



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:45 am GMT

PDB ID : 5F1I
Title : MHC with 9-mer peptide
Authors : Liu, J.; Chai, Y.; QI, J.; Gao, G.F.
Deposited on : 2015-11-30
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

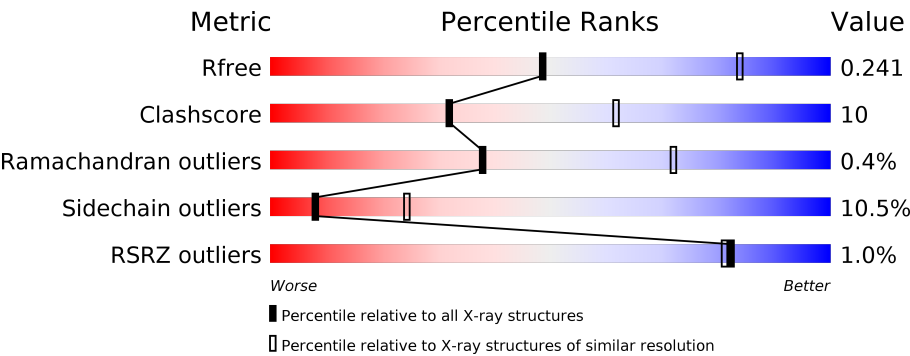
MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

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 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	275	<div><div></div><div>69%25% . .</div></div>
1	D	275	<div><div></div><div>69%28% . .</div></div>
1	G	275	<div><div></div><div>67%28% . .</div></div>
1	J	275	<div><div>%</div><div>67%26%6% .</div></div>
1	M	275	<div><div>%</div><div>75%21% . .</div></div>
1	P	275	<div><div>%</div><div>67%28% . .</div></div>

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Mol	Chain	Length	Quality of chain
1	S	275	
1	V	275	
2	B	99	
2	E	99	
2	H	99	
2	K	99	
2	N	99	
2	Q	99	
2	T	99	
2	W	99	
3	C	9	
3	F	9	
3	I	9	
3	L	9	
3	O	9	
3	R	9	
3	U	9	
3	X	9	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24668 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 MHC class I DLA-88.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2177	1357	390	424	6			
1	D	271	Total	C	N	O	S	0	1	0
			2194	1368	394	426	6			
1	G	271	Total	C	N	O	S	0	0	0
			2184	1362	391	425	6			
1	J	270	Total	C	N	O	S	0	0	0
			2177	1357	390	424	6			
1	M	271	Total	C	N	O	S	0	1	0
			2192	1366	393	427	6			
1	P	271	Total	C	N	O	S	0	0	0
			2184	1362	391	425	6			
1	S	271	Total	C	N	O	S	0	0	0
			2184	1362	391	425	6			
1	V	271	Total	C	N	O	S	0	0	0
			2184	1362	391	425	6			

- Molecule 2 is a protein called Beta2M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	E	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	H	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	K	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	N	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	Q	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	W	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			

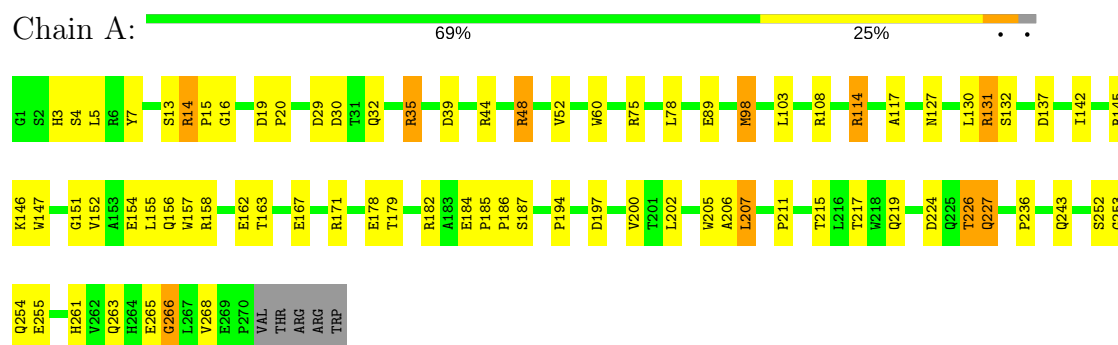
- Molecule 3 is a protein called 9-mer peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			71	47	11	13			
3	F	9	Total	C	N	O	0	0	0
			71	47	11	13			
3	I	9	Total	C	N	O	0	0	0
			71	47	11	13			
3	L	9	Total	C	N	O	0	0	0
			71	47	11	13			
3	O	9	Total	C	N	O	0	0	0
			71	47	11	13			
3	R	9	Total	C	N	O	0	0	0
			71	47	11	13			
3	U	9	Total	C	N	O	0	0	0
			71	47	11	13			
3	X	9	Total	C	N	O	0	0	0
			71	47	11	13			

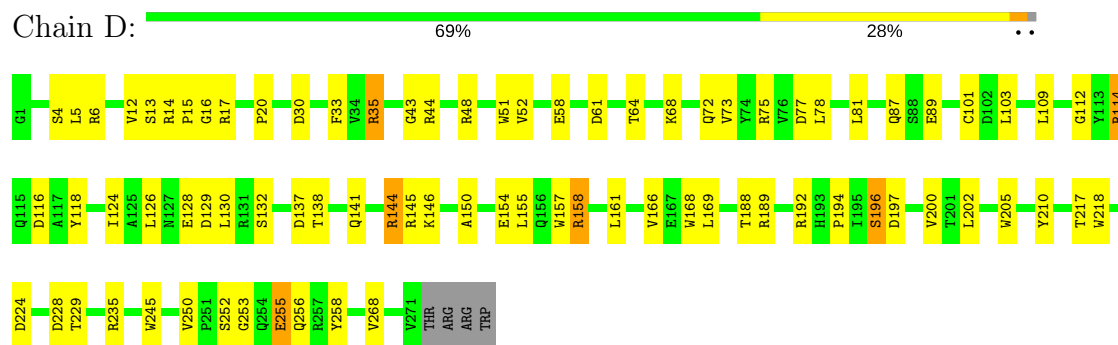
3 Residue-property plots

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

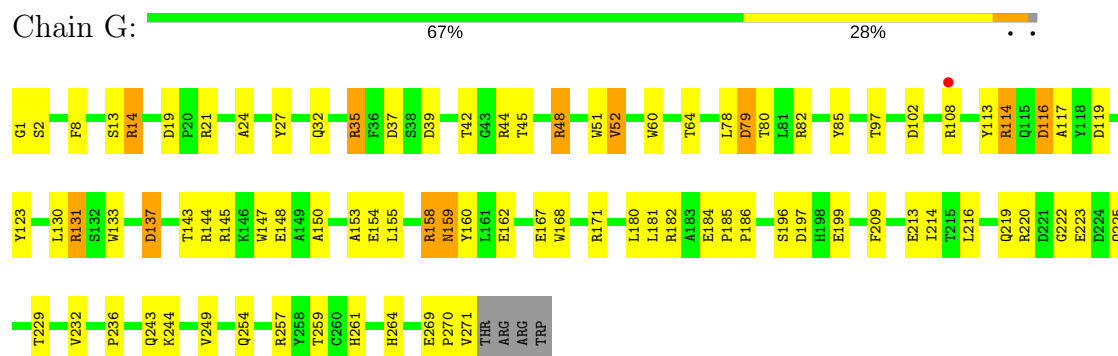
• Molecule 1: MHC class I DLA-88



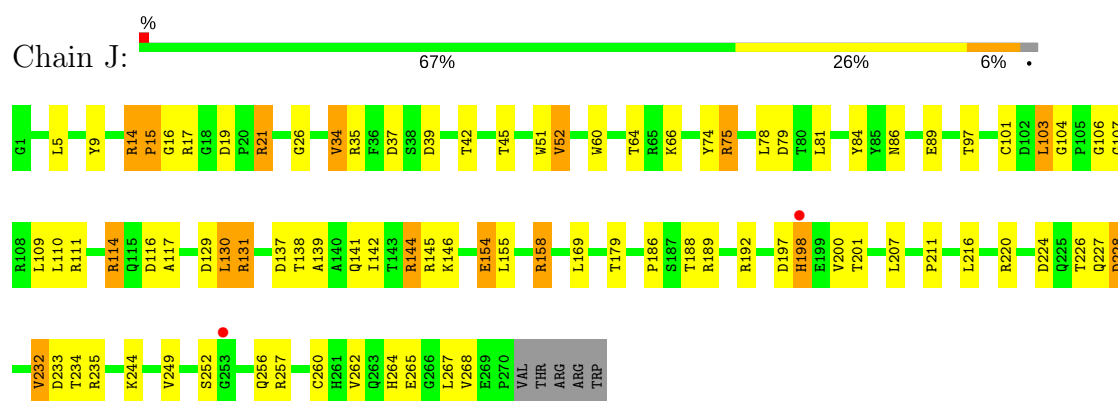
• Molecule 1: MHC class I DLA-88



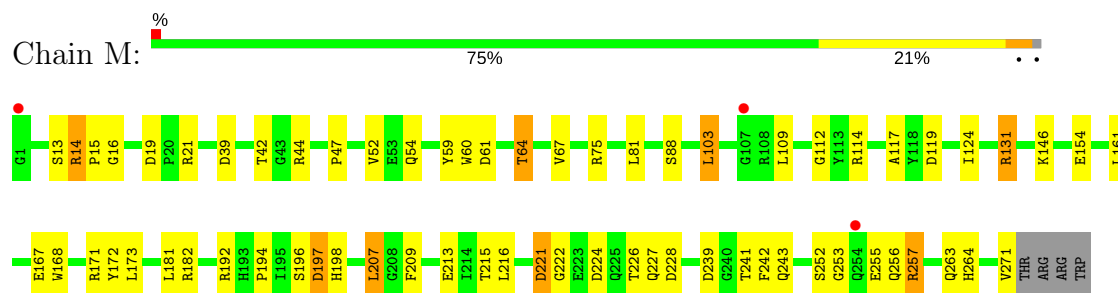
• Molecule 1: MHC class I DLA-88



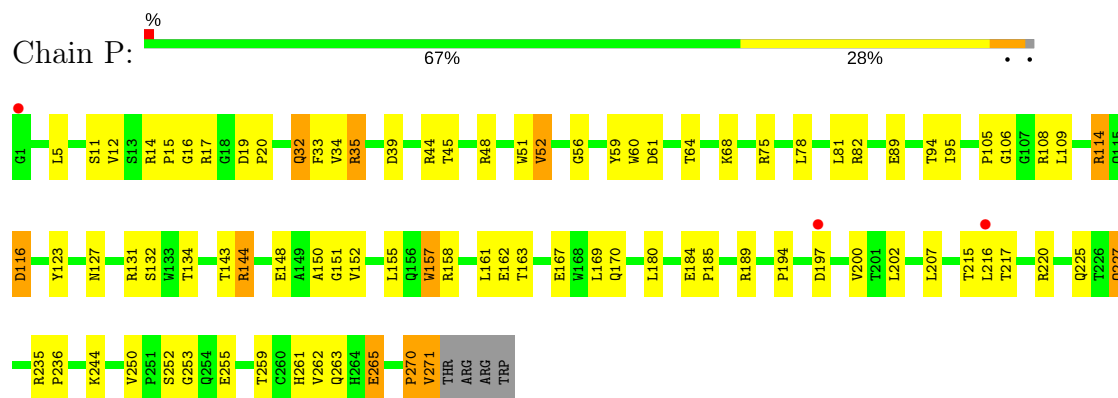
• Molecule 1: MHC class I DLA-88



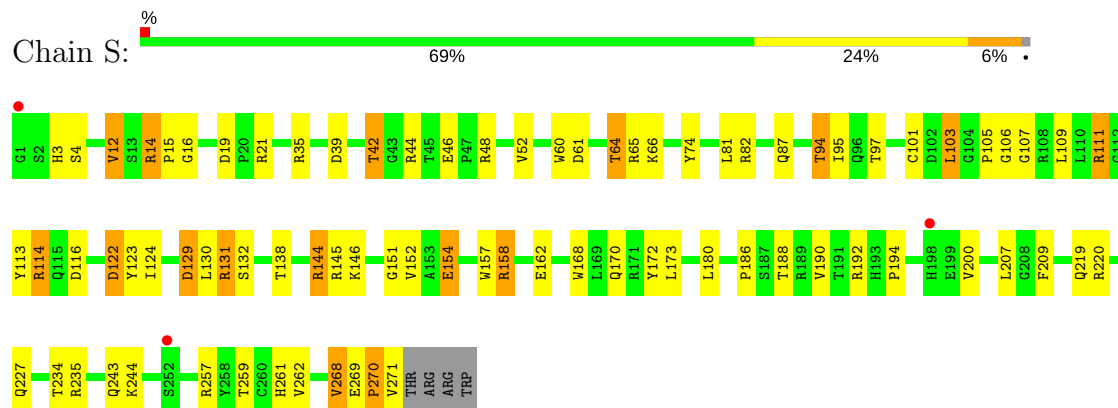
- Molecule 1: MHC class I DLA-88



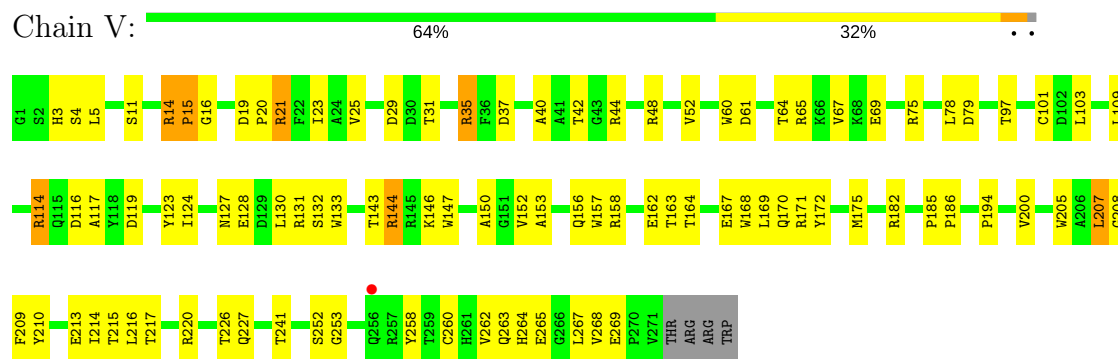
- Molecule 1: MHC class I DLA-88



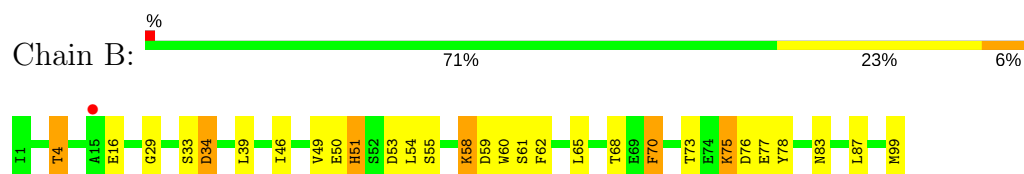
- Molecule 1: MHC class I DLA-88



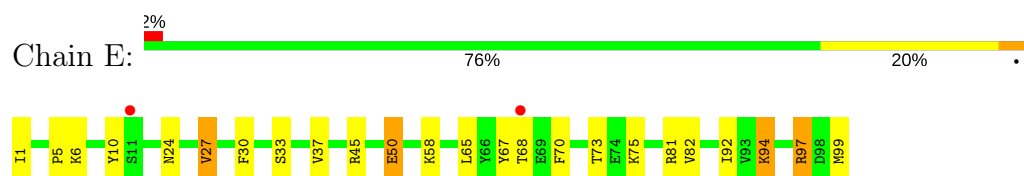
- Molecule 1: MHC class I DLA-88



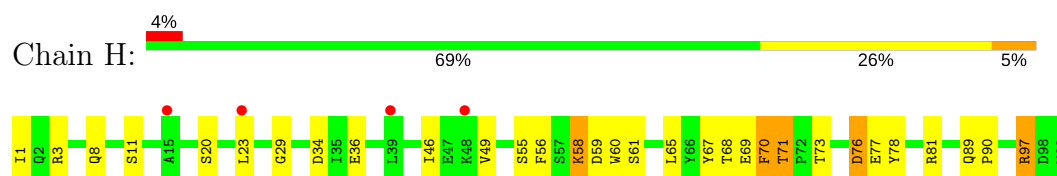
- Molecule 2: Beta2M



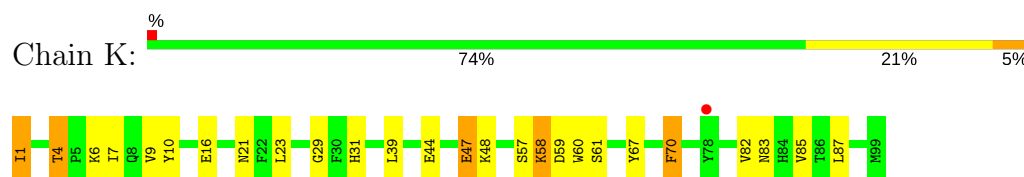
- Molecule 2: Beta2M



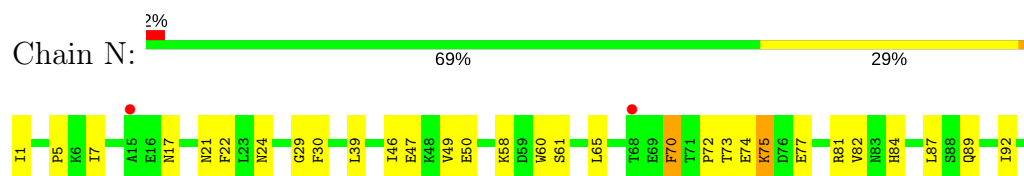
- Molecule 2: Beta2M



- Molecule 2: Beta2M

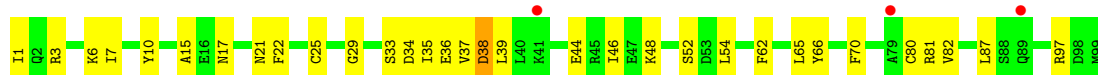


- Molecule 2: Beta2M

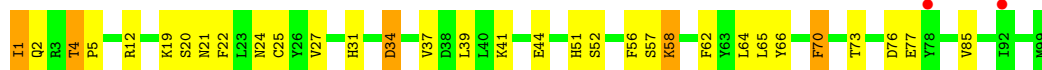


- Molecule 2: Beta2M

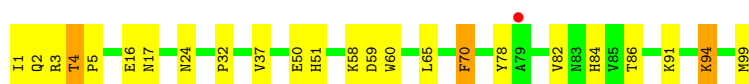
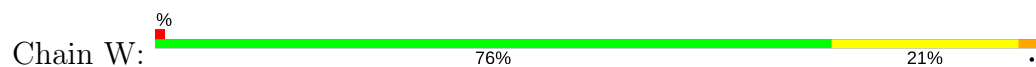




- Molecule 2: Beta2M



- Molecule 2: Beta2M



- Molecule 3: 9-mer peptide



There are no outlier residues recorded for this chain.

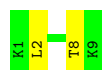
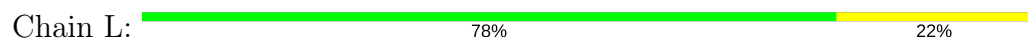
- Molecule 3: 9-mer peptide



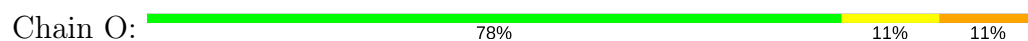
- Molecule 3: 9-mer peptide



- Molecule 3: 9-mer peptide



- Molecule 3: 9-mer peptide



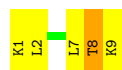
● Molecule 3: 9-mer peptide

Chain R:  56% 33% 11%

● Molecule 3: 9-mer peptide

Chain U:  33% 56% 11%

● Molecule 3: 9-mer peptide

Chain X:  44% 44% 11%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.10Å 94.63Å 124.36Å 84.60° 72.79° 81.61°	Depositor
Resolution (Å)	41.55 – 2.90 48.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (41.55-2.90) 95.0 (48.90-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.208 , 0.240 0.209 , 0.241	Depositor DCC
R_{free} test set	3817 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 28.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24668	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.85% 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	0.46	0/2234	0.65	0/3043
1	D	0.48	0/2252	0.65	0/3068
1	G	0.45	0/2241	0.64	0/3053
1	J	0.44	0/2234	0.65	0/3043
1	M	0.47	0/2249	0.65	0/3064
1	P	0.41	0/2241	0.60	0/3053
1	S	0.43	0/2241	0.63	0/3053
1	V	0.42	0/2241	0.61	0/3053
2	B	0.53	0/851	0.66	0/1152
2	E	0.51	0/851	0.59	0/1152
2	H	0.53	0/851	0.64	0/1152
2	K	0.45	0/851	0.60	0/1152
2	N	0.48	0/851	0.62	0/1152
2	Q	0.44	0/851	0.58	0/1152
2	T	0.46	0/851	0.62	0/1152
2	W	0.45	0/851	0.61	0/1152
3	C	0.42	0/71	0.57	0/92
3	F	0.47	0/71	0.62	0/92
3	I	0.48	0/71	0.53	0/92
3	L	0.48	0/71	0.64	0/92
3	O	0.58	0/71	0.73	0/92
3	R	0.51	0/71	0.65	0/92
3	U	0.56	0/71	0.67	0/92
3	X	0.46	0/71	0.83	0/92
All	All	0.46	0/25309	0.63	0/34382

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2177	0	2040	46	0
1	D	2194	0	2055	48	0
1	G	2184	0	2049	62	0
1	J	2177	0	2040	47	0
1	M	2192	0	2054	37	0
1	P	2184	0	2049	57	0
1	S	2184	0	2049	49	0
1	V	2184	0	2049	60	0
2	B	828	0	794	15	0
2	E	828	0	794	13	0
2	H	828	0	794	18	1
2	K	828	0	794	11	1
2	N	828	0	794	14	0
2	Q	828	0	794	20	0
2	T	828	0	794	18	0
2	W	828	0	794	13	0
3	C	71	0	80	0	0
3	F	71	0	80	6	0
3	I	71	0	80	4	0
3	L	71	0	80	2	0
3	O	71	0	80	3	0
3	R	71	0	80	1	0
3	U	71	0	80	5	0
3	X	71	0	80	6	0
All	All	24668	0	23377	484	1

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 10.

All (484) 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:S:227:GLN:HB3	1:V:144:ARG:HH22	1.35	0.91
1:P:45:THR:H	1:P:64:THR:HG22	1.37	0.90
1:S:35:ARG:HD2	1:S:48:ARG:HD2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:24:ASN:HB3	2:N:65:LEU:HD11	1.62	0.82
2:B:4:THR:H	2:E:1:ILE:HD12	1.44	0.82
1:D:109:LEU:HB3	1:S:131:ARG:HH12	1.46	0.77
1:A:14:ARG:NH2	1:A:39:ASP:OD2	2.18	0.76
1:V:130:LEU:HB2	1:V:158:ARG:HD3	1.66	0.76
2:T:24:ASN:HB3	2:T:65:LEU:HD11	1.68	0.75
1:G:45:THR:H	1:G:64:THR:HG22	1.52	0.74
1:J:74:TYR:HH	1:J:97:THR:HG1	1.35	0.74
1:J:14:ARG:NH2	1:J:39:ASP:OD2	2.23	0.72
1:P:114:ARG:NH1	1:P:116:ASP:OD1	2.23	0.71
1:D:72:GLN:OE1	1:D:75:ARG:NH2	2.23	0.71
1:V:97:THR:OG1	1:V:116:ASP:OD1	2.05	0.71
1:S:194:PRO:HA	1:S:200:VAL:HG22	1.74	0.70
1:J:5:LEU:HB2	1:J:169:LEU:HD13	1.74	0.69
1:A:20:PRO:HG2	1:A:75:ARG:HG3	1.74	0.69
1:G:214:ILE:HG13	1:G:264:HIS:HB2	1.75	0.69
1:G:232:VAL:HB	2:H:8:GLN:HE22	1.58	0.69
1:D:202:LEU:HD11	1:D:255:GLU:HB3	1.76	0.68
2:H:73:THR:OG1	2:H:76:ASP:OD1	2.10	0.68
1:M:59:TYR:HH	1:M:172:TYR:HH	1.41	0.68
1:G:14:ARG:NH2	1:G:39:ASP:OD2	2.25	0.68
1:M:14:ARG:NH2	1:M:39:ASP:OD2	2.21	0.68
1:S:14:ARG:NH2	1:S:39:ASP:OD2	2.27	0.68
1:D:33:PHE:HB2	1:D:52:VAL:HG21	1.75	0.68
1:J:9:TYR:HB2	1:J:97:THR:HB	1.75	0.68
1:S:114:ARG:NH1	1:S:116:ASP:OD1	2.27	0.68
1:V:194:PRO:HA	1:V:200:VAL:HG22	1.75	0.68
1:J:227:GLN:HB3	1:P:144:ARG:HH22	1.57	0.68
1:A:167:GLU:OE1	1:A:171:ARG:NH1	2.26	0.68
1:M:197:ASP:O	1:M:252:SER:OG	2.10	0.67
1:S:144:ARG:NH2	1:V:227:GLN:O	2.26	0.67
1:S:146:LYS:NZ	3:U:8:THR:O	2.24	0.67
1:S:219:GLN:OE1	1:S:261:HIS:NE2	2.27	0.67
1:A:185:PRO:HB3	1:A:266:GLY:O	1.95	0.67
1:V:19:ASP:OD1	1:V:75:ARG:NH1	2.27	0.67
1:A:206:ALA:C	1:A:207:LEU:HD13	2.15	0.67
2:E:97:ARG:HD2	2:E:97:ARG:H	1.58	0.67
1:D:20:PRO:HG2	1:D:75:ARG:HG3	1.77	0.66
1:S:35:ARG:NH2	1:S:46:GLU:OE2	2.27	0.66
1:M:221:ASP:OD1	1:M:257:ARG:NH1	2.29	0.66
1:S:234:THR:OG1	1:S:244:LYS:NZ	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:47:GLU:HG3	2:K:48:LYS:HG3	1.77	0.66
1:S:268:VAL:HA	1:S:269:GLU:HB2	1.76	0.66
1:D:194:PRO:HA	1:D:200:VAL:HG22	1.77	0.66
1:J:109:LEU:O	1:M:131:ARG:NH1	2.29	0.66
1:P:20:PRO:HG2	1:P:75:ARG:HG3	1.77	0.65
2:N:17:ASN:ND2	2:N:74:GLU:OE1	2.28	0.65
1:G:13:SER:HB3	1:G:78:LEU:HD13	1.79	0.65
1:P:270:PRO:O	1:P:271:VAL:HG13	1.96	0.65
1:V:146:LYS:HE2	3:X:7:LEU:HD11	1.79	0.65
1:S:82:ARG:NH1	1:S:87:GLN:O	2.30	0.64
1:P:14:ARG:NH2	1:P:39:ASP:OD2	2.29	0.64
1:S:3:HIS:HB2	1:S:103:LEU:HD22	1.78	0.64
2:T:21:ASN:HB3	2:T:70:PHE:CE1	2.33	0.64
1:V:114:ARG:NH1	1:V:116:ASP:OD2	2.30	0.64
1:G:269:GLU:OE1	1:G:269:GLU:N	2.30	0.64
1:S:129:ASP:OD2	1:S:132:SER:OG	2.17	0.64
2:E:75:LYS:H	2:E:75:LYS:HD2	1.64	0.63
1:S:44:ARG:NH2	1:S:61:ASP:OD1	2.31	0.63
1:D:138:THR:O	1:D:141:GLN:HG2	1.98	0.62
1:V:119:ASP:HB3	2:W:1:ILE:HG13	1.81	0.62
1:D:124:ILE:HD11	1:D:144:ARG:HB3	1.80	0.62
1:G:79:ASP:CG	1:G:82:ARG:HH21	2.03	0.62
1:P:44:ARG:NH2	1:P:61:ASP:OD1	2.30	0.61
1:V:124:ILE:HD11	1:V:133:TRP:HB3	1.83	0.61
2:W:37:VAL:HG22	2:W:82:VAL:HG22	1.82	0.61
2:E:24:ASN:HB3	2:E:65:LEU:HD11	1.83	0.61
1:J:101:CYS:HB2	1:J:109:LEU:HD13	1.83	0.61
1:M:112:GLY:HA3	1:M:161:LEU:HD13	1.83	0.61
1:S:124:ILE:HD11	1:S:144:ARG:HB3	1.81	0.60
1:S:186:PRO:HB3	1:S:209:PHE:HB3	1.83	0.60
1:P:5:LEU:HB2	1:P:169:LEU:HD13	1.82	0.60
1:V:4:SER:N	1:V:29:ASP:OD1	2.30	0.60
1:G:154:GLU:HA	1:G:158:ARG:HB3	1.83	0.60
1:V:3:HIS:H	1:V:103:LEU:HD13	1.67	0.60
2:T:25:CYS:HB2	2:T:39:LEU:HD21	1.84	0.59
2:H:3:ARG:HA	2:N:1:ILE:HG22	1.84	0.59
1:D:116:ASP:HB2	1:D:124:ILE:HG22	1.84	0.59
2:K:7:ILE:HD12	2:K:82:VAL:HG21	1.83	0.58
1:G:131:ARG:NH2	1:P:109:LEU:HD23	2.17	0.58
1:V:150:ALA:HB3	1:V:152:VAL:HG23	1.85	0.58
1:J:130:LEU:HB3	1:J:158:ARG:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:208:GLY:HA2	1:V:241:THR:OG1	2.04	0.58
1:V:37:ASP:HB3	1:V:40:ALA:HB2	1.86	0.58
1:S:168:TRP:HE1	3:U:1:LYS:HZ2	1.49	0.58
1:S:114:ARG:HD2	1:S:157:TRP:CE2	2.38	0.58
1:G:14:ARG:CZ	1:G:21:ARG:HB2	2.34	0.57
1:M:192:ARG:HE	1:M:194:PRO:HG3	1.68	0.57
1:P:216:LEU:HD12	1:P:244:LYS:HD3	1.87	0.57
1:M:192:ARG:NH1	1:M:255:GLU:OE2	2.37	0.57
1:P:270:PRO:C	1:P:271:VAL:HG22	2.25	0.57
1:D:141:GLN:HG3	1:D:145:ARG:NH1	2.20	0.57
1:M:64:THR:HA	1:M:67:VAL:HG12	1.85	0.57
2:B:34:ASP:N	2:B:34:ASP:OD1	2.38	0.57
1:D:202:LEU:HD12	1:D:250:VAL:HG21	1.87	0.57
2:Q:38:ASP:OD2	2:Q:81:ARG:NH1	2.39	0.56
1:G:216:LEU:HD13	1:G:244:LYS:HD3	1.87	0.56
1:A:3:HIS:ND1	1:A:29:ASP:OD2	2.39	0.56
1:G:133:TRP:HB2	1:G:144:ARG:HG3	1.87	0.56
1:S:130:LEU:HD23	1:S:158:ARG:HA	1.87	0.56
1:P:35:ARG:HH11	1:P:48:ARG:NH2	2.04	0.56
1:V:123:TYR:OH	1:V:143:THR:OG1	2.23	0.56
1:V:123:TYR:HH	1:V:143:THR:HG1	1.51	0.56
1:A:265:GLU:O	1:A:268:VAL:HG13	2.05	0.56
2:B:49:VAL:HG22	2:B:68:THR:HB	1.87	0.55
1:D:43:GLY:O	1:D:68:LYS:NZ	2.31	0.55
1:V:35:ARG:HD2	1:V:48:ARG:HD3	1.88	0.55
1:G:44:ARG:NH2	1:G:60:TRP:O	2.40	0.55
2:T:73:THR:OG1	2:T:76:ASP:OD2	2.25	0.55
1:D:77:ASP:CG	3:F:9:LYS:HB3	2.27	0.55
1:S:122:ASP:OD1	1:S:122:ASP:N	2.40	0.55
1:D:35:ARG:HH11	1:D:48:ARG:NH2	2.04	0.55
1:D:61:ASP:HA	1:D:64:THR:HG22	1.89	0.55
1:S:101:CYS:HB2	1:S:109:LEU:HD13	1.87	0.55
1:V:220:ARG:HD2	1:V:258:TYR:CZ	2.42	0.55
2:N:7:ILE:HG12	2:N:82:VAL:HG21	1.88	0.55
2:Q:17:ASN:OD1	2:Q:97:ARG:NH1	2.39	0.55
1:A:215:THR:OG1	1:A:263:GLN:HB2	2.07	0.55
2:E:37:VAL:HG22	2:E:82:VAL:HG22	1.89	0.55
1:P:89:GLU:OE1	1:P:89:GLU:N	2.40	0.54
1:A:145:ARG:HH11	1:D:228:ASP:HA	1.72	0.54
1:D:13:SER:HB3	1:D:78:LEU:HD13	1.89	0.54
1:A:146:LYS:HG2	1:A:147:TRP:HD1	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:37:VAL:HG22	2:Q:82:VAL:HG22	1.89	0.54
1:J:200:VAL:HG23	1:J:252:SER:HB2	1.90	0.54
1:P:202:LEU:HD22	1:P:250:VAL:HG21	1.88	0.54
1:V:147:TRP:HZ2	3:X:9:LYS:HG2	1.72	0.54
1:D:154:GLU:HG2	1:D:155:LEU:N	2.22	0.53
1:G:167:GLU:OE1	1:G:171:ARG:NH1	2.41	0.53
2:B:50:GLU:HG2	2:B:51:HIS:H	1.73	0.53
1:J:216:LEU:HD23	1:J:262:VAL:HG22	1.91	0.53
1:M:213:GLU:O	1:M:264:HIS:HD2	1.91	0.53
1:P:250:VAL:HG11	1:P:255:GLU:HA	1.90	0.53
1:S:60:TRP:O	1:S:64:THR:HG22	2.08	0.53
2:T:21:ASN:HB3	2:T:70:PHE:HE1	1.72	0.53
1:A:130:LEU:HD23	1:A:158:ARG:HA	1.91	0.53
1:D:112:GLY:HA3	1:D:161:LEU:HD13	1.91	0.53
1:V:186:PRO:HB3	1:V:209:PHE:HB3	1.90	0.53
1:G:21:ARG:NE	1:G:37:ASP:OD1	2.42	0.53
2:N:5:PRO:HB3	2:N:30:PHE:HB3	1.91	0.53
1:S:74:TYR:OH	1:S:97:THR:OG1	2.19	0.53
1:D:146:LYS:NZ	3:F:8:THR:HG23	2.24	0.52
1:J:74:TYR:OH	1:J:97:THR:OG1	2.13	0.52
1:A:202:LEU:HD11	1:A:255:GLU:HB2	1.91	0.52
1:S:235:ARG:NH2	1:S:243:GLN:OE1	2.36	0.52
1:A:108:ARG:NH2	1:V:131:ARG:O	2.40	0.52
1:V:127:ASN:HB2	1:V:132:SER:HB3	1.90	0.52
1:A:182:ARG:HE	1:A:184:GLU:HB2	1.75	0.52
2:B:54:LEU:HD11	2:B:62:PHE:CD1	2.44	0.52
1:D:30:ASP:HB2	1:D:210:TYR:HE1	1.74	0.52
2:Q:21:ASN:OD1	2:Q:22:PHE:N	2.36	0.52
1:G:35:ARG:HH11	1:G:48:ARG:CZ	2.23	0.52
1:M:14:ARG:NH2	1:M:21:ARG:HD3	2.25	0.52
1:P:12:VAL:HG22	1:P:94:THR:HG23	1.91	0.52
2:T:56:PHE:HA	2:T:62:PHE:HA	1.91	0.52
1:V:215:THR:HB	1:V:263:GLN:HB2	1.92	0.52
1:M:146:LYS:NZ	3:O:8:THR:HG23	2.26	0.51
1:A:207:LEU:HD12	1:A:243:GLN:HB2	1.92	0.51
1:G:131:ARG:NH1	1:P:109:LEU:HB3	2.25	0.51
2:Q:25:CYS:N	2:Q:66:TYR:O	2.31	0.51
1:V:11:SER:HB3	1:V:78:LEU:HD11	1.93	0.51
1:A:35:ARG:HD2	2:B:53:ASP:OD2	2.10	0.51
1:G:236:PRO:HG2	2:H:65:LEU:HD13	1.92	0.51
1:P:123:TYR:OH	1:P:143:THR:OG1	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:188:THR:HG21	1:S:262:VAL:HG21	1.93	0.51
1:D:138:THR:HG23	1:D:141:GLN:OE1	2.11	0.51
1:G:102:ASP:OD1	1:G:113:TYR:OH	2.20	0.51
1:G:123:TYR:CE2	3:I:9:LYS:HD3	2.45	0.51
2:N:70:PHE:CZ	2:N:72:PRO:HG3	2.46	0.51
1:P:220:ARG:HB3	1:P:225:GLN:HE21	1.75	0.51
2:T:1:ILE:HG23	2:W:3:ARG:HA	1.92	0.51
1:V:20:PRO:HG2	1:V:75:ARG:HG3	1.93	0.51
1:M:119:ASP:O	2:N:1:ILE:HG13	2.11	0.51
1:G:143:THR:HG21	3:I:9:LYS:HG3	1.92	0.50
1:A:44:ARG:HH21	1:A:60:TRP:HB3	1.77	0.50
2:W:32:PRO:O	2:W:84:HIS:NE2	2.36	0.50
1:P:194:PRO:HA	1:P:200:VAL:HG22	1.92	0.50
1:A:131:ARG:HH22	1:V:162:GLU:HG2	1.75	0.50
1:V:25:VAL:HG12	1:V:35:ARG:HB2	1.93	0.50
1:G:108:ARG:NH2	1:P:148:GLU:O	2.45	0.50
1:G:213:GLU:O	1:G:264:HIS:HD2	1.95	0.50
1:P:33:PHE:CD2	1:P:34:VAL:HG13	2.46	0.50
2:Q:33:SER:HB3	2:Q:62:PHE:CE2	2.47	0.50
1:G:14:ARG:HD2	1:G:19:ASP:O	2.12	0.50
2:H:49:VAL:HG22	2:H:68:THR:HB	1.93	0.50
1:S:66:LYS:HG2	3:U:4:SER:HB3	1.93	0.50
1:D:235:ARG:HG3	2:E:10:TYR:CZ	2.46	0.50
1:G:21:ARG:NH2	1:G:37:ASP:OD2	2.41	0.50
1:P:236:PRO:HG2	2:Q:65:LEU:HD13	1.94	0.50
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.94	0.49
2:E:97:ARG:CD	2:E:97:ARG:H	2.25	0.49
1:J:154:GLU:HA	1:J:158:ARG:HB3	1.94	0.49
2:H:58:LYS:HD2	2:H:59:ASP:H	1.78	0.49
1:J:21:ARG:NH2	1:J:37:ASP:OD2	2.44	0.49
2:N:73:THR:OG1	2:N:75:LYS:HG3	2.12	0.49
1:G:130:LEU:HD22	1:P:131:ARG:HH22	1.77	0.49
1:J:114:ARG:NH1	1:J:116:ASP:OD1	2.45	0.49
1:M:44:ARG:NH1	1:M:61:ASP:OD1	2.42	0.49
1:V:44:ARG:HH12	1:V:61:ASP:HA	1.78	0.49
1:J:220:ARG:HD2	1:J:257:ARG:HH21	1.78	0.49
2:T:41:LYS:N	2:T:44:GLU:O	2.45	0.49
1:A:205:TRP:HE3	1:A:207:LEU:HD11	1.77	0.49
1:J:146:LYS:NZ	3:L:8:THR:HG23	2.28	0.49
2:Q:6:LYS:HB2	2:Q:6:LYS:HE3	1.60	0.49
1:S:269:GLU:N	1:S:270:PRO:HD3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:2:GLN:OE1	2:W:2:GLN:NE2	2.45	0.49
1:A:146:LYS:HG2	1:A:147:TRP:CD1	2.48	0.49
1:P:151:GLY:HA3	1:P:155:LEU:HD12	1.95	0.49
1:S:151:GLY:HA2	1:S:154:GLU:OE2	2.13	0.49
1:V:21:ARG:NH2	1:V:23:ILE:HD11	2.28	0.49
1:G:14:ARG:NH2	1:G:21:ARG:HD3	2.28	0.48
1:J:154:GLU:HG2	1:J:155:LEU:H	1.78	0.48
2:T:52:SER:O	2:T:64:LEU:HD22	2.13	0.48
1:A:236:PRO:HG2	2:B:65:LEU:HD13	1.95	0.48
2:E:81:ARG:HG3	2:E:92:ILE:HG12	1.94	0.48
1:J:26:GLY:HA3	1:J:34:VAL:HG23	1.96	0.48
1:V:29:ASP:O	1:V:210:TYR:OH	2.22	0.48
1:J:228:ASP:N	1:J:228:ASP:OD1	2.46	0.48
1:M:271:VAL:HG11	1:P:189:ARG:HA	1.94	0.48
1:S:81:LEU:HD12	1:S:95:ILE:HD11	1.96	0.48
2:K:29:GLY:HA2	2:K:61:SER:OG	2.14	0.48
1:V:168:TRP:CE2	3:X:1:LYS:HD3	2.49	0.48
1:D:103:LEU:HB2	1:D:169:LEU:HD23	1.95	0.48
1:P:56:GLY:O	1:P:60:TRP:HD1	1.97	0.48
1:A:219:GLN:OE1	1:A:261:HIS:NE2	2.47	0.48
1:J:129:ASP:OD1	1:J:131:ARG:HG3	2.14	0.48
1:G:131:ARG:HH22	1:P:109:LEU:HD23	1.76	0.48
1:V:214:ILE:HG13	1:V:264:HIS:HB2	1.95	0.48
1:D:51:TRP:CZ3	1:D:52:VAL:HG22	2.49	0.48
1:M:13:SER:O	1:M:15:PRO:HD3	2.14	0.47
1:M:215:THR:HB	1:M:263:GLN:HB2	1.95	0.47
1:P:35:ARG:HH11	1:P:48:ARG:HH21	1.60	0.47
1:V:147:TRP:CZ2	3:X:9:LYS:HG2	2.49	0.47
1:V:252:SER:HA	1:V:253:GLY:HA2	1.48	0.47
1:D:205:TRP:CZ3	1:D:245:TRP:HD1	2.32	0.47
2:H:89:GLN:HG3	2:H:90:PRO:HD2	1.97	0.47
1:G:271:VAL:HG13	1:J:188:THR:HB	1.96	0.47
1:G:131:ARG:HA	1:G:153:ALA:HB1	1.94	0.47
1:G:155:LEU:O	1:G:159:ASN:HB3	2.15	0.47
1:J:15:PRO:HA	1:J:16:GLY:HA2	1.52	0.47
2:T:4:THR:HG23	2:T:5:PRO:O	2.15	0.47
1:V:117:ALA:HB2	2:W:60:TRP:CE2	2.50	0.47
2:W:94:LYS:H	2:W:94:LYS:NZ	2.12	0.47
1:A:35:ARG:HD3	1:A:48:ARG:HE	1.79	0.47
1:D:161:LEU:O	1:D:166:VAL:HG23	2.14	0.47
1:G:1:GLY:O	1:G:2:SER:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:33:SER:HB3	2:Q:62:PHE:CZ	2.49	0.47
2:B:29:GLY:HA2	2:B:61:SER:OG	2.15	0.47
1:P:15:PRO:HA	1:P:16:GLY:HA2	1.48	0.47
1:P:150:ALA:HB3	1:P:152:VAL:HG23	1.97	0.47
1:S:172:TYR:OH	3:U:1:LYS:N	2.43	0.47
2:T:34:ASP:OD1	2:T:34:ASP:N	2.48	0.47
1:V:14:ARG:NH2	1:V:21:ARG:HD3	2.30	0.47
1:J:104:GLY:CA	1:J:110:LEU:HB2	2.44	0.47
2:K:21:ASN:HB3	2:K:70:PHE:CE1	2.49	0.47
2:E:5:PRO:HB3	2:E:30:PHE:HB3	1.97	0.47
1:J:211:PRO:O	1:J:264:HIS:HE1	1.97	0.47
1:S:173:LEU:HD23	1:S:180:LEU:HD13	1.96	0.47
2:T:12:ARG:HB2	2:T:22:PHE:HB2	1.96	0.47
1:G:114:ARG:HH11	1:G:116:ASP:CG	2.18	0.47
1:J:103:LEU:HB2	1:J:169:LEU:HD23	1.97	0.47
2:K:83:ASN:HA	2:K:87:LEU:HD12	1.97	0.47
1:P:33:PHE:HD2	1:P:52:VAL:HG11	1.80	0.47
2:K:1:ILE:HG23	2:Q:3:ARG:HA	1.96	0.47
1:P:81:LEU:HD12	1:P:95:ILE:HD11	1.97	0.47
1:D:158:ARG:NH1	1:S:162:GLU:OE2	2.46	0.47
2:B:39:LEU:C	2:B:46:ILE:HD12	2.36	0.46
1:V:5:LEU:HB2	1:V:169:LEU:HD13	1.97	0.46
1:G:225:GLN:O	1:G:229:THR:OG1	2.31	0.46
1:J:45:THR:H	1:J:64:THR:HB	1.80	0.46
1:P:216:LEU:HD23	1:P:262:VAL:HG22	1.96	0.46
1:S:152:VAL:HG12	1:S:157:TRP:HD1	1.81	0.46
2:B:75:LYS:H	2:B:75:LYS:HD2	1.79	0.46
1:D:218:TRP:HD1	1:D:229:THR:HG23	1.81	0.46
1:D:168:TRP:CE2	3:F:1:LYS:HD3	2.50	0.46
2:B:73:THR:OG1	2:B:76:ASP:OD2	2.33	0.46
1:P:60:TRP:O	1:P:64:THR:HG23	2.16	0.46
1:V:60:TRP:O	1:V:64:THR:HG22	2.16	0.46
3:X:7:LEU:HD12	3:X:8:THR:N	2.30	0.46
1:G:144:ARG:NH1	1:G:148:GLU:OE1	2.47	0.46
2:W:16:GLU:O	2:W:17:ASN:C	2.54	0.46
1:D:101:CYS:HB2	1:D:109:LEU:HD13	1.98	0.46
2:K:58:LYS:HD2	2:K:59:ASP:N	2.31	0.46
1:S:109:LEU:HD11	1:S:111:ARG:O	2.14	0.46
2:W:24:ASN:HB3	2:W:65:LEU:HD11	1.98	0.46
1:J:131:ARG:NH1	1:M:109:LEU:O	2.25	0.46
2:T:51:HIS:ND1	2:T:51:HIS:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLU:OE1	1:A:89:GLU:N	2.49	0.46
1:J:144:ARG:HG3	1:J:145:ARG:N	2.31	0.46
1:V:205:TRP:CE3	1:V:207:LEU:HD11	2.52	0.46
1:M:168:TRP:CE3	1:M:171:ARG:HD3	2.51	0.45
1:J:75:ARG:HA	1:J:78:LEU:HD12	1.98	0.45
1:M:173:LEU:HD22	1:M:181:LEU:HD21	1.97	0.45
2:N:21:ASN:OD1	2:N:22:PHE:N	2.40	0.45
1:G:131:ARG:HH12	1:P:162:GLU:HG2	1.80	0.45
1:J:60:TRP:O	1:J:64:THR:HG22	2.16	0.45
1:M:252:SER:HA	1:M:253:GLY:HA2	1.64	0.45
1:P:45:THR:HG22	1:P:60:TRP:HZ3	1.81	0.45
1:S:14:ARG:CZ	1:S:21:ARG:HB2	2.47	0.45
2:T:27:VAL:HG21	2:T:37:VAL:HG21	1.97	0.45
2:H:46:ILE:HD13	2:H:68:THR:HG21	1.98	0.45
1:J:81:LEU:HD23	1:J:84:TYR:HD2	1.80	0.45
1:S:107:GLY:HA2	1:S:170:GLN:OE1	2.16	0.45
1:D:44:ARG:HH12	1:D:61:ASP:CG	2.19	0.45
2:H:29:GLY:HA2	2:H:61:SER:OG	2.17	0.45
1:A:114:ARG:HD3	1:A:157:TRP:CZ2	2.52	0.45
1:D:51:TRP:CE3	1:D:52:VAL:HG22	2.52	0.45
1:J:234:THR:OG1	1:J:244:LYS:NZ	2.38	0.45
1:P:127:ASN:ND2	1:P:134:THR:OG1	2.42	0.45
1:J:186:PRO:HD2	1:J:267:LEU:HG	1.99	0.45
1:V:172:TYR:HA	1:V:175:MET:HG2	1.99	0.45
1:A:98:MET:HG3	1:A:98:MET:O	2.16	0.44
1:P:19:ASP:CG	1:P:75:ARG:HH22	2.20	0.44
1:A:15:PRO:HA	1:A:16:GLY:HA2	1.58	0.44
1:A:207:LEU:HD22	1:A:207:LEU:N	2.31	0.44
1:D:150:ALA:HA	1:G:150:ALA:HA	1.99	0.44
1:G:259:THR:OG1	1:G:261:HIS:NE2	2.49	0.44
2:Q:87:LEU:HD23	2:Q:87:LEU:HA	1.73	0.44
1:V:167:GLU:OE1	1:V:171:ARG:NH1	2.50	0.44
1:G:119:ASP:O	2:H:1:ILE:HA	2.17	0.44
1:G:144:ARG:NE	1:M:227:GLN:OE1	2.51	0.44
2:Q:39:LEU:O	2:Q:46:ILE:HG13	2.16	0.44
1:D:5:LEU:HB2	1:D:169:LEU:HD13	1.99	0.44
1:G:114:ARG:NH1	1:G:116:ASP:OD1	2.47	0.44
1:S:270:PRO:O	1:S:271:VAL:HB	2.17	0.44
1:V:15:PRO:HA	1:V:16:GLY:HA2	1.62	0.44
1:V:205:TRP:HB3	1:V:207:LEU:HD21	2.00	0.44
1:A:127:ASN:ND2	1:A:132:SER:OG	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:117:ALA:HB2	2:N:60:TRP:CE2	2.52	0.44
1:V:133:TRP:CZ2	1:V:153:ALA:HB2	2.53	0.44
1:A:131:ARG:NH1	1:V:109:LEU:HB3	2.32	0.44
1:D:30:ASP:HB2	1:D:210:TYR:CE1	2.52	0.44
1:D:101:CYS:HB2	1:D:109:LEU:CD1	2.47	0.44
1:D:35:ARG:HH11	1:D:48:ARG:HH21	1.65	0.44
2:H:70:PHE:HD2	2:H:78:TYR:CZ	2.36	0.44
1:A:154:GLU:HG2	1:A:155:LEU:N	2.33	0.44
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.53	0.44
1:S:65:ARG:HB3	1:S:65:ARG:HE	1.62	0.44
1:A:194:PRO:HA	1:A:200:VAL:HG22	1.98	0.44
1:A:151:GLY:O	1:A:155:LEU:HB2	2.18	0.43
1:D:15:PRO:HA	1:D:16:GLY:HA2	1.56	0.43
1:M:209:PHE:O	1:M:242:PHE:N	2.46	0.43
1:P:265:GLU:HG2	1:P:265:GLU:H	1.64	0.43
1:S:12:VAL:HG13	1:S:94:THR:OG1	2.18	0.43
1:A:207:LEU:HD13	1:A:207:LEU:N	2.31	0.43
2:B:58:LYS:HD2	2:B:59:ASP:H	1.83	0.43
1:G:27:TYR:CE1	1:G:32:GLN:HB2	2.54	0.43
2:H:23:LEU:HD21	2:H:78:TYR:HB3	2.01	0.43
1:J:235:ARG:HD2	2:K:10:TYR:CE1	2.52	0.43
1:J:51:TRP:CZ3	1:J:52:VAL:HG13	2.53	0.43
1:S:234:THR:HG1	1:S:244:LYS:HZ3	1.56	0.43
2:W:4:THR:HG23	2:W:5:PRO:O	2.17	0.43
2:W:70:PHE:HD2	2:W:78:TYR:CE2	2.36	0.43
1:A:162:GLU:OE2	1:V:131:ARG:HD3	2.18	0.43
1:G:145:ARG:NH1	1:M:228:ASP:HA	2.34	0.43
2:Q:6:LYS:HE2	2:Q:29:GLY:HA3	2.00	0.43
3:F:9:LYS:HB2	3:F:9:LYS:HE3	1.79	0.43
1:G:8:PHE:O	1:G:24:ALA:HA	2.18	0.43
2:Q:54:LEU:HD21	2:Q:62:PHE:CE2	2.53	0.43
1:S:15:PRO:HA	1:S:16:GLY:HA2	1.65	0.43
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.53	0.43
1:G:160:TYR:CG	3:I:3:PHE:HD2	2.36	0.43
1:M:221:ASP:OD1	1:M:221:ASP:N	2.49	0.43
2:N:47:GLU:O	2:N:49:VAL:N	2.51	0.43
1:D:73:VAL:HG11	3:F:6:GLU:HG2	2.01	0.43
2:H:20:SER:HA	2:H:71:THR:HG23	2.01	0.43
1:J:109:LEU:HD11	1:J:111:ARG:O	2.18	0.43
1:P:184:GLU:HA	1:P:185:PRO:HD3	1.90	0.43
1:P:215:THR:OG1	1:P:263:GLN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:59:TYR:CD2	3:R:1:LYS:HE3	2.54	0.43
1:A:75:ARG:HH21	1:A:75:ARG:HG2	1.82	0.43
2:E:50:GLU:HB3	2:E:67:TYR:CZ	2.53	0.43
3:F:1:LYS:HD2	3:F:1:LYS:HA	1.82	0.43
1:G:147:TRP:CD1	3:I:7:LEU:HD23	2.54	0.43
1:P:220:ARG:CB	1:P:225:GLN:HE21	2.32	0.43
1:P:252:SER:HA	1:P:253:GLY:HA2	1.66	0.43
1:V:152:VAL:HG12	1:V:157:TRP:HD1	1.83	0.43
1:D:252:SER:HA	1:D:253:GLY:HA2	1.50	0.43
1:A:30:ASP:OD2	1:A:211:PRO:HB2	2.19	0.43
1:G:168:TRP:CE3	1:G:171:ARG:HD3	2.54	0.43
1:G:219:GLN:OE1	1:G:222:GLY:HA2	2.19	0.43
1:M:167:GLU:O	1:M:171:ARG:HG3	2.19	0.43
1:M:255:GLU:HG2	1:M:255:GLU:H	1.60	0.43
2:N:29:GLY:HA2	2:N:61:SER:OG	2.18	0.43
1:P:51:TRP:CZ2	1:P:180:LEU:HD21	2.54	0.42
1:S:81:LEU:HD21	1:S:123:TYR:CZ	2.53	0.42
1:V:265:GLU:O	1:V:268:VAL:HG13	2.19	0.42
1:V:61:ASP:HB3	1:V:65:ARG:NH2	2.35	0.42
2:B:70:PHE:HD2	2:B:78:TYR:CZ	2.37	0.42
2:N:84:HIS:HB3	2:N:87:LEU:HG	2.00	0.42
1:P:114:ARG:HD2	1:P:157:TRP:CH2	2.54	0.42
1:A:226:THR:HA	1:A:227:GLN:HA	1.72	0.42
1:M:103:LEU:HA	1:M:103:LEU:HD23	1.88	0.42
1:G:181:LEU:HD23	1:G:181:LEU:HA	1.91	0.42
3:U:6:GLU:HG3	3:U:7:LEU:O	2.19	0.42
2:K:23:LEU:O	2:K:67:TYR:HA	2.19	0.42
1:P:32:GLN:HB3	1:P:32:GLN:HE21	1.50	0.42
2:Q:54:LEU:HD11	2:Q:62:PHE:CD2	2.55	0.42
1:J:66:LYS:NZ	3:L:2:LEU:O	2.42	0.42
1:M:146:LYS:HZ3	3:O:8:THR:HG23	1.84	0.42
2:B:83:ASN:HA	2:B:87:LEU:HD12	2.01	0.42
1:P:19:ASP:OD1	1:P:75:ARG:NH1	2.40	0.42
2:T:58:LYS:H	2:T:58:LYS:HG3	1.29	0.42
1:D:126:LEU:HD12	1:D:132:SER:O	2.20	0.42
1:G:51:TRP:CZ2	1:G:180:LEU:HD11	2.55	0.42
1:M:207:LEU:HD12	1:M:243:GLN:HB3	2.02	0.42
1:P:82:ARG:CZ	1:P:89:GLU:HG3	2.50	0.42
1:A:152:VAL:HG22	1:A:156:GLN:OE1	2.20	0.42
1:G:85:TYR:OH	1:G:137:ASP:OD1	2.27	0.42
1:G:167:GLU:O	1:G:171:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:TRP:CZ3	1:G:52:VAL:HG13	2.55	0.42
1:P:11:SER:OG	1:P:78:LEU:HD11	2.19	0.42
2:Q:35:ILE:HG13	2:Q:36:GLU:N	2.35	0.42
1:V:133:TRP:CE2	1:V:153:ALA:HB2	2.54	0.42
1:A:158:ARG:HD3	1:V:158:ARG:HH22	1.84	0.42
2:E:94:LYS:H	2:E:94:LYS:HG3	1.43	0.42
1:G:209:PHE:CE2	1:G:243:GLN:HA	2.55	0.42
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.55	0.42
1:J:81:LEU:HD23	1:J:81:LEU:HA	1.75	0.42
3:O:6:GLU:OE2	3:O:6:GLU:HA	2.19	0.42
1:P:235:ARG:HD2	2:Q:10:TYR:CE1	2.55	0.42
1:S:220:ARG:NH2	1:S:257:ARG:HD3	2.34	0.42
1:D:129:ASP:C	1:D:130:LEU:HD12	2.40	0.41
2:H:97:ARG:H	2:H:97:ARG:HD2	1.85	0.41
2:N:39:LEU:HB3	2:N:46:ILE:HD12	2.02	0.41
1:J:232:VAL:HG23	1:J:233:ASP:O	2.20	0.41
1:M:15:PRO:HA	1:M:16:GLY:HA2	1.68	0.41
1:V:213:GLU:O	1:V:264:HIS:HD2	2.03	0.41
1:G:184:GLU:HA	1:G:185:PRO:HD2	1.91	0.41
2:K:4:THR:HB	2:Q:1:ILE:HD13	2.03	0.41
2:H:23:LEU:O	2:H:67:TYR:HA	2.20	0.41
1:S:144:ARG:HG3	1:S:145:ARG:N	2.35	0.41
1:S:42:THR:HG22	1:S:44:ARG:HG2	2.02	0.41
1:A:252:SER:HA	1:A:253:GLY:O	2.20	0.41
1:J:106:GLY:HA2	1:J:107:GLY:HA2	1.75	0.41
1:V:185:PRO:HA	1:V:186:PRO:HD3	1.90	0.41
1:V:220:ARG:NH2	1:V:258:TYR:OH	2.43	0.41
2:E:6:LYS:O	2:E:27:VAL:HA	2.21	0.41
1:G:154:GLU:HG2	1:G:155:LEU:N	2.35	0.41
1:G:162:GLU:OE2	1:P:131:ARG:HD3	2.20	0.41
2:H:55:SER:OG	2:H:56:PHE:N	2.54	0.41
1:M:221:ASP:HB2	1:M:222:GLY:H	1.55	0.41
1:D:114:ARG:HH21	1:D:157:TRP:HE1	1.69	0.41
1:D:250:VAL:HG13	1:D:258:TYR:CE1	2.55	0.41
1:J:201:THR:OG1	1:J:249:VAL:HG22	2.21	0.41
2:W:84:HIS:ND1	2:W:86:THR:HG23	2.35	0.41
1:G:220:ARG:HE	1:G:257:ARG:NH1	2.19	0.41
1:P:105:PRO:HA	1:P:106:GLY:HA2	1.70	0.41
1:P:157:TRP:HD1	1:P:161:LEU:HG	1.86	0.41
2:Q:15:ALA:HB3	2:Q:97:ARG:HG3	2.03	0.41
1:G:185:PRO:HA	1:G:186:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:137:ASP:OD1	1:J:139:ALA:HB3	2.21	0.41
1:S:81:LEU:HA	1:S:81:LEU:HD23	1.70	0.41
2:T:19:LYS:HD3	2:T:19:LYS:HA	1.82	0.41
1:A:185:PRO:HA	1:A:186:PRO:HD3	1.87	0.41
1:A:206:ALA:O	1:A:207:LEU:HD13	2.20	0.41
1:D:196:SER:HB2	1:D:197:ASP:H	1.65	0.41
1:V:67:VAL:HB	3:X:2:LEU:HD13	2.03	0.41
2:E:73:THR:HB	2:E:75:LYS:HD2	2.02	0.40
1:J:14:ARG:CB	1:J:17:ARG:HB2	2.51	0.40
2:Q:7:ILE:HD12	2:Q:82:VAL:HG21	2.02	0.40
1:G:145:ARG:HH11	1:M:228:ASP:HA	1.86	0.40
1:G:269:GLU:HA	1:G:270:PRO:HD2	1.72	0.40
1:M:14:ARG:HH22	1:M:39:ASP:CG	2.18	0.40
1:D:189:ARG:HE	1:D:189:ARG:HB3	1.51	0.40
1:D:81:LEU:HD12	1:D:118:TYR:CD1	2.56	0.40
2:H:97:ARG:HG2	2:H:97:ARG:HH11	1.85	0.40
1:J:189:ARG:HD2	1:J:189:ARG:HH11	1.77	0.40
1:M:239:ASP:OD1	1:M:241:THR:OG1	2.36	0.40
1:M:47:PRO:HB3	1:M:60:TRP:CH2	2.56	0.40
1:P:151:GLY:O	1:P:155:LEU:HB2	2.21	0.40
1:S:105:PRO:HA	1:S:106:GLY:HA2	1.53	0.40
1:V:123:TYR:HD2	1:V:124:ILE:HG22	1.85	0.40
1:V:267:LEU:HA	1:V:267:LEU:HD23	1.87	0.40
1:J:144:ARG:NH1	1:P:227:GLN:HG2	2.37	0.40
1:V:101:CYS:HB2	1:V:109:LEU:HD13	2.03	0.40
2:W:50:GLU:HG2	2:W:51:HIS:H	1.87	0.40
1:A:5:LEU:HD21	1:A:7:TYR:CE2	2.56	0.40
1:J:197:ASP:OD1	1:J:198:HIS:N	2.54	0.40
2:T:51:HIS:HB3	2:T:66:TYR:CD2	2.57	0.40
1:V:3:HIS:CG	1:V:103:LEU:HD13	2.56	0.40

All (1) 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)
2:H:81:ARG:NH2	2:K:44:GLU:OE1[1_545]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	268/275 (98%)	245 (91%)	21 (8%)	2 (1%)	25	60
1	D	270/275 (98%)	245 (91%)	24 (9%)	1 (0%)	38	72
1	G	269/275 (98%)	246 (91%)	21 (8%)	2 (1%)	25	60
1	J	268/275 (98%)	245 (91%)	22 (8%)	1 (0%)	38	72
1	M	270/275 (98%)	241 (89%)	28 (10%)	1 (0%)	38	72
1	P	269/275 (98%)	250 (93%)	17 (6%)	2 (1%)	25	60
1	S	269/275 (98%)	246 (91%)	22 (8%)	1 (0%)	38	72
1	V	269/275 (98%)	246 (91%)	22 (8%)	1 (0%)	38	72
2	B	97/99 (98%)	88 (91%)	9 (9%)	0	100	100
2	E	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	H	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
2	K	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	N	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
2	Q	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
2	T	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
2	W	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
3	I	7/9 (78%)	7 (100%)	0	0	100	100
3	L	7/9 (78%)	7 (100%)	0	0	100	100
3	O	7/9 (78%)	7 (100%)	0	0	100	100
3	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	U	7/9 (78%)	7 (100%)	0	0	100	100
3	X	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
All	All	2984/3064 (97%)	2751 (92%)	222 (7%)	11 (0%)	38	72

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	196	SER
1	D	196	SER
1	S	270	PRO
1	G	254	GLN
1	A	266	GLY
1	P	265	GLU
1	A	254	GLN
1	P	270	PRO
1	V	15	PRO
1	G	196	SER
1	J	15	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	225/230 (98%)	202 (90%)	23 (10%)	8	26
1	D	227/230 (99%)	206 (91%)	21 (9%)	10	31
1	G	226/230 (98%)	207 (92%)	19 (8%)	13	36
1	J	225/230 (98%)	192 (85%)	33 (15%)	3	11
1	M	227/230 (99%)	203 (89%)	24 (11%)	8	24
1	P	226/230 (98%)	204 (90%)	22 (10%)	9	29
1	S	226/230 (98%)	202 (89%)	24 (11%)	8	24
1	V	226/230 (98%)	203 (90%)	23 (10%)	8	26
2	B	94/94 (100%)	83 (88%)	11 (12%)	6	18
2	E	94/94 (100%)	84 (89%)	10 (11%)	8	24
2	H	94/94 (100%)	84 (89%)	10 (11%)	8	24
2	K	94/94 (100%)	82 (87%)	12 (13%)	5	15
2	N	94/94 (100%)	85 (90%)	9 (10%)	10	29
2	Q	94/94 (100%)	87 (93%)	7 (7%)	16	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T	94/94 (100%)	84 (89%)	10 (11%)	8	24
2	W	94/94 (100%)	87 (93%)	7 (7%)	16	42
3	C	8/8 (100%)	8 (100%)	0	100	100
3	F	8/8 (100%)	6 (75%)	2 (25%)	1	2
3	I	8/8 (100%)	8 (100%)	0	100	100
3	L	8/8 (100%)	8 (100%)	0	100	100
3	O	8/8 (100%)	7 (88%)	1 (12%)	5	16
3	R	8/8 (100%)	4 (50%)	4 (50%)	0	0
3	U	8/8 (100%)	6 (75%)	2 (25%)	1	2
3	X	8/8 (100%)	7 (88%)	1 (12%)	5	16
All	All	2624/2656 (99%)	2349 (90%)	275 (10%)	8	24

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	14	ARG
1	A	19	ASP
1	A	32	GLN
1	A	35	ARG
1	A	48	ARG
1	A	52	VAL
1	A	98	MET
1	A	103	LEU
1	A	114	ARG
1	A	131	ARG
1	A	137	ASP
1	A	142	ILE
1	A	163	THR
1	A	178	GLU
1	A	179	THR
1	A	187	SER
1	A	197	ASP
1	A	207	LEU
1	A	217	THR
1	A	224	ASP
1	A	226	THR
1	A	227	GLN

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Mol	Chain	Res	Type
2	B	4	THR
2	B	16	GLU
2	B	33	SER
2	B	34	ASP
2	B	51	HIS
2	B	55	SER
2	B	58	LYS
2	B	70	PHE
2	B	75	LYS
2	B	77	GLU
2	B	99	MET
1	D	4	SER
1	D	6	ARG
1	D	12	VAL
1	D	14	ARG
1	D	17	ARG
1	D	35	ARG
1	D	58	GLU
1	D	87	GLN
1	D	89	GLU
1	D	114	ARG
1	D	128	GLU
1	D	137	ASP
1	D	144	ARG
1	D	158	ARG
1	D	188	THR
1	D	192	ARG
1	D	217	THR
1	D	224	ASP
1	D	255	GLU
1	D	256	GLN
1	D	268	VAL
2	E	27	VAL
2	E	33	SER
2	E	45	ARG
2	E	50	GLU
2	E	58	LYS
2	E	68	THR
2	E	70	PHE
2	E	94	LYS
2	E	97	ARG
2	E	99	MET

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Mol	Chain	Res	Type
3	F	1	LYS
3	F	8	THR
1	G	14	ARG
1	G	35	ARG
1	G	42	THR
1	G	48	ARG
1	G	52	VAL
1	G	79	ASP
1	G	80	THR
1	G	97	THR
1	G	114	ARG
1	G	116	ASP
1	G	131	ARG
1	G	137	ASP
1	G	158	ARG
1	G	159	ASN
1	G	182	ARG
1	G	197	ASP
1	G	199	GLU
1	G	223	GLU
1	G	249	VAL
2	H	11	SER
2	H	34	ASP
2	H	36	GLU
2	H	58	LYS
2	H	69	GLU
2	H	70	PHE
2	H	71	THR
2	H	76	ASP
2	H	77	GLU
2	H	97	ARG
1	J	14	ARG
1	J	19	ASP
1	J	21	ARG
1	J	34	VAL
1	J	35	ARG
1	J	42	THR
1	J	52	VAL
1	J	75	ARG
1	J	79	ASP
1	J	86	ASN
1	J	89	GLU

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Mol	Chain	Res	Type
1	J	103	LEU
1	J	114	ARG
1	J	130	LEU
1	J	131	ARG
1	J	138	THR
1	J	141	GLN
1	J	142	ILE
1	J	144	ARG
1	J	154	GLU
1	J	158	ARG
1	J	179	THR
1	J	192	ARG
1	J	198	HIS
1	J	207	LEU
1	J	224	ASP
1	J	226	THR
1	J	228	ASP
1	J	232	VAL
1	J	256	GLN
1	J	260	CYS
1	J	265	GLU
1	J	268	VAL
2	K	1	ILE
2	K	4	THR
2	K	6	LYS
2	K	9	VAL
2	K	16	GLU
2	K	31	HIS
2	K	39	LEU
2	K	47	GLU
2	K	57	SER
2	K	58	LYS
2	K	70	PHE
2	K	85	VAL
1	M	14	ARG
1	M	19	ASP
1	M	42	THR
1	M	52	VAL
1	M	54	GLN
1	M	64	THR
1	M	75	ARG
1	M	81	LEU

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Mol	Chain	Res	Type
1	M	88	SER
1	M	103	LEU
1	M	114	ARG
1	M	124	ILE
1	M	131	ARG
1	M	154	GLU
1	M	182	ARG
1	M	197	ASP
1	M	198	HIS
1	M	207	LEU
1	M	216	LEU
1	M	221	ASP
1	M	224	ASP
1	M	226	THR
1	M	256	GLN
1	M	257	ARG
2	N	50	GLU
2	N	58	LYS
2	N	70	PHE
2	N	75	LYS
2	N	77	GLU
2	N	81	ARG
2	N	89	GLN
2	N	92	ILE
2	N	99	MET
3	O	6	GLU
1	P	17	ARG
1	P	32	GLN
1	P	35	ARG
1	P	52	VAL
1	P	68	LYS
1	P	108	ARG
1	P	114	ARG
1	P	116	ASP
1	P	132	SER
1	P	144	ARG
1	P	157	TRP
1	P	158	ARG
1	P	163	THR
1	P	167	GLU
1	P	170	GLN
1	P	197	ASP

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Mol	Chain	Res	Type
1	P	207	LEU
1	P	217	THR
1	P	227	GLN
1	P	259	THR
1	P	261	HIS
1	P	271	VAL
2	Q	34	ASP
2	Q	38	ASP
2	Q	44	GLU
2	Q	48	LYS
2	Q	52	SER
2	Q	70	PHE
2	Q	80	CYS
3	R	1	LYS
3	R	6	GLU
3	R	7	LEU
3	R	8	THR
1	S	4	SER
1	S	12	VAL
1	S	14	ARG
1	S	19	ASP
1	S	42	THR
1	S	52	VAL
1	S	64	THR
1	S	94	THR
1	S	103	LEU
1	S	111	ARG
1	S	113	TYR
1	S	114	ARG
1	S	122	ASP
1	S	129	ASP
1	S	131	ARG
1	S	138	THR
1	S	144	ARG
1	S	154	GLU
1	S	158	ARG
1	S	190	VAL
1	S	192	ARG
1	S	207	LEU
1	S	259	THR
1	S	268	VAL
2	T	1	ILE

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Mol	Chain	Res	Type
2	T	4	THR
2	T	20	SER
2	T	31	HIS
2	T	34	ASP
2	T	57	SER
2	T	58	LYS
2	T	70	PHE
2	T	77	GLU
2	T	85	VAL
3	U	1	LYS
3	U	9	LYS
1	V	14	ARG
1	V	21	ARG
1	V	31	THR
1	V	35	ARG
1	V	42	THR
1	V	52	VAL
1	V	69	GLU
1	V	79	ASP
1	V	114	ARG
1	V	128	GLU
1	V	144	ARG
1	V	156	GLN
1	V	163	THR
1	V	164	THR
1	V	170	GLN
1	V	182	ARG
1	V	207	LEU
1	V	216	LEU
1	V	217	THR
1	V	226	THR
1	V	260	CYS
1	V	262	VAL
1	V	269	GLU
2	W	4	THR
2	W	58	LYS
2	W	59	ASP
2	W	70	PHE
2	W	91	LYS
2	W	94	LYS
2	W	99	MET
3	X	8	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	225	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	270/275 (98%)	-0.19	0 100 100	34, 48, 78, 125	0
1	D	271/275 (98%)	-0.18	0 100 100	32, 47, 81, 130	0
1	G	271/275 (98%)	-0.16	1 (0%) 92 92	32, 49, 82, 111	0
1	J	270/275 (98%)	-0.11	2 (0%) 87 86	35, 50, 81, 104	0
1	M	271/275 (98%)	-0.14	3 (1%) 80 79	35, 48, 82, 107	0
1	P	271/275 (98%)	-0.12	3 (1%) 80 79	34, 54, 84, 110	0
1	S	271/275 (98%)	-0.01	3 (1%) 80 79	33, 50, 84, 106	0
1	V	271/275 (98%)	-0.12	1 (0%) 92 92	35, 55, 88, 118	0
2	B	99/99 (100%)	0.18	1 (1%) 82 81	34, 45, 68, 83	0
2	E	99/99 (100%)	-0.06	2 (2%) 65 62	34, 44, 73, 87	0
2	H	99/99 (100%)	0.18	4 (4%) 39 34	33, 45, 74, 90	0
2	K	99/99 (100%)	-0.13	1 (1%) 82 81	35, 47, 77, 97	0
2	N	99/99 (100%)	-0.12	2 (2%) 65 62	34, 46, 75, 98	0
2	Q	99/99 (100%)	0.13	3 (3%) 51 44	36, 51, 80, 105	0
2	T	99/99 (100%)	0.01	2 (2%) 65 62	34, 49, 73, 101	0
2	W	99/99 (100%)	0.08	1 (1%) 82 81	36, 50, 77, 101	0
3	C	9/9 (100%)	-0.10	0 100 100	40, 51, 60, 60	0
3	F	9/9 (100%)	-0.04	0 100 100	34, 45, 53, 77	0
3	I	9/9 (100%)	-0.19	0 100 100	37, 42, 55, 69	0
3	L	9/9 (100%)	0.02	0 100 100	42, 48, 56, 75	0
3	O	9/9 (100%)	-0.12	0 100 100	37, 44, 55, 70	0
3	R	9/9 (100%)	0.01	0 100 100	36, 48, 53, 74	0
3	U	9/9 (100%)	0.05	0 100 100	37, 48, 56, 65	0
3	X	9/9 (100%)	-0.18	0 100 100	42, 48, 61, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3030/3064 (98%)	-0.09	29 (0%) 82 81	32, 49, 82, 130	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	W	79	ALA	4.9
2	N	68	THR	3.3
1	V	256	GLN	2.8
2	E	11	SER	2.8
2	H	23	LEU	2.8
1	J	198	HIS	2.8
2	B	15	ALA	2.8
1	M	254	GLN	2.8
1	S	198	HIS	2.7
2	Q	89	GLN	2.7
2	K	78	TYR	2.7
2	H	15	ALA	2.6
1	M	1	GLY	2.5
2	N	15	ALA	2.5
2	Q	79	ALA	2.4
1	P	1	GLY	2.4
1	S	1	GLY	2.4
2	T	78	TYR	2.4
1	P	197	ASP	2.3
2	T	92	ILE	2.2
1	J	253	GLY	2.2
1	P	216	LEU	2.2
2	H	48	LYS	2.2
1	G	108	ARG	2.2
1	S	252	SER	2.2
2	H	39	LEU	2.1
1	M	107	GLY	2.1
2	E	68	THR	2.0
2	Q	41	LYS	2.0

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

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

6.3 Carbohydrates [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.