Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:22 PM GMT

PDB ID	:	1AFV
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

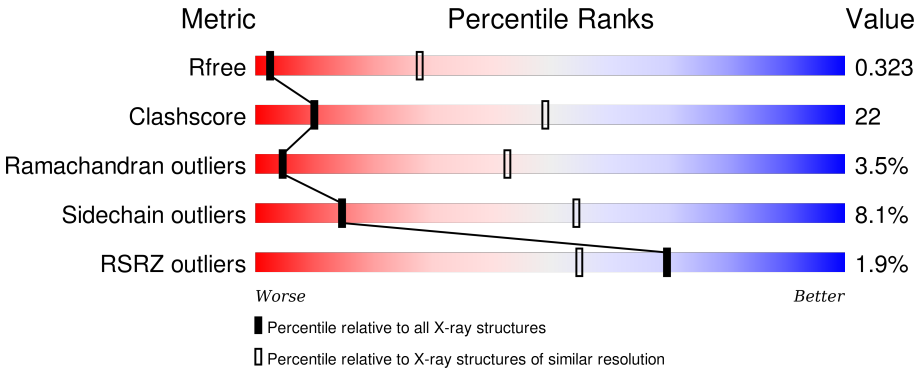
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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 <=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	7%, 42%, 50%, 8%
1	B	151	7%, 42%, 50%, 7%, •
2	L	217	50%, 45%, 5%
2	M	217	53%, 42%, 5%
3	H	220	59%, 37%, •

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Mol	Chain	Length	Quality of chain
3	K	220	

2 Entry composition (i)

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 (three-letter code: PB) (formula: Pb).

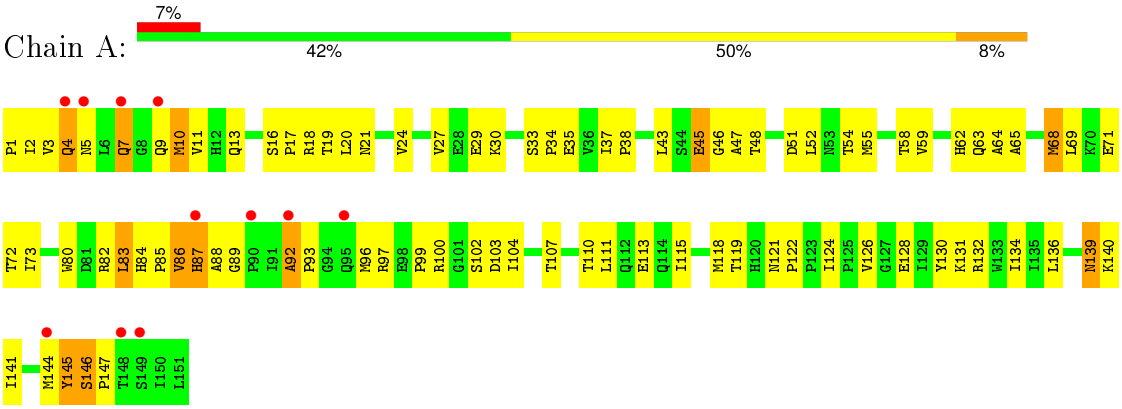
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total Pb 1 1	0	0
4	M	1	Total Pb 1 1	0	0

3 Residue-property plots (i)

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.

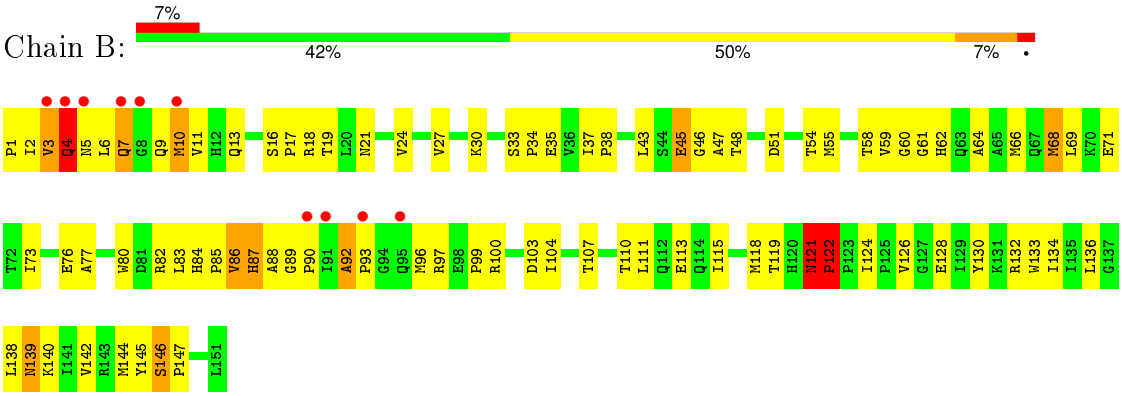
- Molecule 1: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 CAPSID PROTEIN

Chain A:



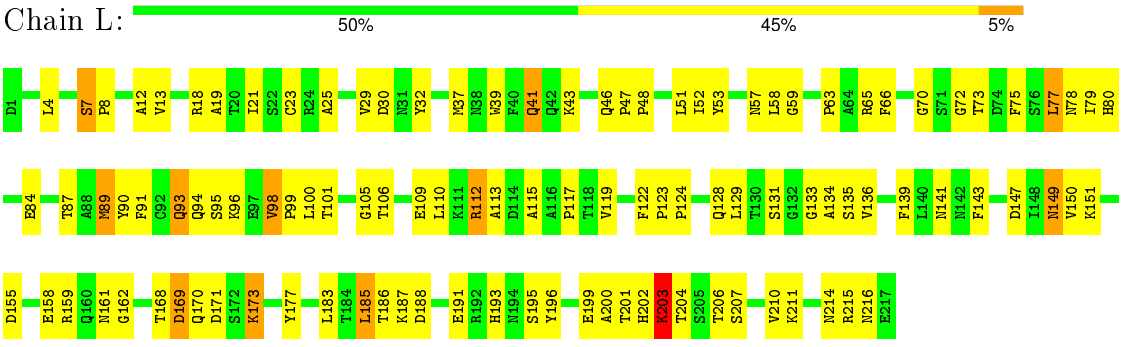
- Molecule 1: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 CAPSID PROTEIN

Chain B:



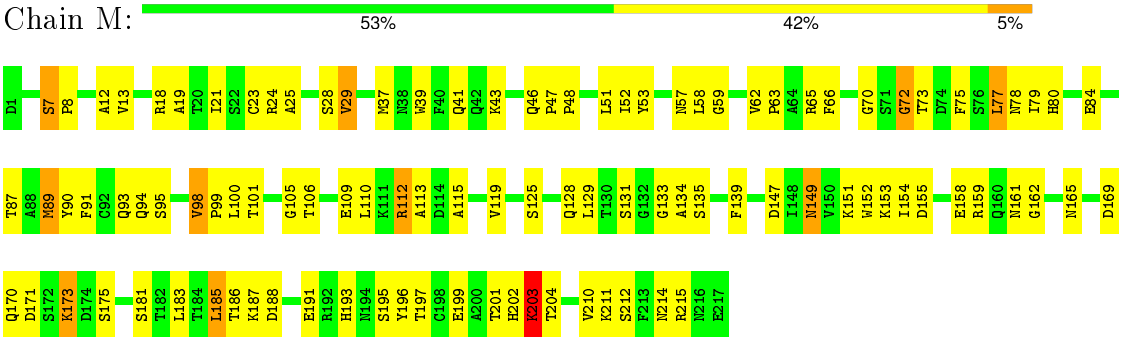
- Molecule 2: ANTIBODY FAB25.3 FRAGMENT (LIGHT CHAIN)

Chain L:



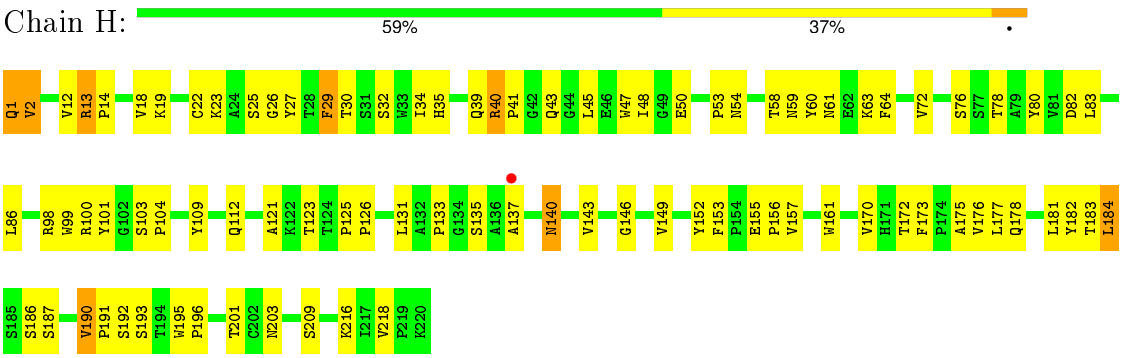
• Molecule 2: ANTIBODY FAB25.3 FRAGMENT (LIGHT CHAIN)

Chain M:



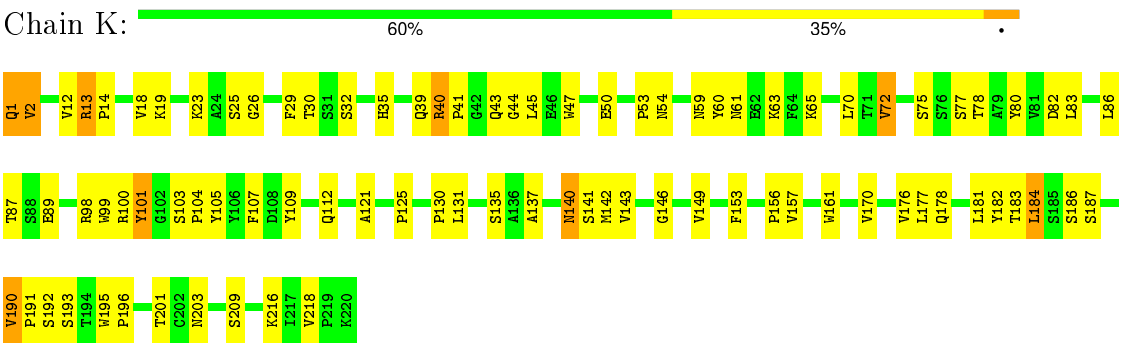
• Molecule 3: ANTIBODY FAB25.3 FRAGMENT (HEAVY CHAIN)

Chain H:



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

Chain K:



4 Data and refinement statistics (i)

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 19.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-3.70) 83.9 (19.98-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.98Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.217 , 0.324 0.257 , 0.323	Depositor DCC
R_{free} test set	861 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	47.3	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 41.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 28315 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	9024	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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 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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.35	0/1201	0.70	2/1635 (0.1%)
1	B	0.36	0/1201	0.65	2/1635 (0.1%)
2	L	0.42	0/1704	0.69	0/2311
2	M	0.41	0/1704	0.69	0/2311
3	H	0.43	0/1722	0.71	0/2360
3	K	0.43	0/1722	0.70	0/2360
All	All	0.41	0/9254	0.69	4/12612 (0.0%)

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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	121	ASN	C-N-CD	-13.21	91.53	120.60
1	B	121	ASN	C-N-CD	-9.51	99.68	120.60
1	A	121	ASN	C-N-CA	7.08	151.75	122.00
1	B	121	ASN	N-CA-C	-5.38	96.48	111.00

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	62	0
1	B	1172	0	1176	67	0
2	L	1667	0	1599	78	0
2	M	1667	0	1599	74	0
3	H	1672	0	1621	69	0
3	K	1672	0	1621	66	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
All	All	9024	0	8792	391	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 (391) 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: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
3:K:143:VAL:HG13	3:K:190:VAL:HG23	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:L:112:ARG:HD3	2:L:113:ALA:O	1.86	0.75
2:L:21:ILE:HD11	2:L:77:LEU:HD12	1.67	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
1:A:17:PRO:HG2	1:B:60:GLY:C	2.08	0.74
3:K:30:THR:HA	3:K:53:PRO:HB2	1.70	0.74
2:M:87:THR:HG21	2:M:170:GLN:HB3	1.70	0.73
1:A:27:VAL:HB	1:A:59:VAL:HG21	1.67	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
2:M:98:VAL:HG12	2:M:99:PRO:HD3	1.78	0.66
1:A:85:PRO:HB3	2:L:98:VAL:HB	1.77	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:K:12:VAL:HG21	3:K:86:LEU:HD13	1.80	0.63
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: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
2:M:199:GLU:HG3	2:M:210:VAL:HG12	1.80	0.63
3:H:149:VAL:HG22	3:H:184:LEU:HG	1.81	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
2:M:147:ASP:O	2:M:202:HIS:HD2	1.82	0.62
1:A:16:SER:OG	1:A:18:ARG:HG2	1.98	0.62
1:A:72:THR:HG23	3:H:103:SER:OG	2.00	0.61
3:K:149:VAL:HG22	3:K:184:LEU:HG	1.82	0.61
1:B:146:SER:HB3	1:B:147:PRO:HD3	1.81	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
3:H:2:VAL:HG21	3:H:98:ARG:HH21	1.64	0.61
1:B:19:THR:HG23	1:B:43:LEU:HD22	1.82	0.61
1:A:110:THR:OG1	1:A:113:GLU:HG3	1.99	0.61
2:L:119:VAL:HG13	2:L:211:LYS:HG2	1.83	0.61
2:L:95:SER:HA	2:L:100:LEU:HD22	1.83	0.61
1:A:54:THR:HG23	1:B:54:THR:HG23	1.82	0.61
3:K:2:VAL:HA	3:K:26:GLY:HA3	1.82	0.61
2:L:46:GLN:HB2	2:L:47:PRO:HD2	1.83	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
2:L:21:ILE:CG2	2:L:106:THR:HG21	2.32	0.60
1:A:20:LEU:HD22	1:B:58:THR:HG23	1.83	0.60
3:H:32:SER:HB3	3:H:99:TRP:O	2.02	0.60
2:L:48:PRO:HG2	3:H:45:LEU:HD11	1.83	0.60
1:A:96:MET:O	1:A:97:ARG:HG2	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:19:ALA:HB3	2:L:79:ILE:HB	1.85	0.59
1:B:1:PRO:N	1:B:13:GLN:O	2.36	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
3:K:2:VAL:HG21	3:K:98:ARG:NH2	2.19	0.58
1:B:111:LEU:O	1:B:115:ILE:HG12	2.02	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
2:M:39:TRP:CD2	2:M:77:LEU:HB2	2.41	0.56
1:B:16:SER:OG	1:B:18:ARG:HG2	2.05	0.56
1:A:146:SER:HB3	1:A:147:PRO:HD3	1.87	0.56
3:H:2:VAL:HG22	3:H:109:TYR:CD2	2.41	0.56
2:L:199:GLU:HG3	2:L:210:VAL:CG1	2.35	0.56
1:B:69:LEU:O	1:B:73:ILE:HG12	2.06	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
3:K:12:VAL:HG21	3:K:86:LEU:CD1	2.36	0.55
1:A:111:LEU:O	1:A:115:ILE:HG12	2.06	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:M:53:TYR:O	2:M:57:ASN:HB2	2.08	0.54
2:L:128:GLN:NE2	2:L:135:SER:H	2.04	0.54
3:H:83:LEU:CB	3:H:86:LEU:HD21	2.38	0.54
3:H:83:LEU:HB3	3:H:86:LEU:HD21	1.90	0.54
2:L:30:ASP:O	2:L:96:LYS:HE3	2.08	0.54
3:H:191:PRO:O	3:H:193:SER:N	2.41	0.53
1:A:80:TRP:O	1:A:84:HIS:HD2	1.90	0.53
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
2:L:12:ALA:HA	2:L:109:GLU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:190:VAL:HG21	3:H:195:TRP:HB3	1.92	0.52
1:B:1:PRO:HA	1:B:47:ALA:HA	1.91	0.52
1:B:100:ARG:HB3	1:B:103:ASP:OD1	2.09	0.52
3:K:191:PRO:O	3:K:193:SER:N	2.43	0.52
2:M:21:ILE:CG2	2:M:106:THR:HG21	2.39	0.52
2:M:21:ILE:HG22	2:M:106:THR:HG21	1.91	0.52
1:A:30:LYS:HG2	1:A:35:GLU:CD	2.30	0.52
3:K:60:TYR:HE2	3:K:70:LEU:H	1.57	0.52
2:L:63:PRO:HG2	2:L:66:PHE:HD2	1.75	0.52
1:B:30:LYS:HG2	1:B:35:GLU:CD	2.30	0.52
2:M:12:ALA:HA	2:M:109:GLU:O	2.09	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:K:190:VAL:HG21	3:K:195:TRP:HB3	1.93	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
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
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
2:L:48:PRO:CG	3:H:45:LEU:HD11	2.41	0.50
1:A:100:ARG:HB3	1:A:103:ASP:OD1	2.11	0.50
1:A:102:SER:HB3	2:L:32:TYR:CE1	2.46	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
1:A:48:THR:HA	1:A:118:MET:HE1	1.94	0.49
3:K:35:HIS:HE1	3:K:99:TRP:HB2	1.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLN:C	1:B:11:VAL:H	2.16	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:K:2:VAL:HG22	3:K:109:TYR:CD2	2.48	0.49
3:H:176:VAL:O	3:H:182:TYR:HA	2.13	0.49
3:H:131:LEU:HB2	3:H:146:GLY:O	2.12	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:M:195:SER:HB3	2:M:214:ASN:OD1	2.13	0.49
2:L:117:PRO:HB3	2:L:143:PHE:HB3	1.95	0.49
1:A:9:GLN:C	1:A:11:VAL:H	2.17	0.49
1:B:136:LEU:O	1:B:139:ASN:ND2	2.46	0.49
1:A:80:TRP:O	1:A:84:HIS:CD2	2.66	0.49
3:H:23:LYS:HA	3:H:78:THR:OG1	2.13	0.49
2:M:191:GLU:HA	2:M:215:ARG:CZ	2.43	0.48
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
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:M:147:ASP:O	2:M:202:HIS:CD2	2.66	0.48
3:K:32:SER:HB3	3:K:99:TRP:O	2.13	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
2:L:159:ARG:HD2	2:L:161:ASN:O	2.14	0.48
2:M:202:HIS:O	2:M:204:THR:N	2.46	0.48
2:M:139:PHE:CE2	3:K:187:SER:HB3	2.49	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: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
1:A:1:PRO:N	1:A:13:GLN:O	2.47	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
2:M:23:CYS:SG	2:M:37:MET:HE3	2.55	0.47
1:B:5:ASN:HB2	1:B:7:GLN:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:48:THR:HA	1:B:118:MET:HE1	1.97	0.47
3:K:29:PHE:HE2	3:K:72:VAL:HG22	1.80	0.47
2:L:23:CYS:SG	2:L:37:MET:HE3	2.55	0.47
2:L:191:GLU:HA	2:L:215:ARG:CZ	2.44	0.47
1:A:33:SER:HB2	1:A:34:PRO:HD2	1.97	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
3:H:12:VAL:HG21	3:H:86:LEU:CD1	2.45	0.46
2:L:162:GLY:O	2:L:183:LEU:HD12	2.15	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
2:L:135:SER:HA	2:L:183:LEU:O	2.15	0.46
2:L:134:ALA:HB3	2:L:185:LEU:HD12	1.98	0.46
2:M:43:LYS:O	2:M:46:GLN:HG2	2.16	0.46
3:H:29:PHE:HE2	3:H:72:VAL:HG22	1.80	0.46
3:H:48:ILE:HA	3:H:64:PHE:CD2	2.50	0.46
2:M:115:ALA:C	2:M:204:THR:HG21	2.37	0.46
2:M:199:GLU:HG3	2:M:210:VAL:CG1	2.46	0.45
3:H:216:LYS:HE3	3:H:218:VAL:CG1	2.46	0.45
3:K:121:ALA:HB3	3:K:153:PHE:CZ	2.51	0.45
1:A:92:ALA:HA	1:A:93:PRO:HD2	1.85	0.45
3:H:155:GLU:OE2	3:H:175:ALA:HB3	2.16	0.45
2:M:112:ARG:NH1	2:M:115:ALA:HB2	2.31	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
1:A:87:HIS:O	1:A:88:ALA:HB3	2.16	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:B:80:TRP:O	1:B:84:HIS:HD2	2.00	0.45
2:M:18:ARG:HD3	2:M:78:ASN:HD21	1.82	0.45
2:M:7:SER:HB2	2:M:8:PRO:HD3	1.98	0.45
1:A:86:VAL:O	1:A:86:VAL:HG13	2.16	0.45
1:B:33:SER:HB2	1:B:34:PRO:HD2	1.99	0.45
3:K:1:GLN:HG2	3:K:1:GLN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:121:ALA:HB3	3:H:153:PHE:CZ	2.51	0.45
1:B:86:VAL:HG13	1:B:86:VAL:O	2.16	0.45
3:K:143:VAL:HG11	3:K:195:TRP:CD1	2.52	0.45
2:M:125:SER:HB3	3:K:130:PRO:O	2.17	0.45
3:H:103:SER:HB2	3:H:104:PRO:HD3	1.99	0.45
2:L:155:ASP:OD2	2:L:193:HIS:HB3	2.17	0.45
2:L:70:GLY:HA3	2:L:75:PHE:CD2	2.51	0.45
1:B:87:HIS:O	1:B:88:ALA:HB3	2.16	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:153:LYS:HB2	2:M:197:THR:HB	2.00	0.44
2:M:70:GLY:HA3	2:M:75:PHE:HA	1.98	0.44
3:K:40:ARG:HD3	3:K:41:PRO:O	2.17	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: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
3:K:83:LEU:CB	3:K:86:LEU:HD21	2.48	0.44
3:H:40:ARG:HG2	3:H:41:PRO:HD2	2.00	0.44
1:A:24:VAL:HG22	1:A:58:THR:CG2	2.48	0.44
3:H:172:THR:HG23	3:H:186:SER:HB2	1.99	0.44
3:H:19:LYS:HE2	3:H:80:TYR:CG	2.52	0.44
1:A:139:ASN:HD22	1:A:140:LYS:N	2.16	0.44
2:L:202:HIS:O	2:L:204:THR:N	2.50	0.44
3:K:40:ARG:C	3:K:40:ARG:HD3	2.38	0.44
3:H:61:ASN:ND2	3:H:63:LYS:HB3	2.33	0.44
1:A:51:ASP:O	1:A:55:MET:HG3	2.18	0.44
3:H:58:THR:HG1	3:H:60:TYR:HE1	1.62	0.44
1:B:18:ARG:N	1:B:18:ARG:NE	2.66	0.44
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
2:M:48:PRO:CG	3:K:45:LEU:HD11	2.48	0.43
1:A:62:HIS:ND1	1:A:64:ALA:HB3	2.33	0.43
1:B:3:VAL:O	1:B:46:GLY:HA3	2.18	0.43
1:A:65:ALA:HB1	1:A:141:ILE:HD13	1.98	0.43
1:A:104:ILE:HG23	1:A:126:VAL:O	2.17	0.43
3:H:40:ARG:C	3:H:40:ARG:HD3	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:126:PRO:HB3	3:H:152:TYR:HB3	2.00	0.43
1:B:92:ALA:HA	1:B:93:PRO:HD2	1.86	0.43
1:A:18:ARG:NH2	1:A:21:ASN:ND2	2.66	0.43
1:B:104:ILE:HG12	1:B:126:VAL:HG12	2.00	0.43
1:B:60:GLY:HA2	1:B:66:MET:SD	2.59	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
1:B:9:GLN:O	1:B:11:VAL:N	2.52	0.43
3:K:101:TYR:N	3:K:101:TYR:CD1	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
3:H:161:TRP:HZ2	3:H:186:SER:O	2.01	0.43
1:A:144:MET:O	1:A:145:TYR:HB2	2.18	0.43
3:K:170:VAL:HA	3:K:187:SER:O	2.19	0.43
2:M:149:ASN:HB3	2:M:201:THR:HG1	1.84	0.43
2:M:63:PRO:HG2	2:M:66:PHE:HD1	1.83	0.43
2:L:93:GLN:HE21	2:L:93:GLN:HB2	1.58	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
2:L:168:THR:HG22	2:L:169:ASP:N	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
2:M:139:PHE:CZ	3:K:187:SER:HB3	2.54	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
3:K:141:SER:O	3:K:142:MET:SD	2.77	0.42
2:M:53:TYR:HE1	2:M:59:GLY:HA2	1.85	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
3:K:157:VAL:HG21	3:K:184:LEU:HD21	2.00	0.42
2:M:63:PRO:HG2	2:M:66:PHE:CD1	2.55	0.42
1:B:68:MET:O	1:B:71:GLU:HG2	2.19	0.42
3:H:152:TYR:CE2	3:H:157:VAL:HG13	2.55	0.42
2:L:206:THR:HG23	2:L:207:SER:N	2.35	0.42
2:L:122:PHE:CE2	3:H:133:PRO:HG3	2.55	0.42
2:L:98:VAL:HG12	2:L:99:PRO:CD	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:100:ARG:NH1	3:K:104:PRO:HD2	2.35	0.42
3:H:123:THR:HA	3:H:153:PHE:O	2.19	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: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:B:5:ASN:C	1:B:7:GLN:H	2.23	0.41
3:K:39:GLN:HG3	3:K:44:GLY:O	2.21	0.41
2:L:7:SER:HB2	2:L:8:PRO:HD3	2.01	0.41
1:A:128:GLU:O	1:A:132:ARG:HG3	2.20	0.41
2:M:29:VAL:O	2:M:29:VAL:HG23	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
1:A:46:GLY:H	1:A:131:LYS:HZ3	1.67	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
3:H:201:THR:HG23	3:H:216:LYS:HA	2.01	0.41
1:B:104:ILE:HG23	1:B:126:VAL:O	2.20	0.41
3:H:143:VAL:HG11	3:H:195:TRP:CD1	2.56	0.41
2:L:119:VAL:HA	2:L:139:PHE:O	2.20	0.41
3:K:1:GLN:N	3:K:1:GLN:OE1	2.50	0.41
2:L:122:PHE:HA	2:L:123:PRO:HD3	1.83	0.41
2:M:155:ASP:OD2	2:M:193:HIS:HB3	2.20	0.41
3:H:170:VAL:HA	3:H:187:SER:O	2.21	0.41
3:H:13:ARG:HD3	3:H:14:PRO:HG2	2.02	0.41
2:L:7:SER:CB	2:L:8:PRO:HD3	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:M:24:ARG:HG3	2:M:73:THR:HG22	2.03	0.41
3:K:40:ARG:HG2	3:K:41:PRO:HD2	2.02	0.41
1:A:144:MET:O	1:A:145:TYR:CB	2.68	0.41
1:A:68:MET:O	1:A:71:GLU:HG2	2.20	0.41
3:K:23:LYS:HA	3:K:78:THR:OG1	2.21	0.41
2:L:195:SER:HA	2:L:214:ASN:HA	2.03	0.41
3:K:61:ASN:ND2	3:K:63:LYS:HB3	2.36	0.41
2:M:43:LYS:HB2	2:M:46:GLN:CD	2.41	0.41
3:K:178:GLN:N	3:K:181:LEU:O	2.54	0.41
3:H:143:VAL:CG1	3:H:190:VAL:HG23	2.43	0.40
2:L:139:PHE:CZ	3:H:187:SER:HB3	2.56	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:4:LEU:HD22	2:L:37:MET:CE	2.51	0.40
3:H:190:VAL:HA	3:H:191:PRO:HD3	1.83	0.40
3:K:177:LEU:HB2	3:K:182:TYR:CE1	2.57	0.40
1:B:9:GLN:C	1:B:11:VAL:N	2.74	0.40
3:H:177:LEU:HB2	3:H:182:TYR:CE1	2.56	0.40
1:B:77:ALA:HA	1:B:133:TRP:CZ3	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%)	2 29
1	B	149/151 (99%)	113 (76%)	27 (18%)	9 (6%)	2 26
2	L	215/217 (99%)	190 (88%)	19 (9%)	6 (3%)	6 47
2	M	215/217 (99%)	187 (87%)	21 (10%)	7 (3%)	5 44
3	H	218/220 (99%)	185 (85%)	27 (12%)	6 (3%)	6 47
3	K	218/220 (99%)	187 (86%)	26 (12%)	5 (2%)	8 52
All	All	1164/1176 (99%)	976 (84%)	147 (13%)	41 (4%)	4 43

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

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Mol	Chain	Res	Type
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 (i)

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%)	119 (93%)	9 (7%)	19 61
1	B	128/128 (100%)	116 (91%)	12 (9%)	11 48
2	L	189/189 (100%)	173 (92%)	16 (8%)	13 53
2	M	189/189 (100%)	175 (93%)	14 (7%)	17 58
3	H	190/190 (100%)	175 (92%)	15 (8%)	15 55
3	K	190/190 (100%)	174 (92%)	16 (8%)	14 53
All	All	1014/1014 (100%)	932 (92%)	82 (8%)	15 54

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	7	GLN
1	A	10	MET
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	B	4	GLN
1	B	6	LEU
1	B	7	GLN
1	B	10	MET
1	B	68	MET
1	B	83	LEU
1	B	86	VAL
1	B	107	THR
1	B	121	ASN
1	B	122	PRO
1	B	139	ASN
1	B	144	MET
2	L	41	GLN
2	L	65	ARG
2	L	77	LEU
2	L	89	MET
2	L	93	GLN

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Mol	Chain	Res	Type
2	L	94	GLN
2	L	98	VAL
2	L	101	THR
2	L	112	ARG
2	L	149	ASN
2	L	169	ASP
2	L	185	LEU
2	L	186	THR
2	L	188	ASP
2	L	203	LYS
2	L	216	ASN
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	76	SER
3	H	82	ASP
3	H	112	GLN
3	H	140	ASN
3	H	156	PRO
3	H	183	THR
3	H	184	LEU
3	H	190	VAL
3	H	203	ASN
2	M	65	ARG
2	M	77	LEU
2	M	89	MET
2	M	93	GLN
2	M	94	GLN
2	M	98	VAL
2	M	101	THR
2	M	112	ARG
2	M	149	ASN
2	M	169	ASP
2	M	185	LEU
2	M	186	THR
2	M	188	ASP
2	M	203	LYS
3	K	1	GLN
3	K	2	VAL

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Mol	Chain	Res	Type
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	82	ASP
3	K	112	GLN
3	K	140	ASN
3	K	156	PRO
3	K	183	THR
3	K	184	LEU
3	K	190	VAL
3	K	203	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	62	HIS
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	139	ASN
2	L	38	ASN
2	L	93	GLN
2	L	128	GLN
2	L	141	ASN
2	L	149	ASN
2	L	165	ASN
3	H	35	HIS
3	H	112	GLN
2	M	38	ASN
2	M	93	GLN
2	M	128	GLN
2	M	149	ASN
2	M	165	ASN
2	M	194	ASN

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Mol	Chain	Res	Type
2	M	216	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 carbohydrates 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, 95^{th} 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%)	0.28	11 (7%) 18 11	37, 37, 37, 37	151 (100%)
1	B	151/151 (100%)	0.28	10 (6%) 22 12	37, 37, 37, 37	151 (100%)
2	L	217/217 (100%)	-0.48	0 100 100	7, 7, 21, 21	0
2	M	217/217 (100%)	-0.39	0 100 100	8, 8, 27, 27	0
3	H	220/220 (100%)	-0.54	1 (0%) 91 86	5, 5, 14, 14	0
3	K	220/220 (100%)	-0.49	0 100 100	9, 9, 21, 21	0
All	All	1176/1176 (100%)	-0.28	22 (1%) 70 55	5, 21, 37, 37	302 (25%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	VAL	5.6
1	B	95	GLN	4.8
1	A	4	GLN	4.3
1	A	95	GLN	3.5
1	A	90	PRO	3.5
1	B	7	GLN	3.2
1	B	10	MET	3.1
1	A	9	GLN	2.9
1	B	5	ASN	2.8
1	B	4	GLN	2.6
1	B	91	ILE	2.6
1	A	5	ASN	2.5
3	H	137	ALA	2.5
1	A	7	GLN	2.5
1	A	149	SER	2.4
1	A	87	HIS	2.4
1	B	90	PRO	2.4
1	B	93	PRO	2.3
1	A	148	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	8	GLY	2.3
1	A	92	ALA	2.2
1	A	144	MET	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	PB	M	218	1/1	0.96	0.04	-	17,17,17,17	1
4	PB	L	218	1/1	0.98	0.06	-	13,13,13,13	1

6.5 Other polymers (i)

There are no such residues in this entry.