Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:28 PM GMT

PDB ID	:	4F37
Title	:	Structure of the tethered N-terminus of Alzheimer's disease A peptide
Authors	:	Nisbet, R.M.; Nuttall, S.D.; Caine, J.M.; Rober, R.; Hittaki, M.; Pearce, L.A.; Davydova, N.; Masters, C.L.; Varghese, J.N.; Streltsov, V.A.
Deposited on	:	2012-05-09
Resolution	:	2.57 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:

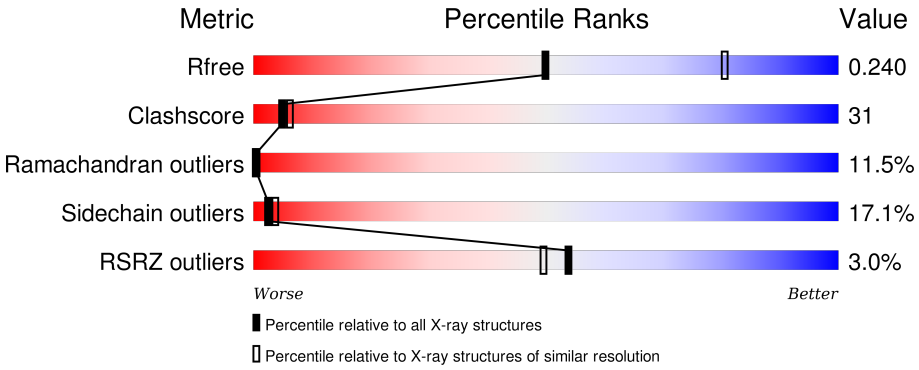
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.57 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	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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	124	2% 27% 41% 14% 18%
1	B	124	2% 39% 29% 14% • 18%
2	F	228	2% 38% 43% 17% ••
2	H	228	3% 38% 47% 13% ••
3	K	219	5% 34% 49% 14% •

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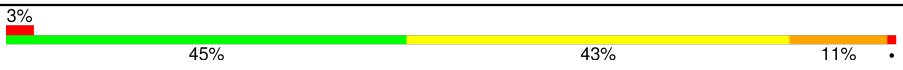
Mol	Chain	Length	Quality of chain
3	L	219	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8769 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 Colicin-E7 immunity protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	0	0	0
			829	520	138	171			
1	B	102	Total	C	N	O	0	0	0
			829	520	138	171			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASP	-	EXPRESSION TAG	UNP Q03708
A	2	ALA	-	EXPRESSION TAG	UNP Q03708
A	3	GLU	-	EXPRESSION TAG	UNP Q03708
A	4	PHE	-	EXPRESSION TAG	UNP Q03708
A	5	ARG	-	EXPRESSION TAG	UNP Q03708
A	6	HIS	-	EXPRESSION TAG	UNP Q03708
A	7	ASP	-	EXPRESSION TAG	UNP Q03708
A	8	SER	-	EXPRESSION TAG	UNP Q03708
A	9	GLY	-	EXPRESSION TAG	UNP Q03708
A	10	TYR	-	EXPRESSION TAG	UNP Q03708
A	11	GLU	-	EXPRESSION TAG	UNP Q03708
A	12	VAL	-	EXPRESSION TAG	UNP Q03708
A	13	HIS	-	EXPRESSION TAG	UNP Q03708
A	14	HIS	-	EXPRESSION TAG	UNP Q03708
A	15	GLN	-	EXPRESSION TAG	UNP Q03708
A	16	LYS	-	EXPRESSION TAG	UNP Q03708
A	17	SER	-	EXPRESSION TAG	UNP Q03708
A	104	ALA	-	EXPRESSION TAG	UNP Q03708
A	105	ALA	-	EXPRESSION TAG	UNP Q03708
A	106	ALA	-	EXPRESSION TAG	UNP Q03708
A	107	ASP	-	EXPRESSION TAG	UNP Q03708
A	108	TYR	-	EXPRESSION TAG	UNP Q03708
A	109	LYS	-	EXPRESSION TAG	UNP Q03708
A	110	ASP	-	EXPRESSION TAG	UNP Q03708
A	111	ASP	-	EXPRESSION TAG	UNP Q03708

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Chain	Residue	Modelled	Actual	Comment	Reference
A	112	ASP	-	EXPRESSION TAG	UNP Q03708
A	113	ASP	-	EXPRESSION TAG	UNP Q03708
A	114	LYS	-	EXPRESSION TAG	UNP Q03708
A	115	ALA	-	EXPRESSION TAG	UNP Q03708
A	116	ALA	-	EXPRESSION TAG	UNP Q03708
A	117	ASP	-	EXPRESSION TAG	UNP Q03708
A	118	TYR	-	EXPRESSION TAG	UNP Q03708
A	119	LYS	-	EXPRESSION TAG	UNP Q03708
A	120	ASP	-	EXPRESSION TAG	UNP Q03708
A	121	ASP	-	EXPRESSION TAG	UNP Q03708
A	122	ASP	-	EXPRESSION TAG	UNP Q03708
A	123	ASP	-	EXPRESSION TAG	UNP Q03708
A	124	LYS	-	EXPRESSION TAG	UNP Q03708
B	1	ASP	-	EXPRESSION TAG	UNP Q03708
B	2	ALA	-	EXPRESSION TAG	UNP Q03708
B	3	GLU	-	EXPRESSION TAG	UNP Q03708
B	4	PHE	-	EXPRESSION TAG	UNP Q03708
B	5	ARG	-	EXPRESSION TAG	UNP Q03708
B	6	HIS	-	EXPRESSION TAG	UNP Q03708
B	7	ASP	-	EXPRESSION TAG	UNP Q03708
B	8	SER	-	EXPRESSION TAG	UNP Q03708
B	9	GLY	-	EXPRESSION TAG	UNP Q03708
B	10	TYR	-	EXPRESSION TAG	UNP Q03708
B	11	GLU	-	EXPRESSION TAG	UNP Q03708
B	12	VAL	-	EXPRESSION TAG	UNP Q03708
B	13	HIS	-	EXPRESSION TAG	UNP Q03708
B	14	HIS	-	EXPRESSION TAG	UNP Q03708
B	15	GLN	-	EXPRESSION TAG	UNP Q03708
B	16	LYS	-	EXPRESSION TAG	UNP Q03708
B	17	SER	-	EXPRESSION TAG	UNP Q03708
B	104	ALA	-	EXPRESSION TAG	UNP Q03708
B	105	ALA	-	EXPRESSION TAG	UNP Q03708
B	106	ALA	-	EXPRESSION TAG	UNP Q03708
B	107	ASP	-	EXPRESSION TAG	UNP Q03708
B	108	TYR	-	EXPRESSION TAG	UNP Q03708
B	109	LYS	-	EXPRESSION TAG	UNP Q03708
B	110	ASP	-	EXPRESSION TAG	UNP Q03708
B	111	ASP	-	EXPRESSION TAG	UNP Q03708
B	112	ASP	-	EXPRESSION TAG	UNP Q03708
B	113	ASP	-	EXPRESSION TAG	UNP Q03708
B	114	LYS	-	EXPRESSION TAG	UNP Q03708
B	115	ALA	-	EXPRESSION TAG	UNP Q03708

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Chain	Residue	Modelled	Actual	Comment	Reference
B	116	ALA	-	EXPRESSION TAG	UNP Q03708
B	117	ASP	-	EXPRESSION TAG	UNP Q03708
B	118	TYR	-	EXPRESSION TAG	UNP Q03708
B	119	LYS	-	EXPRESSION TAG	UNP Q03708
B	120	ASP	-	EXPRESSION TAG	UNP Q03708
B	121	ASP	-	EXPRESSION TAG	UNP Q03708
B	122	ASP	-	EXPRESSION TAG	UNP Q03708
B	123	ASP	-	EXPRESSION TAG	UNP Q03708
B	124	LYS	-	EXPRESSION TAG	UNP Q03708

- Molecule 2 is a protein called Im7 immunity protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	225	Total	C	N	O	S	0	0	0
			1730	1094	292	339	5			
2	H	225	Total	C	N	O	S	0	0	0
			1730	1094	292	339	5			

- Molecule 3 is a protein called Fab WO2 anti-amyloid-beta antibody Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	218	Total	C	N	O	S	0	0	0
			1693	1059	287	341	6			
3	L	218	Total	C	N	O	S	0	0	0
			1693	1059	287	341	6			

- Molecule 4 is water.

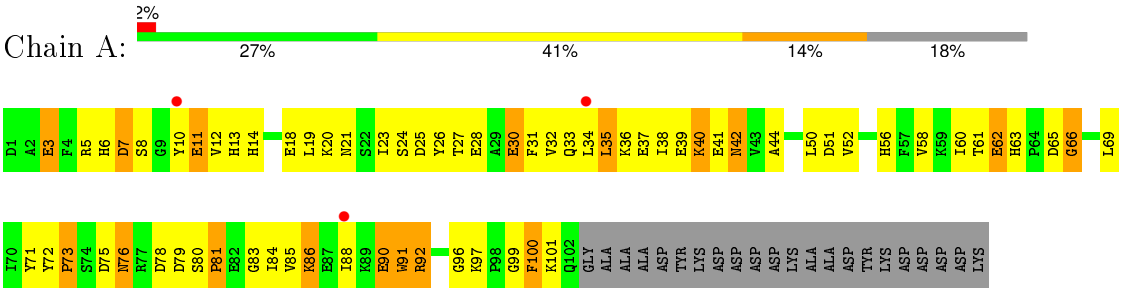
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	34	Total	O	0	0
			34	34		
4	F	53	Total	O	0	0
			53	53		
4	H	50	Total	O	0	0
			50	50		
4	K	42	Total	O	0	0
			42	42		
4	L	54	Total	O	0	0
			54	54		

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.

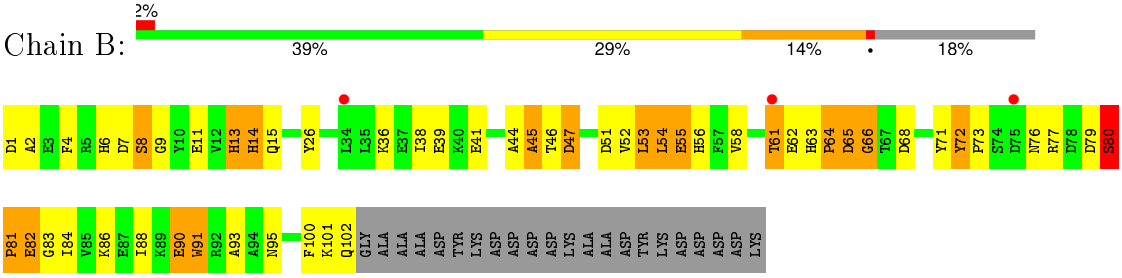
- Molecule 1: Colicin-E7 immunity protein

Chain A:



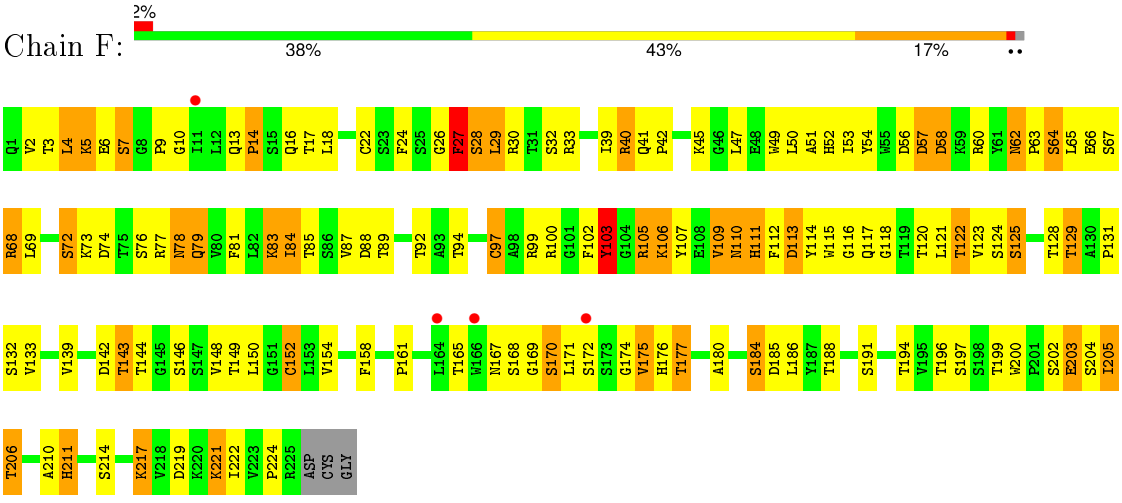
- Molecule 1: Colicin-E7 immunity protein

Chain B:



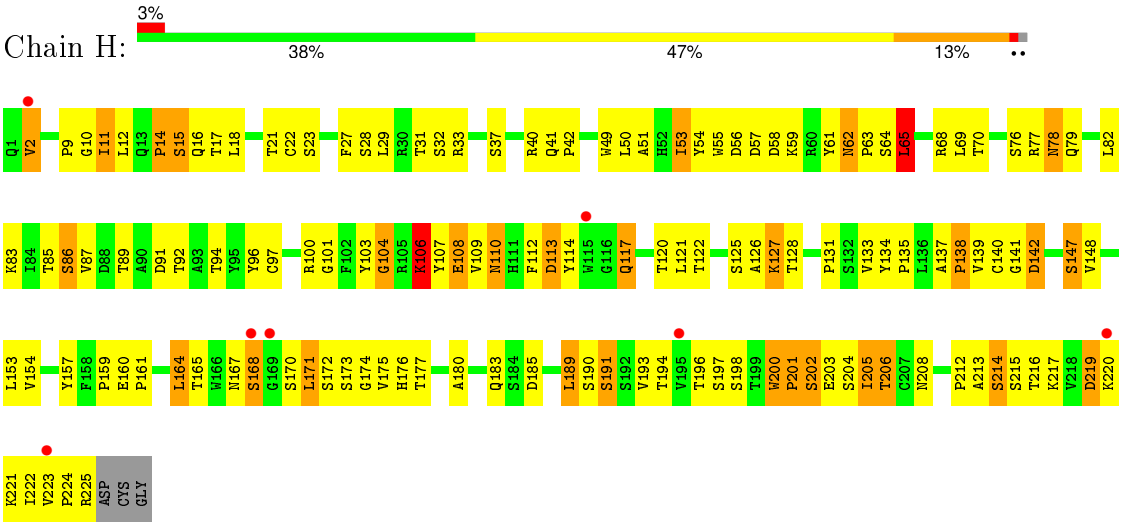
- Molecule 2: Im7 immunity protein

Chain F:



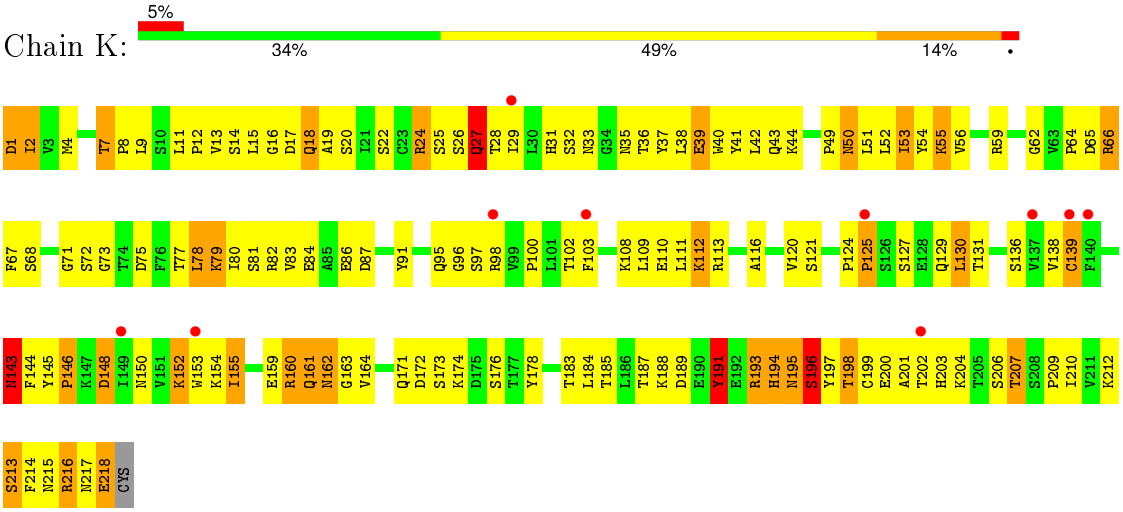
- Molecule 2: Im7 immunity protein

Chain H:



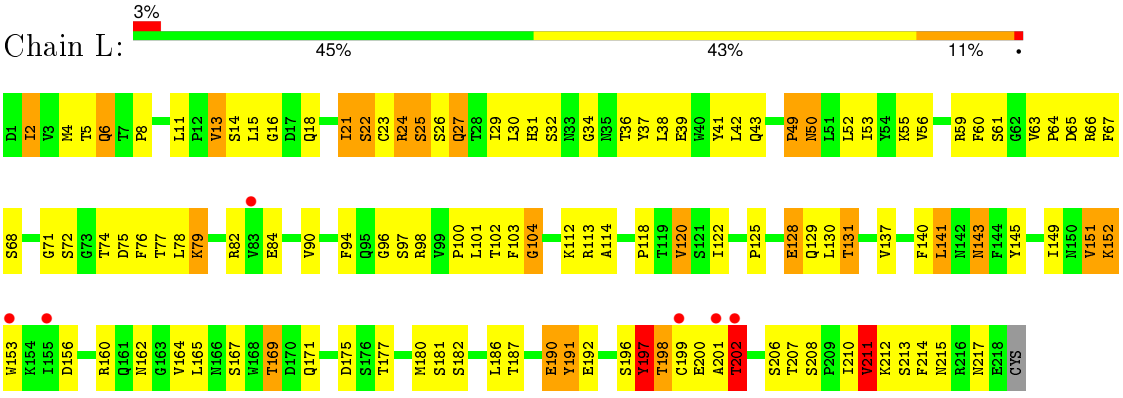
• Molecule 3: Fab WO2 anti-amyloid-beta antibody Fab fragment

Chain K:



• Molecule 3: Fab WO2 anti-amyloid-beta antibody Fab fragment

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	36.64Å 82.84Å 89.20Å 90.05° 92.51° 90.00°	Depositor
Resolution (Å)	44.46 – 2.57 44.56 – 2.50	Depositor EDS
% Data completeness (in resolution range)	77.9 (44.46-2.57) 85.8 (44.56-2.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.223 , 0.269 0.245 , 0.240	Depositor DCC
R_{free} test set	1542 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	54.0	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 24.5	EDS
Estimated twinning fraction	0.489 for H, K, L 0.391 for -H, K, -L 0.120 for -H, -K, L 0.000 for h,-k,-l 0.168 for -h,k,-l 0.000 for -h,-k,l	Xtriage
Reported twinning fraction	0.489 for H, K, L 0.391 for -H, K, -L 0.120 for -H, -K, L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 31156 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8769	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0/847	0.70	0/1145
1	B	0.48	0/847	0.80	2/1145 (0.2%)
2	F	0.52	0/1775	0.72	0/2425
2	H	0.52	0/1775	0.71	0/2425
3	K	0.53	0/1730	0.76	0/2347
3	L	0.55	0/1730	0.75	0/2347
All	All	0.52	0/8704	0.74	2/11834 (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
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	80	SER	C-N-CD	-9.61	99.45	120.60
1	B	80	SER	C-N-CA	5.46	144.93	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	80	SER	Peptide

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	829	0	782	50	0
1	B	829	0	782	39	1
2	F	1730	0	1699	132	1
2	H	1730	0	1699	114	0
3	K	1693	0	1645	114	0
3	L	1693	0	1645	111	0
4	A	32	0	0	2	0
4	B	34	0	0	1	0
4	F	53	0	0	2	0
4	H	50	0	0	4	0
4	K	42	0	0	1	0
4	L	54	0	0	1	1
All	All	8769	0	8252	525	2

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 31.

All (525) 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)
3:L:201:ALA:HB2	3:L:210:ILE:HB	1.28	1.14
2:H:205:ILE:HG23	2:H:221:LYS:HB2	1.16	1.11
2:H:109:VAL:HG23	3:L:55:LYS:HE3	1.24	1.10
2:H:103:TYR:HB2	2:H:109:VAL:HG11	1.36	1.07
2:F:205:ILE:HG21	2:F:222:ILE:HG12	1.32	1.07
3:L:24:ARG:HH11	3:L:24:ARG:HG2	1.18	1.06
2:H:200:TRP:CE3	2:H:201:PRO:HA	1.93	1.03
3:K:171:GLN:HE21	3:K:176:SER:HB3	1.26	0.98
3:K:16:GLY:HA2	3:K:82:ARG:HD2	1.43	0.98
3:K:216:ARG:HG2	3:K:216:ARG:HH21	1.30	0.95
2:F:94:THR:HG23	2:F:120:THR:HG22	1.49	0.94
3:L:2:ILE:HG13	3:L:102:THR:HG21	1.46	0.94
3:K:195:ASN:HD22	3:K:196:SER:H	1.00	0.93
2:F:24:PHE:HD1	2:F:27:PHE:CZ	1.85	0.93
3:K:66:ARG:NH2	3:K:86:GLU:OE2	2.01	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:197:TYR:HD1	3:L:197:TYR:H	1.06	0.93
3:L:191:TYR:CD1	3:L:214:PHE:HZ	1.87	0.92
2:F:184:SER:O	2:F:186:LEU:N	2.03	0.91
3:K:110:GLU:HB2	3:K:171:GLN:OE1	1.71	0.90
3:K:195:ASN:ND2	3:K:196:SER:H	1.68	0.90
2:F:29:LEU:HB2	2:F:78:ASN:OD1	1.70	0.90
3:K:42:LEU:O	3:K:50:ASN:HB2	1.72	0.89
3:K:8:PRO:HG2	3:K:11:LEU:HB2	1.55	0.86
3:L:152:LYS:HG2	3:L:200:GLU:OE1	1.75	0.86
3:K:12:PRO:HA	3:K:110:GLU:O	1.75	0.85
2:H:200:TRP:HE3	2:H:201:PRO:HA	1.42	0.84
2:H:147:SER:HA	2:H:196:THR:HA	1.57	0.84
2:F:24:PHE:CD1	2:F:27:PHE:CZ	2.65	0.84
2:F:103:TYR:HB2	2:F:109:VAL:HG11	1.58	0.83
3:L:49:PRO:HA	3:L:50:ASN:HB2	1.59	0.83
1:A:35:LEU:O	1:A:38:ILE:HG22	1.79	0.82
2:H:200:TRP:HA	2:H:202:SER:H	1.45	0.81
2:F:24:PHE:CD1	2:F:27:PHE:HZ	1.98	0.81
2:F:92:THR:HG23	2:F:122:THR:HA	1.60	0.81
3:K:62:GLY:O	3:K:64:PRO:HD3	1.80	0.81
3:L:191:TYR:HD1	3:L:214:PHE:HZ	1.26	0.80
2:H:59:LYS:HE3	4:H:310:HOH:O	1.82	0.79
3:L:38:LEU:HD12	3:L:94:PHE:O	1.82	0.79
2:F:205:ILE:HG21	2:F:222:ILE:CG1	2.10	0.78
3:L:197:TYR:N	3:L:197:TYR:HD1	1.80	0.78
3:K:2:ILE:O	3:K:102:THR:HG21	1.83	0.78
2:H:94:THR:OG1	2:H:120:THR:HG22	1.84	0.78
3:K:145:TYR:HA	3:K:146:PRO:O	1.83	0.78
2:H:212:PRO:O	2:H:215:SER:OG	2.02	0.77
2:F:112:PHE:O	3:K:51:LEU:HD22	1.84	0.77
3:K:49:PRO:HA	3:K:50:ASN:HB2	1.65	0.77
3:L:24:ARG:CG	3:L:24:ARG:HH11	1.96	0.76
2:F:128:THR:HG23	2:F:158:PHE:O	1.84	0.76
3:L:201:ALA:CB	3:L:210:ILE:HB	2.13	0.76
2:F:205:ILE:HG23	2:F:206:THR:N	2.01	0.75
2:F:6:GLU:HG2	2:F:97:CYS:HB2	1.67	0.75
2:H:205:ILE:CG2	2:H:221:LYS:HB2	2.07	0.75
2:F:24:PHE:HD1	2:F:27:PHE:CE1	2.04	0.75
2:F:28:SER:O	2:F:32:SER:HB3	1.87	0.75
2:F:65:LEU:O	2:F:67:SER:N	2.20	0.74
2:F:24:PHE:HB3	2:F:27:PHE:HE1	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASN:H	1:A:76:ASN:HD22	1.33	0.73
2:H:33:ARG:O	2:H:55:TRP:HB3	1.88	0.73
1:B:63:HIS:HA	1:B:65:ASP:H	1.54	0.73
3:L:206:SER:OG	3:L:208:SER:HB3	1.89	0.72
3:L:8:PRO:HD2	3:L:21:ILE:HG23	1.71	0.72
1:B:4:PHE:HB3	3:K:97:SER:O	1.90	0.72
2:H:103:TYR:CB	2:H:109:VAL:HG11	2.18	0.72
2:F:18:LEU:HD22	2:F:121:LEU:HD22	1.72	0.72
2:H:96:TYR:HE1	2:H:117:GLN:O	1.73	0.71
1:B:53:LEU:HD12	1:B:53:LEU:H	1.53	0.71
2:F:22:CYS:O	2:F:79:GLN:HB3	1.91	0.71
3:K:95:GLN:HE21	3:K:102:THR:HG22	1.56	0.71
3:K:136:SER:HA	3:K:184:LEU:O	1.89	0.71
3:K:216:ARG:CG	3:K:216:ARG:HH21	2.02	0.71
3:K:31:HIS:HD2	3:K:32:SER:H	1.38	0.71
2:F:112:PHE:HD2	3:K:41:TYR:HH	1.38	0.70
2:H:205:ILE:HG23	2:H:221:LYS:CB	2.08	0.70
2:F:150:LEU:HD13	2:F:222:ILE:HG13	1.74	0.70
2:H:205:ILE:HG13	2:H:206:THR:N	2.07	0.70
2:F:133:VAL:HG22	2:F:154:VAL:HG22	1.73	0.70
2:F:205:ILE:CG2	2:F:222:ILE:HG12	2.16	0.69
3:L:191:TYR:CD1	3:L:214:PHE:CZ	2.78	0.69
2:F:57:ASP:HB2	3:L:79:LYS:CE	2.21	0.69
3:L:42:LEU:O	3:L:50:ASN:HB2	1.91	0.69
3:L:59:ARG:NH1	3:L:63:VAL:O	2.24	0.69
2:H:137:ALA:HB2	2:H:222:ILE:HG21	1.74	0.69
3:L:8:PRO:HG2	3:L:11:LEU:HB2	1.73	0.69
1:B:6:HIS:HE1	3:K:96:GLY:O	1.74	0.69
2:F:72:SER:HB2	2:F:81:PHE:HD1	1.57	0.69
2:F:94:THR:HG23	2:F:120:THR:CG2	2.21	0.68
3:K:12:PRO:HB2	3:K:112:LYS:HB2	1.76	0.68
3:L:197:TYR:N	3:L:197:TYR:CD1	2.53	0.68
3:L:4:MET:HB2	3:L:104:GLY:HA2	1.76	0.68
2:H:180:ALA:HA	2:H:189:LEU:HB2	1.76	0.67
3:K:49:PRO:HA	3:K:50:ASN:CB	2.24	0.66
2:F:111:HIS:H	2:F:111:HIS:CD2	2.11	0.66
2:H:2:VAL:HG22	2:H:27:PHE:CD1	2.30	0.66
1:A:71:TYR:O	1:A:73:PRO:HD3	1.94	0.66
3:L:49:PRO:HA	3:L:50:ASN:CB	2.25	0.66
3:K:31:HIS:HD2	3:K:32:SER:N	1.94	0.66
2:F:113:ASP:O	2:F:114:TYR:CD1	2.49	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:24:PHE:HB2	2:F:78:ASN:O	1.96	0.66
2:H:172:SER:OG	4:H:330:HOH:O	2.14	0.66
3:L:141:LEU:HD12	3:L:141:LEU:H	1.62	0.65
3:K:25:SER:OG	3:K:27:GLN:O	2.14	0.65
2:F:57:ASP:HB2	3:L:79:LYS:HE2	1.79	0.65
1:B:8:SER:OG	1:B:9:GLY:N	2.25	0.64
3:K:7:THR:O	3:K:22:SER:OG	2.14	0.64
2:H:109:VAL:CG2	3:L:55:LYS:HE3	2.16	0.64
1:A:6:HIS:HE1	3:L:96:GLY:O	1.80	0.64
1:A:69:LEU:HB3	1:A:84:ILE:HG23	1.80	0.64
2:F:42:PRO:HB2	2:F:45:LYS:HB2	1.79	0.64
1:B:63:HIS:CG	1:B:64:PRO:HA	2.34	0.63
3:K:171:GLN:NE2	3:K:176:SER:HB3	2.07	0.63
3:K:198:THR:HA	3:K:213:SER:HA	1.80	0.63
2:F:58:ASP:OD2	3:L:18:GLN:NE2	2.31	0.63
3:K:195:ASN:HD22	3:K:196:SER:N	1.85	0.63
1:A:6:HIS:HD2	2:H:110:ASN:ND2	1.95	0.62
2:F:14:PRO:HB3	2:F:88:ASP:OD2	1.99	0.62
2:F:24:PHE:HB3	2:F:27:PHE:CE1	2.34	0.62
3:L:43:GLN:HE21	3:L:49:PRO:HG3	1.65	0.62
3:K:198:THR:HA	3:K:213:SER:OG	2.00	0.62
2:H:134:TYR:CE2	3:L:129:GLN:HG3	2.35	0.62
3:L:39:GLU:HB3	3:L:41:TYR:CE1	2.35	0.61
1:A:20:LYS:HB2	1:A:26:TYR:CE1	2.36	0.61
3:L:52:LEU:C	3:L:53:ILE:HD12	2.21	0.61
2:H:109:VAL:HG13	2:H:109:VAL:O	1.98	0.61
2:H:29:LEU:HD22	4:H:306:HOH:O	2.00	0.61
2:H:147:SER:HA	2:H:196:THR:CA	2.29	0.61
3:K:31:HIS:CD2	3:K:32:SER:N	2.69	0.61
1:B:13:HIS:O	1:B:14:HIS:HB2	2.01	0.61
2:H:164:LEU:HA	2:H:208:ASN:O	2.01	0.61
1:A:42:ASN:HB2	1:A:50:LEU:HD13	1.82	0.61
1:A:35:LEU:HD13	1:A:81:PRO:HB2	1.82	0.60
3:K:19:ALA:HB3	3:K:80:ILE:HB	1.83	0.60
3:K:87:ASP:O	3:K:109:LEU:HD23	2.01	0.60
2:F:26:GLY:O	2:F:27:PHE:HB3	2.01	0.60
2:F:205:ILE:HG22	2:F:221:LYS:HA	1.83	0.60
3:K:16:GLY:HA2	3:K:82:ARG:CD	2.26	0.60
2:F:17:THR:HG23	2:F:85:THR:HG22	1.83	0.60
2:H:148:VAL:HG21	2:H:200:TRP:HB3	1.82	0.60
1:A:7:ASP:O	2:H:108:GLU:HB3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:SER:O	1:A:101:LYS:HG3	2.01	0.60
2:F:205:ILE:HG23	2:F:206:THR:H	1.66	0.60
3:L:199:CYS:HB3	3:L:212:LYS:HB2	1.84	0.60
2:H:137:ALA:HB2	2:H:222:ILE:CG2	2.32	0.59
2:H:22:CYS:O	2:H:79:GLN:HB2	2.02	0.59
2:F:9:PRO:HD2	2:F:18:LEU:CD1	2.32	0.59
1:B:101:LYS:O	1:B:102:GLN:HB2	2.03	0.59
3:K:66:ARG:HH22	3:K:86:GLU:CD	2.04	0.59
2:H:174:GLY:O	2:H:175:VAL:HG23	2.02	0.59
2:H:103:TYR:H	2:H:109:VAL:CG1	2.16	0.59
1:A:31:PHE:HD2	1:A:85:VAL:HG22	1.68	0.59
2:H:56:ASP:O	2:H:58:ASP:N	2.36	0.59
1:A:8:SER:HB3	1:A:13:HIS:HE1	1.67	0.59
1:B:80:SER:HB3	1:B:81:PRO:HB2	1.85	0.59
2:H:170:SER:O	2:H:171:LEU:C	2.41	0.58
1:A:19:LEU:HD11	1:A:52:VAL:HG12	1.84	0.58
1:A:31:PHE:CD2	1:A:85:VAL:HG22	2.38	0.58
3:K:171:GLN:HE21	3:K:176:SER:CB	2.08	0.58
1:A:25:ASP:HA	1:A:101:LYS:HE3	1.85	0.58
2:F:53:ILE:O	2:F:53:ILE:HG23	2.04	0.58
2:H:190:SER:OG	3:L:140:PHE:HZ	1.86	0.58
3:L:125:PRO:HD3	3:L:137:VAL:HG22	1.85	0.58
1:A:76:ASN:ND2	1:A:76:ASN:H	2.01	0.57
2:F:18:LEU:CD2	2:F:121:LEU:HD22	2.34	0.57
2:F:131:PRO:HB2	2:F:154:VAL:HG13	1.85	0.57
1:B:54:LEU:O	1:B:58:VAL:HG23	2.03	0.57
2:H:213:ALA:O	2:H:214:SER:HB3	2.05	0.57
3:L:5:THR:O	3:L:23:CYS:HA	2.04	0.57
2:H:69:LEU:HD22	2:H:82:LEU:HD11	1.85	0.57
2:H:96:TYR:CE1	2:H:117:GLN:O	2.56	0.57
3:L:149:ILE:HG13	3:L:202:THR:O	2.05	0.57
3:L:29:ILE:HD11	3:L:38:LEU:HD13	1.86	0.57
1:B:61:THR:OG1	1:B:62:GLU:N	2.37	0.57
3:L:24:ARG:HB2	3:L:74:THR:HG22	1.87	0.57
2:H:53:ILE:HA	2:H:58:ASP:O	2.05	0.57
3:L:24:ARG:HG2	3:L:24:ARG:NH1	2.00	0.57
3:L:27:GLN:HE21	3:L:27:GLN:N	2.03	0.57
3:K:171:GLN:HG3	3:K:178:TYR:CE2	2.40	0.56
3:L:197:TYR:O	3:L:198:THR:HG23	2.03	0.56
1:B:91:TRP:O	1:B:95:ASN:ND2	2.38	0.56
2:H:50:LEU:O	2:H:69:LEU:HD13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:H	1:B:53:LEU:CD1	2.17	0.56
2:F:30:ARG:HE	3:L:75:ASP:CG	2.08	0.56
1:A:3:GLU:OE2	3:L:31:HIS:NE2	2.39	0.56
3:L:190:GLU:C	3:L:192:GLU:H	2.08	0.56
1:A:90:GLU:O	1:A:91:TRP:C	2.43	0.56
3:K:54:TYR:O	3:K:55:LYS:C	2.43	0.56
1:B:53:LEU:HD12	1:B:53:LEU:N	2.20	0.56
2:F:176:HIS:CE1	3:K:143:ASN:OD1	2.59	0.56
2:F:56:ASP:O	2:F:58:ASP:N	2.39	0.55
2:F:205:ILE:CG2	2:F:206:THR:N	2.67	0.55
1:A:6:HIS:CD2	2:H:110:ASN:ND2	2.74	0.55
2:F:68:ARG:NH2	2:F:87:VAL:HA	2.21	0.55
3:K:24:ARG:HG2	3:K:24:ARG:HH11	1.70	0.55
2:H:12:LEU:HD13	2:H:87:VAL:HG21	1.88	0.55
3:L:160:ARG:C	3:L:162:ASN:H	2.08	0.55
2:F:206:THR:HG23	2:F:219:ASP:HB3	1.88	0.55
1:A:8:SER:HB3	1:A:13:HIS:CE1	2.41	0.55
2:F:40:ARG:HG2	2:F:50:LEU:HD21	1.88	0.55
3:L:191:TYR:HD1	3:L:214:PHE:CZ	2.16	0.55
2:H:14:PRO:O	2:H:15:SER:C	2.45	0.55
2:F:139:VAL:HG22	3:K:124:PRO:HD2	1.87	0.55
1:B:54:LEU:C	1:B:56:HIS:H	2.09	0.55
3:L:201:ALA:O	3:L:202:THR:OG1	2.21	0.55
3:K:2:ILE:O	3:K:102:THR:CG2	2.52	0.55
3:K:35:ASN:HD22	3:K:35:ASN:N	2.04	0.55
2:H:190:SER:OG	3:L:140:PHE:CZ	2.59	0.54
2:H:109:VAL:HG23	3:L:55:LYS:CE	2.17	0.54
3:L:143:ASN:HA	3:L:177:THR:HB	1.88	0.54
2:H:68:ARG:NH2	2:H:91:ASP:OD1	2.40	0.54
2:H:18:LEU:HD22	2:H:121:LEU:HD22	1.90	0.54
2:H:147:SER:CA	2:H:196:THR:HA	2.34	0.54
3:K:51:LEU:HG	3:K:52:LEU:N	2.23	0.54
3:K:33:ASN:ND2	3:K:37:TYR:OH	2.40	0.54
2:H:104:GLY:O	2:H:106:LYS:N	2.34	0.54
3:K:197:TYR:HB2	3:K:214:PHE:HB3	1.89	0.54
2:H:135:PRO:HG3	2:H:220:LYS:HD2	1.90	0.54
2:F:105:ARG:O	2:F:107:TYR:N	2.41	0.54
3:K:26:SER:O	3:K:27:GLN:HB3	2.06	0.54
2:F:4:LEU:HD11	2:F:22:CYS:SG	2.47	0.54
2:F:74:ASP:HB2	2:F:81:PHE:CE1	2.44	0.54
3:L:29:ILE:O	3:L:36:THR:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:60:PHE:CG	3:L:61:SER:N	2.76	0.53
3:K:127:SER:O	3:K:130:LEU:N	2.41	0.53
2:F:167:ASN:O	2:F:169:GLY:N	2.41	0.53
3:L:36:THR:O	3:L:36:THR:HG22	2.09	0.53
2:F:74:ASP:HB2	2:F:81:PHE:CZ	2.43	0.53
2:F:139:VAL:HG22	3:K:124:PRO:CD	2.38	0.53
3:L:39:GLU:CB	3:L:41:TYR:CE1	2.91	0.53
2:F:24:PHE:CD1	2:F:27:PHE:CE1	2.91	0.53
3:K:66:ARG:NH2	3:K:87:ASP:OD1	2.41	0.53
3:L:169:THR:OG1	3:L:169:THR:O	2.25	0.53
3:L:71:GLY:HA3	3:L:76:PHE:HA	1.91	0.53
1:B:47:ASP:N	1:B:47:ASP:OD1	2.41	0.53
1:B:63:HIS:HA	1:B:65:ASP:N	2.23	0.53
1:A:34:LEU:O	1:A:37:GLU:CB	2.57	0.53
2:F:18:LEU:HD22	2:F:121:LEU:CD2	2.38	0.53
1:A:10:TYR:O	1:A:11:GLU:HB2	2.09	0.53
2:F:217:LYS:NZ	2:F:219:ASP:OD1	2.36	0.52
1:A:32:VAL:HA	1:A:35:LEU:HD11	1.91	0.52
3:L:66:ARG:HD2	3:L:82:ARG:HB3	1.91	0.52
2:H:113:ASP:HB2	2:H:114:TYR:CD2	2.44	0.52
3:K:203:HIS:O	3:K:206:SER:O	2.27	0.52
1:A:56:HIS:CE1	1:A:60:ILE:HG21	2.45	0.52
2:F:99:ARG:O	2:F:112:PHE:HA	2.08	0.52
3:L:141:LEU:HD13	3:L:180:MET:HB3	1.90	0.52
2:H:40:ARG:HB3	2:H:50:LEU:HD11	1.90	0.52
1:A:34:LEU:O	1:A:37:GLU:HB3	2.09	0.52
2:H:139:VAL:HG12	2:H:140:CYS:N	2.23	0.52
3:L:27:GLN:HE21	3:L:27:GLN:H	1.57	0.52
3:L:42:LEU:HA	3:L:90:VAL:O	2.10	0.52
3:K:1:ASP:O	3:K:2:ILE:HG12	2.10	0.52
1:B:6:HIS:HD2	2:F:110:ASN:HD21	1.57	0.52
3:L:53:ILE:HG13	3:L:59:ARG:HG2	1.90	0.52
2:F:180:ALA:HA	2:F:188:THR:O	2.09	0.51
2:H:9:PRO:HD2	2:H:10:GLY:H	1.76	0.51
3:K:59:ARG:HD3	3:K:67:PHE:O	2.09	0.51
2:H:137:ALA:HB1	2:H:138:PRO:CD	2.41	0.51
3:L:13:VAL:CA	3:L:112:LYS:HB2	2.39	0.51
2:F:54:TYR:HD1	2:F:58:ASP:O	1.92	0.51
3:L:151:VAL:HG22	3:L:200:GLU:O	2.11	0.51
2:F:148:VAL:HG12	2:F:197:SER:HA	1.91	0.51
2:H:10:GLY:HA2	2:H:120:THR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:100:ARG:HG3	2:F:110:ASN:HB2	1.93	0.51
2:F:100:ARG:NH1	3:K:39:GLU:OE1	2.43	0.51
1:A:31:PHE:O	1:A:35:LEU:HG	2.10	0.50
2:F:72:SER:HB2	2:F:81:PHE:CD1	2.43	0.50
2:H:29:LEU:HG	2:H:78:ASN:OD1	2.11	0.50
2:F:77:ARG:O	2:F:78:ASN:HB2	2.12	0.50
2:F:6:GLU:CG	2:F:97:CYS:HB2	2.38	0.50
3:K:129:GLN:C	3:K:131:THR:H	2.14	0.50
2:H:62:ASN:HD22	2:H:63:PRO:HD2	1.76	0.50
2:F:133:VAL:CG1	2:F:152:CYS:SG	2.99	0.50
2:H:113:ASP:HB3	3:L:60:PHE:CE1	2.47	0.50
3:L:8:PRO:CD	3:L:21:ILE:HG23	2.41	0.50
1:A:60:ILE:O	1:A:92:ARG:NH1	2.44	0.50
3:K:152:LYS:HG2	3:K:200:GLU:HG3	1.92	0.50
3:K:161:GLN:O	3:K:162:ASN:C	2.49	0.50
3:K:38:LEU:HD23	3:K:56:VAL:HA	1.93	0.50
2:F:9:PRO:HD2	2:F:18:LEU:HD12	1.92	0.50
2:F:4:LEU:HD12	2:F:5:LYS:N	2.27	0.49
2:F:40:ARG:HG2	2:F:50:LEU:HD11	1.94	0.49
1:B:41:GLU:O	1:B:41:GLU:HG3	2.12	0.49
1:A:27:THR:HG22	1:A:101:LYS:HB3	1.94	0.49
3:L:36:THR:O	3:L:38:LEU:N	2.46	0.49
3:K:40:TRP:O	3:K:52:LEU:HB2	2.12	0.49
3:L:120:VAL:HA	3:L:141:LEU:HA	1.94	0.49
2:F:167:ASN:ND2	2:F:204:SER:O	2.45	0.49
3:K:207:THR:O	3:K:209:PRO:HD3	2.13	0.49
1:A:36:LYS:NZ	4:A:208:HOH:O	2.45	0.49
2:H:94:THR:HA	2:H:120:THR:HA	1.94	0.49
1:B:54:LEU:O	1:B:56:HIS:N	2.45	0.49
3:L:215:ASN:O	3:L:215:ASN:CG	2.51	0.49
2:H:205:ILE:HG13	2:H:206:THR:H	1.75	0.49
3:L:78:LEU:C	3:L:79:LYS:HD3	2.33	0.49
2:F:62:ASN:HD22	2:F:63:PRO:HD2	1.77	0.49
2:F:41:GLN:HB2	2:F:47:LEU:CD2	2.43	0.49
2:H:68:ARG:O	2:H:85:THR:HG23	2.13	0.49
1:A:30:GLU:HA	1:A:33:GLN:HB2	1.94	0.49
3:K:42:LEU:O	3:K:49:PRO:HA	2.13	0.48
3:L:113:ARG:NE	3:L:114:ALA:O	2.46	0.48
3:K:15:LEU:HA	3:K:83:VAL:O	2.13	0.48
2:H:167:ASN:HB2	2:H:206:THR:N	2.28	0.48
2:F:200:TRP:HZ2	2:F:222:ILE:HB	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:77:ARG:O	2:F:78:ASN:CB	2.61	0.48
2:F:14:PRO:HG2	2:F:125:SER:HB2	1.95	0.48
3:L:153:TRP:NE1	3:L:182:SER:OG	2.43	0.48
2:H:200:TRP:CE3	2:H:201:PRO:CA	2.83	0.48
2:H:137:ALA:HB1	2:H:138:PRO:HD2	1.96	0.48
1:A:5:ARG:HB3	2:H:54:TYR:OH	2.13	0.48
1:B:14:HIS:CD2	4:B:201:HOH:O	2.66	0.48
2:F:176:HIS:HE1	3:K:143:ASN:OD1	1.96	0.48
3:K:78:LEU:HG	3:K:78:LEU:O	2.13	0.48
3:K:216:ARG:NH2	3:K:216:ARG:CG	2.69	0.48
1:B:65:ASP:O	1:B:66:GLY:C	2.52	0.48
1:A:31:PHE:HB2	1:A:100:PHE:HE1	1.78	0.48
1:A:76:ASN:HD22	1:A:76:ASN:N	2.08	0.48
3:L:190:GLU:O	3:L:197:TYR:OH	2.30	0.48
3:L:103:PHE:O	3:L:104:GLY:O	2.32	0.48
3:L:160:ARG:HG3	3:L:162:ASN:HB2	1.96	0.48
2:H:85:THR:O	2:H:86:SER:C	2.52	0.48
3:K:138:VAL:HG22	3:K:183:THR:HG23	1.95	0.48
2:F:211:HIS:CE1	2:F:214:SER:HG	2.25	0.48
3:K:59:ARG:HB3	3:K:59:ARG:NH1	2.28	0.48
1:A:35:LEU:HD12	1:A:36:LYS:H	1.79	0.47
2:H:113:ASP:HB3	3:L:60:PHE:HE1	1.78	0.47
2:F:88:ASP:O	2:F:123:VAL:HG11	2.15	0.47
2:F:116:GLY:O	2:F:118:GLY:N	2.47	0.47
3:L:66:ARG:NH1	3:L:84:GLU:CD	2.67	0.47
1:A:32:VAL:HA	1:A:35:LEU:CD1	2.44	0.47
2:H:101:GLY:O	2:H:110:ASN:HA	2.14	0.47
3:K:56:VAL:HG11	3:K:71:GLY:O	2.14	0.47
2:F:124:SER:HB3	2:F:158:PHE:CE1	2.49	0.47
2:H:110:ASN:N	2:H:110:ASN:OD1	2.30	0.47
2:F:39:ILE:CG2	2:F:47:LEU:HD22	2.45	0.47
2:F:199:THR:O	2:F:203:GLU:HB2	2.14	0.47
2:F:115:TRP:N	2:F:115:TRP:CD1	2.82	0.47
2:H:103:TYR:H	2:H:109:VAL:HG12	1.80	0.47
2:H:16:GLN:HB3	2:H:17:THR:H	1.53	0.47
3:K:155:ILE:O	3:K:159:GLU:O	2.32	0.47
3:L:191:TYR:CE1	3:L:214:PHE:HZ	2.29	0.47
2:F:111:HIS:N	2:F:111:HIS:CD2	2.76	0.47
1:B:90:GLU:O	1:B:93:ALA:N	2.48	0.47
3:L:64:PRO:C	3:L:66:ARG:H	2.18	0.47
1:A:83:GLY:HA2	1:A:86:LYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:13:GLN:O	2:F:16:GLN:HG3	2.14	0.47
3:L:152:LYS:N	3:L:152:LYS:HD3	2.30	0.46
2:F:18:LEU:HD23	2:F:84:ILE:HD13	1.97	0.46
1:A:23:ILE:HD11	1:A:61:THR:HG22	1.98	0.46
2:F:200:TRP:CZ2	2:F:222:ILE:HB	2.50	0.46
3:L:2:ILE:HG23	3:L:100:PRO:HD2	1.97	0.46
2:H:133:VAL:O	2:H:135:PRO:HD3	2.15	0.46
2:H:217:LYS:O	2:H:217:LYS:HG2	2.15	0.46
3:L:152:LYS:H	3:L:152:LYS:HD3	1.80	0.46
1:B:8:SER:O	2:F:107:TYR:HD2	1.99	0.46
2:F:144:THR:HB	4:F:343:HOH:O	2.15	0.46
2:H:11:ILE:HG23	2:H:11:ILE:O	2.15	0.46
2:H:103:TYR:HB2	2:H:109:VAL:CG1	2.26	0.46
3:K:148:ASP:N	3:K:148:ASP:OD2	2.48	0.46
3:L:59:ARG:HH12	3:L:63:VAL:C	2.18	0.46
1:B:7:ASP:O	1:B:8:SER:HB2	2.16	0.46
2:H:139:VAL:HG11	4:H:334:HOH:O	2.15	0.46
3:L:130:LEU:HD21	3:L:191:TYR:CE2	2.50	0.46
1:A:36:LYS:O	1:A:39:GLU:HB2	2.16	0.46
3:L:16:GLY:HA2	3:L:82:ARG:HD2	1.96	0.46
2:H:140:CYS:HA	2:H:225:ARG:NH2	2.30	0.46
1:B:72:TYR:CD2	1:B:72:TYR:N	2.83	0.46
2:H:54:TYR:HB2	2:H:58:ASP:HB3	1.98	0.46
1:A:24:SER:HA	1:A:99:GLY:O	2.16	0.46
2:H:177:THR:HA	2:H:191:SER:HA	1.99	0.46
2:H:200:TRP:HA	2:H:202:SER:N	2.24	0.45
2:F:106:LYS:O	2:F:109:VAL:HG12	2.15	0.45
3:L:13:VAL:HA	3:L:112:LYS:HB2	1.97	0.45
2:H:11:ILE:HD12	2:H:159:PRO:HG3	1.97	0.45
2:F:69:LEU:HD23	2:F:84:ILE:HG23	1.97	0.45
3:K:31:HIS:CD2	3:K:32:SER:H	2.24	0.45
2:F:57:ASP:HB2	3:L:79:LYS:HE3	1.98	0.45
3:K:27:GLN:O	3:K:27:GLN:NE2	2.42	0.45
3:K:18:GLN:HG3	3:K:81:SER:HA	1.97	0.45
3:L:128:GLU:HB2	4:L:311:HOH:O	2.16	0.45
2:H:49:TRP:NE1	2:H:51:ALA:O	2.50	0.45
2:F:83:LYS:HG2	2:F:83:LYS:O	2.16	0.45
1:B:71:TYR:O	1:B:73:PRO:HD3	2.16	0.45
2:F:132:SER:O	2:F:133:VAL:C	2.54	0.45
2:H:70:THR:HB	2:H:83:LYS:HB3	1.99	0.45
3:K:82:ARG:NH1	3:K:84:GLU:HG2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:38:LEU:CD1	3:L:94:PHE:O	2.61	0.45
2:F:10:GLY:O	2:F:121:LEU:HD12	2.17	0.45
1:A:7:ASP:O	2:H:108:GLU:CB	2.63	0.45
3:K:120:VAL:HG13	3:K:212:LYS:HE2	1.98	0.45
2:H:107:TYR:O	2:H:109:VAL:N	2.49	0.45
2:F:174:GLY:O	2:F:175:VAL:HB	2.17	0.45
2:F:133:VAL:HG11	2:F:152:CYS:SG	2.56	0.45
2:H:154:VAL:HG21	2:H:164:LEU:HD11	1.97	0.45
3:K:193:ARG:HE	3:K:194:HIS:N	2.14	0.45
1:A:36:LYS:O	1:A:39:GLU:N	2.50	0.45
3:K:199:CYS:HB3	3:K:212:LYS:O	2.17	0.45
2:H:202:SER:HB2	2:H:203:GLU:HG2	1.99	0.45
2:F:107:TYR:O	2:F:110:ASN:ND2	2.37	0.45
3:K:198:THR:HB	3:K:200:GLU:HG2	1.98	0.45
3:K:124:PRO:HA	3:K:125:PRO:HD3	1.77	0.45
2:F:54:TYR:CD1	2:F:58:ASP:O	2.69	0.44
2:H:222:ILE:HG22	2:H:223:VAL:N	2.33	0.44
2:H:134:TYR:HA	2:H:135:PRO:HD2	1.89	0.44
2:H:100:ARG:HB2	2:H:112:PHE:CE1	2.52	0.44
3:K:121:SER:O	3:K:139:CYS:HA	2.18	0.44
3:K:191:TYR:CE1	3:K:214:PHE:HZ	2.36	0.44
2:H:62:ASN:HD22	2:H:63:PRO:CD	2.31	0.44
2:F:63:PRO:HD2	3:K:100:PRO:HB3	2.00	0.44
3:K:22:SER:CB	4:K:308:HOH:O	2.66	0.44
1:B:80:SER:HB2	1:B:83:GLY:H	1.82	0.44
1:B:84:ILE:O	1:B:88:ILE:HD13	2.17	0.44
2:H:147:SER:HB3	2:H:196:THR:HG22	1.98	0.44
3:K:1:ASP:HB2	3:K:2:ILE:H	1.70	0.44
1:B:51:ASP:HA	1:B:54:LEU:HB2	1.99	0.44
3:K:160:ARG:HA	3:K:160:ARG:HD2	1.65	0.44
2:H:23:SER:OG	2:H:79:GLN:NE2	2.49	0.44
3:L:25:SER:OG	3:L:27:GLN:O	2.35	0.44
2:F:148:VAL:HG13	2:F:148:VAL:O	2.18	0.44
1:A:78:ASP:HB2	1:A:83:GLY:HA3	2.00	0.44
2:F:128:THR:HG22	2:F:129:THR:N	2.33	0.44
2:F:110:ASN:H	2:F:110:ASN:ND2	2.16	0.44
2:H:193:VAL:HG13	2:H:193:VAL:O	2.17	0.44
3:L:103:PHE:C	3:L:104:GLY:O	2.56	0.43
1:A:40:LYS:HB3	1:A:41:GLU:H	1.56	0.43
2:F:53:ILE:HG13	2:F:57:ASP:HA	2.00	0.43
3:K:14:SER:O	3:K:17:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:4:MET:HB2	3:K:103:PHE:O	2.17	0.43
2:H:160:GLU:OE1	2:H:161:PRO:HA	2.18	0.43
3:L:191:TYR:CE1	3:L:214:PHE:CZ	3.05	0.43
1:A:84:ILE:O	1:A:88:ILE:HB	2.18	0.43
3:K:216:ARG:NH2	3:K:216:ARG:HG2	2.11	0.43
2:F:41:GLN:HB2	2:F:47:LEU:HD23	1.98	0.43
3:L:206:SER:O	3:L:208:SER:N	2.43	0.43
2:H:29:LEU:HA	2:H:32:SER:OG	2.19	0.43
2:H:77:ARG:O	2:H:78:ASN:CB	2.67	0.43
2:F:9:PRO:O	4:F:330:HOH:O	2.21	0.43
3:K:154:LYS:HD2	3:K:200:GLU:OE1	2.18	0.43
1:A:58:VAL:HG22	1:A:66:GLY:HA3	2.01	0.43
2:H:131:PRO:HB3	2:H:157:TYR:HB3	2.00	0.43
2:H:92:THR:HG23	2:H:122:THR:HA	2.00	0.43
2:F:102:PHE:HD2	2:F:103:TYR:H	1.66	0.43
3:L:52:LEU:O	3:L:53:ILE:HD12	2.18	0.43
2:F:139:VAL:HG13	3:K:124:PRO:HG3	2.00	0.43
2:H:176:HIS:CE1	3:L:143:ASN:OD1	2.72	0.43
2:F:7:SER:OG	2:F:7:SER:O	2.37	0.43
1:B:82:GLU:O	1:B:86:LYS:N	2.51	0.43
3:K:49:PRO:CA	3:K:50:ASN:HB2	2.43	0.43
2:F:2:VAL:HG21	2:F:99:ARG:NH1	2.33	0.43
3:L:78:LEU:O	3:L:79:LYS:HD2	2.19	0.43
3:L:160:ARG:CD	3:L:162:ASN:HD22	2.32	0.43
3:K:13:VAL:HG21	3:K:83:VAL:HG21	1.99	0.43
2:F:69:LEU:CD2	2:F:84:ILE:HG23	2.49	0.42
3:K:187:THR:C	3:K:189:ASP:H	2.22	0.42
3:L:113:ARG:HG2	3:L:145:TYR:CD1	2.53	0.42
2:F:149:THR:HA	2:F:194:THR:HA	1.99	0.42
3:K:35:ASN:ND2	3:K:35:ASN:N	2.66	0.42
3:K:1:ASP:OD1	3:K:1:ASP:N	2.47	0.42
3:L:59:ARG:NH1	3:L:64:PRO:O	2.53	0.42
2:H:213:ALA:O	2:H:214:SER:CB	2.67	0.42
3:L:149:ILE:O	3:L:149:ILE:HG23	2.19	0.42
3:L:2:ILE:HG13	3:L:102:THR:CG2	2.34	0.42
3:L:212:LYS:O	3:L:213:SER:HB2	2.19	0.42
2:F:68:ARG:HH21	2:F:87:VAL:HA	1.85	0.42
2:F:167:ASN:HB3	2:F:170:SER:OG	2.20	0.42
3:K:215:ASN:HD21	3:K:218:GLU:HA	1.83	0.42
1:B:63:HIS:ND1	1:B:91:TRP:CH2	2.87	0.42
3:K:172:ASP:O	3:K:174:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ASP:O	1:B:55:GLU:N	2.53	0.42
2:H:63:PRO:C	2:H:65:LEU:H	2.21	0.42
3:K:116:ALA:HB3	3:K:144:PHE:HA	2.00	0.42
2:F:142:ASP:O	2:F:143:THR:C	2.58	0.42
3:L:118:PRO:HG2	3:L:149:ILE:HD12	2.02	0.42
1:B:54:LEU:C	1:B:56:HIS:N	2.73	0.42
3:K:201:ALA:HB3	3:K:210:ILE:HB	2.02	0.42
1:B:36:LYS:HD2	1:B:39:GLU:OE1	2.20	0.42
3:K:43:GLN:O	3:K:44:LYS:C	2.57	0.42
3:K:129:GLN:NE2	3:K:136:SER:OG	2.40	0.42
2:F:113:ASP:C	2:F:114:TYR:CD1	2.94	0.42
2:H:68:ARG:HA	2:H:85:THR:OG1	2.20	0.42
2:H:142:ASP:OD1	2:H:142:ASP:N	2.44	0.42
2:F:99:ARG:O	2:F:112:PHE:HD1	2.03	0.41
2:F:62:ASN:ND2	2:F:64:SER:OG	2.53	0.41
1:B:26:TYR:O	1:B:100:PHE:HD1	2.02	0.41
2:F:205:ILE:O	2:F:206:THR:CB	2.68	0.41
3:K:39:GLU:HA	3:K:53:ILE:O	2.19	0.41
3:K:143:ASN:N	3:K:143:ASN:OD1	2.52	0.41
1:A:12:VAL:HG12	4:A:203:HOH:O	2.21	0.41
2:H:100:ARG:HB2	2:H:112:PHE:HE1	1.84	0.41
2:F:103:TYR:HB3	2:F:106:LYS:HB2	2.02	0.41
2:F:102:PHE:O	2:F:111:HIS:NE2	2.54	0.41
3:L:31:HIS:O	3:L:34:GLY:N	2.41	0.41
2:F:22:CYS:SG	2:F:24:PHE:HE2	2.44	0.41
3:K:42:LEU:HD13	3:K:91:TYR:CE2	2.55	0.41
3:L:200:GLU:HA	3:L:211:VAL:HG13	2.02	0.41
3:L:56:VAL:HG13	3:L:76:PHE:HD1	1.85	0.41
2:F:49:TRP:NE1	2:F:51:ALA:O	2.52	0.41
1:B:77:ARG:HH21	1:B:79:ASP:HA	1.85	0.41
3:K:113:ARG:HD3	3:K:176:SER:O	2.20	0.41
1:A:5:ARG:O	1:A:6:HIS:CG	2.74	0.41
2:H:139:VAL:HG21	3:L:122:ILE:HG23	2.03	0.41
3:K:64:PRO:C	3:K:66:ARG:H	2.24	0.41
3:K:199:CYS:O	3:K:199:CYS:SG	2.79	0.41
3:K:42:LEU:O	3:K:49:PRO:HB3	2.20	0.41
3:L:160:ARG:O	3:L:164:VAL:HG23	2.21	0.41
3:K:159:GLU:HB3	3:K:194:HIS:HE1	1.86	0.41
3:K:120:VAL:HG11	3:K:210:ILE:HG22	2.03	0.41
3:K:68:SER:HB2	3:K:79:LYS:HB2	2.03	0.41
2:H:134:TYR:HD2	2:H:153:LEU:HD23	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ALA:O	1:B:45:ALA:C	2.59	0.41
2:F:205:ILE:CG2	2:F:221:LYS:HA	2.48	0.40
1:B:90:GLU:O	1:B:91:TRP:C	2.60	0.40
2:F:113:ASP:N	2:F:113:ASP:OD1	2.53	0.40
1:A:92:ARG:HG2	1:A:97:LYS:HB2	2.04	0.40
2:F:52:HIS:HB3	2:F:60:ARG:HB2	2.01	0.40
2:H:41:GLN:HA	2:H:42:PRO:HD2	1.89	0.40
3:L:24:ARG:HA	3:L:74:THR:O	2.21	0.40
3:K:150:ASN:HB2	3:K:202:THR:HB	2.03	0.40
1:A:27:THR:O	1:A:28:GLU:C	2.60	0.40
2:H:126:ALA:O	2:H:127:LYS:C	2.60	0.40
3:K:172:ASP:O	3:K:176:SER:N	2.48	0.40
3:L:21:ILE:HG22	3:L:22:SER:H	1.86	0.40
2:H:28:SER:O	2:H:32:SER:HB3	2.20	0.40
2:H:139:VAL:CG1	2:H:140:CYS:N	2.85	0.40
2:H:63:PRO:O	2:H:65:LEU:N	2.45	0.40
3:L:6:GLN:HB3	3:L:6:GLN:HE21	1.61	0.40
2:F:177:THR:HA	2:F:191:SER:HB2	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:321:HOH:O	4:L:354:HOH:O[1_655]	1.90	0.30
1:B:45:ALA:O	2:F:114:TYR:OH[1_655]	2.08	0.12

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	100/124 (81%)	53 (53%)	26 (26%)	21 (21%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	100/124 (81%)	62 (62%)	20 (20%)	18 (18%)	0	0
2	F	223/228 (98%)	145 (65%)	55 (25%)	23 (10%)	1	0
2	H	223/228 (98%)	155 (70%)	43 (19%)	25 (11%)	0	0
3	K	216/219 (99%)	153 (71%)	42 (19%)	21 (10%)	1	0
3	L	216/219 (99%)	163 (76%)	37 (17%)	16 (7%)	1	1
All	All	1078/1142 (94%)	731 (68%)	223 (21%)	124 (12%)	0	0

All (124) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	14	HIS
1	A	40	LYS
1	A	42	ASN
1	A	73	PRO
1	A	91	TRP
1	A	100	PHE
1	B	11	GLU
1	B	13	HIS
1	B	65	ASP
1	B	81	PRO
1	B	90	GLU
2	F	57	ASP
2	F	66	GLU
2	F	78	ASN
2	F	103	TYR
2	F	106	LYS
2	F	117	GLN
2	F	168	SER
2	F	175	VAL
2	F	185	ASP
2	F	206	THR
2	H	57	ASP
2	H	65	LEU
2	H	86	SER
2	H	108	GLU
3	K	27	GLN
3	K	50	ASN
3	K	146	PRO
3	K	194	HIS

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Mol	Chain	Res	Type
3	L	50	ASN
3	L	197	TYR
3	L	202	THR
1	A	3	GLU
1	A	21	ASN
1	A	44	ALA
1	A	62	GLU
1	A	66	GLY
1	A	90	GLU
1	A	96	GLY
1	B	2	ALA
1	B	45	ALA
1	B	55	GLU
1	B	66	GLY
2	F	143	THR
2	F	184	SER
2	F	221	LYS
2	H	2	VAL
2	H	15	SER
2	H	168	SER
2	H	197	SER
2	H	214	SER
2	H	224	PRO
3	K	55	LYS
3	K	65	ASP
3	K	73	GLY
3	K	143	ASN
3	K	162	ASN
3	K	164	VAL
3	K	173	SER
3	K	217	ASN
3	L	26	SER
3	L	37	TYR
3	L	104	GLY
3	L	131	THR
3	L	143	ASN
3	L	171	GLN
3	L	191	TYR
3	L	207	THR
3	L	211	VAL
1	A	86	LYS
1	B	14	HIS

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Mol	Chain	Res	Type
1	B	52	VAL
1	B	82	GLU
1	B	91	TRP
2	F	27	PHE
2	F	58	ASP
2	F	170	SER
2	F	177	THR
2	F	196	THR
2	F	210	ALA
2	F	224	PRO
2	H	64	SER
2	H	104	GLY
2	H	138	PRO
2	H	171	LEU
2	H	191	SER
2	H	219	ASP
3	K	125	PRO
3	K	161	GLN
3	L	65	ASP
1	A	65	ASP
1	A	80	SER
1	B	15	GLN
1	B	64	PRO
1	B	80	SER
2	F	161	PRO
2	F	211	HIS
2	H	14	PRO
2	H	78	ASN
2	H	89	THR
2	H	173	SER
3	K	2	ILE
3	K	20	SER
3	K	112	LYS
3	K	191	TYR
3	K	196	SER
3	L	217	ASN
1	A	18	GLU
1	A	92	ARG
1	B	54	LEU
2	H	106	LYS
3	K	188	LYS
1	B	8	SER

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Mol	Chain	Res	Type
2	H	11	ILE
2	H	127	LYS
2	H	141	GLY
1	A	72	TYR
2	F	14	PRO
3	K	163	GLY
3	L	151	VAL
3	L	49	PRO
1	A	81	PRO
2	H	201	PRO

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	91/107 (85%)	82 (90%)	9 (10%)	10 17
1	B	91/107 (85%)	82 (90%)	9 (10%)	10 17
2	F	199/201 (99%)	161 (81%)	38 (19%)	2 3
2	H	199/201 (99%)	167 (84%)	32 (16%)	3 5
3	K	195/196 (100%)	156 (80%)	39 (20%)	1 2
3	L	195/196 (100%)	156 (80%)	39 (20%)	1 2
All	All	970/1008 (96%)	804 (83%)	166 (17%)	2 4

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	30	GLU
1	A	35	LEU
1	A	51	ASP
1	A	62	GLU
1	A	63	HIS
1	A	75	ASP
1	A	76	ASN

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Mol	Chain	Res	Type
1	A	79	ASP
1	B	1	ASP
1	B	38	ILE
1	B	46	THR
1	B	47	ASP
1	B	53	LEU
1	B	61	THR
1	B	68	ASP
1	B	72	TYR
1	B	76	ASN
2	F	3	THR
2	F	4	LEU
2	F	5	LYS
2	F	7	SER
2	F	27	PHE
2	F	28	SER
2	F	29	LEU
2	F	33	ARG
2	F	40	ARG
2	F	62	ASN
2	F	64	SER
2	F	68	ARG
2	F	72	SER
2	F	73	LYS
2	F	76	SER
2	F	79	GLN
2	F	83	LYS
2	F	84	ILE
2	F	89	THR
2	F	97	CYS
2	F	103	TYR
2	F	105	ARG
2	F	109	VAL
2	F	110	ASN
2	F	111	HIS
2	F	113	ASP
2	F	122	THR
2	F	125	SER
2	F	129	THR
2	F	146	SER
2	F	152	CYS
2	F	165	THR

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Mol	Chain	Res	Type
2	F	171	LEU
2	F	172	SER
2	F	202	SER
2	F	203	GLU
2	F	205	ILE
2	F	217	LYS
2	H	21	THR
2	H	31	THR
2	H	37	SER
2	H	53	ILE
2	H	61	TYR
2	H	62	ASN
2	H	65	LEU
2	H	76	SER
2	H	97	CYS
2	H	106	LYS
2	H	110	ASN
2	H	113	ASP
2	H	117	GLN
2	H	125	SER
2	H	128	THR
2	H	142	ASP
2	H	147	SER
2	H	164	LEU
2	H	165	THR
2	H	168	SER
2	H	183	GLN
2	H	185	ASP
2	H	189	LEU
2	H	194	THR
2	H	198	SER
2	H	200	TRP
2	H	202	SER
2	H	204	SER
2	H	205	ILE
2	H	206	THR
2	H	216	THR
2	H	219	ASP
3	K	1	ASP
3	K	7	THR
3	K	9	LEU
3	K	18	GLN

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Mol	Chain	Res	Type
3	K	24	ARG
3	K	27	GLN
3	K	28	THR
3	K	29	ILE
3	K	36	THR
3	K	39	GLU
3	K	53	ILE
3	K	66	ARG
3	K	72	SER
3	K	75	ASP
3	K	77	THR
3	K	78	LEU
3	K	79	LYS
3	K	98	ARG
3	K	108	LYS
3	K	111	LEU
3	K	130	LEU
3	K	139	CYS
3	K	143	ASN
3	K	148	ASP
3	K	152	LYS
3	K	153	TRP
3	K	155	ILE
3	K	160	ARG
3	K	185	THR
3	K	191	TYR
3	K	193	ARG
3	K	195	ASN
3	K	196	SER
3	K	198	THR
3	K	204	LYS
3	K	207	THR
3	K	213	SER
3	K	216	ARG
3	K	218	GLU
3	L	2	ILE
3	L	6	GLN
3	L	13	VAL
3	L	14	SER
3	L	15	LEU
3	L	21	ILE
3	L	22	SER

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Mol	Chain	Res	Type
3	L	24	ARG
3	L	25	SER
3	L	27	GLN
3	L	30	LEU
3	L	32	SER
3	L	67	PHE
3	L	68	SER
3	L	72	SER
3	L	77	THR
3	L	79	LYS
3	L	97	SER
3	L	98	ARG
3	L	101	LEU
3	L	120	VAL
3	L	128	GLU
3	L	131	THR
3	L	141	LEU
3	L	152	LYS
3	L	156	ASP
3	L	165	LEU
3	L	167	SER
3	L	169	THR
3	L	175	ASP
3	L	181	SER
3	L	186	LEU
3	L	187	THR
3	L	190	GLU
3	L	196	SER
3	L	197	TYR
3	L	198	THR
3	L	202	THR
3	L	211	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	14	HIS
1	A	56	HIS
1	A	76	ASN
1	B	6	HIS
1	B	14	HIS

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Mol	Chain	Res	Type
1	B	33	GLN
1	B	76	ASN
2	F	62	ASN
2	F	167	ASN
2	F	176	HIS
2	H	16	GLN
2	H	62	ASN
2	H	176	HIS
2	H	208	ASN
3	K	27	GLN
3	K	31	HIS
3	K	35	ASN
3	K	129	GLN
3	K	171	GLN
3	K	195	ASN
3	K	215	ASN
3	L	6	GLN
3	L	27	GLN
3	L	43	GLN
3	L	161	GLN
3	L	162	ASN
3	L	171	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	102/124 (82%)	0.06	3 (2%)	55	51	22, 28, 31, 32	0
1	B	102/124 (82%)	0.21	3 (2%)	55	51	23, 29, 30, 31	0
2	F	225/228 (98%)	0.10	4 (1%)	71	68	18, 22, 29, 34	0
2	H	225/228 (98%)	0.14	7 (3%)	52	48	17, 23, 29, 31	0
3	K	218/219 (99%)	0.11	10 (4%)	36	31	16, 20, 30, 32	0
3	L	218/219 (99%)	0.10	6 (2%)	56	52	15, 18, 30, 33	0
All	All	1090/1142 (95%)	0.12	33 (3%)	54	49	15, 24, 30, 34	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	153	TRP	4.9
3	L	199	CYS	4.9
2	H	223	VAL	4.3
2	H	2	VAL	4.2
3	L	202	THR	4.1
1	B	61	THR	4.1
3	L	201	ALA	3.9
3	K	153	TRP	3.6
3	K	103	PHE	3.6
3	K	137	VAL	3.4
1	B	75	ASP	3.3
2	H	169	GLY	3.1
2	F	11	ILE	2.9
2	H	115	TRP	2.9
2	H	220	LYS	2.8
1	A	34	LEU	2.7
3	K	202	THR	2.6
1	B	34	LEU	2.5
3	K	29	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
3	L	83	VAL	2.5
1	A	88	ILE	2.4
3	K	98	ARG	2.3
2	F	166	TRP	2.2
3	K	125	PRO	2.2
2	F	172	SER	2.2
3	L	155	ILE	2.1
3	K	139	CYS	2.1
2	H	168	SER	2.1
3	K	149	ILE	2.0
2	F	164	LEU	2.0
2	H	195	VAL	2.0
1	A	10	TYR	2.0
3	K	140	PHE	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.