



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 05:48 PM UTC

PDB ID : 8EED / pdb_00008eed
Title : Crystal structure of a NHP anti-ZIKV neutralizing antibody rhMZ107-B in complex with ZIKV E glycoprotein
Authors : Sankhala, R.S.; Joyce, M.G.
Deposited on : 2022-09-07
Resolution : 3.49 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

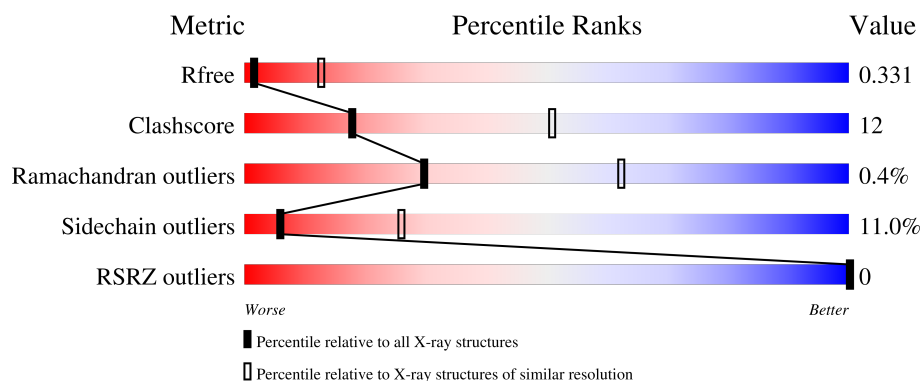
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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.



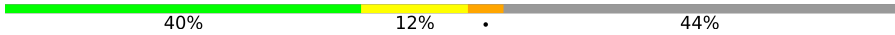
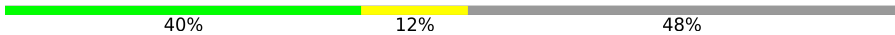
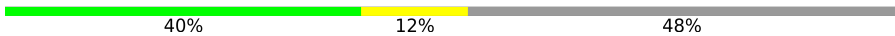
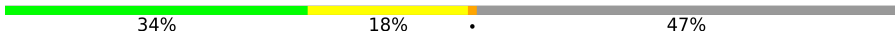
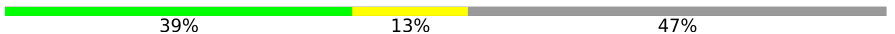
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	405	
1	B	405	
1	C	405	
1	D	405	
2	E	226	

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Mol	Chain	Length	Quality of chain
2	H	226	
2	I	226	
2	M	226	
3	F	220	
3	J	220	
3	L	220	
3	N	220	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 19188 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 Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3030	1896	524	584	26			
1	C	391	Total	C	N	O	S	0	0	0
			2969	1857	517	570	25			
1	D	380	Total	C	N	O	S	0	0	0
			2841	1774	492	551	24			
1	B	403	Total	C	N	O	S	0	0	0
			3069	1916	534	593	26			

- Molecule 2 is a protein called rhMZ107-B antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	126	Total	C	N	O	S	0	0	0
			962	612	157	191	2			
2	M	122	Total	C	N	O	S	0	0	0
			939	600	153	184	2			
2	E	123	Total	C	N	O	S	0	0	0
			945	603	154	186	2			
2	I	125	Total	C	N	O	S	0	0	0
			956	609	156	189	2			

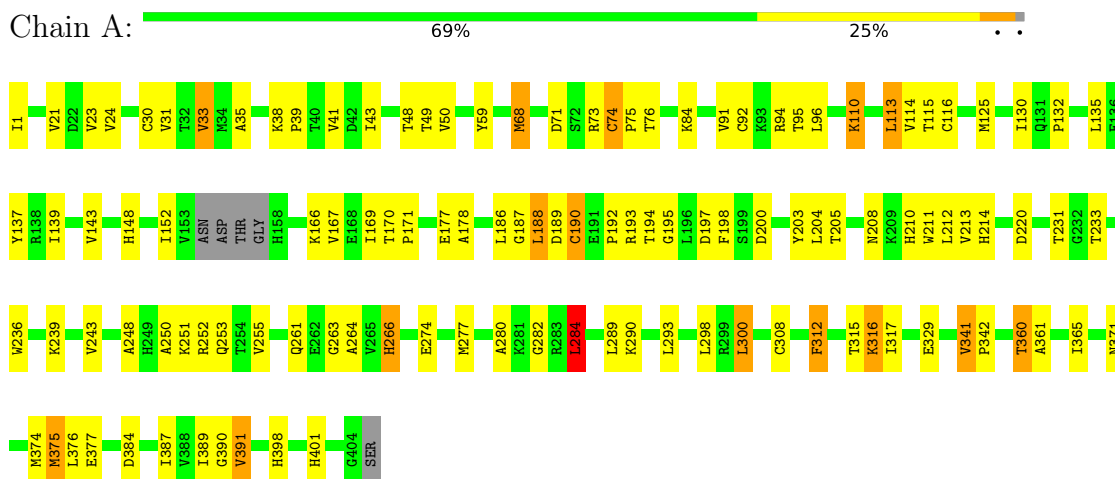
- Molecule 3 is a protein called rhMZ107-B antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	117	Total	C	N	O	S	0	0	0
			878	551	143	181	3			
3	N	116	Total	C	N	O	S	0	0	0
			869	546	141	179	3			
3	F	115	Total	C	N	O	S	0	0	0
			865	544	140	178	3			
3	J	115	Total	C	N	O	S	0	0	0
			865	544	140	178	3			

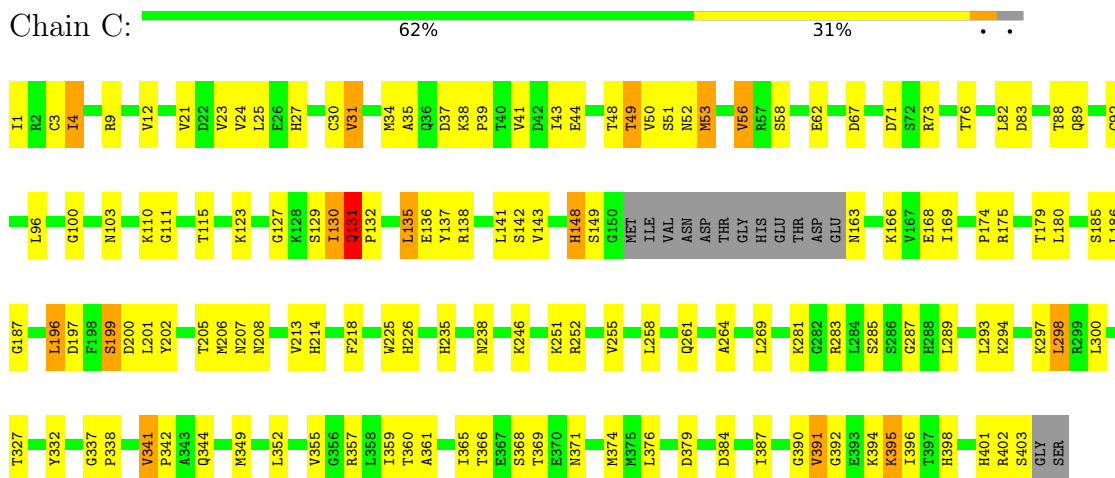
3 Residue-property plots [i](#)

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

- Molecule 1: Envelope protein E

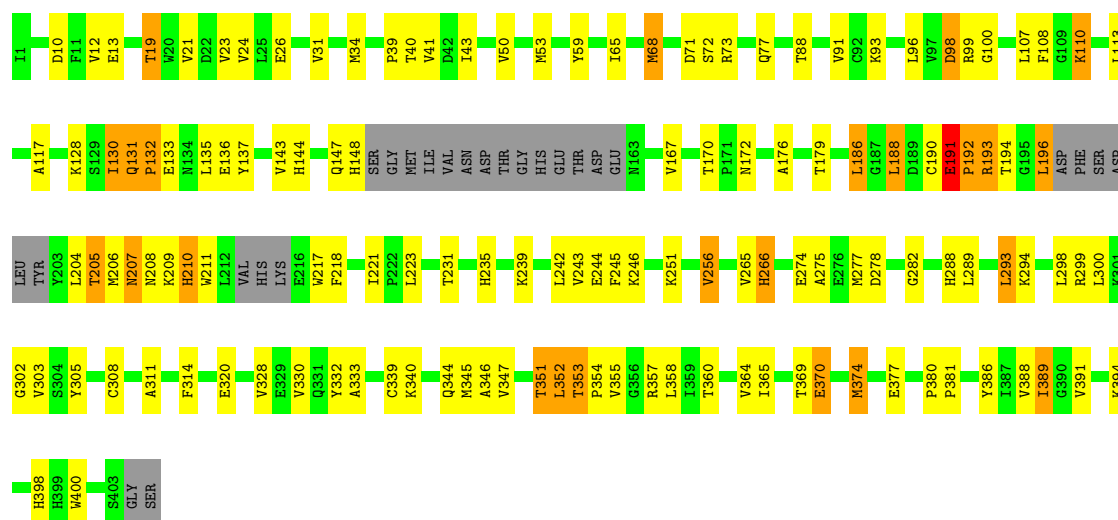


- Molecule 1: Envelope protein E

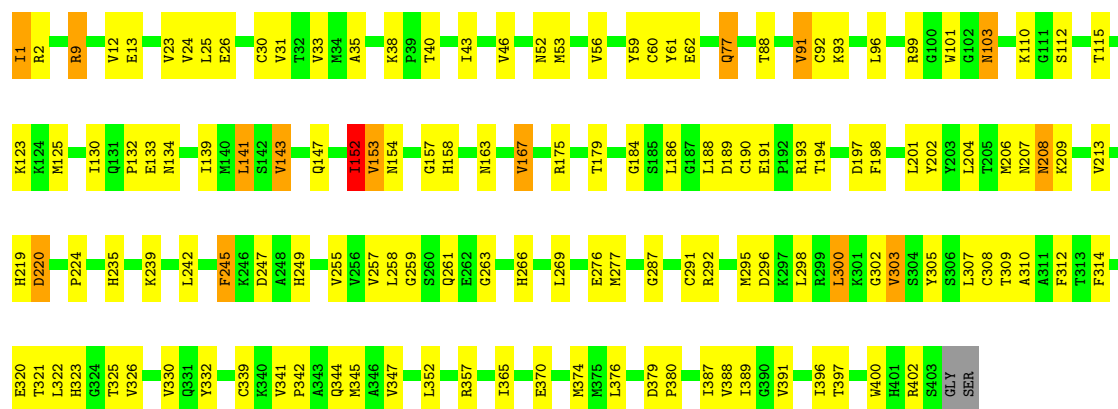


- Molecule 1: Envelope protein E

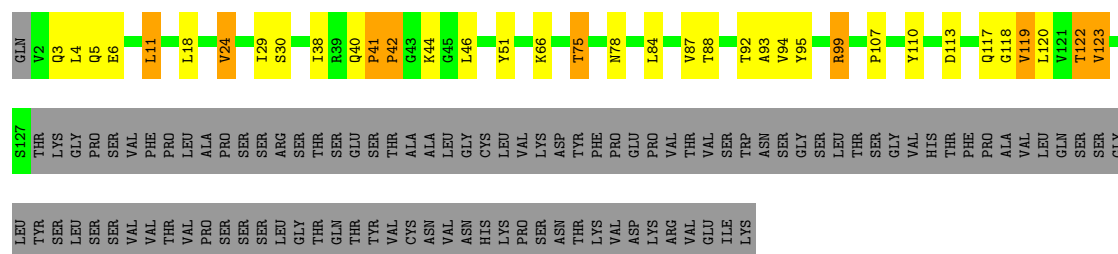




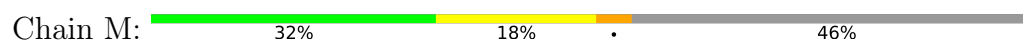
• Molecule 1: Envelope protein E

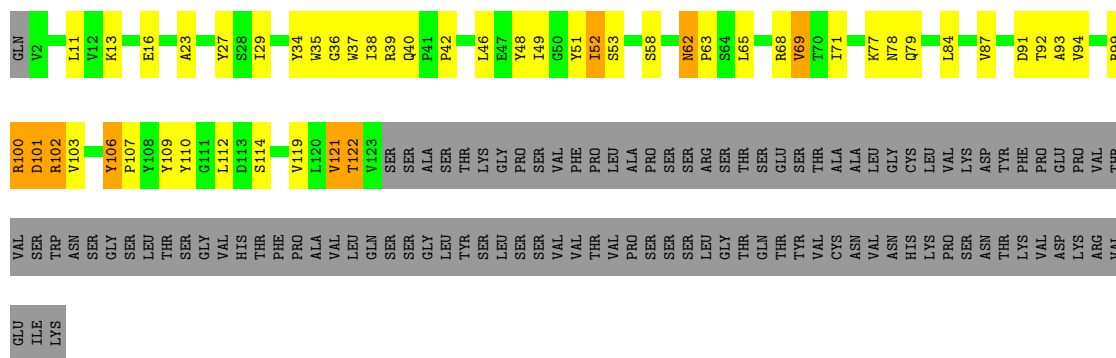


• Molecule 2: rhMZ107-B antibody heavy chain

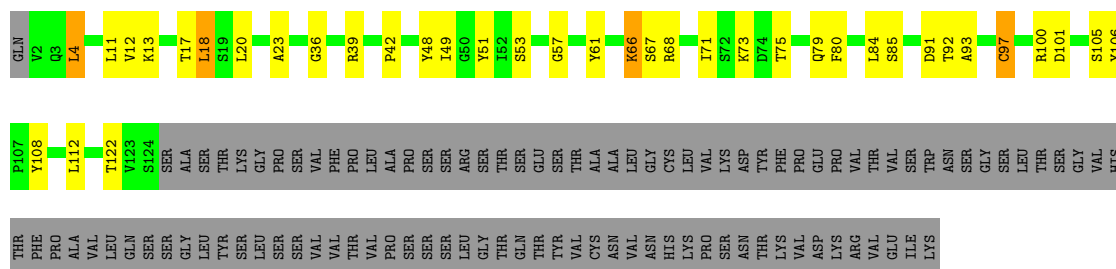
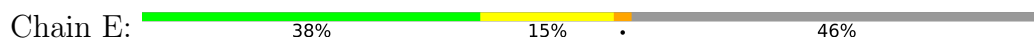


• Molecule 2: rhMZ107-B antibody heavy chain

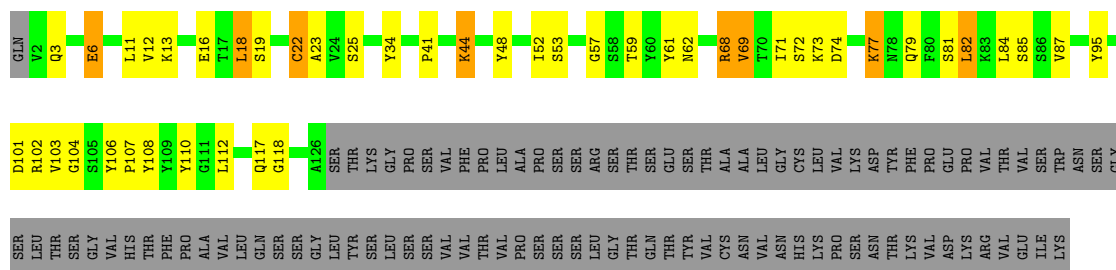
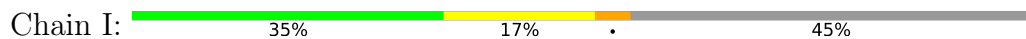




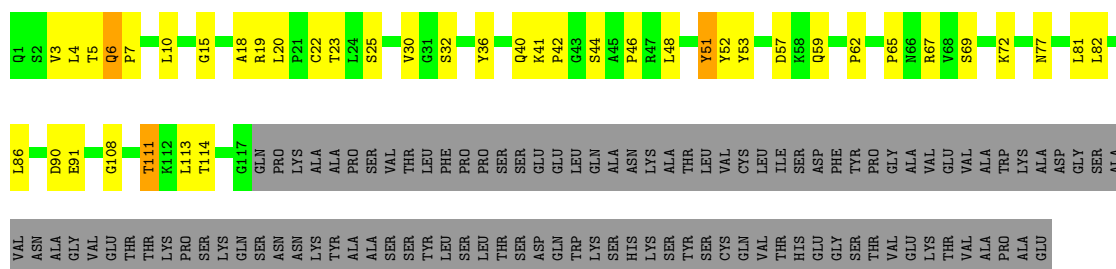
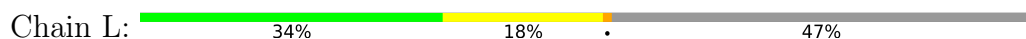
• Molecule 2: rhMZ107-B antibody heavy chain



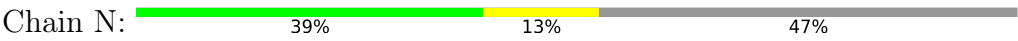
• Molecule 2: rhMZ107-B antibody heavy chain



• Molecule 3: rhMZ107-B antibody light chain

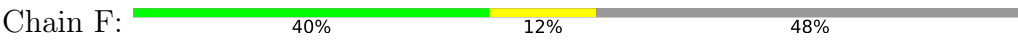


• Molecule 3: rhMZ107-B antibody light chain



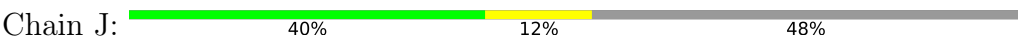
ASN	LYS	LYS	TYR	ALA	ALA	SER	SER	THR	TYR	LEU	LEU	TRP	GLN	LYS	HIS	LYS	SER	TYR	THR	GLU	GLY	THR	THR	VAL	GLU	LYS	THR	VAL	ALA	ALA	PRO	GLU	ALA	ALA	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
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• Molecule 3: rhMZ107-B antibody light chain



GLN	S2	V3	L4	Q6	A18	L24	S25	S26	D27	Q39	Y51	Y52	Y53	S54	D55	K58	K72	E73	T74	S75	S76	L86	Y94	Y95	C96	Q97	D100	N104	D105	V106	F107	G108	K112	L116	GLY	GLN	PRO	LYS	ALA	ALA	PRO	SER	VAL	THR	LEU	PHE
PRO	PRO	SER	SER	GLU	GLU	LEU	GLN	ALA	ASN	LYS	LYS	ALA	THR	LEU	VAL	CYS	GLN	VAL	THR	ILE	SER	ASP	PHE	TYR	PRO	GLY	ALA	VAL	GLU	THR	LYS	ALA	ASP	GLY	GLN	SER	ASN	LYS	ALA	ALA	PRO	SER	VAL	THR	LEU	PHE
SER	LEU	THR	SER	ASP	GLU	TRP	LYS	SER	HIS	LYS	THR	TYR	SER	CYS	GLN	VAL	THR	HIS	GLY	SER	THR	VAL	GLU	LYS	THR	VAL	ALA	ALA	THR	LYS	PRO	SER	LYS	GLN	SER	ASN	LYS	TYR	ALA	ALA	PRO	SER	VAL	THR	LEU	PHE

• Molecule 3: rhMZ107-B antibody light chain



TYR	LEU	SER	LEU	THR	SER	ASP	GLN	TRP	LYS	SER	THR	SER	CYS	GLN	VAL	THR	HIS	GLU	GLY	SER	THR	VAL	GLY	ALA	VAL	VAL	ALA	PRO	ALA	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.03Å 105.63Å 132.38Å 82.52° 70.48° 81.04°	Depositor
Resolution (Å)	48.84 – 3.49 48.84 – 3.49	Depositor EDS
% Data completeness (in resolution range)	80.6 (48.84-3.49) 66.3 (48.84-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.289 , 0.331 0.290 , 0.331	Depositor DCC
R_{free} test set	1996 reflections (3.38%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 17.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	19188	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.13	0/3094	0.42	1/4194 (0.0%)
1	B	0.13	0/3134	0.38	0/4248
1	C	0.19	1/3032 (0.0%)	0.47	3/4110 (0.1%)
1	D	0.14	0/2898	0.43	1/3934 (0.0%)
2	E	0.10	0/970	0.32	0/1320
2	H	0.14	0/987	0.37	0/1343
2	I	0.11	0/981	0.37	0/1335
2	M	0.13	0/964	0.39	0/1312
3	F	0.08	0/886	0.28	0/1207
3	J	0.07	0/886	0.26	0/1207
3	L	0.12	0/899	0.30	0/1224
3	N	0.07	0/890	0.24	0/1212
All	All	0.14	1/19621 (0.0%)	0.39	5/26646 (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
1	C	0	1
1	D	0	2
2	M	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	131	GLN	C-N	7.02	1.50	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	131	GLN	CA-C-N	10.76	133.29	119.84
1	C	131	GLN	C-N-CA	10.76	133.29	119.84
1	C	131	GLN	N-CA-C	-6.01	102.50	110.07
1	A	284	LEU	N-CA-CB	5.51	119.00	110.46
1	D	303	VAL	N-CA-C	-5.06	107.87	112.12

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	152	ILE	Peptide
1	C	130	ILE	Mainchain
1	D	191	GLU	Peptide
1	D	351	THR	Peptide
2	M	106	TYR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3030	0	2947	68	0
1	B	3069	0	2991	76	0
1	C	2969	0	2891	83	0
1	D	2841	0	2730	73	0
2	E	945	0	917	20	0
2	H	962	0	932	27	0
2	I	956	0	927	29	0
2	M	939	0	912	32	0
3	F	865	0	829	17	0
3	J	865	0	829	16	0
3	L	878	0	843	29	0
3	N	869	0	832	19	0
All	All	19188	0	18580	463	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 12.

All (463) 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:53:MET:SD	1:B:130:ILE:HG22	1.36	1.65
1:B:53:MET:SD	1:B:130:ILE:CG2	2.25	1.24
1:C:53:MET:HE2	1:C:130:ILE:HB	1.46	0.94
1:C:53:MET:HE2	1:C:130:ILE:CB	2.07	0.84
1:C:131:GLN:OE1	1:B:77:GLN:NE2	2.12	0.83
1:C:342:PRO:HG2	1:C:391:VAL:HG22	1.63	0.80
1:D:345:MET:HB2	1:D:355:VAL:HG13	1.64	0.79
1:B:99:ARG:HH21	2:E:105:SER:HB2	1.47	0.78
1:C:283:ARG:O	1:C:283:ARG:HG3	1.86	0.73
1:C:252:ARG:NH2	2:I:104:GLY:O	2.21	0.73
1:D:72:SER:OG	1:D:99:ARG:NH2	2.21	0.73
2:H:41:PRO:HB2	2:H:42:PRO:HD3	1.69	0.72
2:M:53:SER:HB3	2:M:58:SER:H	1.54	0.72
3:L:91:GLU:HG3	3:L:114:THR:HA	1.72	0.72
1:D:93:LYS:HD3	1:D:245:PHE:HB2	1.71	0.72
1:C:53:MET:CE	1:C:130:ILE:HD12	2.20	0.71
1:C:67:ASP:OD1	2:I:102:ARG:NH2	2.22	0.71
1:C:58:SER:HB2	1:C:226:HIS:HE1	1.56	0.71
1:A:171:PRO:HA	1:A:192:PRO:HG2	1.73	0.71
3:L:6:GLN:HG2	3:L:22:CYS:HA	1.72	0.71
1:D:191:GLU:O	1:D:193:ARG:N	2.24	0.71
1:A:193:ARG:HH12	1:A:198:PHE:HA	1.55	0.70
1:A:132:PRO:HG3	1:A:193:ARG:HH21	1.56	0.70
1:B:62:GLU:HB2	1:B:123:LYS:HB2	1.74	0.70
1:C:50:VAL:HG11	1:C:130:ILE:HD11	1.73	0.69
1:D:352:LEU:HB2	1:D:354:PRO:HD2	1.73	0.69
1:C:53:MET:HE2	1:C:130:ILE:CG1	2.22	0.69
1:A:41:VAL:HG12	1:A:143:VAL:HG12	1.73	0.69
2:E:68:ARG:NH1	2:E:91:ASP:OD2	2.26	0.69
1:C:31:VAL:HG23	1:C:43:ILE:HG13	1.74	0.68
1:C:360:THR:HG21	1:C:376:LEU:HB2	1.76	0.68
1:B:207:ASN:O	1:B:208:ASN:ND2	2.22	0.68
1:D:302:GLY:HA3	1:D:364:VAL:HG21	1.76	0.68
3:L:40:GLN:HB2	3:L:46:PRO:HB3	1.74	0.68
1:B:202:TYR:HH	1:B:219:HIS:HE2	1.41	0.68
2:H:84:LEU:HG	2:H:87:VAL:HG12	1.75	0.67
3:F:6:GLN:NE2	3:F:96:CYS:SG	2.66	0.67
3:N:4:LEU:HD22	3:N:24:LEU:HG	1.76	0.67
1:C:35:ALA:HB3	1:C:38:LYS:HB2	1.75	0.67
3:N:40:GLN:HB2	3:N:46:PRO:HB3	1.76	0.67
1:A:135:LEU:HD12	1:A:171:PRO:HG3	1.76	0.67
1:B:357:ARG:HB3	1:B:379:ASP:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:6:GLU:O	2:I:117:GLN:NE2	2.28	0.66
1:B:130:ILE:O	1:B:130:ILE:HG13	1.94	0.66
1:B:152:ILE:O	1:B:154:ASN:N	2.28	0.66
2:H:66:LYS:H	2:H:66:LYS:HD3	1.61	0.66
1:A:39:PRO:HA	1:A:361:ALA:HB3	1.78	0.65
1:A:130:ILE:HD11	1:A:203:TYR:HB2	1.79	0.65
1:A:200:ASP:OD2	1:A:214:HIS:ND1	2.26	0.65
1:B:103:ASN:OD1	1:B:103:ASN:N	2.29	0.65
1:B:184:GLY:HA3	1:B:298:LEU:HA	1.79	0.64
1:A:35:ALA:HB3	1:A:38:LYS:HB2	1.79	0.64
1:B:30:CYS:SG	1:B:31:VAL:N	2.69	0.64
2:M:42:PRO:HD3	2:M:93:ALA:HA	1.78	0.64
2:H:41:PRO:HB2	2:H:42:PRO:CD	2.26	0.64
1:D:188:LEU:HA	1:D:293:LEU:HA	1.79	0.64
1:B:1:ILE:HG22	1:B:2:ARG:H	1.64	0.63
1:C:384:ASP:OD1	1:C:401:HIS:ND1	2.30	0.63
2:M:68:ARG:NH2	2:M:91:ASP:OD2	2.31	0.63
1:C:132:PRO:HD3	1:C:199:SER:HA	1.79	0.63
1:A:50:VAL:HG11	1:A:130:ILE:HD12	1.81	0.62
1:C:51:SER:HB2	1:C:281:LYS:HB2	1.80	0.62
1:C:130:ILE:CG2	1:C:201:LEU:O	2.48	0.62
2:M:106:TYR:HB3	2:M:107:PRO:HD3	1.80	0.62
1:D:176:ALA:HB3	1:D:188:LEU:HG	1.81	0.62
1:B:13:GLU:OE1	1:B:357:ARG:NH2	2.33	0.62
1:C:390:GLY:HA3	1:C:395:LYS:HA	1.82	0.62
1:D:77:GLN:NE2	3:N:56:SER:OG	2.33	0.62
3:L:5:THR:O	3:L:6:GLN:NE2	2.32	0.62
1:A:263:GLY:HA2	1:A:266:HIS:HB2	1.81	0.61
1:A:130:ILE:HG21	1:A:197:ASP:OD1	1.99	0.61
1:C:357:ARG:HB2	1:C:379:ASP:HB3	1.82	0.61
1:A:71:ASP:OD2	1:A:73:ARG:NH1	2.33	0.61
1:D:144:HIS:HB3	1:D:360:THR:HG23	1.83	0.61
1:A:33:VAL:HG13	1:A:41:VAL:HG23	1.82	0.61
1:D:53:MET:HB3	1:D:128:LYS:HB3	1.81	0.60
1:B:91:VAL:HG13	1:B:239:LYS:HE2	1.83	0.60
2:H:5:GLN:NE2	2:H:117:GLN:OE1	2.35	0.60
2:M:100:ARG:HB3	2:M:112:LEU:HD23	1.82	0.60
3:L:18:ALA:HB2	3:L:86:LEU:HD11	1.83	0.60
2:I:72:SER:HB2	2:I:81:SER:HB2	1.83	0.60
1:A:360:THR:HG21	1:A:376:LEU:HB2	1.84	0.60
2:I:84:LEU:HG	2:I:87:VAL:HG12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:CYS:HB3	1:B:224:PRO:HG2	1.82	0.60
1:C:30:CYS:SG	1:C:31:VAL:N	2.75	0.60
2:M:99:ARG:HB3	2:M:114:SER:HB3	1.84	0.59
1:A:74:CYS:SG	1:A:75:PRO:HD2	2.41	0.59
1:C:50:VAL:HG12	1:C:135:LEU:HB3	1.84	0.59
1:C:251:LYS:O	1:C:252:ARG:NE	2.35	0.59
1:D:71:ASP:OD2	1:D:73:ARG:NH2	2.36	0.59
2:E:73:LYS:HA	2:E:80:PHE:HA	1.83	0.59
1:C:50:VAL:HG11	1:C:130:ILE:CD1	2.33	0.58
1:C:56:VAL:HG23	1:C:129:SER:HB3	1.84	0.58
3:F:100:ASP:OD1	3:F:104:ASN:N	2.28	0.58
1:C:132:PRO:HA	1:C:135:LEU:HD21	1.86	0.58
1:D:41:VAL:HG22	1:D:143:VAL:HG12	1.84	0.58
1:C:261:GLN:HG3	1:C:264:ALA:HB3	1.85	0.58
1:B:139:ILE:HB	1:B:167:VAL:HG23	1.86	0.58
2:E:42:PRO:HD3	2:E:93:ALA:HA	1.84	0.58
2:I:68:ARG:O	2:I:85:SER:N	2.36	0.58
1:B:344:GLN:NE2	1:B:352:LEU:O	2.37	0.58
2:E:100:ARG:HB3	2:E:112:LEU:HD23	1.86	0.58
1:C:21:VAL:HG22	1:C:293:LEU:HB2	1.85	0.58
1:B:190:CYS:HA	1:B:291:CYS:HA	1.86	0.58
3:L:20:LEU:HD12	3:L:81:LEU:HD23	1.85	0.57
3:F:55:ASP:HA	3:F:58:LYS:HE3	1.86	0.57
1:D:244:GLU:HB2	1:D:256:VAL:HG13	1.85	0.57
2:E:18:LEU:HB2	2:E:84:LEU:HB3	1.86	0.57
3:L:20:LEU:HB2	3:L:81:LEU:HB3	1.85	0.57
2:M:34:TYR:CG	2:M:102:ARG:HB3	2.40	0.56
2:M:36:GLY:HA3	2:M:51:TYR:HD1	1.70	0.56
2:E:53:SER:OG	2:E:57:GLY:N	2.34	0.56
3:L:65:PRO:HG2	3:L:67:ARG:HD3	1.86	0.56
1:B:308:CYS:HB3	1:B:332:TYR:CZ	2.41	0.56
2:E:36:GLY:HA2	2:E:51:TYR:HA	1.88	0.56
1:D:277:MET:HB3	1:D:282:GLY:HA2	1.88	0.55
2:M:37:TRP:HB3	2:M:49:ILE:HD12	1.88	0.55
1:A:342:PRO:HG2	1:A:391:VAL:HG13	1.88	0.55
1:D:314:PHE:HE2	1:D:398:HIS:HB2	1.71	0.55
2:H:41:PRO:HA	2:H:93:ALA:HA	1.87	0.55
3:J:50:LEU:HD22	3:J:68:VAL:HG12	1.89	0.55
1:A:387:ILE:HG12	1:A:398:HIS:HB3	1.89	0.54
1:C:130:ILE:HG22	1:C:202:TYR:HA	1.89	0.54
1:D:346:ALA:HB3	1:D:386:TYR:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:101:ASP:O	2:I:110:TYR:HA	2.07	0.54
1:A:137:TYR:HB2	1:A:169:ILE:HB	1.89	0.54
1:C:1:ILE:H2	1:C:142:SER:HB2	1.72	0.54
1:C:130:ILE:HG23	1:C:130:ILE:O	2.08	0.54
1:C:138:ARG:NH2	1:C:168:GLU:OE1	2.40	0.54
1:D:346:ALA:HB2	1:D:388:VAL:HG23	1.89	0.54
2:I:6:GLU:HA	2:I:22:CYS:HB3	1.90	0.54
1:C:169:ILE:HG23	1:C:174:PRO:HA	1.88	0.54
1:C:58:SER:HB2	1:C:226:HIS:CE1	2.40	0.54
2:H:99:ARG:NH1	2:H:113:ASP:OD2	2.41	0.54
1:B:201:LEU:HA	1:B:213:VAL:O	2.08	0.53
2:I:41:PRO:HG2	2:I:44:LYS:HD3	1.88	0.53
1:A:68:MET:SD	1:A:68:MET:N	2.72	0.53
1:A:212:LEU:HD11	1:A:284:LEU:HD21	1.90	0.53
1:B:380:PRO:HG2	1:B:402:ARG:HH11	1.73	0.53
2:M:69:VAL:HG13	2:M:84:LEU:HD13	1.90	0.53
1:A:132:PRO:O	1:A:171:PRO:HG2	2.07	0.53
1:D:206:MET:HE1	1:D:265:VAL:HG11	1.90	0.53
1:A:190:CYS:SG	1:A:289:LEU:HG	2.48	0.53
2:I:106:TYR:O	2:I:108:TYR:N	2.42	0.53
3:L:6:GLN:HE21	3:L:23:THR:H	1.55	0.53
3:L:67:ARG:NH2	3:L:90:ASP:OD2	2.42	0.53
1:C:52:ASN:HD21	3:F:73:GLU:HA	1.73	0.53
1:A:341:VAL:HG11	1:A:374:MET:HE2	1.91	0.53
1:D:170:THR:HG22	1:D:172:ASN:H	1.73	0.53
1:D:186:LEU:HG	1:D:298:LEU:HD23	1.91	0.53
3:N:67:ARG:NH1	3:N:85:GLY:O	2.42	0.53
2:H:18:LEU:HD23	2:H:84:LEU:HD23	1.91	0.53
1:D:217:TRP:O	1:D:218:PHE:HB3	2.08	0.52
1:D:345:MET:HG3	1:D:381:PRO:HD3	1.91	0.52
2:M:34:TYR:CD1	2:M:53:SER:HA	2.45	0.52
3:L:4:LEU:HB2	3:L:108:GLY:HA2	1.91	0.52
1:B:9:ARG:HB3	1:B:323:HIS:CE1	2.44	0.52
2:H:110:TYR:HB2	3:L:36:TYR:OH	2.09	0.52
1:B:308:CYS:HB3	1:B:332:TYR:CE1	2.45	0.52
1:C:206:MET:O	1:C:208:ASN:N	2.42	0.52
1:B:295:MET:HB3	1:B:298:LEU:HD11	1.92	0.52
1:C:341:VAL:HG11	1:C:374:MET:HE2	1.91	0.52
1:D:347:VAL:HB	1:D:355:VAL:HG11	1.93	0.51
3:L:6:GLN:OE1	3:L:7:PRO:HD3	2.10	0.51
1:A:384:ASP:OD1	1:A:401:HIS:ND1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:PRO:HG3	1:D:196:LEU:HD11	1.92	0.51
2:I:12:VAL:HG11	2:I:18:LEU:HB2	1.91	0.51
1:C:327:THR:HG21	1:D:108:PHE:HE2	1.76	0.51
1:D:190:CYS:O	1:D:192:PRO:HD3	2.09	0.51
1:B:322:LEU:HD12	1:B:322:LEU:H	1.75	0.51
1:A:277:MET:HE3	1:A:280:ALA:H	1.74	0.51
1:D:10:ASP:HB2	1:D:31:VAL:HG22	1.92	0.51
2:H:40:GLN:HB2	2:H:46:LEU:HD23	1.92	0.51
2:I:52:ILE:HD13	2:I:73:LYS:HB3	1.92	0.51
1:C:50:VAL:HG23	1:C:51:SER:H	1.76	0.51
2:H:18:LEU:HB3	2:H:84:LEU:HB3	1.92	0.51
2:M:29:ILE:N	2:M:78:ASN:OD1	2.37	0.51
1:C:53:MET:HE1	1:C:130:ILE:HD12	1.91	0.51
1:D:191:GLU:C	1:D:193:ARG:H	2.16	0.51
1:A:23:VAL:HG11	1:A:43:ILE:HD11	1.91	0.51
1:B:263:GLY:HA2	1:B:266:HIS:HB2	1.93	0.51
2:M:92:THR:HG23	2:M:122:THR:HA	1.93	0.51
1:B:257:VAL:HG23	1:B:259:GLY:H	1.75	0.51
2:M:36:GLY:HA3	2:M:51:TYR:CD1	2.46	0.51
3:L:30:VAL:HB	3:L:77:ASN:HB2	1.93	0.51
1:A:277:MET:HA	1:A:282:GLY:HA2	1.93	0.50
1:B:35:ALA:HB3	1:B:38:LYS:HB2	1.93	0.50
3:L:32:SER:HA	3:L:53:TYR:HE1	1.76	0.50
1:C:96:LEU:HB3	1:C:110:LYS:HB3	1.92	0.50
1:C:129:SER:O	1:C:129:SER:OG	2.26	0.50
1:D:23:VAL:HG11	1:D:43:ILE:HD11	1.93	0.50
1:D:65:ILE:HG23	1:D:117:ALA:HB1	1.92	0.50
2:M:62:ASN:ND2	2:M:63:PRO:O	2.44	0.50
1:D:211:TRP:HE3	1:D:274:GLU:HB3	1.75	0.50
2:M:34:TYR:CD1	2:M:102:ARG:HB3	2.47	0.50
1:C:50:VAL:HB	1:C:53:MET:HE3	1.93	0.50
3:L:19:ARG:HG2	3:L:82:LEU:HD22	1.94	0.50
3:J:34:ASN:ND2	3:J:99:TYR:OH	2.40	0.50
1:D:91:VAL:HG13	1:D:239:LYS:HE2	1.94	0.50
2:H:6:GLU:OE1	2:H:118:GLY:N	2.42	0.50
1:C:41:VAL:HG22	1:C:143:VAL:HG12	1.93	0.49
2:I:69:VAL:HG13	2:I:84:LEU:HD13	1.94	0.49
1:C:49:THR:O	1:C:136:GLU:N	2.45	0.49
1:C:187:GLY:HA3	1:C:294:LYS:HB3	1.94	0.49
1:B:188:LEU:HA	1:B:292:ARG:O	2.11	0.49
2:I:53:SER:OG	2:I:57:GLY:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:119:VAL:HG12	2:M:121:VAL:HG22	1.95	0.49
1:C:374:MET:HE1	1:C:376:LEU:HD23	1.93	0.49
1:B:314:PHE:HA	1:B:330:VAL:HG12	1.94	0.49
1:A:312:PHE:HZ	1:A:342:PRO:HD2	1.78	0.49
1:B:43:ILE:HG22	1:B:141:LEU:HD23	1.95	0.49
1:B:152:ILE:HG23	1:B:157:GLY:HA3	1.94	0.49
1:A:177:GLU:HA	1:A:187:GLY:HA2	1.93	0.49
1:C:175:ARG:H	1:C:175:ARG:HD3	1.78	0.49
1:C:185:SER:HB2	1:C:297:LYS:HB3	1.94	0.49
1:D:39:PRO:HD2	1:D:298:LEU:HD13	1.95	0.48
1:B:132:PRO:HB3	1:B:193:ARG:HD3	1.94	0.48
1:B:310:ALA:N	1:B:332:TYR:OH	2.46	0.48
1:B:330:VAL:HG11	1:B:389:ILE:HD11	1.94	0.48
2:I:23:ALA:HB2	2:I:79:GLN:HG2	1.95	0.48
2:I:104:GLY:HA2	2:I:110:TYR:OH	2.13	0.48
1:A:211:TRP:CD1	1:A:274:GLU:HG2	2.48	0.48
1:C:3:CYS:HB3	1:C:9:ARG:HD2	1.94	0.48
2:M:39:ARG:HB3	2:M:49:ILE:HD11	1.95	0.48
3:N:73:GLU:HB2	3:N:80:PHE:HE2	1.78	0.48
1:C:53:MET:CE	1:C:130:ILE:CG1	2.91	0.48
2:M:11:LEU:HD13	2:M:122:THR:HB	1.95	0.48
1:C:1:ILE:O	1:C:142:SER:OG	2.30	0.48
1:B:88:THR:HB	1:B:235:HIS:ND1	2.29	0.48
3:F:73:GLU:OE1	3:F:76:SER:OG	2.29	0.48
1:A:210:HIS:NE2	1:A:277:MET:HB3	2.28	0.48
1:D:100:GLY:HA3	1:D:108:PHE:CD1	2.49	0.48
2:I:74:ASP:CG	2:I:77:LYS:HD2	2.38	0.48
1:C:88:THR:OG1	1:C:235:HIS:ND1	2.37	0.48
2:M:94:VAL:HA	2:M:119:VAL:O	2.14	0.48
2:E:23:ALA:HA	2:E:79:GLN:HG2	1.95	0.48
1:A:23:VAL:HG13	1:A:31:VAL:HG11	1.95	0.48
1:B:339:CYS:H	1:B:365:ILE:HG22	1.79	0.48
1:C:71:ASP:OD2	1:C:73:ARG:NH2	2.47	0.48
1:D:39:PRO:HG3	1:D:300:LEU:HA	1.96	0.48
1:A:186:LEU:HD11	1:A:293:LEU:HD12	1.94	0.47
3:F:6:GLN:HE21	3:F:108:GLY:HA3	1.79	0.47
3:J:4:LEU:HD22	3:J:24:LEU:HG	1.96	0.47
1:D:19:THR:O	1:D:294:LYS:HA	2.14	0.47
3:N:18:ALA:HB2	3:N:86:LEU:HD11	1.96	0.47
1:A:91:VAL:HG21	1:A:243:VAL:HG11	1.94	0.47
1:D:194:THR:OG1	1:D:288:HIS:O	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:100:ARG:NH1	3:F:105:ASP:OD2	2.47	0.47
1:C:332:TYR:O	1:C:371:ASN:HA	2.15	0.47
1:D:205:THR:HB	1:D:210:HIS:ND1	2.29	0.47
1:D:339:CYS:H	1:D:365:ILE:HG22	1.80	0.47
1:B:374:MET:HB2	1:B:374:MET:HE2	1.74	0.47
3:N:51:TYR:OH	3:N:57:ASP:OD2	2.29	0.47
3:N:93:ASP:OD2	3:N:112:LYS:NZ	2.44	0.47
3:J:39:GLN:NE2	3:J:47:ARG:HH21	2.12	0.47
1:C:100:GLY:N	1:C:103:ASN:OD1	2.47	0.47
3:N:4:LEU:HD11	3:N:98:VAL:HG22	1.96	0.47
1:A:48:THR:O	1:A:284:LEU:HB2	2.15	0.47
2:M:48:TYR:CD1	3:N:105:ASP:HB2	2.49	0.47
1:C:338:PRO:HA	1:C:365:ILE:O	2.15	0.47
1:D:88:THR:O	1:D:239:LYS:NZ	2.48	0.47
1:D:345:MET:HG3	1:D:380:PRO:HA	1.97	0.47
1:B:220:ASP:OD1	1:B:220:ASP:N	2.47	0.47
3:L:6:GLN:NE2	3:L:23:THR:H	2.12	0.47
1:D:23:VAL:HG21	1:D:43:ILE:HD11	1.97	0.47
2:E:66:LYS:HD2	2:E:67:SER:H	1.79	0.47
1:A:50:VAL:HG11	1:A:130:ILE:CD1	2.42	0.47
1:A:91:VAL:O	1:A:116:CYS:HA	2.15	0.47
1:C:196:LEU:HD13	1:C:287:GLY:HA2	1.97	0.47
2:E:17:THR:HA	2:E:85:SER:HA	1.97	0.47
3:N:25:SER:OG	3:N:27:ASP:OD1	2.27	0.47
1:A:139:ILE:HB	1:A:167:VAL:HB	1.98	0.46
3:F:97:GLN:HA	3:F:106:VAL:O	2.15	0.46
2:I:13:LYS:HD2	2:I:13:LYS:N	2.30	0.46
1:D:308:CYS:HB3	1:D:332:TYR:CE1	2.50	0.46
2:M:27:TYR:O	2:M:78:ASN:ND2	2.43	0.46
1:A:167:VAL:HG11	1:A:188:LEU:HD11	1.98	0.46
2:M:23:ALA:HA	2:M:79:GLN:HG2	1.97	0.46
1:C:359:ILE:HG13	1:C:379:ASP:HB2	1.96	0.46
3:N:65:PRO:HB2	3:N:67:ARG:HG2	1.98	0.46
2:M:52:ILE:HD12	2:M:71:ILE:HG22	1.97	0.46
3:F:4:LEU:HD22	3:F:24:LEU:HG	1.97	0.46
1:B:387:ILE:O	1:B:397:THR:HA	2.16	0.46
3:J:25:SER:OG	3:J:27:ASP:OD1	2.21	0.46
1:C:201:LEU:HA	1:C:214:HIS:HA	1.96	0.46
2:M:110:TYR:HB2	3:N:36:TYR:OH	2.16	0.46
1:D:311:ALA:HB2	1:D:394:LYS:HB3	1.97	0.46
1:C:39:PRO:HD2	1:C:298:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:MET:CE	1:C:130:ILE:CD1	2.91	0.46
1:C:83:ASP:OD2	3:J:101:GLY:HA2	2.16	0.46
1:B:25:LEU:HD21	1:B:43:ILE:HG13	1.97	0.46
2:H:99:ARG:HH11	2:H:99:ARG:HB3	1.81	0.46
2:E:92:THR:HG23	2:E:122:THR:HA	1.96	0.45
1:A:248:ALA:O	1:A:250:ALA:N	2.49	0.45
1:A:312:PHE:HE1	1:A:390:GLY:HA2	1.81	0.45
1:C:344:GLN:OE1	1:C:352:LEU:HB3	2.16	0.45
1:D:206:MET:HE3	1:D:206:MET:HB2	1.55	0.45
1:B:77:GLN:OE1	3:F:54:SER:OG	2.35	0.45
2:I:3:GLN:HB2	2:I:25:SER:O	2.16	0.45
1:A:96:LEU:HB3	1:A:110:LYS:HB3	1.98	0.45
1:A:132:PRO:HG3	1:A:193:ARG:NH2	2.27	0.45
3:L:52:TYR:HE2	3:L:72:LYS:HG3	1.82	0.45
1:A:92:CYS:HA	1:A:115:THR:O	2.16	0.45
1:C:92:CYS:HA	1:C:115:THR:O	2.17	0.45
2:E:18:LEU:HD23	2:E:20:LEU:HG	1.98	0.45
1:A:94:ARG:HG2	1:A:114:VAL:HB	1.99	0.45
1:D:330:VAL:HG11	1:D:389:ILE:HD13	1.98	0.45
1:B:96:LEU:HB3	1:B:110:LYS:HB3	1.99	0.45
2:I:108:TYR:HE1	3:J:48:LEU:HG	1.81	0.45
1:B:312:PHE:CZ	1:B:341:VAL:HG13	2.51	0.45
1:B:320:GLU:HB2	1:B:400:TRP:CZ2	2.52	0.45
2:E:108:TYR:HD1	3:F:51:TYR:HB3	1.81	0.45
1:A:193:ARG:C	1:A:195:GLY:H	2.25	0.44
2:H:95:TYR:O	2:H:118:GLY:HA2	2.16	0.44
3:F:18:ALA:HB2	3:F:86:LEU:HD11	1.99	0.44
1:D:34:MET:HA	1:D:40:THR:HG22	1.99	0.44
3:L:41:LYS:HB2	3:L:44:SER:OG	2.16	0.44
3:F:52:TYR:HE2	3:F:72:LYS:HG3	1.81	0.44
2:I:69:VAL:HA	2:I:84:LEU:HA	1.99	0.44
1:A:315:THR:HG22	1:A:316:LYS:HD3	1.99	0.44
1:C:43:ILE:HG22	1:C:141:LEU:HG	2.00	0.44
1:D:320:GLU:HB2	1:D:400:TRP:CZ2	2.52	0.44
1:B:345:MET:HE1	1:B:380:PRO:HB3	2.00	0.44
3:L:7:PRO:HD2	3:L:111:THR:HG22	1.99	0.44
2:E:39:ARG:HB3	2:E:49:ILE:HD11	1.98	0.44
1:D:300:LEU:HD12	1:D:300:LEU:H	1.83	0.44
1:B:23:VAL:HG21	1:B:31:VAL:HG11	1.99	0.44
3:L:20:LEU:HD11	3:L:113:LEU:HD22	2.00	0.44
3:N:37:TRP:HA	3:N:95:TYR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:GLY:HA2	1:C:368:SER:HA	1.99	0.44
1:B:26:GLU:HB2	1:B:287:GLY:O	2.18	0.44
1:B:152:ILE:O	1:B:152:ILE:HG23	2.18	0.44
1:A:59:TYR:HB2	1:A:125:MET:HG3	1.99	0.44
1:C:127:GLY:HA3	1:C:218:PHE:CZ	2.53	0.44
1:D:88:THR:HB	1:D:235:HIS:CD2	2.53	0.44
1:B:9:ARG:HB3	1:B:323:HIS:HE1	1.82	0.44
1:B:52:ASN:HA	3:J:74:THR:HG22	1.98	0.44
1:B:175:ARG:HA	1:B:189:ASP:HA	1.99	0.44
2:H:120:LEU:HD23	2:H:120:LEU:H	1.82	0.44
2:E:61:TYR:HE1	2:E:71:ILE:HG13	1.83	0.44
2:M:68:ARG:HH21	2:M:84:LEU:HD11	1.83	0.44
3:J:4:LEU:HD22	3:J:24:LEU:HA	2.00	0.44
3:L:15:GLY:H	3:L:86:LEU:HB2	1.82	0.43
2:I:48:TYR:O	2:I:62:ASN:ND2	2.51	0.43
1:C:129:SER:HA	1:C:202:TYR:HD1	1.82	0.43
2:H:29:ILE:HG22	2:H:30:SER:H	1.83	0.43
1:A:329:GLU:HB2	1:B:101:TRP:HZ3	1.82	0.43
1:C:53:MET:HG2	1:C:130:ILE:HA	2.00	0.43
1:C:225:TRP:NE1	1:C:238:ASN:HD21	2.16	0.43
2:I:34:TYR:CE1	2:I:53:SER:HB3	2.53	0.43
1:D:131:GLN:O	1:D:132:PRO:C	2.62	0.43
1:D:207:ASN:HB3	1:D:209:LYS:HE2	2.01	0.43
1:A:312:PHE:CD1	1:A:389:ILE:HG22	2.54	0.43
1:C:39:PRO:HA	1:C:361:ALA:HB3	2.01	0.43
1:B:61:TYR:CD1	1:B:206:MET:HE2	2.53	0.43
1:B:302:GLY:HA2	1:B:305:TYR:CD1	2.53	0.43
1:B:326:VAL:HG23	1:B:380:PRO:HD3	2.01	0.43
3:N:40:GLN:HE21	3:N:46:PRO:HD3	1.83	0.43
2:I:19:SER:HA	2:I:82:LEU:O	2.19	0.43
1:A:236:TRP:O	1:A:239:LYS:HE3	2.19	0.43
1:B:59:TYR:HB2	1:B:125:MET:HE3	2.00	0.43
2:H:11:LEU:HD21	2:H:122:THR:HB	2.01	0.43
3:L:3:VAL:O	3:L:25:SER:OG	2.35	0.43
3:J:7:PRO:HG3	3:J:21:PRO:HD2	2.01	0.43
3:J:20:LEU:HB2	3:J:81:LEU:HB3	2.00	0.43
1:D:353:THR:O	1:D:355:VAL:N	2.50	0.43
2:H:29:ILE:HG13	2:H:78:ASN:OD1	2.19	0.43
1:A:113:LEU:HD11	1:A:253:GLN:HG2	2.01	0.43
1:A:211:TRP:HD1	1:A:274:GLU:HG2	1.84	0.43
1:D:137:TYR:CE1	1:D:289:LEU:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:VAL:HB	3:L:62:PRO:HB3	2.01	0.43
2:H:24:VAL:HG13	2:H:78:ASN:ND2	2.34	0.43
3:N:29:SER:O	3:N:33:LYS:HG2	2.18	0.43
2:M:38:ILE:HG12	2:M:48:TYR:HB2	2.00	0.43
3:J:20:LEU:HD22	3:J:81:LEU:HD23	2.00	0.43
1:A:312:PHE:CZ	1:A:341:VAL:HG23	2.54	0.42
1:D:251:LYS:O	2:M:106:TYR:HE2	2.02	0.42
1:D:333:ALA:HA	1:D:370:GLU:O	2.17	0.42
1:B:125:MET:SD	1:B:204:LEU:HD11	2.58	0.42
3:J:4:LEU:HD11	3:J:98:VAL:HG22	2.00	0.42
1:A:148:HIS:O	1:A:375:MET:HB2	2.19	0.42
1:A:293:LEU:HD23	1:A:293:LEU:H	1.84	0.42
1:D:147:GLN:HB3	1:D:374:MET:HA	2.00	0.42
1:C:148:HIS:CG	1:C:149:SER:H	2.37	0.42
1:D:59:TYR:HD2	1:D:223:LEU:HB2	1.84	0.42
1:C:88:THR:O	1:C:89:GLN:HG2	2.20	0.42
1:D:110:LYS:H	1:D:110:LYS:HD2	1.85	0.42
1:B:143:VAL:HG23	1:B:163:ASN:HA	2.01	0.42
3:L:41:LYS:HB3	3:L:42:PRO:HD2	2.02	0.42
2:E:4:LEU:HD12	2:E:97:CYS:HB3	2.00	0.42
3:F:25:SER:OG	3:F:27:ASP:OD1	2.23	0.42
1:A:125:MET:HE3	1:A:204:LEU:HD21	2.01	0.42
1:A:167:VAL:HG22	1:A:178:ALA:HB2	2.00	0.42
1:C:62:GLU:HB3	1:C:123:LYS:HB2	1.99	0.42
1:B:92:CYS:HA	1:B:115:THR:O	2.20	0.42
1:B:388:VAL:HA	1:B:396:ILE:O	2.20	0.42
2:I:52:ILE:HD11	2:I:73:LYS:HD3	2.02	0.42
1:C:48:THR:HG23	1:C:137:TYR:CE1	2.54	0.42
1:D:130:ILE:HD12	1:D:131:GLN:H	1.85	0.42
1:B:300:LEU:HB3	1:B:303:VAL:HG13	2.01	0.42
2:M:40:GLN:HB2	2:M:46:LEU:HD23	2.01	0.42
2:E:48:TYR:OH	3:F:104:ASN:ND2	2.37	0.42
3:J:19:ARG:HG2	3:J:82:LEU:HD22	2.02	0.42
3:F:39:GLN:NE2	3:F:94:TYR:OH	2.52	0.42
1:A:374:MET:HE1	1:A:376:LEU:HD22	2.01	0.42
1:C:82:LEU:HD23	1:C:82:LEU:HA	1.92	0.42
1:C:402:ARG:NH1	1:C:403:SER:HB3	2.35	0.42
1:D:26:GLU:HA	1:D:288:HIS:H	1.85	0.42
1:B:103:ASN:HB3	2:E:106:TYR:CE1	2.54	0.42
3:J:52:TYR:OH	3:J:55:ASP:OD1	2.34	0.42
1:A:95:THR:OG1	1:A:96:LEU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:TYR:HB2	1:D:340:LYS:HG3	2.01	0.42
1:B:61:TYR:HB2	1:B:261:GLN:HB3	2.02	0.42
1:B:321:THR:OG1	1:B:325:THR:OG1	2.23	0.42
1:D:73:ARG:HD2	3:N:53:TYR:CE2	2.54	0.41
1:B:345:MET:HE2	1:B:345:MET:HB3	1.92	0.41
1:A:360:THR:HG22	1:A:377:GLU:O	2.20	0.41
1:D:218:PHE:HA	1:D:221:ILE:HG13	2.02	0.41
2:H:6:GLU:OE1	2:H:117:GLN:N	2.53	0.41
2:M:101:ASP:HB3	2:M:109:TYR:O	2.20	0.41
1:A:371:ASN:OD1	1:A:371:ASN:N	2.52	0.41
1:B:307:LEU:HD23	1:B:307:LEU:HA	1.93	0.41
2:H:29:ILE:HB	2:H:75:THR:HG23	2.02	0.41
2:I:95:TYR:O	2:I:118:GLY:HA2	2.20	0.41
1:C:52:ASN:OD1	3:F:74:THR:HG22	2.20	0.41
1:C:96:LEU:HA	1:C:111:GLY:O	2.20	0.41
1:D:98:ASP:OD1	1:D:98:ASP:N	2.53	0.41
1:B:191:GLU:O	1:B:191:GLU:HG3	2.20	0.41
3:L:51:TYR:HD2	3:L:59:GLN:HB3	1.85	0.41
1:D:302:GLY:HA2	1:D:305:TYR:CD1	2.56	0.41
2:H:40:GLN:HG3	2:H:44:LYS:O	2.21	0.41
1:D:347:VAL:H	1:D:355:VAL:HG11	1.85	0.41
2:H:4:LEU:HG	2:H:24:VAL:HA	2.02	0.41
1:A:24:VAL:HG22	1:A:290:LYS:HD2	2.03	0.41
1:A:135:LEU:HD13	1:A:137:TYR:OH	2.21	0.41
1:C:4:ILE:HG23	1:D:108:PHE:CE1	2.56	0.41
1:C:163:ASN:ND2	1:C:180:LEU:O	2.54	0.41
1:D:91:VAL:HG21	1:D:243:VAL:HG11	2.03	0.41
1:B:93:LYS:HB2	1:B:245:PHE:CE1	2.56	0.41
1:B:309:THR:N	1:B:332:TYR:OH	2.53	0.41
2:H:107:PRO:HB2	3:L:51:TYR:CZ	2.56	0.41
3:L:51:TYR:OH	3:L:57:ASP:OD1	2.29	0.41
3:N:60:LEU:HB2	3:N:64:VAL:HB	2.02	0.41
3:J:67:ARG:NH2	3:J:90:ASP:OD2	2.53	0.41
1:A:251:LYS:HG2	1:A:252:ARG:N	2.36	0.41
1:B:312:PHE:CZ	1:B:342:PRO:HD2	2.55	0.41
3:N:33:LYS:O	3:N:72:LYS:NZ	2.38	0.41
2:I:18:LEU:HB3	2:I:87:VAL:HG11	2.03	0.41
1:A:39:PRO:HD3	1:A:300:LEU:HG	2.03	0.40
2:M:29:ILE:HG23	2:M:35:TRP:NE1	2.35	0.40
2:I:71:ILE:HA	2:I:82:LEU:HA	2.04	0.40
1:D:68:MET:SD	2:M:102:ARG:NH2	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:LYS:HE3	1:D:266:HIS:NE2	2.35	0.40
1:B:209:LYS:HE2	1:B:209:LYS:HB3	1.88	0.40
3:L:10:LEU:HD23	3:L:10:LEU:HA	1.86	0.40
1:A:261:GLN:HG3	1:A:264:ALA:HB3	2.03	0.40
1:D:210:HIS:HB2	1:D:275:ALA:O	2.22	0.40
1:B:312:PHE:HZ	1:B:342:PRO:HD2	1.86	0.40
2:H:92:THR:HB	2:H:123:VAL:HG23	2.03	0.40
2:H:94:VAL:HA	2:H:119:VAL:O	2.21	0.40
1:C:392:GLY:C	1:C:394:LYS:H	2.30	0.40
2:H:93:ALA:HB3	2:H:95:TYR:CE1	2.56	0.40
2:I:59:THR:HB	2:I:61:TYR:CE1	2.57	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	396/405 (98%)	358 (90%)	38 (10%)	0	100	100
1	B	401/405 (99%)	369 (92%)	31 (8%)	1 (0%)	43	74
1	C	387/405 (96%)	351 (91%)	35 (9%)	1 (0%)	36	67
1	D	372/405 (92%)	338 (91%)	29 (8%)	5 (1%)	9	39
2	E	121/226 (54%)	113 (93%)	8 (7%)	0	100	100
2	H	124/226 (55%)	113 (91%)	9 (7%)	2 (2%)	7	36
2	I	123/226 (54%)	114 (93%)	8 (6%)	1 (1%)	16	49
2	M	120/226 (53%)	108 (90%)	12 (10%)	0	100	100
3	F	113/220 (51%)	108 (96%)	5 (4%)	0	100	100
3	J	113/220 (51%)	109 (96%)	4 (4%)	0	100	100
3	L	115/220 (52%)	107 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	N	114/220 (52%)	109 (96%)	5 (4%)	0	100	100
All	All	2499/3404 (73%)	2297 (92%)	192 (8%)	10 (0%)	30	62

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	192	PRO
1	B	153	VAL
1	D	193	ARG
2	H	42	PRO
2	H	41	PRO
1	C	207	ASN
1	D	191	GLU
2	I	107	PRO
1	D	131	GLN
1	D	132	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/338 (97%)	291 (88%)	38 (12%)	5	24
1	B	335/338 (99%)	292 (87%)	43 (13%)	4	21
1	C	322/338 (95%)	278 (86%)	44 (14%)	3	19
1	D	304/338 (90%)	256 (84%)	48 (16%)	2	14
2	E	104/196 (53%)	95 (91%)	9 (9%)	9	33
2	H	106/196 (54%)	95 (90%)	11 (10%)	7	28
2	I	105/196 (54%)	93 (89%)	12 (11%)	5	24
2	M	103/196 (53%)	89 (86%)	14 (14%)	3	20
3	F	98/185 (53%)	97 (99%)	1 (1%)	68	75
3	J	98/185 (53%)	94 (96%)	4 (4%)	27	53
3	L	99/185 (54%)	94 (95%)	5 (5%)	21	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	N	98/185 (53%)	96 (98%)	2 (2%)	48 66
All	All	2101/2876 (73%)	1870 (89%)	231 (11%)	6 26

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	21	VAL
1	A	30	CYS
1	A	33	VAL
1	A	49	THR
1	A	68	MET
1	A	74	CYS
1	A	76	THR
1	A	84	LYS
1	A	110	LYS
1	A	113	LEU
1	A	152	ILE
1	A	166	LYS
1	A	170	THR
1	A	188	LEU
1	A	189	ASP
1	A	190	CYS
1	A	194	THR
1	A	205	THR
1	A	208	ASN
1	A	213	VAL
1	A	220	ASP
1	A	231	THR
1	A	233	THR
1	A	255	VAL
1	A	266	HIS
1	A	284	LEU
1	A	298	LEU
1	A	300	LEU
1	A	308	CYS
1	A	312	PHE
1	A	316	LYS
1	A	317	ILE
1	A	341	VAL
1	A	360	THR
1	A	365	ILE

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Mol	Chain	Res	Type
1	A	375	MET
1	A	391	VAL
1	C	4	ILE
1	C	12	VAL
1	C	23	VAL
1	C	24	VAL
1	C	25	LEU
1	C	27	HIS
1	C	31	VAL
1	C	34	MET
1	C	37	ASP
1	C	44	GLU
1	C	49	THR
1	C	53	MET
1	C	56	VAL
1	C	76	THR
1	C	131	GLN
1	C	135	LEU
1	C	148	HIS
1	C	166	LYS
1	C	179	THR
1	C	186	LEU
1	C	196	LEU
1	C	197	ASP
1	C	199	SER
1	C	200	ASP
1	C	205	THR
1	C	213	VAL
1	C	246	LYS
1	C	255	VAL
1	C	258	LEU
1	C	269	LEU
1	C	285	SER
1	C	289	LEU
1	C	298	LEU
1	C	300	LEU
1	C	341	VAL
1	C	349	MET
1	C	355	VAL
1	C	366	THR
1	C	369	THR
1	C	387	ILE

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Mol	Chain	Res	Type
1	C	391	VAL
1	C	395	LYS
1	C	396	ILE
1	C	398	HIS
1	D	12	VAL
1	D	13	GLU
1	D	19	THR
1	D	21	VAL
1	D	24	VAL
1	D	50	VAL
1	D	68	MET
1	D	96	LEU
1	D	98	ASP
1	D	107	LEU
1	D	110	LYS
1	D	113	LEU
1	D	130	ILE
1	D	133	GLU
1	D	135	LEU
1	D	136	GLU
1	D	148	HIS
1	D	167	VAL
1	D	179	THR
1	D	186	LEU
1	D	188	LEU
1	D	196	LEU
1	D	204	LEU
1	D	205	THR
1	D	207	ASN
1	D	208	ASN
1	D	210	HIS
1	D	231	THR
1	D	242	LEU
1	D	246	LYS
1	D	256	VAL
1	D	266	HIS
1	D	278	ASP
1	D	293	LEU
1	D	299	ARG
1	D	328	VAL
1	D	344	GLN
1	D	351	THR

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Mol	Chain	Res	Type
1	D	352	LEU
1	D	353	THR
1	D	357	ARG
1	D	358	LEU
1	D	369	THR
1	D	370	GLU
1	D	374	MET
1	D	377	GLU
1	D	389	ILE
1	D	391	VAL
1	B	1	ILE
1	B	9	ARG
1	B	12	VAL
1	B	24	VAL
1	B	33	VAL
1	B	40	THR
1	B	46	VAL
1	B	56	VAL
1	B	77	GLN
1	B	91	VAL
1	B	103	ASN
1	B	112	SER
1	B	133	GLU
1	B	134	ASN
1	B	141	LEU
1	B	143	VAL
1	B	147	GLN
1	B	152	ILE
1	B	158	HIS
1	B	167	VAL
1	B	179	THR
1	B	186	LEU
1	B	194	THR
1	B	197	ASP
1	B	198	PHE
1	B	208	ASN
1	B	220	ASP
1	B	242	LEU
1	B	245	PHE
1	B	247	ASP
1	B	249	HIS
1	B	255	VAL

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Mol	Chain	Res	Type
1	B	258	LEU
1	B	269	LEU
1	B	276	GLU
1	B	277	MET
1	B	296	ASP
1	B	300	LEU
1	B	303	VAL
1	B	347	VAL
1	B	370	GLU
1	B	376	LEU
1	B	391	VAL
2	H	3	GLN
2	H	11	LEU
2	H	24	VAL
2	H	38	ILE
2	H	51	TYR
2	H	75	THR
2	H	88	THR
2	H	99	ARG
2	H	119	VAL
2	H	122	THR
2	H	123	VAL
2	M	13	LYS
2	M	16	GLU
2	M	52	ILE
2	M	62	ASN
2	M	65	LEU
2	M	69	VAL
2	M	77	LYS
2	M	87	VAL
2	M	100	ARG
2	M	101	ASP
2	M	102	ARG
2	M	103	VAL
2	M	121	VAL
2	M	122	THR
3	L	6	GLN
3	L	48	LEU
3	L	51	TYR
3	L	69	SER
3	L	111	THR
2	E	4	LEU

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Mol	Chain	Res	Type
2	E	11	LEU
2	E	12	VAL
2	E	13	LYS
2	E	18	LEU
2	E	66	LYS
2	E	75	THR
2	E	97	CYS
2	E	101	ASP
3	N	48	LEU
3	N	60	LEU
3	F	112	LYS
2	I	6	GLU
2	I	11	LEU
2	I	16	GLU
2	I	18	LEU
2	I	22	CYS
2	I	44	LYS
2	I	68	ARG
2	I	69	VAL
2	I	77	LYS
2	I	82	LEU
2	I	103	VAL
2	I	112	LEU
3	J	6	GLN
3	J	10	LEU
3	J	41	LYS
3	J	48	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	77	GLN
1	A	131	GLN
1	A	237	ASN
1	A	253	GLN
1	A	398	HIS
1	C	226	HIS
1	C	238	ASN
1	C	323	HIS
1	D	77	GLN
1	B	131	GLN

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Mol	Chain	Res	Type
1	B	249	HIS
2	H	3	GLN
2	M	40	GLN
3	L	40	GLN
2	E	79	GLN
3	N	40	GLN
3	F	6	GLN
3	J	34	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	400/405 (98%)	-1.32	0 100 100	16, 40, 70, 93	0
1	B	403/405 (99%)	-1.29	0 100 100	20, 41, 75, 101	0
1	C	391/405 (96%)	-1.32	0 100 100	20, 43, 72, 108	0
1	D	380/405 (93%)	-1.33	0 100 100	18, 40, 78, 104	0
2	E	123/226 (54%)	-1.13	0 100 100	38, 69, 85, 96	0
2	H	126/226 (55%)	-1.30	0 100 100	24, 59, 75, 84	0
2	I	125/226 (55%)	-1.14	0 100 100	39, 82, 102, 116	0
2	M	122/226 (53%)	-1.34	0 100 100	33, 60, 79, 96	0
3	F	115/220 (52%)	-1.21	0 100 100	29, 53, 72, 98	0
3	J	115/220 (52%)	-1.23	0 100 100	34, 52, 79, 88	0
3	L	117/220 (53%)	-1.40	0 100 100	22, 41, 58, 67	0
3	N	116/220 (52%)	-1.29	0 100 100	23, 42, 62, 71	0
All	All	2533/3404 (74%)	-1.29	0 100 100	16, 47, 81, 116	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.