.1
1	G	191	HIS	4.0
1	A	255	GLN	4.0
1	C	247	VAL	4.0
1	A	247	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	180	LEU	3.9
1	A	272	LEU	3.9
1	G	41	GLU	3.9
1	C	193	PRO	3.9
1	E	252	GLY	3.9
1	C	254	GLU	3.8
1	C	192	HIS	3.8
1	G	217	TRP	3.8
1	A	196	LYS	3.8
1	G	246	SER	3.7
1	G	248	VAL	3.7
1	G	260	ARG	3.7
1	E	217	TRP	3.7
1	E	193	PRO	3.7
1	E	248	VAL	3.7
1	G	200	THR	3.7
1	C	227	ASP	3.7
1	G	226	GLN	3.7
1	C	228	MET	3.6
1	G	254	GLU	3.6
2	B	46	ILE	3.6
1	C	226	GLN	3.6
1	E	40	ALA	3.5
1	A	222	GLU	3.5
1	E	254	GLU	3.5
1	G	198	GLU	3.5
1	E	181	ARG	3.5
1	A	219	LEU	3.5
1	A	221	GLY	3.5
1	E	258	THR	3.5
2	F	44	LYS	3.4
1	E	273	ARG	3.4
1	G	17	LEU	3.4
1	A	194	ARG	3.4
1	C	181	ARG	3.3
1	G	273	ARG	3.3
1	A	224	LEU	3.3
2	F	48	LYS	3.3
1	E	272	LEU	3.2
1	A	257	TYR	3.2
1	C	273	ARG	3.1
1	E	222	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	228	MET	3.1
1	A	271	THR	3.1
1	E	201	LEU	3.1
1	A	225	THR	3.1
1	E	53	GLU	3.0
2	D	47	PRO	3.0
1	C	198	GLU	3.0
1	E	230	LEU	3.0
1	E	16	GLY	3.0
1	A	198	GLU	3.0
1	C	191	HIS	3.0
1	G	192	HIS	3.0
1	C	15	PRO	2.9
1	E	259	CYS	2.9
2	H	47	PRO	2.9
1	C	258	THR	2.9
1	C	17	LEU	2.8
1	C	272	LEU	2.8
2	F	71	THR	2.8
2	H	48	LYS	2.8
1	C	189	VAL	2.8
1	A	181	ARG	2.8
1	E	251	LEU	2.8
1	G	270	LEU	2.8
1	E	199	VAL	2.8
1	G	181	ARG	2.7
1	G	16	GLY	2.7
2	B	1	ILE	2.7
1	E	246	SER	2.7
1	A	15	PRO	2.6
2	D	1	ILE	2.6
1	E	198	GLU	2.6
1	A	251	LEU	2.6
1	C	201	LEU	2.6
1	E	225	THR	2.6
2	H	1	ILE	2.6
1	A	16	GLY	2.5
1	C	54	GLN	2.5
1	E	39	ASP	2.5
2	F	49	VAL	2.5
1	E	18	GLU	2.4
1	E	176	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	262	TYR	2.4
1	G	229	GLU	2.4
2	F	45	LYS	2.4
1	A	18	GLU	2.4
2	D	48	LYS	2.4
1	E	51	TRP	2.3
2	D	45	LYS	2.3
1	C	218	GLN	2.3
1	E	229	GLU	2.3
2	H	19	LYS	2.3
1	C	167	TRP	2.3
1	E	200	THR	2.3
1	A	248	VAL	2.3
1	C	223	GLU	2.3
1	A	250	PRO	2.2
1	C	217	TRP	2.2
1	A	259	CYS	2.2
1	G	259	CYS	2.2
1	E	270	LEU	2.2
1	A	217	TRP	2.2
1	E	44	ARG	2.1
2	B	71	THR	2.1
1	E	15	PRO	2.1
2	F	94	TYR	2.1
1	A	230	LEU	2.1
1	G	202	ARG	2.1
1	C	175	GLY	2.1
2	B	75	THR	2.0
1	E	260	ARG	2.0
2	F	23	LEU	2.0
1	C	62	ARG	2.0
1	E	215	LEU	2.0
1	A	218	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.