



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:31 pm BST

PDB ID : 6M8S
Title : Crystal structure of the KCTD12 H1 domain in complex with Gbeta1gamma2 subunits
Authors : Zheng, S.; Kruse, A.C.
Deposited on : 2018-08-22
Resolution : 3.71 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

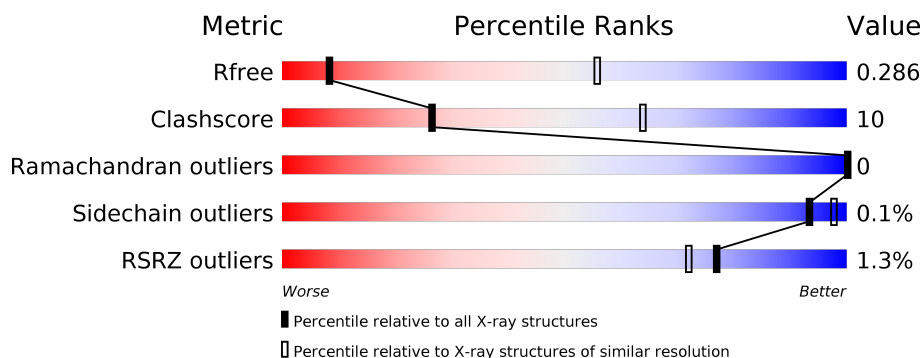
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 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.








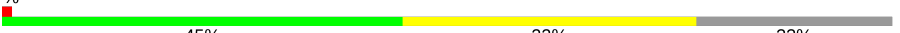



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

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 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	C	350	<div> <div></div> <div>78% 17% 5%</div> </div>
1	D	350	<div> <div>2%</div> <div>74% 21% 5%</div> </div>
1	G	350	<div> <div>2%</div> <div>78% 17% 5%</div> </div>
1	H	350	<div> <div>%</div> <div>74% 21% 5%</div> </div>
1	K	350	<div> <div>%</div> <div>75% 20% 5%</div> </div>
2	E	71	<div> <div></div> <div>68% 10% 23%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	71	 69%8%23%
2	I	71	%  65%13%23%
2	J	71	%  62%15%23%
2	L	71	%  62%14%24%
3	A	129	2%  49%32%19%
3	B	129	%  45%33%22%
3	M	129	2%  50%30%••18%
3	O	129	%  53%29%19%
3	P	129	 55%25%•19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18981 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 Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	333	Total	C	N	O	S	0	0	0
			2536	1569	446	500	21			
1	D	333	Total	C	N	O	S	0	0	0
			2554	1578	455	500	21			
1	G	334	Total	C	N	O	S	0	0	0
			2555	1580	453	501	21			
1	H	332	Total	C	N	O	S	0	0	0
			2537	1569	448	499	21			
1	K	332	Total	C	N	O	S	0	0	0
			2549	1575	454	499	21			

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	MET	-	expression tag	UNP P62873
C	-8	HIS	-	expression tag	UNP P62873
C	-7	HIS	-	expression tag	UNP P62873
C	-6	HIS	-	expression tag	UNP P62873
C	-5	HIS	-	expression tag	UNP P62873
C	-4	HIS	-	expression tag	UNP P62873
C	-3	HIS	-	expression tag	UNP P62873
C	-2	GLY	-	expression tag	UNP P62873
C	-1	SER	-	expression tag	UNP P62873
C	0	SER	-	expression tag	UNP P62873
C	1	GLY	-	expression tag	UNP P62873
D	-9	MET	-	expression tag	UNP P62873
D	-8	HIS	-	expression tag	UNP P62873
D	-7	HIS	-	expression tag	UNP P62873
D	-6	HIS	-	expression tag	UNP P62873
D	-5	HIS	-	expression tag	UNP P62873
D	-4	HIS	-	expression tag	UNP P62873
D	-3	HIS	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP P62873
D	-1	SER	-	expression tag	UNP P62873
D	0	SER	-	expression tag	UNP P62873
D	1	GLY	-	expression tag	UNP P62873
G	-9	MET	-	expression tag	UNP P62873
G	-8	HIS	-	expression tag	UNP P62873
G	-7	HIS	-	expression tag	UNP P62873
G	-6	HIS	-	expression tag	UNP P62873
G	-5	HIS	-	expression tag	UNP P62873
G	-4	HIS	-	expression tag	UNP P62873
G	-3	HIS	-	expression tag	UNP P62873
G	-2	GLY	-	expression tag	UNP P62873
G	-1	SER	-	expression tag	UNP P62873
G	0	SER	-	expression tag	UNP P62873
G	1	GLY	-	expression tag	UNP P62873
H	-9	MET	-	expression tag	UNP P62873
H	-8	HIS	-	expression tag	UNP P62873
H	-7	HIS	-	expression tag	UNP P62873
H	-6	HIS	-	expression tag	UNP P62873
H	-5	HIS	-	expression tag	UNP P62873
H	-4	HIS	-	expression tag	UNP P62873
H	-3	HIS	-	expression tag	UNP P62873
H	-2	GLY	-	expression tag	UNP P62873
H	-1	SER	-	expression tag	UNP P62873
H	0	SER	-	expression tag	UNP P62873
H	1	GLY	-	expression tag	UNP P62873
K	-9	MET	-	expression tag	UNP P62873
K	-8	HIS	-	expression tag	UNP P62873
K	-7	HIS	-	expression tag	UNP P62873
K	-6	HIS	-	expression tag	UNP P62873
K	-5	HIS	-	expression tag	UNP P62873
K	-4	HIS	-	expression tag	UNP P62873
K	-3	HIS	-	expression tag	UNP P62873
K	-2	GLY	-	expression tag	UNP P62873
K	-1	SER	-	expression tag	UNP P62873
K	0	SER	-	expression tag	UNP P62873
K	1	GLY	-	expression tag	UNP P62873

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	55	Total	C	N	O	S	0	0	0
			418	263	72	80	3			
2	J	55	Total	C	N	O	S	0	0	0
			418	263	72	80	3			
2	L	54	Total	C	N	O	S	0	0	0
			413	260	71	79	3			
2	E	55	Total	C	N	O	S	0	0	0
			424	266	75	80	3			
2	F	55	Total	C	N	O	S	0	0	0
			418	263	72	80	3			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	68	SER	CYS	conflict	UNP P59768
J	68	SER	CYS	conflict	UNP P59768
L	68	SER	CYS	conflict	UNP P59768
E	68	SER	CYS	conflict	UNP P59768
F	68	SER	CYS	conflict	UNP P59768

- Molecule 3 is a protein called BTB/POZ domain-containing protein KCTD12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	104	Total	C	N	O	S	0	0	0
			833	527	142	159	5			
3	O	105	Total	C	N	O	S	0	0	0
			840	530	142	163	5			
3	P	104	Total	C	N	O	S	0	0	0
			830	524	139	162	5			
3	B	101	Total	C	N	O	S	0	0	0
			812	515	138	154	5			
3	M	106	Total	C	N	O	S	0	0	0
			844	532	143	164	5			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	GLY	-	expression tag	UNP Q96CX2
A	198	PRO	-	expression tag	UNP Q96CX2
A	199	GLU	-	expression tag	UNP Q96CX2
O	197	GLY	-	expression tag	UNP Q96CX2
O	198	PRO	-	expression tag	UNP Q96CX2
O	199	GLU	-	expression tag	UNP Q96CX2

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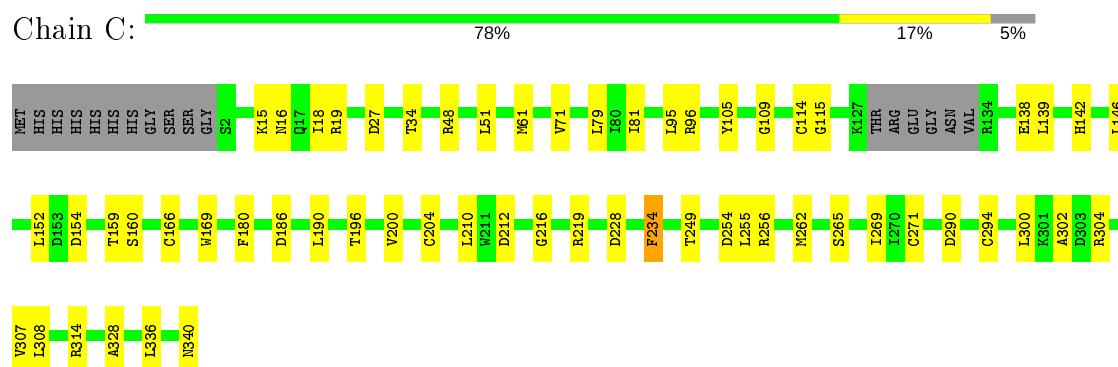
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Chain	Residue	Modelled	Actual	Comment	Reference
P	197	GLY	-	expression tag	UNP Q96CX2
P	198	PRO	-	expression tag	UNP Q96CX2
P	199	GLU	-	expression tag	UNP Q96CX2
B	197	GLY	-	expression tag	UNP Q96CX2
B	198	PRO	-	expression tag	UNP Q96CX2
B	199	GLU	-	expression tag	UNP Q96CX2
M	197	GLY	-	expression tag	UNP Q96CX2
M	198	PRO	-	expression tag	UNP Q96CX2
M	199	GLU	-	expression tag	UNP Q96CX2

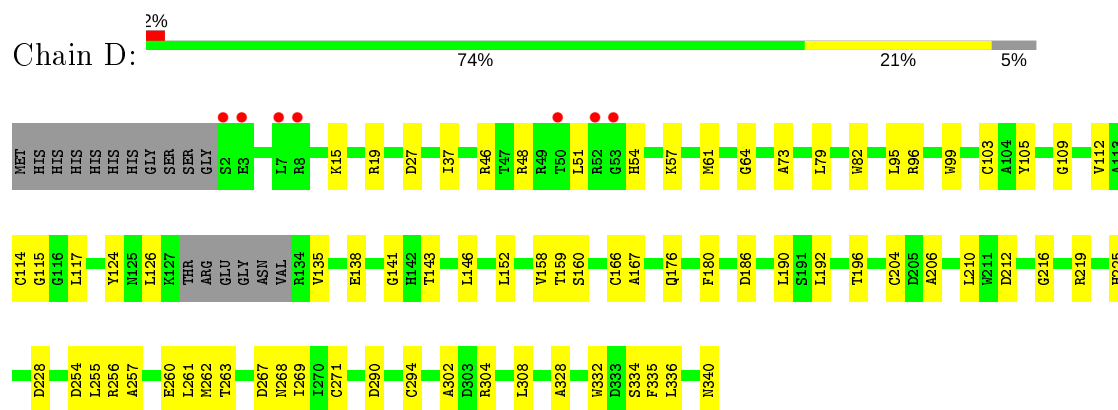
3 Residue-property plots

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.

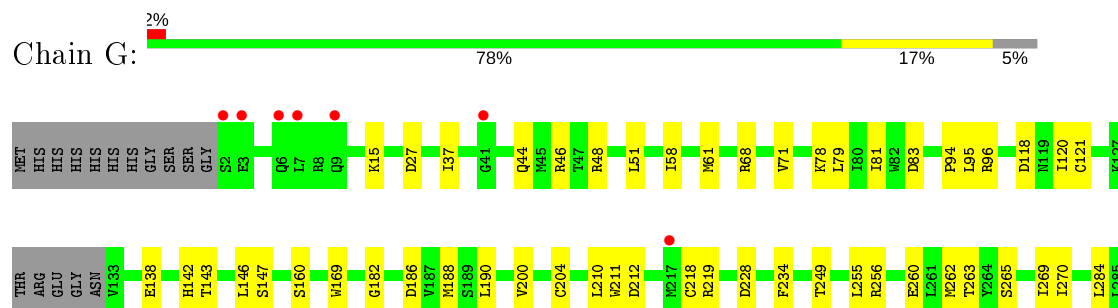
- Molecule 1: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

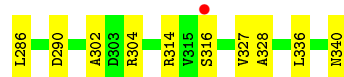


- Molecule 1: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

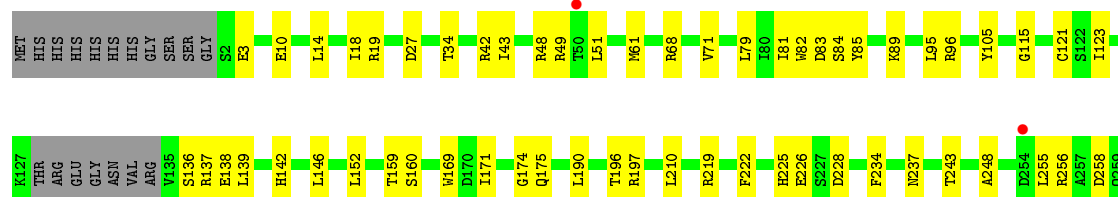
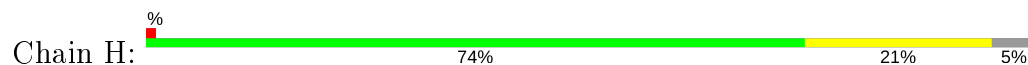


- Molecule 1: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

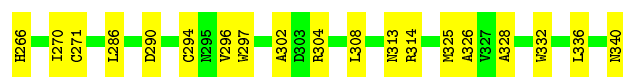
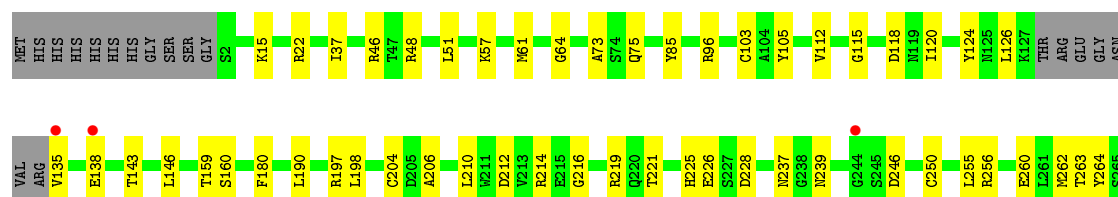
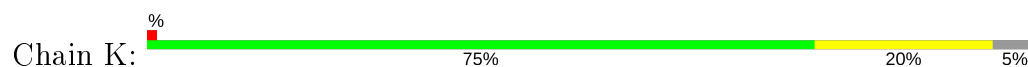




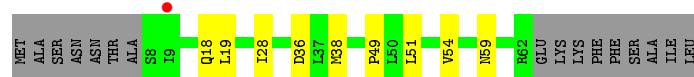
- Molecule 1: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 1: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2





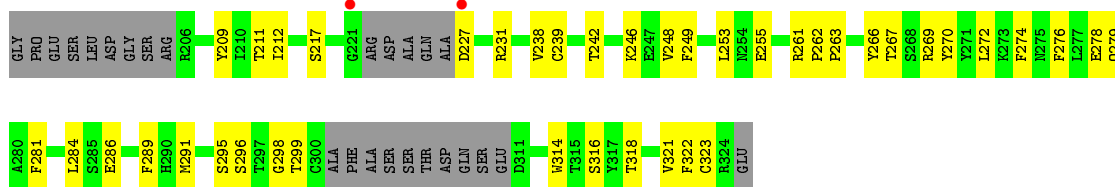
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



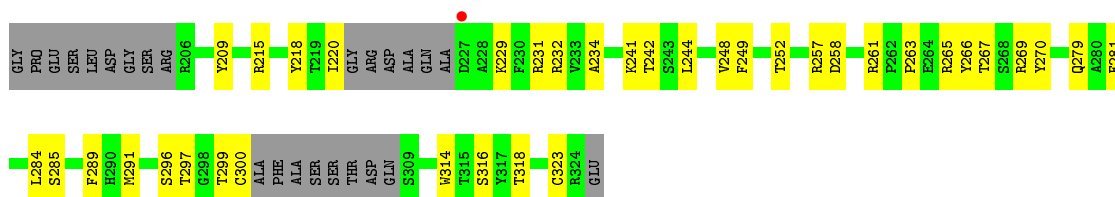
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



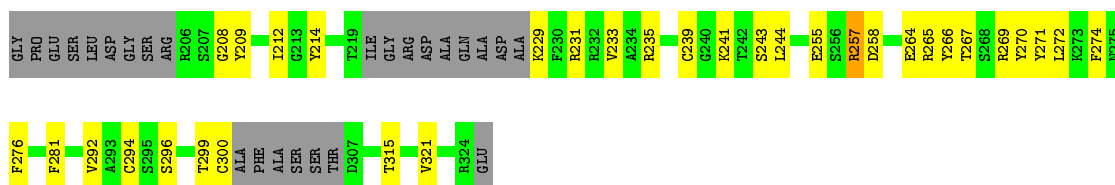
- Molecule 3: BTB/POZ domain-containing protein KCTD12



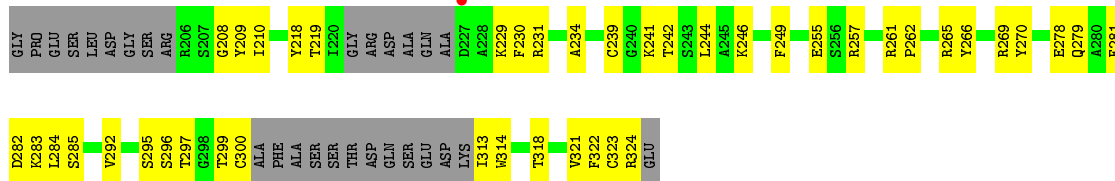
- Molecule 3: BTB/POZ domain-containing protein KCTD12



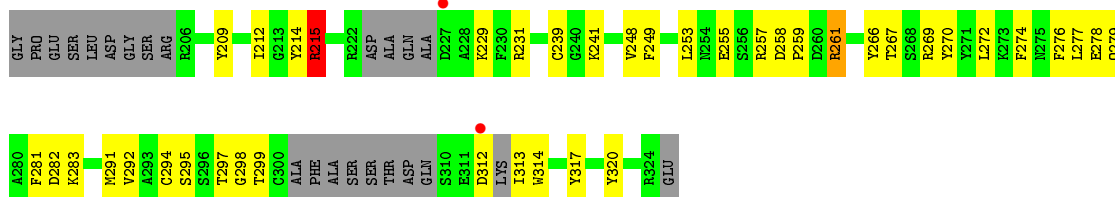
- Molecule 3: BTB/POZ domain-containing protein KCTD12



- Molecule 3: BTB/POZ domain-containing protein KCTD12



- Molecule 3: BTB/POZ domain-containing protein KCTD12



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.09Å 121.99Å 206.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.41 – 3.71 48.41 – 3.71	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.41-3.71) 81.5 (48.41-3.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.47 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.14_3211: ???)	Depositor
R, R_{free}	0.251 , 0.287 0.251 , 0.286	Depositor DCC
R_{free} test set	1959 reflections (6.74%)	wwPDB-VP
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.598	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	18981	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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 [i](#)

5.1 Standard geometry [i](#)

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	C	0.25	0/2582	0.49	0/3504
1	D	0.25	0/2600	0.49	0/3525
1	G	0.25	0/2601	0.50	0/3528
1	H	0.25	0/2583	0.52	0/3504
1	K	0.25	0/2595	0.50	0/3518
2	E	0.25	0/430	0.40	0/580
2	F	0.24	0/424	0.40	0/573
2	I	0.24	0/424	0.43	0/573
2	J	0.25	0/424	0.41	0/573
2	L	0.29	0/419	0.48	0/566
3	A	0.27	0/851	0.53	0/1145
3	B	0.29	0/830	0.55	0/1118
3	M	0.33	0/862	0.96	5/1161 (0.4%)
3	O	0.29	0/858	0.59	0/1156
3	P	0.29	0/848	0.60	1/1142 (0.1%)
All	All	0.26	0/19331	0.53	6/26166 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	M	0	2
3	P	0	1
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	261	ARG	NE-CZ-NH2	-16.67	111.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	215	ARG	CD-NE-CZ	13.52	142.53	123.60
3	M	215	ARG	NE-CZ-NH2	-7.90	116.35	120.30
3	M	215	ARG	NE-CZ-NH1	-7.63	116.49	120.30
3	P	257	ARG	NE-CZ-NH2	-7.25	116.67	120.30
3	M	261	ARG	CD-NE-CZ	5.30	131.02	123.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	215	ARG	Sidechain
3	M	261	ARG	Sidechain
3	P	257	ARG	Sidechain

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	C	2536	0	2421	43	1
1	D	2554	0	2454	53	0
1	G	2555	0	2452	44	0
1	H	2537	0	2430	58	1
1	K	2549	0	2452	55	0
2	E	424	0	436	5	1
2	F	418	0	425	5	0
2	I	418	0	425	10	0
2	J	418	0	425	8	1
2	L	413	0	423	11	0
3	A	833	0	789	37	0
3	B	812	0	769	41	0
3	M	844	0	789	37	0
3	O	840	0	786	39	0
3	P	830	0	772	32	0
All	All	18981	0	18248	382	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (382) 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:K:256:ARG:NH2	2:L:36:ASP:OD2	1.98	0.97
1:D:115:GLY:HA3	1:D:146:LEU:HD23	1.55	0.88
1:K:115:GLY:HA3	1:K:146:LEU:HD23	1.55	0.87
1:H:115:GLY:HA3	1:H:146:LEU:HD23	1.55	0.86
1:G:256:ARG:NH2	2:I:36:ASP:OD2	2.10	0.85
1:C:115:GLY:HA3	1:C:146:LEU:HD23	1.57	0.85
1:H:256:ARG:NH2	2:J:36:ASP:OD2	2.12	0.83
1:K:212:ASP:OD2	1:K:219:ARG:NH2	2.13	0.82
1:G:44:GLN:NE2	1:H:175:GLN:OE1	2.14	0.81
1:H:228:ASP:OD1	3:B:269:ARG:NH1	2.16	0.78
1:D:212:ASP:OD2	1:D:219:ARG:NH2	2.17	0.78
1:D:228:ASP:OD1	3:M:269:ARG:NH1	2.18	0.76
3:B:292:VAL:HG11	3:M:291:MET:HB3	1.68	0.75
3:A:209:TYR:CD2	3:P:281:PHE:HB3	2.20	0.75
3:O:248:VAL:HG21	3:O:284:LEU:HD23	1.68	0.74
1:G:340:ASN:HD21	2:I:59:ASN:HD21	1.36	0.73
1:C:96:ARG:NH1	1:C:138:GLU:OE2	2.20	0.73
1:G:212:ASP:OD2	1:G:219:ARG:NH2	2.22	0.73
3:O:231:ARG:NH1	3:P:239:CYS:SG	2.61	0.73
1:K:48:ARG:NH2	1:K:340:ASN:OD1	2.22	0.72
3:B:239:CYS:SG	3:M:231:ARG:NH1	2.62	0.72
3:O:248:VAL:HG13	3:O:249:PHE:CD1	2.26	0.71
3:O:261:ARG:HH11	3:O:265:ARG:HG2	1.56	0.70
1:K:239:ASN:HD22	1:K:256:ARG:HH11	1.40	0.70
1:C:71:VAL:HG22	1:C:81:ILE:HG12	1.71	0.70
3:A:231:ARG:NH1	3:M:239:CYS:SG	2.65	0.70
1:D:256:ARG:NH2	2:F:36:ASP:OD2	2.26	0.69
1:C:105:TYR:HE1	1:C:109:GLY:HA2	1.57	0.68
1:D:99:TRP:HB3	1:D:117:LEU:HD13	1.76	0.68
3:O:209:TYR:CD2	3:B:281:PHE:HB3	2.28	0.68
1:G:44:GLN:OE1	1:H:175:GLN:NE2	2.24	0.68
1:K:250:CYS:HB2	1:K:264:TYR:HB2	1.75	0.67
1:D:176:GLN:NE2	1:H:42:ARG:HH22	1.92	0.67
1:K:228:ASP:OD1	3:P:269:ARG:NH1	2.27	0.67
1:D:160:SER:HB3	1:D:190:LEU:HD23	1.75	0.67
1:G:68:ARG:NE	1:G:83:ASP:OD1	2.28	0.67
1:H:49:ARG:HH12	1:H:85:TYR:HA	1.59	0.67
3:A:299:THR:HA	3:M:299:THR:HG21	1.78	0.66
1:G:260:GLU:OE2	1:G:263:THR:OG1	2.13	0.66
3:O:291:MET:HB3	3:P:292:VAL:HG11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:246:LYS:NZ	3:B:255:GLU:OE2	2.21	0.66
1:K:246:ASP:O	3:O:232:ARG:NH2	2.29	0.66
1:C:228:ASP:OD1	3:A:269:ARG:NH1	2.28	0.65
1:C:51:LEU:HB2	1:C:336:LEU:HB2	1.78	0.65
1:G:340:ASN:ND2	2:I:59:ASN:HD21	1.94	0.65
1:G:270:ILE:HD12	3:B:234:ALA:HB1	1.78	0.65
3:O:258:ASP:OD2	3:O:261:ARG:HG3	1.97	0.64
3:A:295:SER:HB2	3:P:296:SER:HB3	1.80	0.64
1:G:160:SER:HB3	1:G:190:LEU:HD23	1.79	0.64
1:K:57:LYS:HB3	1:K:332:TRP:HE3	1.62	0.64
1:H:256:ARG:HB3	2:J:28:ILE:HD12	1.78	0.64
1:K:180:PHE:HE1	1:K:216:GLY:HA2	1.62	0.64
1:K:326:ALA:HB2	2:L:61:PHE:HE2	1.62	0.64
1:C:256:ARG:HB3	2:E:28:ILE:HD12	1.80	0.64
1:D:141:GLY:HA3	1:H:42:ARG:HD3	1.79	0.64
1:G:228:ASP:OD1	3:O:269:ARG:NH1	2.32	0.62
3:A:291:MET:HB3	3:M:292:VAL:HG11	1.82	0.62
1:K:57:LYS:HB3	1:K:332:TRP:CE3	2.34	0.62
1:H:71:VAL:HG22	1:H:81:ILE:HG12	1.80	0.62
3:A:209:TYR:HE1	3:A:323:CYS:HG	1.45	0.62
3:B:218:TYR:O	3:B:314:TRP:N	2.32	0.62
1:D:262:MET:SD	1:D:302:ALA:HB2	2.40	0.62
3:A:209:TYR:HD2	3:P:281:PHE:HB3	1.65	0.61
1:H:260:GLU:OE2	1:H:263:THR:OG1	2.18	0.61
3:M:258:ASP:OD2	3:M:267:THR:OG1	2.13	0.61
1:C:210:LEU:HD22	1:C:255:LEU:HD22	1.83	0.60
1:K:160:SER:HB3	1:K:190:LEU:HD23	1.81	0.60
3:O:218:TYR:HB2	3:O:314:TRP:HB3	1.83	0.60
1:K:226:GLU:OE2	3:P:265:ARG:NH2	2.34	0.60
3:B:297:THR:HG22	3:M:314:TRP:HZ2	1.67	0.60
1:K:271:CYS:HB2	1:K:290:ASP:HB2	1.84	0.59
2:L:54:VAL:HG23	2:L:59:ASN:HB2	1.83	0.59
1:D:210:LEU:HD22	1:D:255:LEU:HD22	1.83	0.59
1:D:158:VAL:HG21	1:D:192:LEU:HD21	1.84	0.59
3:A:239:CYS:SG	3:P:231:ARG:NH1	2.75	0.59
1:D:143:THR:HB	1:H:304:ARG:HH21	1.67	0.59
1:H:68:ARG:HH21	1:H:68:ARG:HG3	1.67	0.59
1:G:286:LEU:HD22	1:G:327:VAL:HG11	1.85	0.58
1:H:160:SER:HB3	1:H:190:LEU:HD23	1.85	0.58
2:J:17:GLU:HA	2:J:20:LYS:HE3	1.85	0.58
3:O:285:SER:HB2	3:P:209:TYR:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:MET:HE3	1:G:328:ALA:HB3	1.86	0.57
3:B:299:THR:HG21	3:M:299:THR:HA	1.85	0.57
1:K:262:MET:SD	1:K:302:ALA:HB2	2.44	0.57
1:K:290:ASP:HA	1:K:314:ARG:HB2	1.85	0.57
1:H:48:ARG:NH1	1:H:340:ASN:O	2.37	0.57
3:B:255:GLU:HG2	3:B:270:TYR:CE1	2.40	0.57
1:K:260:GLU:OE2	1:K:263:THR:OG1	2.21	0.57
1:C:271:CYS:HB2	1:C:290:ASP:HB2	1.85	0.57
1:C:160:SER:HB3	1:C:190:LEU:HD23	1.88	0.56
1:G:46:ARG:HB3	1:G:48:ARG:NH1	2.19	0.56
1:H:262:MET:SD	1:H:302:ALA:HB2	2.45	0.56
1:K:51:LEU:HB2	1:K:336:LEU:HB2	1.88	0.56
1:H:174:GLY:O	1:H:175:GLN:HG3	2.06	0.56
3:A:212:ILE:HG22	3:A:238:VAL:HG12	1.87	0.56
2:F:16:VAL:HG12	2:F:20:LYS:HE3	1.88	0.56
1:G:262:MET:SD	1:G:302:ALA:HB2	2.45	0.56
3:B:209:TYR:CD2	3:M:281:PHE:HB3	2.41	0.56
1:H:18:ILE:HG23	2:J:27:ARG:NH2	2.20	0.56
3:O:249:PHE:HB3	3:O:252:THR:OG1	2.06	0.56
3:B:300:CYS:HB3	3:B:314:TRP:CD1	2.41	0.55
3:O:241:LYS:HB2	3:O:266:TYR:CE2	2.42	0.55
1:C:61:MET:HE3	1:C:328:ALA:HB3	1.88	0.55
1:H:3:GLU:N	1:H:3:GLU:OE1	2.37	0.55
1:G:256:ARG:HB3	2:I:28:ILE:HD12	1.89	0.55
1:D:37:ILE:HD11	2:F:38:MET:SD	2.47	0.55
1:D:256:ARG:HB3	2:F:28:ILE:HD12	1.89	0.55
1:D:54:HIS:O	1:D:334:SER:HB2	2.07	0.55
1:H:49:ARG:NH1	1:H:84:SER:O	2.40	0.55
1:D:146:LEU:HD11	1:D:159:THR:HB	1.88	0.55
1:K:198:LEU:HB3	1:K:210:LEU:HD11	1.89	0.55
3:A:276:PHE:HB2	3:A:279:GLN:HE21	1.73	0.54
1:H:226:GLU:HA	3:B:261:ARG:HH22	1.72	0.54
1:G:340:ASN:HD21	2:I:59:ASN:ND2	2.03	0.54
3:O:267:THR:HG21	3:O:270:TYR:CE2	2.42	0.54
1:H:49:ARG:HH11	1:H:49:ARG:HG3	1.72	0.54
1:H:329:THR:O	1:H:336:LEU:HD12	2.07	0.54
3:O:285:SER:HB2	3:P:209:TYR:HE2	1.69	0.54
1:H:146:LEU:HD11	1:H:159:THR:HB	1.90	0.54
3:A:261:ARG:HD3	3:A:262:PRO:HD2	1.88	0.54
1:C:71:VAL:HG23	1:C:105:TYR:HD2	1.73	0.54
1:G:121:CYS:HB2	1:G:146:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:10:GLU:O	1:H:14:LEU:HD13	2.07	0.54
3:A:299:THR:HG21	3:P:299:THR:HA	1.91	0.53
3:M:258:ASP:N	3:M:259:PRO:HD3	2.24	0.53
1:C:254:ASP:OD2	2:E:33:ALA:HB1	2.08	0.53
1:H:283:ARG:HB3	2:J:51:LEU:HD11	1.90	0.53
1:K:61:MET:HE3	1:K:328:ALA:HB3	1.89	0.53
3:B:210:ILE:HD11	3:B:244:LEU:HB3	1.90	0.53
1:C:212:ASP:OD2	1:C:219:ARG:NH2	2.41	0.53
1:H:61:MET:HE3	1:H:328:ALA:HB3	1.91	0.53
1:K:270:ILE:HD12	3:O:234:ALA:HB1	1.90	0.53
3:B:321:VAL:HG11	3:M:291:MET:SD	2.49	0.52
1:D:61:MET:HE3	1:D:328:ALA:HB3	1.91	0.52
1:K:180:PHE:CE1	1:K:216:GLY:HA2	2.43	0.52
3:B:284:LEU:HD22	3:B:322:PHE:CD2	2.45	0.52
1:H:68:ARG:HH22	1:H:85:TYR:HB2	1.73	0.52
3:P:267:THR:HG21	3:P:270:TYR:HE2	1.74	0.52
1:H:237:ASN:HD21	2:J:37:LEU:HD23	1.73	0.52
1:K:256:ARG:HB3	2:L:28:ILE:HD12	1.91	0.52
3:M:312:ASP:OD1	3:M:313:ILE:N	2.42	0.52
1:C:16:ASN:HA	1:C:19:ARG:HD2	1.92	0.52
3:O:281:PHE:HB3	3:P:209:TYR:CD2	2.45	0.52
3:P:214:TYR:HB2	3:P:233:VAL:HG23	1.91	0.52
1:G:71:VAL:HG22	1:G:81:ILE:HG12	1.91	0.52
3:B:219:THR:HG22	3:B:313:ILE:HA	1.92	0.52
1:D:152:LEU:HD22	1:D:196:THR:HB	1.90	0.52
3:P:267:THR:HG21	3:P:270:TYR:CE2	2.45	0.51
1:K:204:CYS:O	3:P:269:ARG:NH1	2.43	0.51
1:C:105:TYR:CE1	1:C:109:GLY:HA2	2.41	0.51
1:D:271:CYS:HB2	1:D:290:ASP:HB2	1.92	0.51
3:A:298:GLY:HA2	3:A:316:SER:HA	1.93	0.51
3:M:241:LYS:HB2	3:M:266:TYR:CE2	2.45	0.51
1:G:269:ILE:HD11	1:G:304:ARG:NH1	2.26	0.50
1:G:79:LEU:HG	1:G:95:LEU:HD21	1.93	0.50
1:C:79:LEU:HG	1:C:95:LEU:HD21	1.92	0.50
1:D:180:PHE:HE1	1:D:216:GLY:HA2	1.76	0.50
1:D:143:THR:HB	1:H:304:ARG:NH2	2.25	0.50
3:O:209:TYR:HE1	3:O:323:CYS:HB2	1.74	0.50
1:G:37:ILE:HD11	2:I:38:MET:HG3	1.92	0.50
1:H:210:LEU:HD22	1:H:255:LEU:HD22	1.93	0.50
1:K:146:LEU:HD11	1:K:159:THR:HB	1.94	0.50
1:H:68:ARG:NH2	1:H:83:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:239:ASN:ND2	1:K:256:ARG:HH11	2.08	0.50
3:M:248:VAL:HG23	3:M:249:PHE:CD2	2.47	0.50
3:A:211:THR:HG22	3:A:321:VAL:HA	1.93	0.50
1:D:260:GLU:OE2	1:D:263:THR:OG1	2.30	0.50
1:D:294:CYS:HB3	1:D:308:LEU:HB2	1.94	0.50
1:C:304:ARG:HH21	1:K:143:THR:HB	1.77	0.49
3:A:299:THR:HG21	3:P:300:CYS:H	1.76	0.49
3:B:219:THR:HG22	3:B:313:ILE:HG22	1.93	0.49
3:O:297:THR:OG1	3:B:296:SER:HB2	2.13	0.49
1:D:57:LYS:HA	1:D:332:TRP:O	2.12	0.49
3:M:267:THR:HG21	3:M:270:TYR:CE2	2.48	0.49
1:C:294:CYS:HB3	1:C:308:LEU:HB2	1.94	0.49
1:G:210:LEU:HD22	1:G:255:LEU:HD22	1.93	0.49
1:C:71:VAL:HG23	1:C:105:TYR:CD2	2.48	0.49
3:P:235:ARG:HD3	3:P:271:TYR:CG	2.47	0.49
3:A:209:TYR:HE1	3:A:323:CYS:SG	2.35	0.49
1:K:46:ARG:HB3	1:K:48:ARG:NH2	2.26	0.49
1:K:57:LYS:HG2	1:K:332:TRP:HB3	1.93	0.49
1:C:152:LEU:HD22	1:C:196:THR:HB	1.94	0.49
1:D:27:ASP:N	1:D:27:ASP:OD1	2.38	0.49
1:D:176:GLN:CD	1:H:42:ARG:HH22	2.16	0.48
1:H:290:ASP:HA	1:H:314:ARG:HB2	1.94	0.48
3:A:267:THR:HG21	3:A:270:TYR:CE2	2.48	0.48
3:O:209:TYR:CE2	3:B:285:SER:HB2	2.48	0.48
1:D:51:LEU:HB2	1:D:336:LEU:HB2	1.95	0.48
3:A:281:PHE:HB3	3:M:209:TYR:CD2	2.49	0.48
3:B:296:SER:HA	3:B:318:THR:HG22	1.96	0.48
1:C:27:ASP:N	1:C:27:ASP:OD1	2.40	0.48
1:H:152:LEU:HD22	1:H:196:THR:HB	1.95	0.48
2:L:8:SER:O	2:L:11:GLN:N	2.35	0.48
3:A:272:LEU:HD13	3:A:274:PHE:CZ	2.49	0.48
1:G:46:ARG:HB3	1:G:48:ARG:HH11	1.77	0.48
1:H:27:ASP:OD1	1:H:27:ASP:N	2.40	0.48
3:A:238:VAL:HG23	3:A:270:TYR:HB2	1.95	0.48
1:D:79:LEU:HG	1:D:95:LEU:HD21	1.96	0.48
1:G:182:GLY:H	1:G:211:TRP:HH2	1.62	0.48
1:D:112:VAL:HG13	1:D:126:LEU:HD11	1.95	0.48
2:I:49:PRO:HB3	2:I:54:VAL:HG13	1.96	0.48
3:M:257:ARG:HB3	3:M:269:ARG:HH11	1.79	0.48
3:M:272:LEU:HD13	3:M:274:PHE:CZ	2.49	0.48
3:A:298:GLY:HA3	3:M:297:THR:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:LYS:HE2	1:C:15:LYS:HB2	1.69	0.47
1:D:254:ASP:HB3	1:D:257:ALA:HB3	1.96	0.47
1:G:249:THR:HG22	1:G:265:SER:HB3	1.96	0.47
1:K:112:VAL:HG13	1:K:126:LEU:HD11	1.96	0.47
3:A:248:VAL:HG23	3:A:249:PHE:CD2	2.49	0.47
1:H:248:ALA:HA	1:H:271:CYS:O	2.14	0.47
3:A:217:SER:HA	3:A:314:TRP:O	2.14	0.47
1:D:96:ARG:NH1	1:D:138:GLU:OE2	2.48	0.47
1:H:51:LEU:HD12	1:H:336:LEU:HD23	1.97	0.47
3:B:242:THR:O	3:B:246:LYS:HG2	2.15	0.47
1:C:34:THR:HG21	1:C:300:LEU:HB3	1.97	0.47
3:B:257:ARG:O	3:B:269:ARG:NH2	2.49	0.46
1:C:304:ARG:NH2	1:K:143:THR:HB	2.30	0.46
1:H:142:HIS:CD2	1:H:169:TRP:HZ2	2.33	0.46
1:C:262:MET:SD	1:C:302:ALA:HB2	2.55	0.46
1:H:270:ILE:O	1:H:270:ILE:HG22	2.15	0.46
1:H:68:ARG:NH2	1:H:85:TYR:HB2	2.31	0.46
3:B:297:THR:HG23	3:M:298:GLY:HA3	1.96	0.46
3:P:255:GLU:HG3	3:P:270:TYR:HE1	1.81	0.46
1:G:186:ASP:HB2	1:G:204:CYS:SG	2.55	0.46
1:G:68:ARG:NH2	1:G:83:ASP:OD2	2.48	0.46
1:H:43:ILE:HG21	2:J:50:LEU:O	2.15	0.46
1:K:237:ASN:HD21	2:L:37:LEU:HD23	1.80	0.46
3:O:257:ARG:HG3	3:B:230:PHE:CE2	2.50	0.46
1:K:124:TYR:CE1	1:K:135:VAL:HG22	2.51	0.46
3:B:231:ARG:HH12	3:B:278:GLU:CD	2.18	0.46
1:G:96:ARG:NH1	1:G:138:GLU:OE2	2.49	0.46
1:H:34:THR:HG21	1:H:300:LEU:HB3	1.97	0.46
1:K:37:ILE:HD11	2:L:38:MET:SD	2.56	0.46
1:G:200:VAL:HG22	1:G:234:PHE:CE2	2.51	0.45
1:K:73:ALA:HB2	1:K:103:CYS:HB3	1.97	0.45
3:A:231:ARG:HH12	3:A:278:GLU:CD	2.20	0.45
3:B:208:GLY:HA3	3:B:244:LEU:HD11	1.98	0.45
1:H:61:MET:SD	1:H:336:LEU:HD11	2.56	0.45
1:C:249:THR:HG22	1:C:265:SER:HB3	1.99	0.45
1:G:15:LYS:NZ	2:I:19:LEU:HD11	2.31	0.45
3:B:255:GLU:HG2	3:B:270:TYR:HE1	1.80	0.45
1:K:294:CYS:HB3	1:K:308:LEU:HB2	1.98	0.45
3:O:244:LEU:HD23	3:O:289:PHE:HZ	1.82	0.45
1:H:96:ARG:NH1	1:H:138:GLU:OE2	2.49	0.45
1:D:105:TYR:HD1	1:D:112:VAL:HG12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:249:PHE:HB2	3:M:253:LEU:HG	1.98	0.45
1:D:64:GLY:HA2	1:D:105:TYR:CD2	2.52	0.45
1:K:313:ASN:ND2	1:K:332:TRP:HB2	2.31	0.45
3:B:266:TYR:HE2	3:M:282:ASP:OD2	2.00	0.45
3:O:261:ARG:NH1	3:O:266:TYR:O	2.50	0.45
3:P:243:SER:OG	3:P:264:GLU:N	2.50	0.45
3:O:215:ARG:NH1	3:B:229:LYS:O	2.43	0.44
3:B:241:LYS:HB2	3:B:266:TYR:CE2	2.52	0.44
3:B:295:SER:HB3	3:M:294:CYS:SG	2.57	0.44
1:C:186:ASP:HB2	1:C:204:CYS:SG	2.57	0.44
1:C:146:LEU:HD11	1:C:159:THR:HB	2.00	0.44
1:C:200:VAL:HG22	1:C:234:PHE:CE2	2.52	0.44
1:H:197:ARG:HH22	1:H:219:ARG:HH22	1.66	0.44
1:C:269:ILE:HD11	1:C:304:ARG:NH1	2.32	0.44
1:D:166:CYS:HB2	1:D:180:PHE:HB2	1.99	0.44
1:D:15:LYS:O	1:D:19:ARG:HG3	2.17	0.44
1:D:141:GLY:CA	1:H:42:ARG:HD3	2.47	0.44
3:M:279:GLN:O	3:M:283:LYS:HG3	2.16	0.44
3:A:266:TYR:HB2	3:P:276:PHE:CD2	2.52	0.44
1:H:19:ARG:HH12	3:B:262:PRO:HA	1.83	0.44
1:K:105:TYR:HD1	1:K:112:VAL:HG12	1.83	0.44
1:D:51:LEU:HB3	1:D:82:TRP:CZ3	2.53	0.44
1:G:27:ASP:OD1	1:G:27:ASP:N	2.42	0.44
2:J:10:ALA:O	2:J:14:LYS:HG3	2.17	0.44
1:K:266:HIS:HB2	1:K:297:TRP:HH2	1.83	0.44
1:G:284:LEU:HG	2:I:51:LEU:HD11	1.99	0.44
1:K:64:GLY:HA2	1:K:105:TYR:CD2	2.53	0.44
1:K:85:TYR:CD1	2:L:61:PHE:HE1	2.36	0.44
3:P:208:GLY:HA3	3:P:244:LEU:HD11	1.99	0.44
3:A:246:LYS:HE2	3:A:255:GLU:OE2	2.17	0.43
3:M:214:TYR:O	3:M:317:TYR:HD1	2.00	0.43
3:P:241:LYS:HB2	3:P:266:TYR:CE1	2.53	0.43
1:K:96:ARG:NH1	1:K:138:GLU:OE2	2.52	0.43
3:M:255:GLU:O	3:M:259:PRO:HG3	2.18	0.43
3:O:261:ARG:NH1	3:O:265:ARG:HG2	2.28	0.43
3:O:299:THR:O	3:O:300:CYS:HB2	2.19	0.43
1:D:117:LEU:H	1:D:117:LEU:HD12	1.82	0.43
1:G:218:CYS:HB3	2:I:18:GLN:OE1	2.17	0.43
1:C:48:ARG:NH1	1:C:340:ASN:O	2.51	0.43
1:K:118:ASP:O	1:K:120:ILE:HG12	2.18	0.43
3:O:266:TYR:HE2	3:B:282:ASP:OD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:49:ARG:NH1	1:H:49:ARG:HG3	2.33	0.43
1:C:166:CYS:HB2	1:C:180:PHE:HB2	2.01	0.43
3:P:229:LYS:HD3	3:P:229:LYS:HA	1.87	0.43
1:K:197:ARG:HH12	1:K:214:ARG:HD2	1.84	0.43
1:C:307:VAL:HG12	1:K:143:THR:HA	2.01	0.43
1:D:267:ASP:OD1	1:D:268:ASN:N	2.52	0.43
3:P:212:ILE:HD11	3:P:281:PHE:CE1	2.54	0.43
1:G:204:CYS:HB3	3:O:257:ARG:NH2	2.34	0.43
3:P:300:CYS:SG	3:P:315:THR:OG1	2.69	0.43
1:C:18:ILE:HG23	2:E:27:ARG:NH2	2.34	0.43
1:G:147:SER:HB3	1:G:188:MET:O	2.18	0.43
2:L:60:PRO:O	2:L:61:PHE:HB2	2.19	0.43
3:A:296:SER:HB3	3:M:295:SER:HB2	2.01	0.42
3:M:229:LYS:HD3	3:M:229:LYS:HA	1.87	0.42
3:B:265:ARG:HD2	3:B:265:ARG:HA	1.83	0.42
3:B:249:PHE:CZ	3:B:284:LEU:HD11	2.53	0.42
1:G:51:LEU:HB2	1:G:336:LEU:HB2	2.00	0.42
3:O:229:LYS:HA	3:O:229:LYS:HD3	1.83	0.42
1:C:180:PHE:CE1	1:C:216:GLY:HA2	2.54	0.42
3:M:212:ILE:HG13	3:M:320:TYR:HB2	2.01	0.42
1:C:139:LEU:HB3	1:C:169:TRP:CE3	2.54	0.42
1:D:206:ALA:HB1	1:D:225:HIS:O	2.18	0.42
1:C:340:ASN:ND2	2:E:59:ASN:HD21	2.17	0.42
1:H:222:PHE:HE2	1:H:258:ASP:HA	1.85	0.42
1:C:142:HIS:CD2	1:C:169:TRP:HZ2	2.38	0.42
3:O:220:ILE:HD12	3:O:220:ILE:HA	1.90	0.42
3:O:249:PHE:HB3	3:O:252:THR:HG1	1.83	0.42
1:G:142:HIS:CD2	1:G:169:TRP:HZ2	2.38	0.42
1:G:78:LYS:NZ	1:G:94:PRO:HG3	2.34	0.42
1:H:123:ILE:O	1:H:136:SER:HB2	2.20	0.42
1:G:143:THR:HB	1:K:304:ARG:HH21	1.85	0.42
2:L:59:ASN:HA	2:L:60:PRO:HD3	1.90	0.42
3:A:212:ILE:HD11	3:A:281:PHE:CE1	2.55	0.42
1:H:137:ARG:HG3	1:H:171:ILE:O	2.19	0.42
1:H:331:SER:HB3	1:H:333:ASP:OD1	2.19	0.42
3:O:296:SER:CB	3:O:318:THR:HG22	2.49	0.42
3:A:227:ASP:HB2	3:M:215:ARG:HG2	2.02	0.42
3:A:296:SER:HA	3:A:318:THR:HA	2.01	0.42
1:K:325:MET:HE2	2:L:60:PRO:HD2	2.02	0.42
3:O:279:GLN:HB2	3:P:266:TYR:CD2	2.54	0.42
3:O:291:MET:SD	3:P:321:VAL:HG11	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:LEU:HB3	1:H:82:TRP:CZ3	2.54	0.41
1:G:290:ASP:HA	1:G:314:ARG:HB2	2.02	0.41
1:C:79:LEU:HD11	1:C:114:CYS:SG	2.59	0.41
1:K:124:TYR:HE1	1:K:135:VAL:HG22	1.86	0.41
1:K:22:ARG:NH2	1:K:221:THR:O	2.47	0.41
1:K:206:ALA:HB1	1:K:225:HIS:O	2.21	0.41
3:O:258:ASP:OD2	3:O:261:ARG:CG	2.65	0.41
3:P:272:LEU:HD13	3:P:274:PHE:CZ	2.55	0.41
3:B:323:CYS:SG	3:B:324:ARG:N	2.93	0.41
3:A:286:GLU:O	3:A:286:GLU:HG3	2.20	0.41
1:K:15:LYS:HB3	1:K:15:LYS:HE3	1.79	0.41
1:K:57:LYS:O	1:K:75:GLN:N	2.47	0.41
3:A:295:SER:HB3	3:P:294:CYS:SG	2.60	0.41
1:D:79:LEU:HD11	1:D:114:CYS:SG	2.60	0.41
1:K:210:LEU:HD22	1:K:255:LEU:HD22	2.03	0.41
3:O:242:THR:HG23	3:O:263:PRO:HA	2.03	0.41
1:C:180:PHE:HE1	1:C:216:GLY:HA2	1.86	0.41
1:G:118:ASP:O	1:G:120:ILE:HG12	2.20	0.41
3:M:278:GLU:HA	3:M:281:PHE:HB2	2.02	0.41
3:A:291:MET:HB2	3:A:322:PHE:CE1	2.56	0.41
3:B:279:GLN:O	3:B:283:LYS:HG3	2.20	0.41
1:D:167:ALA:HB1	1:D:176:GLN:HG2	2.02	0.41
1:H:225:HIS:NE2	1:H:243:THR:OG1	2.40	0.41
3:P:299:THR:O	3:P:300:CYS:SG	2.76	0.41
3:B:262:PRO:O	3:B:265:ARG:HB2	2.20	0.41
3:B:265:ARG:HH11	3:M:276:PHE:HE2	1.68	0.41
1:D:46:ARG:HB3	1:D:48:ARG:NH1	2.35	0.41
1:H:79:LEU:HG	1:H:95:LEU:HD21	2.02	0.41
1:D:73:ALA:HB2	1:D:103:CYS:HB3	2.03	0.41
1:D:335:PHE:CD1	1:D:335:PHE:N	2.88	0.41
2:E:18:GLN:HE21	2:E:22:GLU:HG3	1.85	0.41
1:D:204:CYS:O	3:M:269:ARG:NH1	2.54	0.41
3:M:212:ILE:HD11	3:M:281:PHE:CE1	2.56	0.41
1:D:105:TYR:CZ	1:D:109:GLY:HA2	2.56	0.40
1:D:124:TYR:CE1	1:D:135:VAL:HG22	2.55	0.40
1:D:269:ILE:HD11	1:D:304:ARG:NH1	2.36	0.40
1:G:58:ILE:O	1:G:316:SER:OG	2.31	0.40
1:H:121:CYS:HB3	1:H:139:LEU:HB2	2.02	0.40
3:O:266:TYR:CE2	3:B:282:ASP:OD2	2.74	0.40
3:O:314:TRP:NE1	3:O:316:SER:HB3	2.36	0.40
3:A:242:THR:HG23	3:A:263:PRO:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:ASP:OD1	3:M:257:ARG:NH1	2.52	0.40
1:D:254:ASP:HB2	1:D:261:LEU:HD11	2.03	0.40
1:G:269:ILE:HD11	1:G:304:ARG:HH11	1.87	0.40
1:K:286:LEU:HD22	1:K:296:VAL:HG22	2.04	0.40
3:M:277:LEU:HD21	3:M:320:TYR:CE2	2.57	0.40
3:A:284:LEU:HB3	3:A:289:PHE:HB2	2.03	0.40
1:C:146:LEU:HD12	1:C:160:SER:O	2.22	0.40
1:D:64:GLY:HA2	1:D:105:TYR:HD2	1.85	0.40
1:H:314:ARG:O	1:H:331:SER:OG	2.39	0.40
3:A:253:LEU:HA	3:A:272:LEU:HD23	2.03	0.40
1:C:290:ASP:HA	1:C:314:ARG:HB2	2.03	0.40
1:D:340:ASN:HD22	2:F:59:ASN:HD21	1.70	0.40
3:O:296:SER:HA	3:O:318:THR:HA	2.04	0.40
3:P:258:ASP:HB2	3:P:269:ARG:HB2	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89:LYS:NZ	2:E:17:GLU:OE2[3_554]	2.05	0.15
1:C:154:ASP:OD2	2:J:26:ASP:OD2[1_455]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	329/350 (94%)	321 (98%)	8 (2%)	0	100	100
1	D	329/350 (94%)	323 (98%)	6 (2%)	0	100	100
1	G	330/350 (94%)	324 (98%)	6 (2%)	0	100	100
1	H	328/350 (94%)	321 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	328/350 (94%)	320 (98%)	8 (2%)	0	100	100
2	E	53/71 (75%)	51 (96%)	2 (4%)	0	100	100
2	F	53/71 (75%)	50 (94%)	3 (6%)	0	100	100
2	I	53/71 (75%)	52 (98%)	1 (2%)	0	100	100
2	J	53/71 (75%)	52 (98%)	1 (2%)	0	100	100
2	L	52/71 (73%)	50 (96%)	2 (4%)	0	100	100
3	A	98/129 (76%)	93 (95%)	5 (5%)	0	100	100
3	B	95/129 (74%)	93 (98%)	2 (2%)	0	100	100
3	M	100/129 (78%)	97 (97%)	3 (3%)	0	100	100
3	O	99/129 (77%)	96 (97%)	3 (3%)	0	100	100
3	P	98/129 (76%)	94 (96%)	4 (4%)	0	100	100
All	All	2398/2750 (87%)	2337 (98%)	61 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	C	273/291 (94%)	272 (100%)	1 (0%)	91	95
1	D	276/291 (95%)	276 (100%)	0	100	100
1	G	276/291 (95%)	276 (100%)	0	100	100
1	H	274/291 (94%)	272 (99%)	2 (1%)	84	91
1	K	276/291 (95%)	276 (100%)	0	100	100
2	E	45/58 (78%)	45 (100%)	0	100	100
2	F	44/58 (76%)	44 (100%)	0	100	100
2	I	44/58 (76%)	44 (100%)	0	100	100
2	J	44/58 (76%)	44 (100%)	0	100	100
2	L	44/58 (76%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	89/110 (81%)	89 (100%)	0	100	100
3	B	87/110 (79%)	87 (100%)	0	100	100
3	M	90/110 (82%)	90 (100%)	0	100	100
3	O	90/110 (82%)	90 (100%)	0	100	100
3	P	89/110 (81%)	89 (100%)	0	100	100
All	All	2041/2295 (89%)	2038 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	234	PHE
1	H	105	TYR
1	H	234	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	17	GLN
1	C	75	GLN
1	C	340	ASN
1	D	17	GLN
1	D	75	GLN
1	D	266	HIS
1	D	340	ASN
1	G	75	GLN
1	G	340	ASN
1	H	9	GLN
1	H	16	ASN
1	H	17	GLN
1	H	239	ASN
2	I	24	ASN
2	J	24	ASN
2	J	44	HIS
1	K	9	GLN
1	K	17	GLN
1	K	75	GLN
1	K	239	ASN
2	L	24	ASN
2	L	44	HIS

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Mol	Chain	Res	Type
3	A	275	ASN
3	A	279	GLN
3	P	279	GLN
3	B	279	GLN
2	E	24	ASN
2	F	24	ASN
2	F	44	HIS

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	C	333/350 (95%)	0.03	0 100 100	67, 85, 115, 150	0
1	D	333/350 (95%)	0.13	7 (2%) 63 56	69, 86, 119, 158	0
1	G	334/350 (95%)	0.11	8 (2%) 59 51	62, 85, 119, 166	0
1	H	332/350 (94%)	0.20	4 (1%) 79 74	67, 87, 115, 133	0
1	K	332/350 (94%)	0.10	3 (0%) 84 80	71, 90, 130, 168	0
2	E	55/71 (77%)	-0.09	0 100 100	90, 105, 130, 132	0
2	F	55/71 (77%)	0.05	0 100 100	84, 104, 137, 147	0
2	I	55/71 (77%)	0.06	1 (1%) 68 62	80, 109, 137, 147	0
2	J	55/71 (77%)	-0.08	1 (1%) 68 62	84, 102, 127, 140	0
2	L	54/71 (76%)	0.03	1 (1%) 66 60	87, 115, 141, 147	0
3	A	104/129 (80%)	0.11	2 (1%) 66 60	76, 92, 121, 128	0
3	B	101/129 (78%)	0.18	1 (0%) 82 78	70, 90, 116, 137	0
3	M	106/129 (82%)	0.20	2 (1%) 66 60	74, 94, 119, 129	0
3	O	105/129 (81%)	0.09	1 (0%) 82 78	70, 90, 124, 140	0
3	P	104/129 (80%)	0.03	0 100 100	79, 92, 127, 141	0
All	All	2458/2750 (89%)	0.10	31 (1%) 77 72	62, 90, 126, 168	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	2	SER	4.3
1	G	41	GLY	4.1
1	G	6	GLN	3.7
1	D	2	SER	3.5
3	O	227	ASP	3.4
1	G	3	GLU	3.3
1	D	3	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
3	A	221	GLY	3.0
2	L	10	ALA	3.0
2	J	8	SER	2.9
3	M	227	ASP	2.7
3	A	227	ASP	2.6
3	M	312	ASP	2.5
2	I	9	ILE	2.5
1	G	217	MET	2.5
1	G	316	SER	2.4
1	G	9	GLN	2.4
1	K	138	GLU	2.3
1	H	325	MET	2.3
1	H	50	THR	2.3
1	H	254	ASP	2.3
1	D	52	ARG	2.3
1	D	50	THR	2.3
1	K	244	GLY	2.2
1	G	7	LEU	2.2
1	H	337	LYS	2.2
1	D	8	ARG	2.1
3	B	227	ASP	2.1
1	D	7	LEU	2.1
1	K	135	VAL	2.0
1	D	53	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.