



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:34 AM UTC

PDB ID : 1AFV / pdb_00001afv
Title : HIV-1 CAPSID PROTEIN (P24) COMPLEX WITH FAB25.3
Authors : Momany, C.; Kovari, L.C.; Prongay, A.J.; Keller, W.; Gitti, R.K.; Lee, B.M.; Gorbalenya, A.E.; Tong, L.; McClure, J.; Ehrlich, L.S.; Summers, M.F.; Carter, C.; Rossmann, M.G.
Deposited on : 1997-03-14
Resolution : 3.70 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

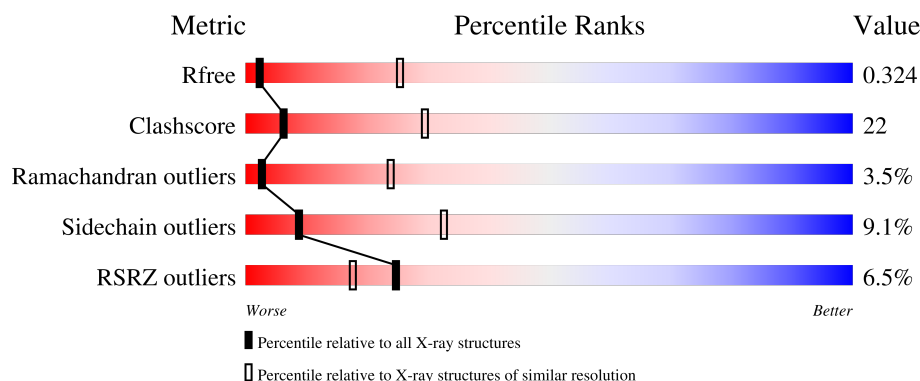
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	151	17% 43% 46% 11%
1	B	151	15% 40% 49% 8%
2	L	217	% 47% 46% 6%
2	M	217	3% 50% 43% 5%
3	H	220	4% 60% 35% 5%

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Mol	Chain	Length	Quality of chain
3	K	220	4% 60% 35%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9024 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 HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 CAPSID PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1172	742	205	217	8			
1	B	151	Total	C	N	O	S	0	0	0
			1172	742	205	217	8			

- Molecule 2 is a protein called ANTIBODY FAB25.3 FRAGMENT (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	217	Total	C	N	O	S	0	0	0
			1667	1038	281	340	8			
2	M	217	Total	C	N	O	S	0	0	0
			1667	1038	281	340	8			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	4	LEU	MET	conflict	UNP 600718
L	18	ARG	SER	conflict	UNP 600718
L	19	ALA	VAL	conflict	UNP 600718
L	30	ASP	GLU	conflict	UNP 600718
L	31	ASN	TYR	conflict	UNP 600718
L	34	ILE	THR	conflict	UNP 600718
L	36	PHE	LEU	conflict	UNP 600718
L	38	ASN	GLN	conflict	UNP 600718
L	40	PHE	TYR	conflict	UNP 600718
L	54	ALA	GLY	conflict	UNP 600718
L	58	LEU	VAL	conflict	UNP 600718
L	59	GLY	GLU	conflict	UNP 600718
L	82	MET	VAL	conflict	UNP 600718
L	85	GLU	ASP	conflict	UNP 600718
L	87	THR	ILE	conflict	UNP 600718
L	89	MET	ILE	conflict	UNP 600718

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Chain	Residue	Modelled	Actual	Comment	Reference
L	96	LYS	ARG	conflict	UNP 600718
L	97	GLU	LYS	conflict	UNP 600718
L	100	LEU	ALA	conflict	UNP 600718
L	104	ALA	SER	conflict	UNP 600718
L	108	VAL	LEU	conflict	UNP 600718
L	110	LEU	ILE	conflict	UNP 600718
M	4	LEU	MET	conflict	UNP 600718
M	18	ARG	SER	conflict	UNP 600718
M	19	ALA	VAL	conflict	UNP 600718
M	30	ASP	GLU	conflict	UNP 600718
M	31	ASN	TYR	conflict	UNP 600718
M	34	ILE	THR	conflict	UNP 600718
M	36	PHE	LEU	conflict	UNP 600718
M	38	ASN	GLN	conflict	UNP 600718
M	40	PHE	TYR	conflict	UNP 600718
M	54	ALA	GLY	conflict	UNP 600718
M	58	LEU	VAL	conflict	UNP 600718
M	59	GLY	GLU	conflict	UNP 600718
M	82	MET	VAL	conflict	UNP 600718
M	85	GLU	ASP	conflict	UNP 600718
M	87	THR	ILE	conflict	UNP 600718
M	89	MET	ILE	conflict	UNP 600718
M	96	LYS	ARG	conflict	UNP 600718
M	97	GLU	LYS	conflict	UNP 600718
M	100	LEU	ALA	conflict	UNP 600718
M	104	ALA	SER	conflict	UNP 600718
M	108	VAL	LEU	conflict	UNP 600718
M	110	LEU	ILE	conflict	UNP 600718

- Molecule 3 is a protein called ANTIBODY FAB25.3 FRAGMENT (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	220	Total	C	N	O	S	0	0	0
			1672	1062	275	330	5			
3	K	220	Total	C	N	O	S	0	0	0
			1672	1062	275	330	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	GLN	GLU	conflict	UNP Q99LC4
H	3	GLN	LYS	conflict	UNP Q99LC4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	5	GLN	HIS	conflict	UNP Q99LC4
H	6	GLN	GLU	conflict	UNP Q99LC4
H	7	PRO	SER	conflict	UNP Q99LC4
H	9	SER	PRO	conflict	UNP Q99LC4
H	10	VAL	GLY	conflict	UNP Q99LC4
H	16	ALA	THR	conflict	UNP Q99LC4
H	20	LEU	ILE	conflict	UNP Q99LC4
H	31	SER	ASN	conflict	UNP Q99LC4
H	32	SER	TYR	conflict	UNP Q99LC4
H	34	ILE	LEU	conflict	UNP Q99LC4
H	35	HIS	GLY	conflict	UNP Q99LC4
H	37	ALA	VAL	conflict	UNP Q99LC4
H	43	GLN	HIS	conflict	UNP Q99LC4
H	50	GLU	ASP	conflict	UNP Q99LC4
H	52	HIS	TYR	conflict	UNP Q99LC4
H	54	ASN	GLY	conflict	UNP Q99LC4
H	55	SER	GLY	conflict	UNP Q99LC4
H	57	ASN	TYR	conflict	UNP Q99LC4
H	72	VAL	ALA	conflict	UNP Q99LC4
H	81	VAL	MET	conflict	UNP Q99LC4
H	82	ASP	GLN	conflict	UNP Q99LC4
H	95	TYR	PHE	conflict	UNP Q99LC4
H	99	TRP	PHE	conflict	UNP Q99LC4
H	100	ARG	TYR	conflict	UNP Q99LC4
H	104	PRO	SER	conflict	UNP Q99LC4
H	?	-	TRP	deletion	UNP Q99LC4
H	109	TYR	VAL	conflict	UNP Q99LC4
H	116	LEU	VAL	conflict	UNP Q99LC4
K	1	GLN	GLU	conflict	UNP Q99LC4
K	3	GLN	LYS	conflict	UNP Q99LC4
K	5	GLN	HIS	conflict	UNP Q99LC4
K	6	GLN	GLU	conflict	UNP Q99LC4
K	7	PRO	SER	conflict	UNP Q99LC4
K	9	SER	PRO	conflict	UNP Q99LC4
K	10	VAL	GLY	conflict	UNP Q99LC4
K	16	ALA	THR	conflict	UNP Q99LC4
K	20	LEU	ILE	conflict	UNP Q99LC4
K	31	SER	ASN	conflict	UNP Q99LC4
K	32	SER	TYR	conflict	UNP Q99LC4
K	34	ILE	LEU	conflict	UNP Q99LC4
K	35	HIS	GLY	conflict	UNP Q99LC4
K	37	ALA	VAL	conflict	UNP Q99LC4

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Chain	Residue	Modelled	Actual	Comment	Reference
K	43	GLN	HIS	conflict	UNP Q99LC4
K	50	GLU	ASP	conflict	UNP Q99LC4
K	52	HIS	TYR	conflict	UNP Q99LC4
K	54	ASN	GLY	conflict	UNP Q99LC4
K	55	SER	GLY	conflict	UNP Q99LC4
K	57	ASN	TYR	conflict	UNP Q99LC4
K	72	VAL	ALA	conflict	UNP Q99LC4
K	81	VAL	MET	conflict	UNP Q99LC4
K	82	ASP	GLN	conflict	UNP Q99LC4
K	95	TYR	PHE	conflict	UNP Q99LC4
K	99	TRP	PHE	conflict	UNP Q99LC4
K	100	ARG	TYR	conflict	UNP Q99LC4
K	104	PRO	SER	conflict	UNP Q99LC4
K	?	-	TRP	deletion	UNP Q99LC4
K	109	TYR	VAL	conflict	UNP Q99LC4
K	116	LEU	VAL	conflict	UNP Q99LC4

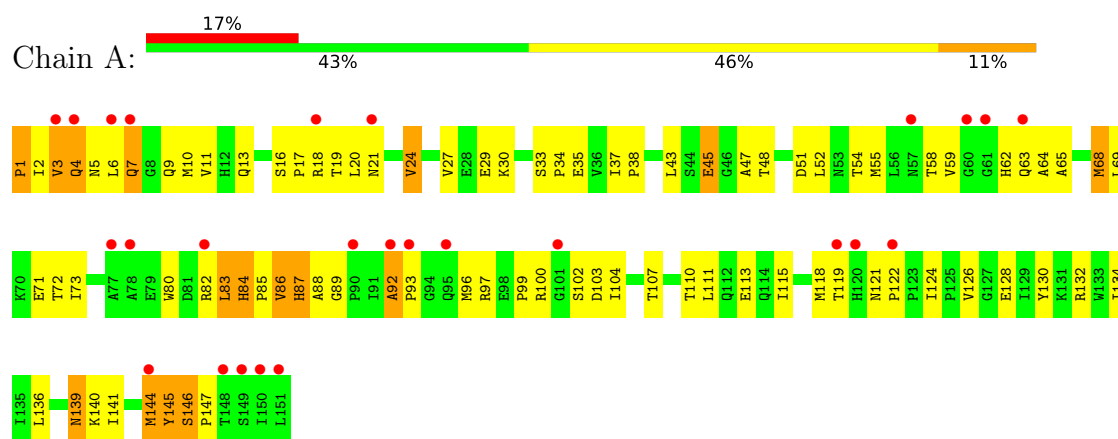
- Molecule 4 is LEAD (II) ION (CCD ID: PB) (formula: Pb).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total Pb 1 1	0	0
4	M	1	Total Pb 1 1	0	0

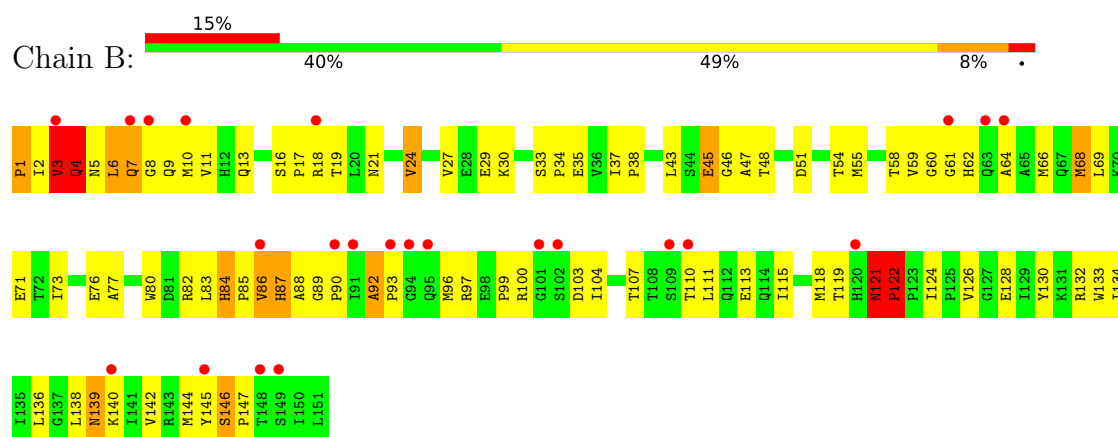
3 Residue-property plots

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.

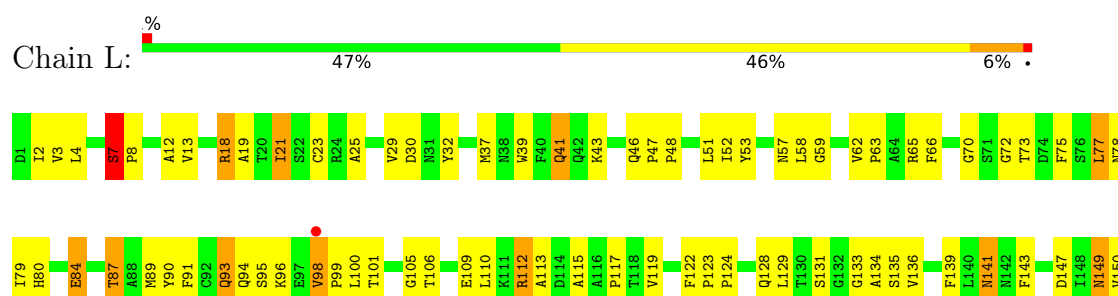
• Molecule 1: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 CAPSID PROTEIN



• Molecule 1: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 CAPSID PROTEIN

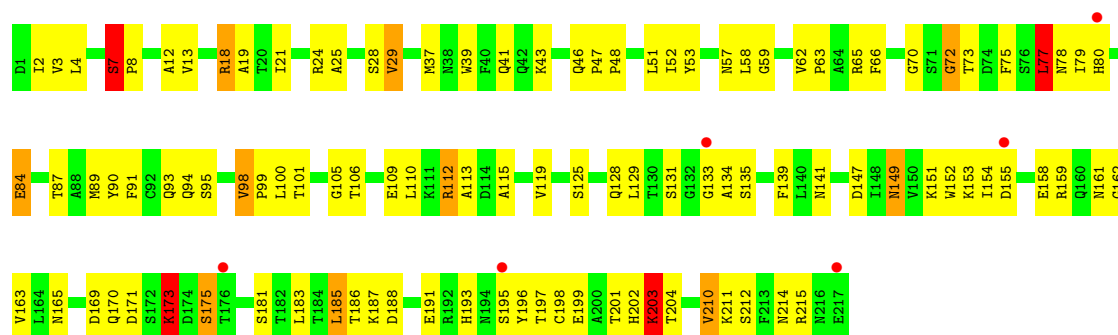


• Molecule 2: ANTIBODY FAB25.3 FRAGMENT (LIGHT CHAIN)

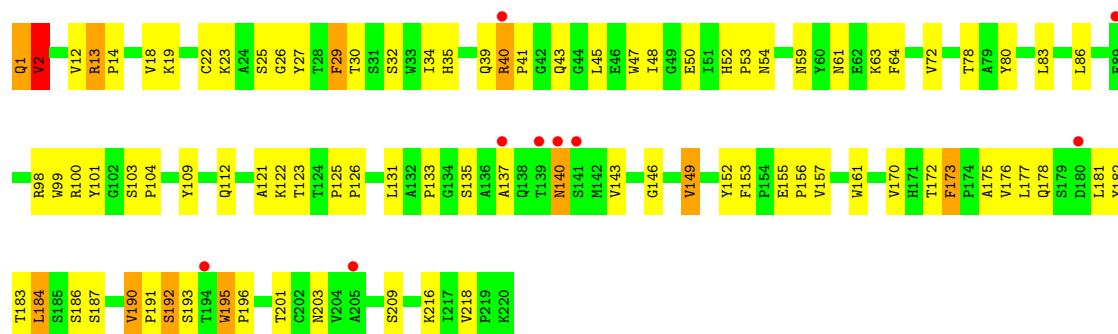




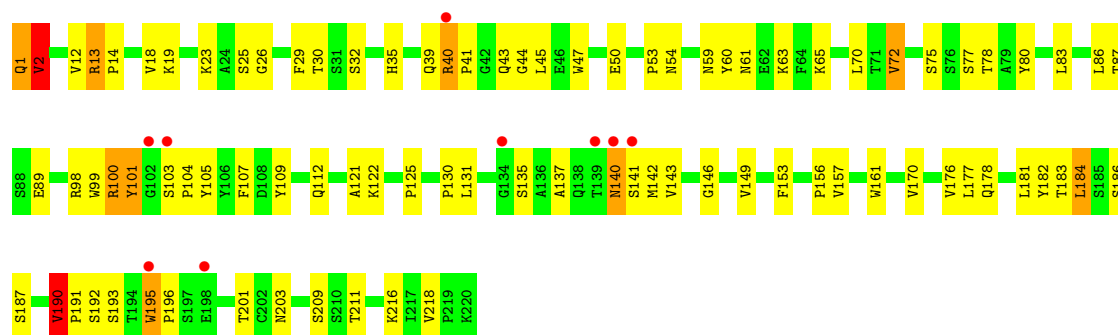
• Molecule 2: ANTIBODY FAB25.3 FRAGMENT (LIGHT CHAIN)



• Molecule 3: ANTIBODY FAB25.3 FRAGMENT (HEAVY CHAIN)



• Molecule 3: ANTIBODY FAB25.3 FRAGMENT (HEAVY CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.90Å 92.30Å 149.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.70 12.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-3.70) 91.4 (12.00-3.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.98Å)	Xtrriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.217 , 0.324 0.263 , 0.324	Depositor DCC
R_{free} test set	1433 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtrriage
Anisotropy	0.343	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9024	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.98 % 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 7.9592e-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

Bond lengths and bond angles in the following residue types are not validated in this section: PB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	0/1201	1.07	5/1635 (0.3%)
1	B	0.48	0/1201	1.07	8/1635 (0.5%)
2	L	0.50	0/1704	1.02	11/2311 (0.5%)
2	M	0.48	0/1704	1.00	10/2311 (0.4%)
3	H	0.53	0/1722	1.02	6/2360 (0.3%)
3	K	0.52	0/1722	1.01	6/2360 (0.3%)
All	All	0.50	0/9254	1.03	46/12612 (0.4%)

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
3	H	0	1
3	K	0	1
All	All	0	2

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ASN	C-N-CD	-13.21	91.53	120.60
1	B	121	ASN	CA-C-N	10.86	131.56	120.38
1	B	121	ASN	C-N-CA	10.86	131.56	120.38
1	B	121	ASN	N-CA-C	-10.64	96.48	109.57
1	A	121	ASN	CA-C-N	10.31	151.75	127.00
1	A	121	ASN	C-N-CA	10.31	151.75	127.00
3	H	2	VAL	N-CA-C	-8.64	98.50	109.30
3	K	2	VAL	N-CA-C	-7.53	99.89	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	3	VAL	N-CA-C	6.96	119.46	109.51
2	L	7	SER	CA-C-N	-6.83	111.31	119.84
2	L	7	SER	C-N-CA	-6.83	111.31	119.84
2	L	141	ASN	N-CA-C	6.63	120.69	110.42
2	L	87	THR	N-CA-C	-6.51	100.02	109.59
2	M	141	ASN	N-CA-C	6.51	120.51	110.42
3	K	195	TRP	CA-C-N	-6.39	113.56	119.82
3	K	195	TRP	C-N-CA	-6.39	113.56	119.82
1	B	121	ASN	C-N-CD	-6.17	99.68	125.00
1	B	122	PRO	N-CA-C	-6.11	103.25	110.70
2	M	198	CYS	N-CA-C	-6.08	99.33	109.24
3	H	52	HIS	CA-C-N	6.04	126.21	119.32
3	H	52	HIS	C-N-CA	6.04	126.21	119.32
2	L	3	VAL	N-CA-C	6.00	118.08	109.51
2	L	198	CYS	N-CA-C	-5.89	99.63	109.24
3	H	173	PHE	CA-C-N	5.72	125.67	119.78
3	H	173	PHE	C-N-CA	5.72	125.67	119.78
2	M	77	LEU	N-CA-C	-5.68	99.99	109.24
3	K	190	VAL	CA-C-N	5.64	126.89	119.84
3	K	190	VAL	C-N-CA	5.64	126.89	119.84
1	A	84	HIS	CA-C-N	5.63	126.88	119.84
1	A	84	HIS	C-N-CA	5.63	126.88	119.84
2	M	7	SER	CA-C-N	-5.59	112.86	119.84
2	M	7	SER	C-N-CA	-5.59	112.86	119.84
1	B	84	HIS	CA-C-N	5.42	126.62	119.84
1	B	84	HIS	C-N-CA	5.42	126.62	119.84
3	H	195	TRP	N-CA-C	5.37	120.91	113.45
1	B	122	PRO	CA-N-CD	-5.36	104.50	112.00
2	L	84	GLU	N-CA-C	5.30	120.12	111.37
2	L	175	SER	N-CA-C	5.29	119.03	112.47
2	L	209	ILE	N-CA-C	-5.18	100.31	108.23
2	M	84	GLU	N-CA-C	5.09	119.71	111.37
2	L	62	VAL	N-CA-C	-5.08	101.57	107.61
2	M	175	SER	N-CA-C	5.08	118.77	112.47
2	L	18	ARG	N-CA-C	5.08	116.80	108.52
2	M	18	ARG	N-CA-C	5.05	116.76	108.52
3	K	100	ARG	N-CA-C	5.05	117.67	110.24
2	M	210	VAL	N-CA-C	5.03	117.05	108.86

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	101	TYR	Sidechain
3	K	101	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	1172	0	1176	63	0
1	B	1172	0	1176	70	0
2	L	1667	0	1599	79	0
2	M	1667	0	1599	74	0
3	H	1672	0	1621	70	0
3	K	1672	0	1621	67	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
All	All	9024	0	8792	398	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 22.

All (398) 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:B:85:PRO:HB3	2:M:98:VAL:HB	1.51	0.93
2:L:203:LYS:H	2:L:203:LYS:HD3	1.37	0.89
1:A:99:PRO:HG3	1:A:124:ILE:HG21	1.58	0.86
1:B:99:PRO:HG3	1:B:124:ILE:HG21	1.59	0.85
2:L:84:GLU:HA	2:L:110:LEU:HD13	1.59	0.85
3:K:30:THR:HB	3:K:54:ASN:HB2	1.59	0.84
1:B:10:MET:HA	1:B:119:THR:HG21	1.58	0.84
1:A:10:MET:HA	1:A:119:THR:HG21	1.59	0.82
2:M:203:LYS:H	2:M:203:LYS:HD3	1.42	0.82
2:L:98:VAL:HG12	2:L:99:PRO:HD3	1.61	0.82
2:M:112:ARG:HD3	2:M:113:ALA:O	1.80	0.82
2:L:4:LEU:HD22	2:L:37:MET:HE1	1.62	0.82
2:M:52:ILE:HD13	2:M:58:LEU:HA	1.63	0.81
2:L:52:ILE:HD13	2:L:58:LEU:HA	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:143:VAL:HG13	3:K:190:VAL:HG23	1.63	0.80
2:M:84:GLU:HA	2:M:110:LEU:HD13	1.64	0.80
3:H:30:THR:HB	3:H:54:ASN:HB2	1.64	0.79
1:A:17:PRO:HG2	1:B:60:GLY:C	2.08	0.79
3:K:35:HIS:CE1	3:K:99:TRP:HB2	2.18	0.78
3:H:35:HIS:CE1	3:H:99:TRP:HB2	2.18	0.78
1:B:110:THR:OG1	1:B:113:GLU:HG3	1.83	0.77
2:L:87:THR:HG21	2:L:170:GLN:HB3	1.66	0.76
2:M:4:LEU:HD22	2:M:37:MET:HE1	1.68	0.76
2:L:21:ILE:HD11	2:L:77:LEU:HD12	1.67	0.75
2:L:112:ARG:HD3	2:L:113:ALA:O	1.86	0.75
3:H:143:VAL:HG13	3:H:190:VAL:HG23	1.68	0.75
1:B:27:VAL:HB	1:B:59:VAL:HG21	1.68	0.74
2:M:21:ILE:HD11	2:M:77:LEU:HD12	1.69	0.74
3:K:30:THR:HA	3:K:53:PRO:HB2	1.70	0.74
1:A:27:VAL:HB	1:A:59:VAL:HG21	1.67	0.73
2:M:87:THR:HG21	2:M:170:GLN:HB3	1.70	0.73
2:M:13:VAL:HG21	2:M:19:ALA:HB2	1.71	0.73
2:M:95:SER:HA	2:M:100:LEU:HD22	1.71	0.72
2:M:193:HIS:HB2	2:M:196:TYR:OH	1.90	0.72
1:A:20:LEU:HD13	1:B:58:THR:HA	1.70	0.71
2:M:89:MET:HG2	2:M:91:PHE:CZ	2.26	0.71
2:L:13:VAL:HG21	2:L:19:ALA:HB2	1.71	0.70
3:H:18:VAL:HG12	3:H:86:LEU:HD11	1.74	0.70
3:H:100:ARG:HD3	3:H:104:PRO:O	1.90	0.70
1:B:27:VAL:HG21	1:B:59:VAL:HG11	1.74	0.70
1:A:4:GLN:HG2	1:A:45:GLU:HB3	1.74	0.69
3:H:2:VAL:HA	3:H:26:GLY:HA3	1.75	0.69
1:A:19:THR:HG23	1:A:43:LEU:HD22	1.76	0.68
1:B:96:MET:O	1:B:97:ARG:HG2	1.93	0.68
3:K:18:VAL:HG12	3:K:86:LEU:HD11	1.75	0.68
2:L:199:GLU:HG3	2:L:210:VAL:HG12	1.76	0.68
2:L:13:VAL:HG21	2:L:19:ALA:CB	2.23	0.67
1:A:27:VAL:HG21	1:A:59:VAL:HG11	1.76	0.67
2:L:89:MET:HG2	2:L:91:PHE:CZ	2.30	0.66
1:A:85:PRO:HB3	2:L:98:VAL:HB	1.77	0.66
2:M:98:VAL:HG12	2:M:99:PRO:HD3	1.78	0.66
2:L:193:HIS:HB2	2:L:196:TYR:OH	1.96	0.66
1:B:4:GLN:HG2	1:B:45:GLU:HB3	1.77	0.65
3:H:30:THR:HA	3:H:53:PRO:HB2	1.78	0.65
2:L:25:ALA:O	2:L:73:THR:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ASN:CB	1:B:122:PRO:HD2	2.27	0.64
1:B:37:ILE:HB	1:B:38:PRO:HD3	1.79	0.64
2:M:119:VAL:HG13	2:M:211:LYS:HG2	1.80	0.64
2:M:13:VAL:HG21	2:M:19:ALA:CB	2.27	0.64
1:A:37:ILE:HB	1:A:38:PRO:HD3	1.80	0.63
1:B:5:ASN:HB2	1:B:7:GLN:HG3	1.79	0.63
3:K:12:VAL:HG21	3:K:86:LEU:HD13	1.80	0.63
1:B:48:THR:HG22	1:B:118:MET:HE1	1.79	0.63
3:H:40:ARG:HE	3:H:41:PRO:HG2	1.63	0.63
3:K:100:ARG:HD3	3:K:104:PRO:O	1.99	0.63
3:H:149:VAL:HG22	3:H:184:LEU:HG	1.81	0.63
2:M:199:GLU:HG3	2:M:210:VAL:HG12	1.80	0.63
3:K:195:TRP:CD1	3:K:196:PRO:HD3	2.35	0.62
3:H:2:VAL:HG21	3:H:98:ARG:NH2	2.15	0.62
2:M:25:ALA:O	2:M:73:THR:HG23	1.99	0.62
1:A:16:SER:OG	1:A:18:ARG:HG2	1.98	0.62
2:M:147:ASP:O	2:M:202:HIS:HD2	1.82	0.62
1:A:72:THR:HG23	3:H:103:SER:OG	2.00	0.61
1:B:146:SER:HB3	1:B:147:PRO:HD3	1.81	0.61
3:K:149:VAL:HG22	3:K:184:LEU:HG	1.82	0.61
1:A:5:ASN:HB2	1:A:7:GLN:HG3	1.82	0.61
1:A:17:PRO:HG2	1:B:61:GLY:N	2.16	0.61
1:A:110:THR:OG1	1:A:113:GLU:HG3	1.99	0.61
1:B:19:THR:HG23	1:B:43:LEU:HD22	1.82	0.61
3:H:2:VAL:HG21	3:H:98:ARG:HH21	1.64	0.61
2:L:95:SER:HA	2:L:100:LEU:HD22	1.83	0.61
2:L:119:VAL:HG13	2:L:211:LYS:HG2	1.83	0.61
1:A:54:THR:HG23	1:B:54:THR:HG23	1.82	0.61
2:L:46:GLN:HB2	2:L:47:PRO:HD2	1.83	0.61
3:K:2:VAL:HA	3:K:26:GLY:HA3	1.82	0.61
3:H:195:TRP:CD1	3:H:196:PRO:HD3	2.35	0.61
1:A:69:LEU:O	1:A:73:ILE:HG12	2.02	0.60
1:A:136:LEU:O	1:A:140:LYS:HG2	2.02	0.60
1:B:85:PRO:O	1:B:86:VAL:HG12	2.00	0.60
1:A:20:LEU:HD22	1:B:58:THR:HG23	1.83	0.60
2:L:21:ILE:CG2	2:L:106:THR:HG21	2.32	0.60
1:A:96:MET:O	1:A:97:ARG:HG2	2.01	0.60
2:L:48:PRO:HG2	3:H:45:LEU:HD11	1.83	0.60
3:H:32:SER:HB3	3:H:99:TRP:O	2.02	0.60
2:L:112:ARG:NH1	2:L:115:ALA:HB2	2.16	0.59
2:L:147:ASP:O	2:L:202:HIS:HD2	1.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:HG13	1:A:89:GLY:HA2	1.85	0.59
1:B:136:LEU:O	1:B:140:LYS:HG2	2.03	0.59
3:K:35:HIS:HD2	3:K:47:TRP:HE1	1.51	0.59
3:H:35:HIS:HD2	3:H:47:TRP:HE1	1.51	0.59
1:A:17:PRO:HB2	1:A:18:ARG:HH21	1.67	0.59
1:B:1:PRO:N	1:B:13:GLN:O	2.36	0.59
2:L:19:ALA:HB3	2:L:79:ILE:HB	1.85	0.59
2:L:171:ASP:OD1	2:L:173:LYS:HB3	2.03	0.58
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.85	0.58
2:M:41:GLN:HB3	2:M:51:LEU:HD11	1.84	0.58
1:B:111:LEU:O	1:B:115:ILE:HG12	2.02	0.58
3:K:2:VAL:HG21	3:K:98:ARG:NH2	2.19	0.58
1:B:17:PRO:HB2	1:B:18:ARG:HH21	1.68	0.57
2:L:21:ILE:HG22	2:L:106:THR:HG21	1.86	0.57
2:L:39:TRP:CD2	2:L:77:LEU:HB2	2.38	0.57
1:B:86:VAL:HG13	1:B:89:GLY:HA2	1.87	0.57
1:A:30:LYS:HG2	1:A:35:GLU:CD	2.30	0.57
1:B:30:LYS:HG2	1:B:35:GLU:CD	2.30	0.56
2:M:39:TRP:CD2	2:M:77:LEU:HB2	2.41	0.56
1:A:146:SER:HB3	1:A:147:PRO:HD3	1.87	0.56
1:B:16:SER:OG	1:B:18:ARG:HG2	2.05	0.56
3:H:2:VAL:HG22	3:H:109:TYR:CD2	2.41	0.56
1:B:69:LEU:O	1:B:73:ILE:HG12	2.06	0.56
2:L:199:GLU:HG3	2:L:210:VAL:CG1	2.35	0.56
3:K:143:VAL:CG1	3:K:190:VAL:HG23	2.33	0.56
2:L:41:GLN:HB3	2:L:51:LEU:HD11	1.86	0.56
1:A:85:PRO:O	1:A:86:VAL:HG12	2.06	0.56
3:K:13:ARG:HD3	3:K:14:PRO:HD2	1.87	0.56
1:A:104:ILE:HG22	1:A:130:TYR:HB2	1.88	0.55
1:A:111:LEU:O	1:A:115:ILE:HG12	2.06	0.55
3:K:12:VAL:HG21	3:K:86:LEU:CD1	2.36	0.55
1:A:1:PRO:HA	1:A:47:ALA:HA	1.89	0.55
2:M:171:ASP:OD1	2:M:173:LYS:HB3	2.06	0.55
1:B:104:ILE:HG22	1:B:130:TYR:HB2	1.90	0.54
2:L:128:GLN:NE2	2:L:135:SER:H	2.04	0.54
2:M:53:TYR:O	2:M:57:ASN:HB2	2.08	0.54
3:H:83:LEU:CB	3:H:86:LEU:HD21	2.38	0.54
2:L:30:ASP:O	2:L:96:LYS:HE3	2.08	0.54
3:H:83:LEU:HB3	3:H:86:LEU:HD21	1.90	0.54
1:A:80:TRP:O	1:A:84:HIS:HD2	1.90	0.53
3:H:191:PRO:O	3:H:193:SER:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:40:ARG:HE	3:K:41:PRO:HG2	1.73	0.53
2:L:149:ASN:HB3	2:L:201:THR:OG1	2.08	0.53
2:M:28:SER:HA	2:M:72:GLY:O	2.09	0.53
2:M:19:ALA:HB3	2:M:79:ILE:HB	1.91	0.53
1:B:9:GLN:C	1:B:11:VAL:H	2.16	0.53
2:L:12:ALA:HA	2:L:109:GLU:O	2.08	0.53
1:B:1:PRO:HA	1:B:47:ALA:HA	1.91	0.52
3:H:190:VAL:HG21	3:H:195:TRP:HB3	1.92	0.52
1:B:100:ARG:HB3	1:B:103:ASP:OD1	2.09	0.52
2:M:21:ILE:CG2	2:M:106:THR:HG21	2.39	0.52
3:K:191:PRO:O	3:K:193:SER:N	2.43	0.52
2:M:21:ILE:HG22	2:M:106:THR:HG21	1.91	0.52
2:L:63:PRO:HG2	2:L:66:PHE:HD2	1.75	0.52
3:K:60:TYR:HE2	3:K:70:LEU:H	1.57	0.52
2:M:12:ALA:HA	2:M:109:GLU:O	2.09	0.52
1:A:9:GLN:C	1:A:11:VAL:H	2.17	0.52
2:L:63:PRO:HG2	2:L:66:PHE:CD2	2.45	0.52
3:K:2:VAL:HG21	3:K:98:ARG:HH21	1.74	0.51
1:A:24:VAL:HG22	1:A:58:THR:HG21	1.93	0.51
2:L:53:TYR:O	2:L:57:ASN:HB2	2.09	0.51
1:B:82:ARG:NH1	3:K:99:TRP:CE2	2.78	0.51
2:L:151:LYS:N	2:L:199:GLU:O	2.44	0.51
2:M:48:PRO:HG2	3:K:45:LEU:HD11	1.93	0.51
2:M:159:ARG:HD2	2:M:161:ASN:O	2.11	0.51
3:H:27:TYR:CZ	3:H:98:ARG:HD3	2.44	0.51
2:M:152:TRP:O	2:M:153:LYS:HD2	2.11	0.51
3:K:190:VAL:HG21	3:K:195:TRP:HB3	1.93	0.51
1:A:48:THR:HG22	1:A:118:MET:HE1	1.92	0.51
2:M:149:ASN:HB3	2:M:201:THR:OG1	2.11	0.51
3:H:157:VAL:HG21	3:H:184:LEU:HD21	1.92	0.51
1:A:73:ILE:HD11	1:A:134:ILE:HA	1.92	0.51
1:B:73:ILE:HD11	1:B:134:ILE:HA	1.92	0.51
1:B:24:VAL:HG22	1:B:58:THR:HG21	1.93	0.50
2:L:18:ARG:HB2	2:L:80:HIS:HB2	1.93	0.50
3:H:125:PRO:HG3	3:H:209:SER:HB2	1.93	0.50
2:M:135:SER:HA	2:M:183:LEU:O	2.11	0.50
2:M:115:ALA:C	2:M:204:THR:HG21	2.37	0.50
1:B:124:ILE:HG22	1:B:126:VAL:HG13	1.94	0.50
2:M:197:THR:HG23	2:M:212:SER:HB3	1.93	0.50
2:M:46:GLN:HB2	2:M:47:PRO:HD2	1.93	0.50
1:A:100:ARG:HB3	1:A:103:ASP:OD1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:SER:HB3	2:L:32:TYR:CE1	2.46	0.50
2:L:48:PRO:CG	3:H:45:LEU:HD11	2.41	0.50
2:L:128:GLN:O	2:L:131:SER:HB2	2.11	0.50
3:H:1:GLN:HG2	3:H:1:GLN:O	2.12	0.50
2:M:128:GLN:O	2:M:131:SER:HB2	2.11	0.49
3:K:35:HIS:HE1	3:K:99:TRP:HB2	1.70	0.49
3:K:35:HIS:CG	3:K:107:PHE:HE1	2.29	0.49
3:K:39:GLN:HB2	3:K:45:LEU:HD23	1.94	0.49
3:K:125:PRO:HG3	3:K:209:SER:HB2	1.94	0.49
2:L:187:LYS:O	2:L:191:GLU:HG2	2.13	0.49
3:H:131:LEU:HB2	3:H:146:GLY:O	2.12	0.49
3:H:176:VAL:O	3:H:182:TYR:HA	2.13	0.49
3:K:2:VAL:HG22	3:K:109:TYR:CD2	2.48	0.49
2:L:149:ASN:O	2:L:200:ALA:HA	2.13	0.49
1:A:136:LEU:O	1:A:139:ASN:ND2	2.46	0.49
2:L:117:PRO:HB3	2:L:143:PHE:HB3	1.95	0.49
2:M:195:SER:HB3	2:M:214:ASN:OD1	2.13	0.49
1:A:80:TRP:O	1:A:84:HIS:CD2	2.66	0.49
1:B:136:LEU:O	1:B:139:ASN:ND2	2.46	0.49
3:H:23:LYS:HA	3:H:78:THR:OG1	2.13	0.49
3:H:201:THR:HG23	3:H:216:LYS:N	2.28	0.48
2:M:165:ASN:HD22	2:M:181:SER:HA	1.78	0.48
2:M:191:GLU:HA	2:M:215:ARG:CZ	2.43	0.48
3:K:40:ARG:HD3	3:K:40:ARG:C	2.38	0.48
3:H:35:HIS:HE1	3:H:99:TRP:HB2	1.71	0.48
2:L:53:TYR:HE1	2:L:59:GLY:HA2	1.78	0.48
2:L:170:GLN:HB2	2:L:177:TYR:CE1	2.48	0.48
3:H:13:ARG:HG2	3:H:14:PRO:HD2	1.95	0.48
2:M:18:ARG:HB2	2:M:80:HIS:HB2	1.95	0.48
2:L:159:ARG:HD2	2:L:161:ASN:O	2.14	0.48
3:H:40:ARG:C	3:H:40:ARG:HD3	2.39	0.48
2:M:147:ASP:O	2:M:202:HIS:CD2	2.66	0.48
2:M:151:LYS:N	2:M:199:GLU:O	2.46	0.48
2:M:162:GLY:O	2:M:183:LEU:HD12	2.14	0.48
3:K:32:SER:HB3	3:K:99:TRP:O	2.13	0.48
2:M:139:PHE:CE2	3:K:187:SER:HB3	2.49	0.48
2:M:202:HIS:O	2:M:204:THR:N	2.46	0.48
1:A:83:LEU:HA	2:L:98:VAL:HG23	1.96	0.48
2:M:165:ASN:ND2	2:M:181:SER:HA	2.28	0.48
3:K:19:LYS:HE2	3:K:80:TYR:CG	2.47	0.48
1:A:1:PRO:N	1:A:13:GLN:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ILE:HG22	1:A:126:VAL:HG13	1.95	0.47
3:H:39:GLN:HB2	3:H:45:LEU:HD23	1.96	0.47
2:L:43:LYS:O	2:L:46:GLN:HG2	2.14	0.47
2:M:134:ALA:HB3	2:M:185:LEU:HD12	1.96	0.47
1:B:5:ASN:HB2	1:B:7:GLN:CG	2.44	0.47
1:B:24:VAL:HG22	1:B:58:THR:CG2	2.44	0.47
2:M:58:LEU:HD21	2:M:62:VAL:O	2.15	0.47
3:K:131:LEU:HB2	3:K:146:GLY:O	2.14	0.47
3:K:29:PHE:HE2	3:K:72:VAL:HG22	1.80	0.47
1:A:33:SER:HB2	1:A:34:PRO:HD2	1.97	0.47
2:L:191:GLU:HA	2:L:215:ARG:CZ	2.44	0.47
1:B:100:ARG:O	1:B:103:ASP:HB2	2.15	0.47
2:M:195:SER:HA	2:M:214:ASN:HA	1.97	0.47
1:B:59:VAL:HG13	1:B:59:VAL:O	2.15	0.46
2:L:162:GLY:O	2:L:183:LEU:HD12	2.15	0.46
3:H:12:VAL:HG21	3:H:86:LEU:CD1	2.45	0.46
2:M:154:ILE:HD12	2:M:159:ARG:HE	1.80	0.46
3:H:201:THR:HG23	3:H:216:LYS:CA	2.44	0.46
2:M:187:LYS:O	2:M:191:GLU:HG2	2.16	0.46
1:B:18:ARG:NH2	1:B:21:ASN:ND2	2.63	0.46
2:L:141:ASN:HD21	3:H:173:PHE:HZ	1.63	0.46
1:B:5:ASN:C	1:B:7:GLN:H	2.23	0.46
2:L:134:ALA:HB3	2:L:185:LEU:HD12	1.98	0.46
2:L:135:SER:HA	2:L:183:LEU:O	2.15	0.46
3:H:29:PHE:HE2	3:H:72:VAL:HG22	1.80	0.46
2:M:43:LYS:O	2:M:46:GLN:HG2	2.16	0.46
3:H:48:ILE:HA	3:H:64:PHE:CD2	2.50	0.46
2:M:43:LYS:HB2	2:M:46:GLN:CD	2.41	0.46
1:A:92:ALA:HA	1:A:93:PRO:HD2	1.85	0.45
1:B:9:GLN:C	1:B:11:VAL:N	2.74	0.45
3:H:216:LYS:HE3	3:H:218:VAL:CG1	2.46	0.45
2:M:199:GLU:HG3	2:M:210:VAL:CG1	2.46	0.45
3:K:121:ALA:HB3	3:K:153:PHE:CZ	2.51	0.45
3:H:155:GLU:OE2	3:H:175:ALA:HB3	2.16	0.45
1:A:87:HIS:O	1:A:88:ALA:HB3	2.16	0.45
2:L:139:PHE:CE2	3:H:187:SER:HB3	2.52	0.45
2:M:90:TYR:O	2:M:105:GLY:HA2	2.16	0.45
2:M:112:ARG:NH1	2:M:115:ALA:HB2	2.31	0.45
3:K:50:GLU:HG2	3:K:59:ASN:HB2	1.98	0.45
3:K:201:THR:HG23	3:K:216:LYS:N	2.32	0.45
1:A:9:GLN:C	1:A:11:VAL:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:TRP:O	1:B:84:HIS:HD2	2.00	0.45
2:M:7:SER:HB2	2:M:8:PRO:HD3	1.98	0.45
2:M:18:ARG:HD3	2:M:78:ASN:HD21	1.82	0.45
1:A:86:VAL:HG13	1:A:86:VAL:O	2.16	0.45
1:B:33:SER:HB2	1:B:34:PRO:HD2	1.99	0.45
3:H:121:ALA:HB3	3:H:153:PHE:CZ	2.51	0.45
3:K:1:GLN:O	3:K:1:GLN:HG2	2.16	0.45
1:B:86:VAL:HG13	1:B:86:VAL:O	2.16	0.45
2:M:4:LEU:CD2	2:M:37:MET:HE1	2.43	0.45
2:M:125:SER:HB3	3:K:130:PRO:O	2.17	0.45
3:K:143:VAL:HG11	3:K:195:TRP:CD1	2.52	0.45
1:B:87:HIS:O	1:B:88:ALA:HB3	2.16	0.45
2:L:70:GLY:HA3	2:L:75:PHE:CD2	2.51	0.45
2:L:155:ASP:OD2	2:L:193:HIS:HB3	2.17	0.45
3:H:103:SER:HB2	3:H:104:PRO:HD3	1.99	0.45
2:L:21:ILE:HG21	2:L:106:THR:HG21	1.99	0.45
3:H:27:TYR:OH	3:H:34:ILE:HD11	2.17	0.45
2:M:119:VAL:HA	2:M:139:PHE:O	2.16	0.45
3:H:178:GLN:N	3:H:181:LEU:O	2.50	0.45
2:M:129:LEU:HA	2:M:133:GLY:O	2.17	0.45
3:K:176:VAL:O	3:K:182:TYR:HA	2.17	0.45
2:M:70:GLY:HA3	2:M:75:PHE:HA	1.98	0.44
2:M:153:LYS:HB2	2:M:197:THR:HB	2.00	0.44
2:L:18:ARG:HD3	2:L:78:ASN:HD21	1.82	0.44
2:L:90:TYR:O	2:L:105:GLY:HA2	2.17	0.44
3:K:40:ARG:HD3	3:K:41:PRO:O	2.17	0.44
3:K:161:TRP:HZ2	3:K:186:SER:O	2.01	0.44
1:B:128:GLU:O	1:B:132:ARG:HG3	2.17	0.44
1:A:24:VAL:HG22	1:A:58:THR:CG2	2.48	0.44
3:H:40:ARG:HG2	3:H:41:PRO:HD2	2.00	0.44
3:H:172:THR:HG23	3:H:186:SER:HB2	1.99	0.44
3:K:83:LEU:CB	3:K:86:LEU:HD21	2.48	0.44
3:H:19:LYS:HE2	3:H:80:TYR:CG	2.52	0.44
1:A:51:ASP:O	1:A:55:MET:HG3	2.18	0.44
1:A:139:ASN:HD22	1:A:140:LYS:N	2.16	0.44
1:B:29:GLU:C	1:B:30:LYS:HD2	2.42	0.44
2:L:202:HIS:O	2:L:204:THR:N	2.50	0.44
3:H:61:ASN:ND2	3:H:63:LYS:HB3	2.33	0.44
3:K:54:ASN:O	3:K:54:ASN:CG	2.61	0.44
1:B:18:ARG:N	1:B:18:ARG:NE	2.66	0.44
2:L:115:ALA:C	2:L:204:THR:HG21	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:129:LEU:HA	2:L:133:GLY:O	2.18	0.44
1:A:29:GLU:HB3	1:A:30:LYS:HD2	2.00	0.43
1:A:62:HIS:ND1	1:A:64:ALA:HB3	2.33	0.43
1:A:65:ALA:HB1	1:A:141:ILE:HD13	1.98	0.43
1:B:3:VAL:O	1:B:46:GLY:HA3	2.18	0.43
2:M:48:PRO:CG	3:K:45:LEU:HD11	2.48	0.43
1:A:104:ILE:HG23	1:A:126:VAL:O	2.17	0.43
1:B:92:ALA:HA	1:B:93:PRO:HD2	1.86	0.43
3:H:126:PRO:HB3	3:H:152:TYR:HB3	2.00	0.43
1:A:18:ARG:NH2	1:A:21:ASN:ND2	2.66	0.43
1:B:9:GLN:O	1:B:11:VAL:N	2.52	0.43
1:B:60:GLY:HA2	1:B:66:MET:SD	2.59	0.43
1:B:104:ILE:HG12	1:B:126:VAL:HG12	2.00	0.43
2:L:193:HIS:O	2:L:215:ARG:HD3	2.18	0.43
2:M:119:VAL:CG1	2:M:211:LYS:HG2	2.47	0.43
2:M:128:GLN:NE2	2:M:135:SER:H	2.16	0.43
3:K:101:TYR:CD1	3:K:101:TYR:N	2.85	0.43
1:B:76:GLU:OE2	3:K:103:SER:HA	2.17	0.43
1:A:5:ASN:HB2	1:A:7:GLN:CG	2.46	0.43
3:K:216:LYS:HE3	3:K:218:VAL:CG1	2.48	0.43
1:A:18:ARG:N	1:A:18:ARG:NE	2.67	0.43
1:A:144:MET:O	1:A:145:TYR:HB2	2.18	0.43
3:H:161:TRP:HZ2	3:H:186:SER:O	2.01	0.43
2:L:93:GLN:HE21	2:L:93:GLN:HB2	1.58	0.43
2:M:63:PRO:HG2	2:M:66:PHE:HD1	1.83	0.43
3:K:170:VAL:HA	3:K:187:SER:O	2.19	0.43
1:A:82:ARG:HD2	2:L:100:LEU:HD21	2.00	0.43
1:B:62:HIS:ND1	1:B:64:ALA:HB3	2.34	0.42
1:B:139:ASN:HD22	1:B:140:LYS:N	2.18	0.42
3:K:87:THR:HB	3:K:89:GLU:OE2	2.19	0.42
1:B:82:ARG:NH1	3:K:99:TRP:NE1	2.68	0.42
1:B:146:SER:HB3	1:B:147:PRO:CD	2.49	0.42
3:H:50:GLU:HG2	3:H:59:ASN:HB2	2.01	0.42
2:M:139:PHE:CZ	3:K:187:SER:HB3	2.54	0.42
2:M:53:TYR:HE1	2:M:59:GLY:HA2	1.85	0.42
3:K:141:SER:O	3:K:142:MET:SD	2.77	0.42
1:B:86:VAL:HG21	1:B:90:PRO:HD3	2.02	0.42
3:K:103:SER:HB2	3:K:104:PRO:HD3	2.00	0.42
3:K:103:SER:O	3:K:105:TYR:CD2	2.72	0.42
2:M:63:PRO:HG2	2:M:66:PHE:CD1	2.55	0.42
3:K:157:VAL:HG21	3:K:184:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:MET:O	1:B:71:GLU:HG2	2.19	0.42
1:A:85:PRO:C	1:A:87:HIS:N	2.77	0.42
2:L:122:PHE:CE2	3:H:133:PRO:HG3	2.55	0.42
2:L:206:THR:HG23	2:L:207:SER:N	2.35	0.42
3:H:152:TYR:CE2	3:H:157:VAL:HG13	2.55	0.42
2:L:98:VAL:HG12	2:L:99:PRO:CD	2.41	0.42
2:L:168:THR:HG22	2:L:169:ASP:N	2.34	0.42
3:H:123:THR:HA	3:H:153:PHE:O	2.19	0.42
3:K:100:ARG:NH1	3:K:104:PRO:HD2	2.35	0.42
2:L:150:VAL:HA	2:L:199:GLU:O	2.20	0.42
3:H:40:ARG:HD3	3:H:41:PRO:O	2.19	0.42
1:B:3:VAL:C	1:B:46:GLY:HA3	2.45	0.41
1:B:86:VAL:CG2	1:B:90:PRO:HD3	2.50	0.41
3:H:100:ARG:NH1	3:H:104:PRO:HD2	2.35	0.41
1:A:128:GLU:O	1:A:132:ARG:HG3	2.20	0.41
1:B:6:LEU:C	1:B:8:GLY:H	2.29	0.41
2:L:7:SER:HB2	2:L:8:PRO:HD3	2.01	0.41
2:M:29:VAL:O	2:M:29:VAL:HG23	2.21	0.41
3:K:39:GLN:HG3	3:K:44:GLY:O	2.21	0.41
3:K:65:LYS:HD2	3:K:65:LYS:HA	1.76	0.41
1:A:47:ALA:HB3	1:A:52:LEU:CD1	2.51	0.41
3:H:201:THR:HG23	3:H:216:LYS:HA	2.01	0.41
3:K:142:MET:SD	3:K:191:PRO:HA	2.60	0.41
3:K:190:VAL:HA	3:K:191:PRO:HD3	1.80	0.41
1:B:104:ILE:HG23	1:B:126:VAL:O	2.20	0.41
2:L:119:VAL:HA	2:L:139:PHE:O	2.20	0.41
2:L:122:PHE:HA	2:L:123:PRO:HD3	1.83	0.41
3:H:143:VAL:HG11	3:H:195:TRP:CD1	2.56	0.41
3:K:1:GLN:OE1	3:K:1:GLN:N	2.50	0.41
1:B:51:ASP:O	1:B:55:MET:HG3	2.21	0.41
1:B:138:LEU:O	1:B:142:VAL:HG23	2.20	0.41
2:L:7:SER:CB	2:L:8:PRO:HD3	2.50	0.41
3:H:13:ARG:HD3	3:H:14:PRO:HG2	2.02	0.41
3:H:170:VAL:HA	3:H:187:SER:O	2.21	0.41
2:M:155:ASP:OD2	2:M:193:HIS:HB3	2.20	0.41
1:A:68:MET:O	1:A:71:GLU:HG2	2.20	0.41
1:A:144:MET:O	1:A:145:TYR:CB	2.68	0.41
2:L:179:MET:HE3	2:L:179:MET:HB2	1.98	0.41
2:L:195:SER:HA	2:L:214:ASN:HA	2.03	0.41
2:M:24:ARG:HG3	2:M:73:THR:HG22	2.03	0.41
3:K:23:LYS:HA	3:K:78:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:40:ARG:HG2	3:K:41:PRO:HD2	2.02	0.41
3:K:61:ASN:ND2	3:K:63:LYS:HB3	2.36	0.41
3:K:178:GLN:N	3:K:181:LEU:O	2.54	0.41
1:A:100:ARG:O	1:A:103:ASP:HB2	2.21	0.40
2:L:124:PRO:HD3	2:L:136:VAL:HG22	2.03	0.40
2:L:139:PHE:CZ	3:H:187:SER:HB3	2.56	0.40
3:H:54:ASN:O	3:H:54:ASN:CG	2.64	0.40
3:H:143:VAL:CG1	3:H:190:VAL:HG23	2.43	0.40
3:H:83:LEU:HB2	3:H:86:LEU:HD21	2.03	0.40
2:L:23:CYS:HB2	2:L:39:TRP:CH2	2.56	0.40
3:H:190:VAL:HA	3:H:191:PRO:HD3	1.83	0.40
3:H:191:PRO:O	3:H:192:SER:C	2.64	0.40
3:K:177:LEU:HB2	3:K:182:TYR:CE1	2.57	0.40
1:B:77:ALA:HA	1:B:133:TRP:CZ3	2.56	0.40
3:H:177:LEU:HB2	3:H:182:TYR:CE1	2.56	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	149/151 (99%)	114 (76%)	27 (18%)	8 (5%)	1	16
1	B	149/151 (99%)	113 (76%)	27 (18%)	9 (6%)	1	15
2	L	215/217 (99%)	190 (88%)	19 (9%)	6 (3%)	4	27
2	M	215/217 (99%)	187 (87%)	21 (10%)	7 (3%)	3	25
3	H	218/220 (99%)	185 (85%)	27 (12%)	6 (3%)	4	27
3	K	218/220 (99%)	187 (86%)	26 (12%)	5 (2%)	5	30
All	All	1164/1176 (99%)	976 (84%)	147 (13%)	41 (4%)	3	24

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	145	TYR
1	B	45	GLU
1	B	122	PRO
1	B	145	TYR
2	L	7	SER
2	L	203	LYS
3	H	140	ASN
3	H	192	SER
2	M	7	SER
2	M	203	LYS
3	K	140	ASN
3	K	192	SER
1	A	2	ILE
1	A	87	HIS
1	A	146	SER
1	B	2	ILE
1	B	87	HIS
1	B	146	SER
3	H	137	ALA
3	K	137	ALA
2	L	173	LYS
3	H	29	PHE
3	H	135	SER
2	M	173	LYS
1	A	92	ALA
1	B	4	GLN
1	B	92	ALA
2	L	72	GLY
2	L	158	GLU
2	M	158	GLU
3	K	77	SER
1	A	63	GLN
3	H	22	CYS
2	M	175	SER
3	K	135	SER
1	A	3	VAL
1	B	3	VAL
2	M	72	GLY
2	L	29	VAL
2	M	29	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	128/128 (100%)	115 (90%)	13 (10%)	7	29
1	B	128/128 (100%)	114 (89%)	14 (11%)	6	26
2	L	189/189 (100%)	172 (91%)	17 (9%)	9	33
2	M	189/189 (100%)	173 (92%)	16 (8%)	10	35
3	H	190/190 (100%)	175 (92%)	15 (8%)	11	37
3	K	190/190 (100%)	173 (91%)	17 (9%)	9	33
All	All	1014/1014 (100%)	922 (91%)	92 (9%)	9	33

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

Mol	Chain	Res	Type
1	A	1	PRO
1	A	3	VAL
1	A	4	GLN
1	A	6	LEU
1	A	7	GLN
1	A	24	VAL
1	A	68	MET
1	A	83	LEU
1	A	86	VAL
1	A	107	THR
1	A	122	PRO
1	A	139	ASN
1	A	144	MET
1	B	1	PRO
1	B	3	VAL
1	B	4	GLN
1	B	6	LEU
1	B	7	GLN
1	B	24	VAL
1	B	68	MET
1	B	83	LEU
1	B	86	VAL

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Mol	Chain	Res	Type
1	B	107	THR
1	B	121	ASN
1	B	122	PRO
1	B	139	ASN
1	B	144	MET
2	L	2	ILE
2	L	21	ILE
2	L	41	GLN
2	L	65	ARG
2	L	77	LEU
2	L	93	GLN
2	L	94	GLN
2	L	98	VAL
2	L	101	THR
2	L	112	ARG
2	L	149	ASN
2	L	163	VAL
2	L	169	ASP
2	L	173	LYS
2	L	185	LEU
2	L	186	THR
2	L	203	LYS
3	H	1	GLN
3	H	2	VAL
3	H	13	ARG
3	H	25	SER
3	H	40	ARG
3	H	43	GLN
3	H	112	GLN
3	H	122	LYS
3	H	140	ASN
3	H	149	VAL
3	H	156	PRO
3	H	183	THR
3	H	184	LEU
3	H	190	VAL
3	H	203	ASN
2	M	2	ILE
2	M	65	ARG
2	M	77	LEU
2	M	93	GLN
2	M	94	GLN

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Mol	Chain	Res	Type
2	M	98	VAL
2	M	101	THR
2	M	112	ARG
2	M	149	ASN
2	M	163	VAL
2	M	169	ASP
2	M	173	LYS
2	M	185	LEU
2	M	186	THR
2	M	188	ASP
2	M	203	LYS
3	K	1	GLN
3	K	2	VAL
3	K	13	ARG
3	K	25	SER
3	K	40	ARG
3	K	43	GLN
3	K	72	VAL
3	K	75	SER
3	K	112	GLN
3	K	122	LYS
3	K	140	ASN
3	K	156	PRO
3	K	183	THR
3	K	184	LEU
3	K	190	VAL
3	K	203	ASN
3	K	211	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	84	HIS
1	A	139	ASN
1	B	4	GLN
1	B	21	ASN
1	B	53	ASN
1	B	57	ASN
1	B	84	HIS
1	B	87	HIS
1	B	139	ASN

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Mol	Chain	Res	Type
2	L	38	ASN
2	L	93	GLN
2	L	94	GLN
2	L	128	GLN
2	L	141	ASN
2	L	149	ASN
2	L	165	ASN
3	H	35	HIS
3	H	43	GLN
3	H	57	ASN
3	H	112	GLN
2	M	38	ASN
2	M	93	GLN
2	M	94	GLN
2	M	141	ASN
2	M	149	ASN
2	M	165	ASN
3	K	35	HIS
3	K	112	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	151/151 (100%)	1.15	26 (17%) 4 5	33, 33, 33, 33	151 (100%)
1	B	151/151 (100%)	1.08	23 (15%) 5 7	33, 33, 33, 33	151 (100%)
2	L	217/217 (100%)	0.27	3 (1%) 73 48	7, 7, 21, 21	0
2	M	217/217 (100%)	0.43	6 (2%) 55 34	8, 8, 27, 27	0
3	H	220/220 (100%)	0.28	9 (4%) 41 26	5, 5, 14, 14	0
3	K	220/220 (100%)	0.40	9 (4%) 41 26	9, 9, 21, 21	0
All	All	1176/1176 (100%)	0.54	76 (6%) 25 18	5, 21, 33, 33	302 (25%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	141	SER	5.6
3	K	140	ASN	5.6
1	A	95	GLN	5.6
3	H	137	ALA	5.3
1	B	3	VAL	5.1
1	B	63	GLN	4.5
3	K	139	THR	4.3
1	B	95	GLN	4.2
1	B	101	GLY	3.8
1	B	7	GLN	3.7
1	A	7	GLN	3.6
3	H	139	THR	3.6
2	M	155	ASP	3.4
1	A	149	SER	3.4
3	H	140	ASN	3.3
3	H	141	SER	3.3
2	M	217	GLU	3.3
1	B	102	SER	3.1
1	A	148	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	6	LEU	3.0
1	A	101	GLY	3.0
1	B	148	THR	2.9
1	A	60	GLY	2.9
1	A	90	PRO	2.9
3	H	205	ALA	2.9
1	A	144	MET	2.9
1	A	4	GLN	2.8
1	B	110	THR	2.8
1	A	63	GLN	2.8
1	B	61	GLY	2.7
1	B	8	GLY	2.6
1	B	109	SER	2.6
2	M	195	SER	2.6
1	B	145	TYR	2.6
1	A	21	ASN	2.6
2	L	155	ASP	2.6
1	A	120	HIS	2.6
1	B	18	ARG	2.6
2	M	133	GLY	2.6
1	A	122	PRO	2.5
1	A	57	ASN	2.5
1	B	86	VAL	2.5
1	A	77	ALA	2.5
1	A	3	VAL	2.5
1	A	92	ALA	2.4
1	B	91	ILE	2.4
1	A	151	LEU	2.4
1	B	149	SER	2.4
2	M	80	HIS	2.4
1	B	10	MET	2.4
3	K	103	SER	2.4
3	K	195	TRP	2.3
3	K	40	ARG	2.3
1	B	64	ALA	2.3
1	B	90	PRO	2.3
1	B	93	PRO	2.3
3	K	134	GLY	2.3
1	A	18	ARG	2.3
2	L	198	CYS	2.2
1	A	61	GLY	2.2
2	M	176	THR	2.2

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Mol	Chain	Res	Type	RSRZ
3	H	194	THR	2.2
1	B	140	LYS	2.2
3	H	180	ASP	2.2
3	K	102	GLY	2.1
3	H	40	ARG	2.1
1	B	120	HIS	2.1
1	A	78	ALA	2.1
1	B	94	GLY	2.1
3	H	89	GLU	2.1
3	K	198	GLU	2.1
1	A	119	THR	2.1
1	A	150	ILE	2.1
2	L	98	VAL	2.1
1	A	82	ARG	2.0
1	A	93	PRO	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PB	L	218	1/1	0.95	0.05	13,13,13,13	1
4	PB	M	218	1/1	0.98	0.04	17,17,17,17	1

6.5 Other polymers [i](#)

There are no such residues in this entry.