



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2026 – 11:47 pm BST

PDB ID : 9SOL / pdb_00009sol
Title : Structure of TCR-581 in complex with Peptide-HLA
Authors : Karuppiah, V.; Rangel, V.L.
Deposited on : 2025-09-14
Resolution : 2.93 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

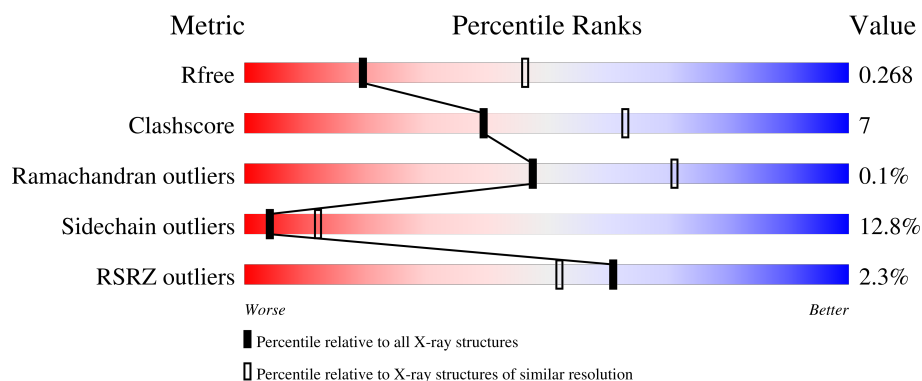
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	276	 79% 18% ..
1	F	276	 79% 18% .
1	K	276	 80% 17% .
1	P	276	 78% 19% .
2	B	100	 84% 12% .

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Mol	Chain	Length	Quality of chain
2	G	100	2% 84% 13% .
2	L	100	% 79% 14% 6% .
2	Q	100	% 84% 12% .
3	C	9	67% 33%
3	H	9	56% 44%
3	M	9	56% 44%
3	R	9	44% 33% 22%
4	D	208	2% 67% 19% 7% 6%
4	I	208	4% 65% 22% 6% 6%
4	N	208	4% 68% 21% 5% 6%
4	S	208	3% 65% 20% 8% 6%
5	E	242	2% 73% 23% ...
5	J	242	6% 70% 23% . ..
5	O	242	2% 75% 22% ..
5	T	242	4% 71% 23% . ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26430 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 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	F	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	K	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	P	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	G	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	L	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	Q	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769
L	0	MET	-	initiating methionine	UNP P61769
Q	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Piwi-like protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			80	52	13	15			
3	H	9	Total	C	N	O	0	0	0
			80	52	13	15			
3	M	9	Total	C	N	O	0	0	0
			80	52	13	15			
3	R	9	Total	C	N	O	0	0	0
			80	52	13	15			

- Molecule 4 is a protein called TCR alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	195	Total	C	N	O	S	0	0	0
			1512	936	254	314	8			
4	I	195	Total	C	N	O	S	0	0	0
			1512	936	254	314	8			
4	N	195	Total	C	N	O	S	0	0	0
			1512	936	254	314	8			
4	S	195	Total	C	N	O	S	0	0	0
			1512	936	254	314	8			

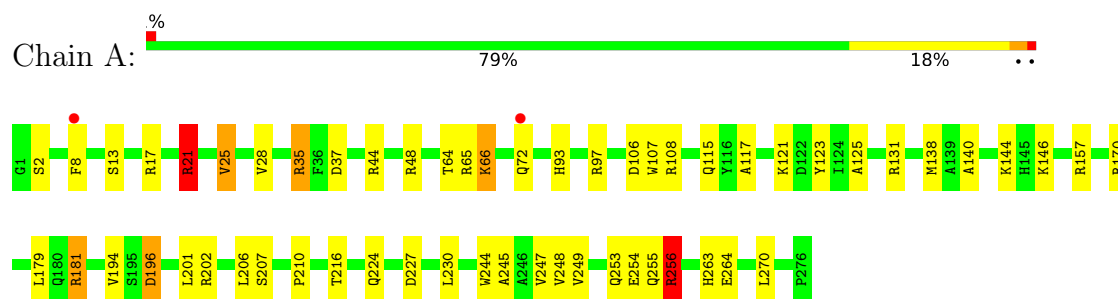
- Molecule 5 is a protein called TCR beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	240	Total	C	N	O	S	0	0	0
			1927	1214	346	358	9			
5	J	239	Total	C	N	O	S	0	0	0
			1922	1211	345	357	9			
5	O	240	Total	C	N	O	S	0	0	0
			1927	1214	346	358	9			
5	T	239	Total	C	N	O	S	0	0	0
			1922	1211	345	357	9			

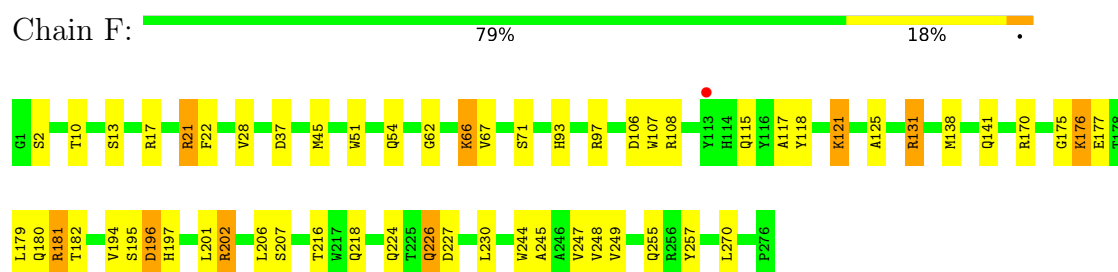
3 Residue-property plots

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

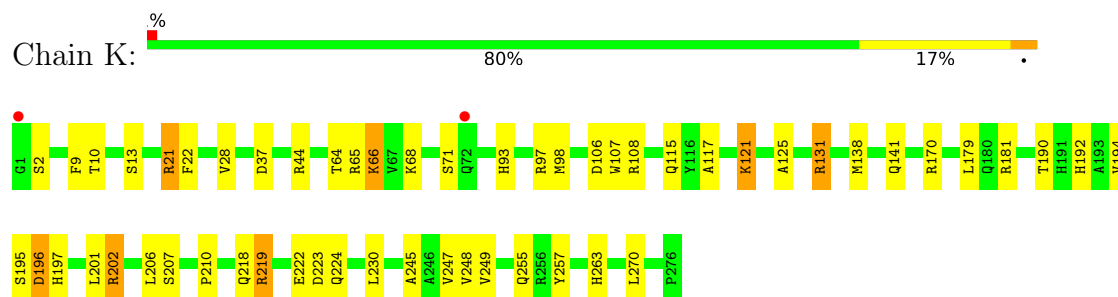
- Molecule 1: MHC class I antigen



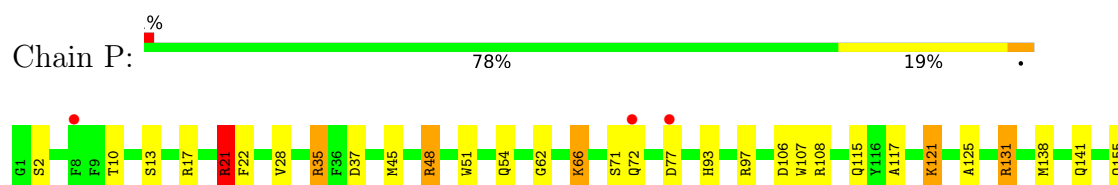
- Molecule 1: MHC class I antigen



- Molecule 1: MHC class I antigen

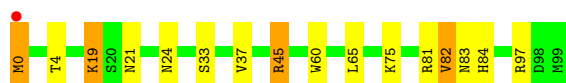
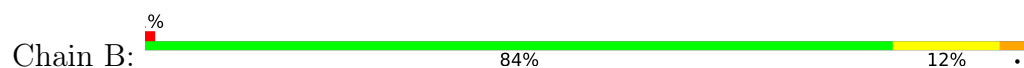


- Molecule 1: MHC class I antigen

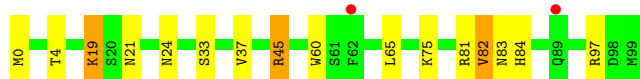
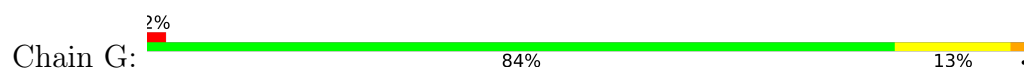




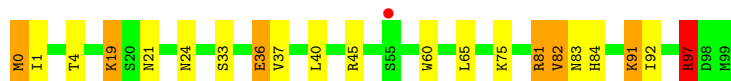
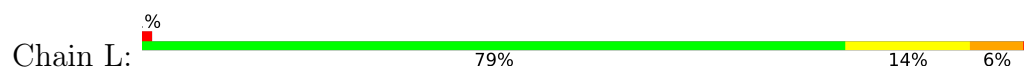
- Molecule 2: Beta-2-microglobulin



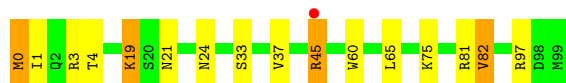
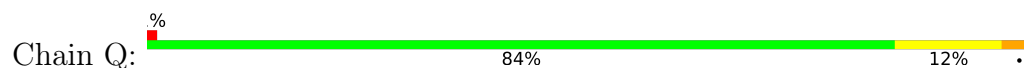
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



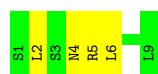
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Piwi-like protein 1

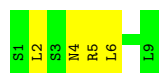


- Molecule 3: Piwi-like protein 1

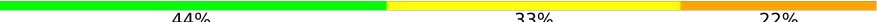


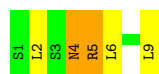
- Molecule 3: Piwi-like protein 1

Chain M:  56% 44%



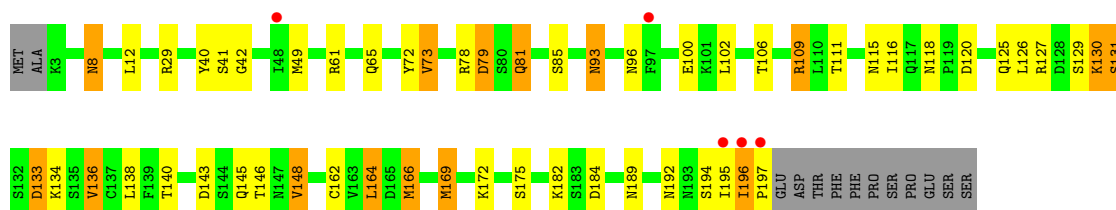
- Molecule 3: Piwi-like protein 1

Chain R:  44% 33% 22%



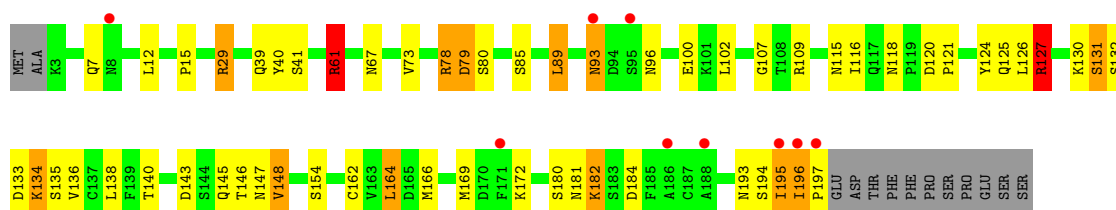
- Molecule 4: TCR alpha

Chain D:  2% 67% 19% 7% 6%



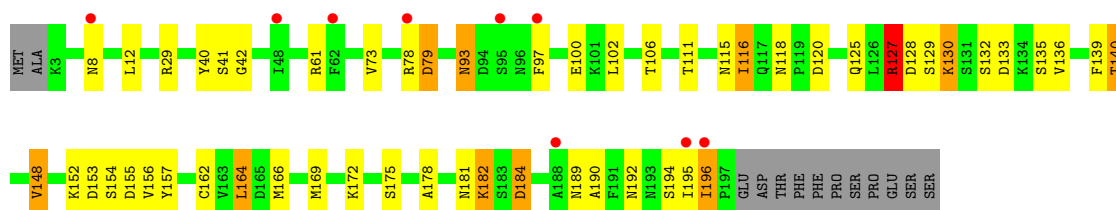
- Molecule 4: TCR alpha

Chain I:  4% 65% 22% 6% 6%



- Molecule 4: TCR alpha

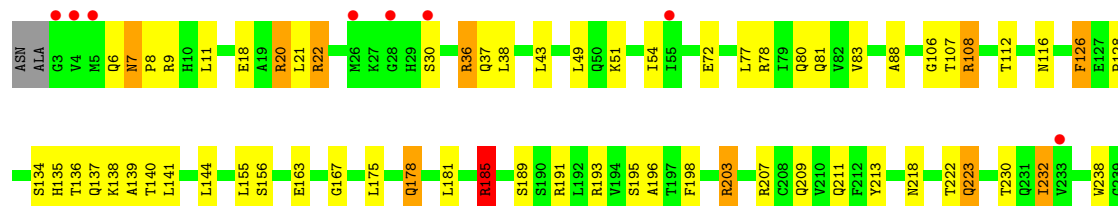
Chain N:  4% 68% 21% 5% 6%



- Molecule 4: TCR alpha

Chain S:  3% 65% 20% 8% 6%







4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	237.23Å 238.08Å 175.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	168.05 – 2.93 168.05 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.8 (168.05-2.93) 99.8 (168.05-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.232 , 0.270 0.240 , 0.268	Depositor DCC
R_{free} test set	5318 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	90.8	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 84.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h-1/2*k+1,-1/2*h-1/2*k-l,1/2 *h-1/2*k 0.000 for -1/2*h-1/2*k-l,-1/2*h-1/2*k+1,-1/ 2*h+1/2*k 0.000 for -1/2*h+1/2*k-l,1/2*h-1/2*k-l,-1/2 *h-1/2*k 0.000 for -1/2*h+1/2*k+1,1/2*h-1/2*k+1,1 /2*h+1/2*k 0.165 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	26430	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6169e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.70	0/2320	1.15	1/3149 (0.0%)
1	F	0.65	0/2320	1.16	0/3149
1	K	0.66	0/2320	1.17	0/3149
1	P	0.69	0/2320	1.16	0/3149
2	B	0.58	0/860	1.05	0/1162
2	G	0.54	0/860	1.02	0/1162
2	L	0.61	0/860	1.06	0/1162
2	Q	0.58	0/860	1.05	0/1162
3	C	0.79	0/81	1.17	0/107
3	H	0.74	0/81	1.12	0/107
3	M	0.77	0/81	1.16	0/107
3	R	0.72	0/81	1.22	0/107
4	D	0.73	0/1541	1.09	1/2087 (0.0%)
4	I	0.76	0/1541	1.16	1/2087 (0.0%)
4	N	0.75	0/1541	1.12	0/2087
4	S	0.73	0/1541	1.12	1/2087 (0.0%)
5	E	0.69	0/1980	1.13	0/2687
5	J	0.72	0/1975	1.17	1/2680 (0.0%)
5	O	0.64	0/1980	1.12	0/2687
5	T	0.66	0/1975	1.14	2/2680 (0.1%)
All	All	0.68	0/27118	1.13	7/36754 (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	A	0	9
1	F	0	5
1	K	0	6
1	P	0	9
2	B	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	2
2	L	0	1
2	Q	0	3
3	C	0	1
3	H	0	1
3	M	0	1
3	R	0	1
4	D	0	3
4	I	0	4
4	N	0	2
4	S	0	4
5	E	0	4
5	J	0	8
5	O	0	4
5	T	0	6
All	All	0	76

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ASP	N-CA-C	-6.29	104.87	113.30
5	T	106	GLY	CA-C-O	-5.83	118.20	122.23
5	J	106	GLY	CA-C-O	-5.74	118.27	122.23
4	D	133	ASP	N-CA-C	-5.44	106.14	112.89
5	T	126	PHE	CB-CA-C	5.40	118.71	109.80
4	I	107	GLY	CA-C-O	-5.37	118.45	122.37
4	S	193	ASN	N-CA-C	-5.17	105.76	111.71

There are no chirality outliers.

All (76) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	ARG	Sidechain
1	A	17	ARG	Sidechain
1	A	170	ARG	Sidechain
1	A	181	ARG	Sidechain
1	A	21	ARG	Sidechain
1	A	256	ARG	Sidechain
1	A	35	ARG	Sidechain
1	A	65	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	97	ARG	Sidechain
2	B	45	ARG	Sidechain
2	B	81	ARG	Sidechain
3	C	5	ARG	Sidechain
4	D	109	ARG	Sidechain
4	D	127	ARG	Sidechain
4	D	61	ARG	Sidechain
5	E	14	ARG	Sidechain
5	E	185	ARG	Sidechain
5	E	20	ARG	Sidechain
5	E	203	ARG	Sidechain
1	F	131	ARG	Sidechain
1	F	17	ARG	Sidechain
1	F	170	ARG	Sidechain
1	F	181	ARG	Sidechain
1	F	97	ARG	Sidechain
2	G	45	ARG	Sidechain
2	G	81	ARG	Sidechain
3	H	5	ARG	Sidechain
4	I	127	ARG	Sidechain
4	I	29	ARG	Sidechain
4	I	61	ARG	Sidechain
4	I	78	ARG	Sidechain
5	J	14	ARG	Sidechain
5	J	185	ARG	Sidechain
5	J	193	ARG	Sidechain
5	J	20	ARG	Sidechain
5	J	203	ARG	Sidechain
5	J	240	ARG	Sidechain
5	J	36	ARG	Sidechain
5	J	78	ARG	Sidechain
1	K	131	ARG	Sidechain
1	K	170	ARG	Sidechain
1	K	181	ARG	Sidechain
1	K	202	ARG	Sidechain
1	K	219	ARG	Sidechain
1	K	65	ARG	Sidechain
2	L	97	ARG	Sidechain
3	M	5	ARG	Sidechain
4	N	127	ARG	Sidechain
4	N	61	ARG	Sidechain
5	O	14	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	O	185	ARG	Sidechain
5	O	20	ARG	Sidechain
5	O	78	ARG	Sidechain
1	P	131	ARG	Sidechain
1	P	17	ARG	Sidechain
1	P	170	ARG	Sidechain
1	P	181	ARG	Sidechain
1	P	21	ARG	Sidechain
1	P	219	ARG	Sidechain
1	P	35	ARG	Sidechain
1	P	48	ARG	Sidechain
1	P	97	ARG	Sidechain
2	Q	3	ARG	Sidechain
2	Q	45	ARG	Sidechain
2	Q	81	ARG	Sidechain
3	R	5	ARG	Sidechain
4	S	109	ARG	Sidechain
4	S	127	ARG	Sidechain
4	S	61	ARG	Sidechain
4	S	78	ARG	Sidechain
5	T	108	ARG	Sidechain
5	T	185	ARG	Sidechain
5	T	20	ARG	Sidechain
5	T	22	ARG	Sidechain
5	T	78	ARG	Sidechain
5	T	9	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2254	0	2103	19	0
1	F	2254	0	2103	26	0
1	K	2254	0	2103	24	0
1	P	2254	0	2103	27	0
2	B	837	0	803	7	0
2	G	837	0	803	6	0
2	L	837	0	803	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	837	0	803	7	0
3	C	80	0	82	0	0
3	H	80	0	82	1	0
3	M	80	0	82	1	0
3	R	80	0	82	4	0
4	D	1512	0	1431	30	0
4	I	1512	0	1431	27	0
4	N	1512	0	1431	28	0
4	S	1512	0	1431	38	0
5	E	1927	0	1851	32	0
5	J	1922	0	1846	39	0
5	O	1927	0	1851	27	0
5	T	1922	0	1846	31	0
All	All	26430	0	25070	345	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 7.

All (345) 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)
5:T:36:ARG:HD3	5:T:38:LEU:HG	1.62	0.81
5:T:38:LEU:HD23	5:T:88:ALA:HB2	1.65	0.77
1:K:138:MET:HE3	1:K:141:GLN:HG3	1.68	0.76
1:P:138:MET:HE3	1:P:141:GLN:HG3	1.68	0.75
1:F:138:MET:HE3	1:F:141:GLN:HG3	1.68	0.75
5:J:36:ARG:HD3	5:J:38:LEU:HG	1.71	0.73
5:E:51:LYS:HG2	5:E:71:LYS:HA	1.70	0.72
1:P:35:ARG:HG2	1:P:48:ARG:HD3	1.72	0.70
4:D:126:LEU:HB3	5:E:126:PHE:HB3	1.74	0.70
5:E:38:LEU:HD23	5:E:88:ALA:HB2	1.75	0.69
4:S:189:ASN:HA	4:S:192:ASN:HB2	1.75	0.69
1:A:35:ARG:HG2	1:A:48:ARG:HD3	1.75	0.68
2:L:40:LEU:HD11	2:L:81:ARG:HB2	1.74	0.67
4:S:196:ILE:HG13	4:S:197:PRO:HD2	1.77	0.67
5:O:38:LEU:HD23	5:O:88:ALA:HB2	1.76	0.66
5:O:21:LEU:HD22	5:O:107:THR:HG21	1.78	0.66
4:D:189:ASN:HA	4:D:192:ASN:HB2	1.76	0.66
5:T:128:PRO:HB3	5:T:139:ALA:HB1	1.77	0.65
5:J:38:LEU:HD23	5:J:88:ALA:HB2	1.77	0.65
5:O:178:GLN:HG3	5:O:181:LEU:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:164:LEU:HD22	5:T:193:ARG:CZ	2.28	0.64
5:E:36:ARG:HD3	5:E:38:LEU:HG	1.79	0.64
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.79	0.64
1:K:28:VAL:HG11	1:K:179:LEU:HD13	1.80	0.64
5:T:185:ARG:HH11	5:T:185:ARG:HG3	1.62	0.64
5:O:36:ARG:HD3	5:O:38:LEU:HG	1.80	0.64
5:J:132:GLU:HB3	5:J:139:ALA:HA	1.82	0.62
5:E:185:ARG:HH11	5:E:185:ARG:HG3	1.64	0.62
4:N:164:LEU:HD22	5:O:193:ARG:CZ	2.30	0.62
5:T:21:LEU:HD22	5:T:107:THR:HG21	1.81	0.62
5:O:185:ARG:HH11	5:O:185:ARG:HG3	1.64	0.61
1:F:28:VAL:HG11	1:F:179:LEU:HD13	1.82	0.61
5:J:185:ARG:HH11	5:J:185:ARG:HG3	1.65	0.60
4:D:148:VAL:HA	4:D:194:SER:HB3	1.82	0.60
4:N:189:ASN:HA	4:N:192:ASN:HB2	1.84	0.60
4:S:192:ASN:HA	4:S:196:ILE:HD13	1.84	0.60
5:T:178:GLN:HG3	5:T:181:LEU:HD12	1.84	0.60
5:J:178:GLN:HG3	5:J:181:LEU:HD12	1.83	0.60
5:E:178:GLN:HG3	5:E:181:LEU:HD12	1.83	0.59
5:T:207:ARG:NH2	5:T:209:GLN:OE1	2.34	0.59
1:A:202:ARG:HD3	1:A:244:TRP:CD2	2.38	0.59
4:S:164:LEU:HD12	5:T:167:GLY:O	2.03	0.59
5:O:207:ARG:NH2	5:O:209:GLN:OE1	2.34	0.59
4:D:196:ILE:HG13	4:D:197:PRO:HD2	1.85	0.58
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.38	0.58
5:E:128:PRO:HB3	5:E:139:ALA:HB1	1.87	0.57
5:E:37:GLN:HB2	5:E:43:LEU:HD12	1.87	0.57
1:P:202:ARG:HD3	1:P:244:TRP:CD2	2.39	0.57
5:J:197:THR:O	5:J:198:PHE:C	2.48	0.57
1:P:195:SER:C	1:P:197:HIS:H	2.12	0.57
4:D:164:LEU:HD12	5:E:167:GLY:O	2.04	0.57
1:A:249:VAL:HG11	1:A:254:GLU:HA	1.85	0.56
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.40	0.56
4:S:188:ALA:C	4:S:190:ALA:H	2.13	0.56
1:K:195:SER:C	1:K:197:HIS:H	2.13	0.56
4:S:125:GLN:HE22	4:S:127:ARG:HD3	1.70	0.56
1:F:195:SER:C	1:F:197:HIS:H	2.12	0.56
4:I:126:LEU:HB3	5:J:126:PHE:HB3	1.87	0.56
4:I:196:ILE:O	4:I:197:PRO:C	2.48	0.56
5:J:21:LEU:HD22	5:J:107:THR:HG21	1.87	0.56
5:T:49:LEU:HD23	5:T:54:ILE:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:196:ASP:OD1	1:P:196:ASP:N	2.39	0.56
4:N:78:ARG:O	4:N:79:ASP:C	2.48	0.55
1:K:13:SER:HB2	1:K:93:HIS:H	1.71	0.55
1:K:66:LYS:HG3	4:N:97:PHE:HE1	1.72	0.55
5:E:21:LEU:HD22	5:E:107:THR:HG21	1.87	0.55
1:A:13:SER:HB2	1:A:93:HIS:H	1.72	0.55
1:P:13:SER:HB2	1:P:93:HIS:H	1.70	0.55
5:J:195:SER:O	5:J:196:ALA:C	2.50	0.55
5:E:201:ASP:HB3	5:E:203:ARG:HG3	1.88	0.55
5:E:207:ARG:NH2	5:E:209:GLN:OE1	2.33	0.55
5:J:207:ARG:NH2	5:J:209:GLN:OE1	2.35	0.54
1:F:202:ARG:HD3	1:F:244:TRP:CD2	2.42	0.54
4:S:78:ARG:O	4:S:79:ASP:C	2.49	0.54
1:A:106:ASP:OD2	1:A:108:ARG:HD3	2.07	0.54
1:F:106:ASP:OD2	1:F:108:ARG:HD3	2.08	0.54
5:J:213:TYR:HA	5:J:230:THR:HG23	1.89	0.54
1:K:218:GLN:HG2	1:K:223:ASP:HA	1.89	0.54
5:T:213:TYR:HA	5:T:230:THR:HG23	1.88	0.54
1:P:106:ASP:OD2	1:P:108:ARG:HD3	2.07	0.54
4:N:115:ASN:O	4:N:116:ILE:C	2.50	0.54
5:E:202:PRO:HA	5:E:239:GLY:HA3	1.89	0.53
5:O:128:PRO:HB3	5:O:139:ALA:HB1	1.89	0.53
3:R:4:ASN:ND2	4:S:96:ASN:OD1	2.41	0.53
4:D:164:LEU:HD22	5:E:193:ARG:CZ	2.38	0.53
5:E:213:TYR:HA	5:E:230:THR:HG23	1.89	0.53
1:K:196:ASP:OD1	1:K:196:ASP:N	2.41	0.53
4:I:166:MET:HE1	5:J:138:LYS:HD2	1.91	0.53
4:N:140:THR:HG22	4:N:175:SER:HB3	1.91	0.53
5:O:213:TYR:HA	5:O:230:THR:HG23	1.89	0.53
2:Q:24:ASN:HB3	2:Q:65:LEU:HD11	1.90	0.53
1:K:106:ASP:OD2	1:K:108:ARG:HD3	2.09	0.52
1:K:121:LYS:HG2	2:L:1:ILE:HG12	1.92	0.52
4:N:164:LEU:HD12	5:O:167:GLY:O	2.09	0.52
4:D:115:ASN:ND2	4:I:67:ASN:HD21	2.07	0.52
4:D:116:ILE:HG21	4:D:143:ASP:HA	1.92	0.52
1:K:117:ALA:HB2	2:L:60:TRP:CE2	2.45	0.52
2:L:37:VAL:HG22	2:L:82:VAL:HB	1.92	0.52
4:S:116:ILE:HG21	4:S:143:ASP:HA	1.92	0.52
2:G:24:ASN:HB3	2:G:65:LEU:HD11	1.91	0.52
4:I:148:VAL:HA	4:I:194:SER:HB3	1.91	0.52
4:N:42:GLY:O	5:O:108:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:153:ASP:HB3	4:S:156:VAL:HB	1.92	0.51
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.92	0.51
4:D:42:GLY:O	5:E:108:ARG:NH2	2.43	0.51
5:J:159:VAL:HG11	5:J:198:PHE:HE2	1.75	0.51
1:K:192:HIS:HE1	1:K:202:ARG:HE	1.57	0.51
5:O:140:THR:HG23	5:O:193:ARG:HG2	1.93	0.51
4:I:78:ARG:O	4:I:80:SER:N	2.44	0.51
5:T:37:GLN:HB2	5:T:43:LEU:HD12	1.91	0.51
4:D:126:LEU:HB2	4:D:136:VAL:HG12	1.93	0.51
4:I:116:ILE:HG21	4:I:143:ASP:HA	1.93	0.51
2:L:83:ASN:OD1	2:L:84:HIS:N	2.43	0.51
1:P:117:ALA:HB2	2:Q:60:TRP:CE2	2.46	0.50
2:L:24:ASN:HB3	2:L:65:LEU:HD11	1.93	0.50
5:T:140:THR:HG23	5:T:193:ARG:HG2	1.94	0.50
5:J:132:GLU:HB3	5:J:138:LYS:O	2.11	0.50
5:E:140:THR:HG23	5:E:193:ARG:HG2	1.94	0.50
2:B:83:ASN:OD1	2:B:84:HIS:N	2.43	0.50
4:N:128:ASP:C	4:N:130:LYS:H	2.20	0.49
4:S:131:SER:O	4:S:133:ASP:N	2.45	0.49
4:S:147:ASN:HB2	4:S:195:ILE:HG13	1.93	0.49
1:F:51:TRP:O	1:F:54:GLN:HG2	2.12	0.49
4:N:182:LYS:C	4:N:184:ASP:H	2.20	0.49
5:E:137:GLN:O	5:E:196:ALA:N	2.39	0.49
5:J:140:THR:HG23	5:J:193:ARG:HG2	1.93	0.49
1:P:51:TRP:O	1:P:54:GLN:HG2	2.12	0.49
1:P:202:ARG:HD3	1:P:244:TRP:CE3	2.47	0.49
5:O:21:LEU:HD12	5:O:77:LEU:HD23	1.95	0.49
4:S:49:MET:HE2	4:S:49:MET:HB3	1.76	0.49
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.48	0.49
4:D:49:MET:HE2	4:D:49:MET:HB3	1.70	0.49
5:J:128:PRO:HG2	5:J:139:ALA:HB1	1.95	0.49
4:I:164:LEU:HD11	4:I:166:MET:HE2	1.95	0.48
4:I:164:LEU:HD22	5:J:193:ARG:CZ	2.43	0.48
1:K:249:VAL:HG22	1:K:257:TYR:CZ	2.48	0.48
1:P:249:VAL:HG22	1:P:257:TYR:CZ	2.48	0.48
1:F:13:SER:HB2	1:F:93:HIS:H	1.78	0.48
4:D:164:LEU:HD11	4:D:166:MET:HE2	1.94	0.48
1:F:196:ASP:OD1	1:F:196:ASP:N	2.39	0.48
1:F:22:PHE:CE2	1:F:71:SER:HA	2.49	0.48
1:F:249:VAL:HG22	1:F:257:TYR:CZ	2.48	0.48
5:O:137:GLN:O	5:O:196:ALA:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:175:GLY:O	1:P:176:LYS:C	2.56	0.48
4:S:188:ALA:C	4:S:190:ALA:N	2.72	0.48
5:J:158:TRP:HA	5:J:162:LYS:O	2.14	0.48
1:A:44:ARG:HA	1:A:64:THR:HG23	1.96	0.47
4:I:124:TYR:CE2	5:J:132:GLU:HG3	2.49	0.47
5:J:129:SER:N	5:J:132:GLU:OE1	2.47	0.47
4:S:125:GLN:NE2	4:S:127:ARG:HD3	2.28	0.47
4:S:152:LYS:HA	4:S:152:LYS:HD3	1.66	0.47
4:S:40:TYR:O	4:S:41:SER:C	2.57	0.47
1:F:202:ARG:HD3	1:F:244:TRP:CE3	2.49	0.47
1:P:28:VAL:HG11	1:P:179:LEU:HD13	1.95	0.47
4:D:120:ASP:OD2	5:E:135:HIS:CD2	2.67	0.47
1:F:118:TYR:O	1:F:121:LYS:HG3	2.14	0.47
2:G:83:ASN:OD1	2:G:84:HIS:N	2.43	0.47
4:I:145:GLN:O	4:I:146:THR:C	2.58	0.47
1:K:22:PHE:CE2	1:K:71:SER:HA	2.50	0.47
1:P:22:PHE:CE2	1:P:71:SER:HA	2.50	0.47
4:S:126:LEU:HB2	4:S:136:VAL:HG12	1.96	0.47
4:D:93:ASN:OD1	4:D:100:GLU:HA	2.14	0.47
4:N:93:ASN:OD1	4:N:100:GLU:HA	2.15	0.47
1:P:21:ARG:NH1	1:P:37:ASP:OD1	2.48	0.47
1:P:121:LYS:HG2	2:Q:1:ILE:HG12	1.96	0.47
4:I:40:TYR:O	4:I:41:SER:C	2.57	0.47
4:S:164:LEU:HD11	4:S:166:MET:HE2	1.97	0.47
4:N:139:PHE:O	4:N:175:SER:HA	2.15	0.47
4:N:153:ASP:HB3	4:N:156:VAL:HB	1.97	0.46
4:D:145:GLN:O	4:D:146:THR:C	2.58	0.46
5:T:137:GLN:O	5:T:196:ALA:N	2.40	0.46
5:T:80:GLN:O	5:T:81:GLN:C	2.58	0.46
1:A:210:PRO:HD2	1:A:263:HIS:CE1	2.51	0.46
4:D:175:SER:OG	5:E:193:ARG:NH1	2.48	0.46
4:I:164:LEU:HD12	5:J:167:GLY:O	2.15	0.46
5:T:21:LEU:HD12	5:T:77:LEU:HD23	1.97	0.46
4:S:39:GLN:HB2	4:S:89:LEU:HD11	1.97	0.46
1:A:21:ARG:NH1	1:A:37:ASP:OD1	2.49	0.46
5:O:240:ARG:HH11	5:O:240:ARG:HG2	1.81	0.46
4:I:127:ARG:HD2	4:I:127:ARG:HA	1.69	0.46
1:K:210:PRO:HD2	1:K:263:HIS:CE1	2.50	0.46
2:L:0:MET:HB2	2:L:0:MET:HE2	1.64	0.46
4:S:139:PHE:O	4:S:175:SER:HA	2.15	0.46
4:N:40:TYR:O	4:N:41:SER:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:148:VAL:HA	4:N:194:SER:HB3	1.97	0.46
4:D:40:TYR:O	4:D:41:SER:C	2.59	0.46
1:F:45:MET:CE	3:H:2:LEU:HD11	2.46	0.46
5:J:134:SER:OG	5:J:135:HIS:N	2.48	0.46
4:D:130:LYS:HB2	4:D:131:SER:H	1.49	0.46
1:F:175:GLY:O	1:F:176:LYS:C	2.59	0.46
2:G:19:LYS:HE2	2:G:21:ASN:ND2	2.31	0.46
5:J:240:ARG:HE	5:J:240:ARG:HB3	1.62	0.46
4:D:130:LYS:O	4:D:131:SER:C	2.59	0.45
5:J:199:TRP:O	5:J:200:GLN:C	2.59	0.45
1:F:176:LYS:HA	1:F:180:GLN:HG3	1.99	0.45
1:K:230:LEU:HD12	1:K:245:ALA:HB2	1.99	0.45
1:P:45:MET:CE	3:R:2:LEU:HD11	2.46	0.45
4:S:134:LYS:HB3	4:S:134:LYS:HE2	1.58	0.45
5:E:80:GLN:O	5:E:81:GLN:C	2.59	0.45
2:L:19:LYS:HE2	2:L:21:ASN:ND2	2.31	0.45
4:I:182:LYS:HB3	4:I:182:LYS:HE2	1.36	0.45
2:Q:19:LYS:HE2	2:Q:21:ASN:ND2	2.31	0.45
1:F:106:ASP:O	1:F:107:TRP:HB2	2.16	0.45
4:I:115:ASN:O	4:I:116:ILE:C	2.60	0.45
5:J:37:GLN:HB2	5:J:43:LEU:HD12	1.98	0.45
1:F:117:ALA:HB2	2:G:60:TRP:CD2	2.52	0.45
5:E:240:ARG:HH11	5:E:240:ARG:HG2	1.81	0.45
4:S:126:LEU:HB3	5:T:126:PHE:HB3	1.98	0.45
1:F:230:LEU:HD12	1:F:245:ALA:HB2	1.99	0.45
1:P:230:LEU:HD12	1:P:245:ALA:HB2	1.99	0.45
5:T:240:ARG:HG2	5:T:240:ARG:HH11	1.82	0.45
2:B:19:LYS:HE2	2:B:21:ASN:ND2	2.32	0.45
5:E:50:GLN:O	5:E:51:LYS:C	2.60	0.45
1:P:158:ALA:O	1:P:159:TYR:C	2.60	0.45
4:S:127:ARG:HA	4:S:127:ARG:HD2	1.68	0.45
5:J:197:THR:OG1	5:J:198:PHE:N	2.49	0.44
1:K:64:THR:HG22	1:K:68:LYS:HD2	1.99	0.44
1:P:210:PRO:HD2	1:P:263:HIS:CE1	2.52	0.44
4:D:72:TYR:CG	4:I:15:PRO:HG2	2.52	0.44
4:I:39:GLN:HB2	4:I:89:LEU:HD11	1.99	0.44
4:N:189:ASN:O	4:N:190:ALA:C	2.60	0.44
4:I:134:LYS:HB3	4:I:134:LYS:HE2	1.67	0.44
2:L:91:LYS:HE2	2:L:91:LYS:HB2	1.85	0.44
4:N:127:ARG:O	5:O:126:PHE:HA	2.18	0.44
5:E:14:ARG:HB2	5:E:115:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:21:ARG:NH1	1:K:37:ASP:OD1	2.50	0.44
4:S:132:SER:O	4:S:133:ASP:C	2.60	0.44
4:N:128:ASP:C	4:N:130:LYS:N	2.73	0.44
5:J:185:ARG:HG3	5:J:185:ARG:NH1	2.33	0.44
5:T:8:PRO:HG2	5:T:11:LEU:HB2	1.99	0.44
5:E:26:MET:O	5:E:27:LYS:C	2.60	0.44
5:J:201:ASP:HB2	5:J:203:ARG:NH1	2.32	0.44
1:K:44:ARG:HA	1:K:64:THR:HG23	1.98	0.44
5:O:26:MET:O	5:O:27:LYS:C	2.61	0.44
3:M:2:LEU:HD23	3:M:2:LEU:HA	1.84	0.44
4:N:157:TYR:O	4:N:178:ALA:HA	2.17	0.44
4:D:115:ASN:O	4:D:116:ILE:C	2.60	0.43
4:S:166:MET:HE3	4:S:166:MET:HB2	1.91	0.43
5:J:80:GLN:O	5:J:81:GLN:C	2.60	0.43
5:T:195:SER:O	5:T:196:ALA:C	2.61	0.43
5:E:185:ARG:HG3	5:E:185:ARG:NH1	2.33	0.43
1:F:226:GLN:HB3	1:F:227:ASP:H	1.64	0.43
4:N:182:LYS:C	4:N:184:ASP:N	2.76	0.43
5:O:195:SER:O	5:O:196:ALA:C	2.61	0.43
2:B:37:VAL:HG22	2:B:82:VAL:HB	2.00	0.43
1:F:21:ARG:NH1	1:F:37:ASP:OD1	2.51	0.43
4:I:147:ASN:O	4:I:195:ILE:HB	2.19	0.43
4:N:166:MET:HE3	4:N:166:MET:HB2	1.92	0.43
1:P:62:GLY:O	1:P:66:LYS:HB2	2.19	0.43
4:S:157:TYR:O	4:S:178:ALA:HA	2.18	0.43
5:T:185:ARG:HH11	5:T:185:ARG:CG	2.29	0.43
4:N:155:ASP:HB3	4:N:181:ASN:HD22	1.83	0.43
4:S:115:ASN:O	4:S:116:ILE:C	2.60	0.43
4:S:128:ASP:OD1	4:S:132:SER:N	2.51	0.43
4:S:152:LYS:HG2	4:S:193:ASN:HB3	2.00	0.43
1:F:115:GLN:HG2	1:F:125:ALA:HB1	2.01	0.43
5:O:80:GLN:O	5:O:81:GLN:C	2.62	0.43
5:E:134:SER:C	5:E:135:HIS:CG	2.97	0.43
5:T:128:PRO:HD3	5:T:141:LEU:HG	2.01	0.43
4:D:8:ASN:OD1	4:D:8:ASN:N	2.51	0.43
5:J:31:HIS:ND1	5:J:48:TYR:OH	2.45	0.43
5:T:7:ASN:HB2	5:T:22:ARG:CZ	2.48	0.43
5:T:116:ASN:OD1	5:T:223:GLN:HG3	2.19	0.43
5:E:195:SER:O	5:E:196:ALA:C	2.61	0.42
1:K:106:ASP:O	1:K:107:TRP:HB2	2.19	0.42
5:E:20:ARG:HE	5:E:20:ARG:HB3	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:196:ALA:O	5:J:197:THR:C	2.62	0.42
5:T:134:SER:C	5:T:135:HIS:CG	2.97	0.42
2:G:37:VAL:HG22	2:G:82:VAL:HB	2.02	0.42
5:J:196:ALA:O	5:J:200:GLN:N	2.41	0.42
5:J:204:ASN:O	5:J:238:TRP:HA	2.19	0.42
5:O:121:PRO:HD3	5:O:212:PHE:HB2	2.01	0.42
1:K:121:LYS:HE2	1:K:121:LYS:HB2	1.39	0.42
1:P:51:TRP:CD1	1:P:51:TRP:H	2.37	0.42
1:P:106:ASP:O	1:P:107:TRP:HB2	2.18	0.42
4:D:166:MET:HE3	4:D:166:MET:HB2	1.95	0.42
4:I:79:ASP:O	4:I:80:SER:C	2.63	0.42
5:J:185:ARG:HH11	5:J:185:ARG:CG	2.30	0.42
5:O:198:PHE:O	5:O:203:ARG:NH1	2.51	0.42
4:S:128:ASP:C	4:S:130:LYS:H	2.27	0.42
1:A:117:ALA:HB2	2:B:60:TRP:CD2	2.54	0.42
4:D:196:ILE:HD12	4:D:196:ILE:HA	1.89	0.42
1:F:62:GLY:O	1:F:66:LYS:HB2	2.20	0.42
4:N:164:LEU:HD11	4:N:166:MET:HE2	2.02	0.42
5:T:155:LEU:HD13	5:T:156:SER:N	2.35	0.42
1:K:9:PHE:CD2	1:K:97:ARG:HD2	2.55	0.42
5:T:198:PHE:O	5:T:203:ARG:NH1	2.51	0.42
4:N:164:LEU:HD13	5:O:193:ARG:CG	2.50	0.42
1:A:230:LEU:HD12	1:A:245:ALA:HB2	2.01	0.42
1:A:253:GLN:HB3	1:A:256:ARG:HD3	2.00	0.42
1:P:195:SER:C	1:P:197:HIS:N	2.75	0.42
5:E:155:LEU:HD13	5:E:156:SER:N	2.35	0.41
1:P:77:ASP:HB3	3:R:9:LEU:HD12	2.02	0.41
1:A:8:PHE:HB2	1:A:25:VAL:HG23	2.02	0.41
1:A:106:ASP:O	1:A:107:TRP:HB2	2.20	0.41
1:K:97:ARG:HG2	1:K:98:MET:N	2.35	0.41
2:L:36:GLU:HG3	2:L:83:ASN:HB3	2.02	0.41
4:N:164:LEU:HD13	5:O:193:ARG:CD	2.50	0.41
1:F:51:TRP:H	1:F:51:TRP:CD1	2.37	0.41
4:I:131:SER:OG	4:I:132:SER:N	2.52	0.41
1:K:115:GLN:HG2	1:K:125:ALA:HB1	2.03	0.41
4:S:128:ASP:OD1	4:S:134:LYS:HB2	2.20	0.41
5:E:185:ARG:HH11	5:E:185:ARG:CG	2.30	0.41
4:I:132:SER:C	4:I:134:LYS:N	2.77	0.41
5:J:46:MET:HE2	5:J:46:MET:HB3	1.97	0.41
5:O:116:ASN:OD1	5:O:223:GLN:HG3	2.21	0.41
4:D:78:ARG:O	4:D:79:ASP:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:14:ARG:HB2	5:J:115:LEU:HD21	2.02	0.41
4:D:164:LEU:HD23	4:D:164:LEU:O	2.20	0.41
4:D:169:MET:HE2	4:D:169:MET:HB2	1.93	0.41
1:F:22:PHE:CD2	1:F:71:SER:HA	2.55	0.41
4:I:124:TYR:HE2	5:J:132:GLU:HG3	1.86	0.41
5:O:155:LEU:HD13	5:O:156:SER:N	2.36	0.41
4:S:128:ASP:C	4:S:130:LYS:N	2.79	0.41
4:S:164:LEU:HD13	5:T:193:ARG:CD	2.51	0.41
5:T:138:LYS:CG	5:T:193:ARG:HB3	2.51	0.41
1:A:123:TYR:CZ	1:A:140:ALA:HA	2.56	0.41
4:I:61:ARG:O	4:I:78:ARG:HG2	2.20	0.41
5:O:185:ARG:HH11	5:O:185:ARG:CG	2.30	0.41
5:T:211:GLN:NE2	5:T:232:ILE:HG22	2.36	0.41
1:F:45:MET:HE2	1:F:67:VAL:HB	2.02	0.41
1:K:190:THR:HG1	1:K:192:HIS:CE1	2.38	0.41
1:A:66:LYS:HB2	1:A:66:LYS:HE3	1.57	0.41
1:A:115:GLN:HG2	1:A:125:ALA:HB1	2.03	0.41
2:L:97:ARG:H	2:L:97:ARG:HG3	1.56	0.41
1:P:115:GLN:HG2	1:P:125:ALA:HB1	2.03	0.41
2:Q:0:MET:HE3	2:Q:0:MET:HB2	1.64	0.41
2:Q:19:LYS:HE2	2:Q:21:ASN:HD22	1.86	0.41
2:Q:37:VAL:HG22	2:Q:82:VAL:HB	2.02	0.41
4:S:65:GLN:O	4:S:73:VAL:HA	2.21	0.41
2:B:0:MET:HE3	2:B:0:MET:HB2	1.61	0.40
5:J:211:GLN:NE2	5:J:232:ILE:HG22	2.36	0.40
4:N:196:ILE:HD12	4:N:196:ILE:HA	1.78	0.40
1:P:155:GLN:HB3	3:R:5:ARG:HH11	1.86	0.40
4:D:65:GLN:O	4:D:73:VAL:HA	2.21	0.40
5:J:159:VAL:HG22	5:J:206:PHE:HD1	1.85	0.40
2:L:19:LYS:HE2	2:L:21:ASN:HD22	1.86	0.40
4:N:164:LEU:O	4:N:164:LEU:HD23	2.21	0.40
4:S:164:LEU:O	4:S:164:LEU:HD23	2.21	0.40
4:S:175:SER:OG	5:T:191:ARG:HD2	2.21	0.40
4:D:175:SER:OG	5:E:191:ARG:HD2	2.20	0.40
4:I:93:ASN:OD1	4:I:100:GLU:HA	2.21	0.40
4:D:79:ASP:O	4:D:81:GLN:NE2	2.54	0.40
4:I:120:ASP:O	4:I:121:PRO:C	2.64	0.40
4:N:164:LEU:HD13	5:O:193:ARG:HG3	2.03	0.40

There are no symmetry-related clashes.

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	274/276 (99%)	259 (94%)	15 (6%)	0	100	100
1	F	274/276 (99%)	259 (94%)	15 (6%)	0	100	100
1	K	274/276 (99%)	262 (96%)	12 (4%)	0	100	100
1	P	274/276 (99%)	257 (94%)	17 (6%)	0	100	100
2	B	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
2	G	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	L	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	Q	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	7 (100%)	0	0	100	100
3	M	7/9 (78%)	7 (100%)	0	0	100	100
3	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	193/208 (93%)	173 (90%)	19 (10%)	1 (0%)	24	49
4	I	193/208 (93%)	170 (88%)	22 (11%)	1 (0%)	24	49
4	N	193/208 (93%)	179 (93%)	13 (7%)	1 (0%)	24	49
4	S	193/208 (93%)	175 (91%)	17 (9%)	1 (0%)	24	49
5	E	238/242 (98%)	218 (92%)	20 (8%)	0	100	100
5	J	237/242 (98%)	215 (91%)	22 (9%)	0	100	100
5	O	238/242 (98%)	218 (92%)	20 (8%)	0	100	100
5	T	237/242 (98%)	217 (92%)	20 (8%)	0	100	100
All	All	3238/3340 (97%)	3003 (93%)	231 (7%)	4 (0%)	48	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	79	ASP

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Mol	Chain	Res	Type
4	N	79	ASP
4	S	79	ASP
4	D	79	ASP

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	232/232 (100%)	207 (89%)	25 (11%)	6	17
1	F	232/232 (100%)	208 (90%)	24 (10%)	7	18
1	K	232/232 (100%)	214 (92%)	18 (8%)	11	28
1	P	232/232 (100%)	211 (91%)	21 (9%)	9	22
2	B	95/95 (100%)	87 (92%)	8 (8%)	10	25
2	G	95/95 (100%)	87 (92%)	8 (8%)	10	25
2	L	95/95 (100%)	83 (87%)	12 (13%)	4	12
2	Q	95/95 (100%)	87 (92%)	8 (8%)	10	25
3	C	9/9 (100%)	7 (78%)	2 (22%)	1	2
3	H	9/9 (100%)	7 (78%)	2 (22%)	1	2
3	M	9/9 (100%)	7 (78%)	2 (22%)	1	2
3	R	9/9 (100%)	7 (78%)	2 (22%)	1	2
4	D	174/186 (94%)	142 (82%)	32 (18%)	1	4
4	I	174/186 (94%)	139 (80%)	35 (20%)	1	3
4	N	174/186 (94%)	143 (82%)	31 (18%)	2	4
4	S	174/186 (94%)	141 (81%)	33 (19%)	1	3
5	E	207/209 (99%)	180 (87%)	27 (13%)	4	11
5	J	207/209 (99%)	180 (87%)	27 (13%)	4	11
5	O	207/209 (99%)	181 (87%)	26 (13%)	4	12
5	T	207/209 (99%)	183 (88%)	24 (12%)	5	15
All	All	2868/2924 (98%)	2501 (87%)	367 (13%)	4	12

All (367) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	21	ARG
1	A	25	VAL
1	A	66	LYS
1	A	72	GLN
1	A	121	LYS
1	A	131	ARG
1	A	138	MET
1	A	144	LYS
1	A	146	LYS
1	A	181	ARG
1	A	194	VAL
1	A	196	ASP
1	A	201	LEU
1	A	206	LEU
1	A	207	SER
1	A	216	THR
1	A	224	GLN
1	A	227	ASP
1	A	247	VAL
1	A	248	VAL
1	A	255	GLN
1	A	256	ARG
1	A	264	GLU
1	A	270	LEU
2	B	0	MET
2	B	4	THR
2	B	19	LYS
2	B	33	SER
2	B	45	ARG
2	B	75	LYS
2	B	82	VAL
2	B	97	ARG
3	C	4	ASN
3	C	6	LEU
4	D	8	ASN
4	D	12	LEU
4	D	29	ARG
4	D	73	VAL
4	D	81	GLN
4	D	85	SER
4	D	93	ASN

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Mol	Chain	Res	Type
4	D	96	ASN
4	D	102	LEU
4	D	106	THR
4	D	109	ARG
4	D	111	THR
4	D	118	ASN
4	D	125	GLN
4	D	129	SER
4	D	130	LYS
4	D	131	SER
4	D	133	ASP
4	D	134	LYS
4	D	136	VAL
4	D	138	LEU
4	D	140	THR
4	D	148	VAL
4	D	162	CYS
4	D	164	LEU
4	D	166	MET
4	D	169	MET
4	D	172	LYS
4	D	182	LYS
4	D	184	ASP
4	D	195	ILE
4	D	196	ILE
5	E	6	GLN
5	E	18	GLU
5	E	20	ARG
5	E	30	SER
5	E	36	ARG
5	E	51	LYS
5	E	54	ILE
5	E	71	LYS
5	E	83	VAL
5	E	112	THR
5	E	136	THR
5	E	144	LEU
5	E	146	THR
5	E	163	GLU
5	E	173	GLN
5	E	175	LEU
5	E	178	GLN

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Mol	Chain	Res	Type
5	E	185	ARG
5	E	189	SER
5	E	203	ARG
5	E	218	ASN
5	E	220	GLU
5	E	222	THR
5	E	223	GLN
5	E	232	ILE
5	E	236	GLU
5	E	238	TRP
1	F	2	SER
1	F	10	THR
1	F	21	ARG
1	F	66	LYS
1	F	121	LYS
1	F	131	ARG
1	F	176	LYS
1	F	177	GLU
1	F	181	ARG
1	F	182	THR
1	F	194	VAL
1	F	196	ASP
1	F	201	LEU
1	F	202	ARG
1	F	206	LEU
1	F	207	SER
1	F	216	THR
1	F	218	GLN
1	F	224	GLN
1	F	226	GLN
1	F	247	VAL
1	F	248	VAL
1	F	255	GLN
1	F	270	LEU
2	G	0	MET
2	G	4	THR
2	G	19	LYS
2	G	33	SER
2	G	45	ARG
2	G	75	LYS
2	G	82	VAL
2	G	97	ARG

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Mol	Chain	Res	Type
3	H	4	ASN
3	H	6	LEU
4	I	7	GLN
4	I	12	LEU
4	I	29	ARG
4	I	61	ARG
4	I	73	VAL
4	I	85	SER
4	I	89	LEU
4	I	93	ASN
4	I	96	ASN
4	I	102	LEU
4	I	109	ARG
4	I	118	ASN
4	I	125	GLN
4	I	127	ARG
4	I	130	LYS
4	I	131	SER
4	I	133	ASP
4	I	134	LYS
4	I	135	SER
4	I	136	VAL
4	I	138	LEU
4	I	140	THR
4	I	148	VAL
4	I	154	SER
4	I	162	CYS
4	I	164	LEU
4	I	169	MET
4	I	172	LYS
4	I	180	SER
4	I	181	ASN
4	I	182	LYS
4	I	184	ASP
4	I	193	ASN
4	I	195	ILE
4	I	196	ILE
5	J	18	GLU
5	J	30	SER
5	J	72	GLU
5	J	83	VAL
5	J	108	ARG

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Mol	Chain	Res	Type
5	J	112	THR
5	J	133	ILE
5	J	136	THR
5	J	138	LYS
5	J	141	LEU
5	J	144	LEU
5	J	162	LYS
5	J	163	GLU
5	J	175	LEU
5	J	178	GLN
5	J	185	ARG
5	J	189	SER
5	J	198	PHE
5	J	203	ARG
5	J	204	ASN
5	J	217	GLU
5	J	218	ASN
5	J	222	THR
5	J	223	GLN
5	J	232	ILE
5	J	238	TRP
5	J	240	ARG
1	K	2	SER
1	K	10	THR
1	K	21	ARG
1	K	66	LYS
1	K	121	LYS
1	K	131	ARG
1	K	194	VAL
1	K	196	ASP
1	K	201	LEU
1	K	206	LEU
1	K	207	SER
1	K	219	ARG
1	K	222	GLU
1	K	224	GLN
1	K	247	VAL
1	K	248	VAL
1	K	255	GLN
1	K	270	LEU
2	L	0	MET
2	L	4	THR

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Mol	Chain	Res	Type
2	L	19	LYS
2	L	33	SER
2	L	36	GLU
2	L	45	ARG
2	L	75	LYS
2	L	81	ARG
2	L	82	VAL
2	L	91	LYS
2	L	92	ILE
2	L	97	ARG
3	M	4	ASN
3	M	6	LEU
4	N	8	ASN
4	N	12	LEU
4	N	29	ARG
4	N	73	VAL
4	N	93	ASN
4	N	102	LEU
4	N	106	THR
4	N	111	THR
4	N	116	ILE
4	N	118	ASN
4	N	120	ASP
4	N	125	GLN
4	N	127	ARG
4	N	129	SER
4	N	130	LYS
4	N	132	SER
4	N	133	ASP
4	N	135	SER
4	N	136	VAL
4	N	140	THR
4	N	148	VAL
4	N	152	LYS
4	N	154	SER
4	N	162	CYS
4	N	164	LEU
4	N	169	MET
4	N	172	LYS
4	N	182	LYS
4	N	184	ASP
4	N	195	ILE

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Mol	Chain	Res	Type
4	N	196	ILE
5	O	5	MET
5	O	13	ARG
5	O	18	GLU
5	O	26	MET
5	O	36	ARG
5	O	41	GLU
5	O	72	GLU
5	O	83	VAL
5	O	112	THR
5	O	136	THR
5	O	141	LEU
5	O	144	LEU
5	O	146	THR
5	O	163	GLU
5	O	170	THR
5	O	175	LEU
5	O	178	GLN
5	O	185	ARG
5	O	189	SER
5	O	203	ARG
5	O	218	ASN
5	O	222	THR
5	O	223	GLN
5	O	232	ILE
5	O	236	GLU
5	O	238	TRP
1	P	2	SER
1	P	10	THR
1	P	21	ARG
1	P	66	LYS
1	P	72	GLN
1	P	121	LYS
1	P	131	ARG
1	P	176	LYS
1	P	177	GLU
1	P	182	THR
1	P	194	VAL
1	P	196	ASP
1	P	201	LEU
1	P	202	ARG
1	P	206	LEU

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Mol	Chain	Res	Type
1	P	207	SER
1	P	247	VAL
1	P	248	VAL
1	P	255	GLN
1	P	264	GLU
1	P	270	LEU
2	Q	0	MET
2	Q	4	THR
2	Q	19	LYS
2	Q	33	SER
2	Q	45	ARG
2	Q	75	LYS
2	Q	82	VAL
2	Q	97	ARG
3	R	4	ASN
3	R	6	LEU
4	S	8	ASN
4	S	61	ARG
4	S	73	VAL
4	S	85	SER
4	S	89	LEU
4	S	93	ASN
4	S	95	SER
4	S	102	LEU
4	S	109	ARG
4	S	118	ASN
4	S	125	GLN
4	S	127	ARG
4	S	130	LYS
4	S	131	SER
4	S	133	ASP
4	S	134	LYS
4	S	135	SER
4	S	136	VAL
4	S	140	THR
4	S	146	THR
4	S	148	VAL
4	S	150	GLN
4	S	152	LYS
4	S	162	CYS
4	S	164	LEU
4	S	169	MET

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Mol	Chain	Res	Type
4	S	172	LYS
4	S	182	LYS
4	S	184	ASP
4	S	187	CYS
4	S	193	ASN
4	S	195	ILE
4	S	196	ILE
5	T	6	GLN
5	T	7	ASN
5	T	18	GLU
5	T	20	ARG
5	T	30	SER
5	T	36	ARG
5	T	51	LYS
5	T	72	GLU
5	T	83	VAL
5	T	108	ARG
5	T	112	THR
5	T	136	THR
5	T	144	LEU
5	T	163	GLU
5	T	175	LEU
5	T	178	GLN
5	T	185	ARG
5	T	189	SER
5	T	203	ARG
5	T	218	ASN
5	T	222	THR
5	T	223	GLN
5	T	232	ILE
5	T	238	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	74	HIS
1	A	255	GLN
1	A	260	HIS
3	C	4	ASN
4	D	39	GLN
4	D	65	GLN

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Mol	Chain	Res	Type
4	D	115	ASN
5	E	6	GLN
5	E	101	GLN
5	E	211	GLN
1	F	70	HIS
1	F	188	HIS
1	F	218	GLN
3	H	4	ASN
4	I	8	ASN
4	I	39	GLN
4	I	115	ASN
5	J	6	GLN
5	J	101	GLN
5	J	135	HIS
5	J	137	GLN
5	J	211	GLN
5	J	231	GLN
1	K	70	HIS
1	K	87	GLN
3	M	4	ASN
4	N	39	GLN
4	N	99	ASN
4	N	115	ASN
4	N	150	GLN
4	N	174	ASN
4	N	181	ASN
5	O	6	GLN
5	O	37	GLN
5	O	101	GLN
5	O	211	GLN
1	P	32	GLN
1	P	70	HIS
1	P	72	GLN
1	P	188	HIS
3	R	4	ASN
4	S	39	GLN
4	S	81	GLN
4	S	96	ASN
4	S	115	ASN
4	S	189	ASN
5	T	101	GLN
5	T	211	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 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 ⓘ

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	276/276 (100%)	-0.08	2 (0%) 84 79	57, 79, 108, 130	0
1	F	276/276 (100%)	-0.08	1 (0%) 88 86	60, 81, 115, 143	0
1	K	276/276 (100%)	-0.10	2 (0%) 84 79	52, 74, 104, 125	0
1	P	276/276 (100%)	-0.11	4 (1%) 73 66	48, 73, 105, 128	0
2	B	100/100 (100%)	0.03	1 (1%) 79 74	54, 82, 135, 152	0
2	G	100/100 (100%)	0.06	2 (2%) 65 56	62, 83, 134, 162	0
2	L	100/100 (100%)	-0.02	1 (1%) 79 74	55, 79, 130, 155	0
2	Q	100/100 (100%)	-0.05	1 (1%) 79 74	51, 77, 125, 155	0
3	C	9/9 (100%)	0.55	0 100 100	58, 72, 92, 104	0
3	H	9/9 (100%)	-0.06	0 100 100	62, 66, 83, 85	0
3	M	9/9 (100%)	0.38	0 100 100	55, 66, 84, 92	0
3	R	9/9 (100%)	-0.30	0 100 100	56, 64, 74, 80	0
4	D	195/208 (93%)	0.31	5 (2%) 57 48	62, 100, 169, 270	0
4	I	195/208 (93%)	0.57	9 (4%) 37 30	68, 104, 200, 263	0
4	N	195/208 (93%)	0.24	9 (4%) 37 30	60, 96, 180, 274	0
4	S	195/208 (93%)	0.32	7 (3%) 46 38	55, 93, 202, 278	0
5	E	240/242 (99%)	0.34	5 (2%) 63 54	57, 96, 172, 199	0
5	J	239/242 (98%)	0.43	14 (5%) 28 23	67, 98, 183, 233	0
5	O	240/242 (99%)	0.20	5 (2%) 63 54	54, 90, 165, 206	0
5	T	239/242 (98%)	0.47	9 (3%) 44 36	52, 100, 184, 206	0
All	All	3278/3340 (98%)	0.16	77 (2%) 61 52	48, 86, 166, 278	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	204	ASN	4.6
5	O	94	SER	4.1
5	T	3	GLY	3.9
4	N	196	ILE	3.8
5	T	5	MET	3.8
5	T	4	VAL	3.5
4	N	48	ILE	3.4
5	T	28	GLY	3.3
4	I	196	ILE	3.3
5	J	238	TRP	3.3
5	J	202	PRO	3.2
5	O	96	ALA	3.2
4	D	97	PHE	3.2
4	N	97	PHE	3.1
4	I	197	PRO	3.1
5	J	161	GLY	3.1
4	D	196	ILE	3.0
5	O	241	ALA	2.9
4	I	195	ILE	2.9
4	D	197	PRO	2.8
1	F	113	TYR	2.8
4	S	195	ILE	2.8
5	J	141	LEU	2.8
5	O	233	VAL	2.8
4	N	95	SER	2.8
4	N	195	ILE	2.8
5	T	241	ALA	2.7
5	E	194	VAL	2.7
5	J	205	HIS	2.7
5	T	55	ILE	2.7
1	A	8	PHE	2.7
4	I	171	PHE	2.7
2	G	62	PHE	2.6
5	J	203	ARG	2.5
2	L	55	SER	2.5
4	N	62	PHE	2.5
4	S	96	ASN	2.5
4	I	95	SER	2.4
2	G	89	GLN	2.4
1	P	77	ASP	2.4
5	E	139	ALA	2.4
5	J	139	ALA	2.4
2	B	0	MET	2.4

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Mol	Chain	Res	Type	RSRZ
4	S	196	ILE	2.4
1	K	1	GLY	2.3
5	T	26	MET	2.3
5	J	135	HIS	2.3
5	J	193	ARG	2.3
5	J	94	SER	2.3
5	E	233	VAL	2.3
4	S	95	SER	2.3
5	E	39	PRO	2.3
4	N	8	ASN	2.2
5	E	241	ALA	2.2
5	T	30	SER	2.2
4	I	8	ASN	2.2
1	A	72	GLN	2.2
1	K	72	GLN	2.2
4	S	78	ARG	2.2
4	S	89	LEU	2.2
4	N	188	ALA	2.2
4	D	48	ILE	2.2
4	S	30	GLY	2.2
1	P	8	PHE	2.2
4	D	195	ILE	2.1
4	I	188	ALA	2.1
1	P	72	GLN	2.1
5	J	196	ALA	2.1
5	J	133	ILE	2.1
5	T	233	VAL	2.1
4	I	186	ALA	2.1
1	P	182	THR	2.1
5	O	98	THR	2.1
5	J	241	ALA	2.1
4	I	93	ASN	2.0
2	Q	45	ARG	2.0
4	N	78	ARG	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 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.