



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:03 am BST

PDB ID : 4GX5  
Title : GsuK Channel  
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Deposited on : 2012-09-03  
Resolution : 3.70 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](mailto: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.

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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

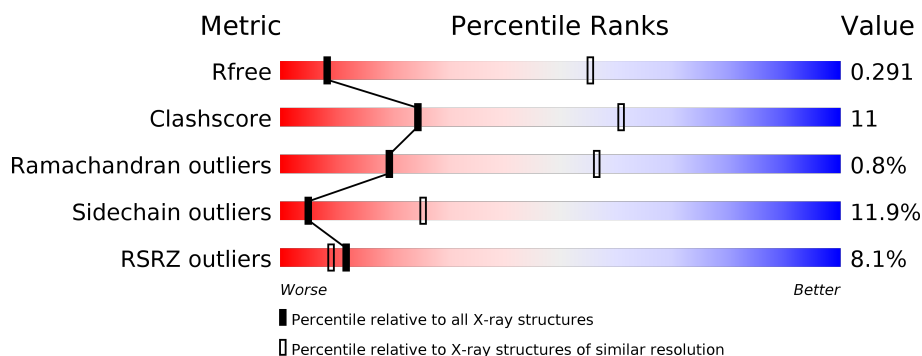
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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  $\geq 3$ , 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	565	<div> <div>4%</div> <div> <div>48%</div> <div>15%</div> <div>•</div> <div>34%</div> </div> </div>
1	B	565	<div> <div>11%</div> <div> <div>66%</div> <div>26%</div> <div>5%</div> <div>•</div> </div> </div>
1	C	565	<div> <div>10%</div> <div> <div>65%</div> <div>28%</div> <div>•</div> <div>•</div> </div> </div>
1	D	565	<div> <div>2%</div> <div> <div>47%</div> <div>15%</div> <div>•</div> <div>33%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	K	C	608	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14266 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 TrkA domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2922	1882	506	523	11			
1	B	548	Total	C	N	O	S	0	0	0
			4208	2695	729	769	15			
1	C	546	Total	C	N	O	S	0	0	0
			4188	2684	723	766	15			
1	D	376	Total	C	N	O	S	0	0	0
			2928	1885	507	525	11			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	EXPRESSION TAG	UNP Q74FS9
A	5	GLN	-	EXPRESSION TAG	UNP Q74FS9
A	6	ARG	-	EXPRESSION TAG	UNP Q74FS9
A	7	GLY	-	EXPRESSION TAG	UNP Q74FS9
A	8	SER	-	EXPRESSION TAG	UNP Q74FS9
A	52	ALA	GLU	ENGINEERED MUTATION	UNP Q74FS9
A	77	GLU	GLN	ENGINEERED MUTATION	UNP Q74FS9
A	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
A	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
A	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
A	568	ARG	-	EXPRESSION TAG	UNP Q74FS9
B	4	MET	-	EXPRESSION TAG	UNP Q74FS9
B	5	GLN	-	EXPRESSION TAG	UNP Q74FS9
B	6	ARG	-	EXPRESSION TAG	UNP Q74FS9
B	7	GLY	-	EXPRESSION TAG	UNP Q74FS9
B	8	SER	-	EXPRESSION TAG	UNP Q74FS9
B	52	ALA	GLU	ENGINEERED MUTATION	UNP Q74FS9
B	77	GLU	GLN	ENGINEERED MUTATION	UNP Q74FS9
B	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
B	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
B	567	PRO	-	EXPRESSION TAG	UNP Q74FS9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	568	ARG	-	EXPRESSION TAG	UNP Q74FS9
C	4	MET	-	EXPRESSION TAG	UNP Q74FS9
C	5	GLN	-	EXPRESSION TAG	UNP Q74FS9
C	6	ARG	-	EXPRESSION TAG	UNP Q74FS9
C	7	GLY	-	EXPRESSION TAG	UNP Q74FS9
C	8	SER	-	EXPRESSION TAG	UNP Q74FS9
C	52	ALA	GLU	ENGINEERED MUTATION	UNP Q74FS9
C	77	GLU	GLN	ENGINEERED MUTATION	UNP Q74FS9
C	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
C	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
C	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
C	568	ARG	-	EXPRESSION TAG	UNP Q74FS9
D	4	MET	-	EXPRESSION TAG	UNP Q74FS9
D	5	GLN	-	EXPRESSION TAG	UNP Q74FS9
D	6	ARG	-	EXPRESSION TAG	UNP Q74FS9
D	7	GLY	-	EXPRESSION TAG	UNP Q74FS9
D	8	SER	-	EXPRESSION TAG	UNP Q74FS9
D	52	ALA	GLU	ENGINEERED MUTATION	UNP Q74FS9
D	77	GLU	GLN	ENGINEERED MUTATION	UNP Q74FS9
D	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
D	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
D	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
D	568	ARG	-	EXPRESSION TAG	UNP Q74FS9

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total K 6 6	0	0
2	C	6	Total K 6 6	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

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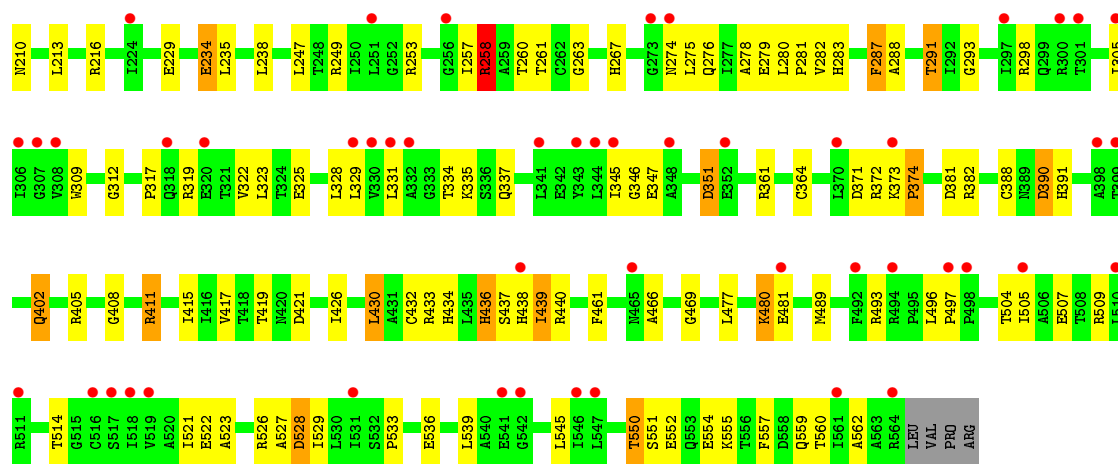
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Zn	0	0
			1	1		

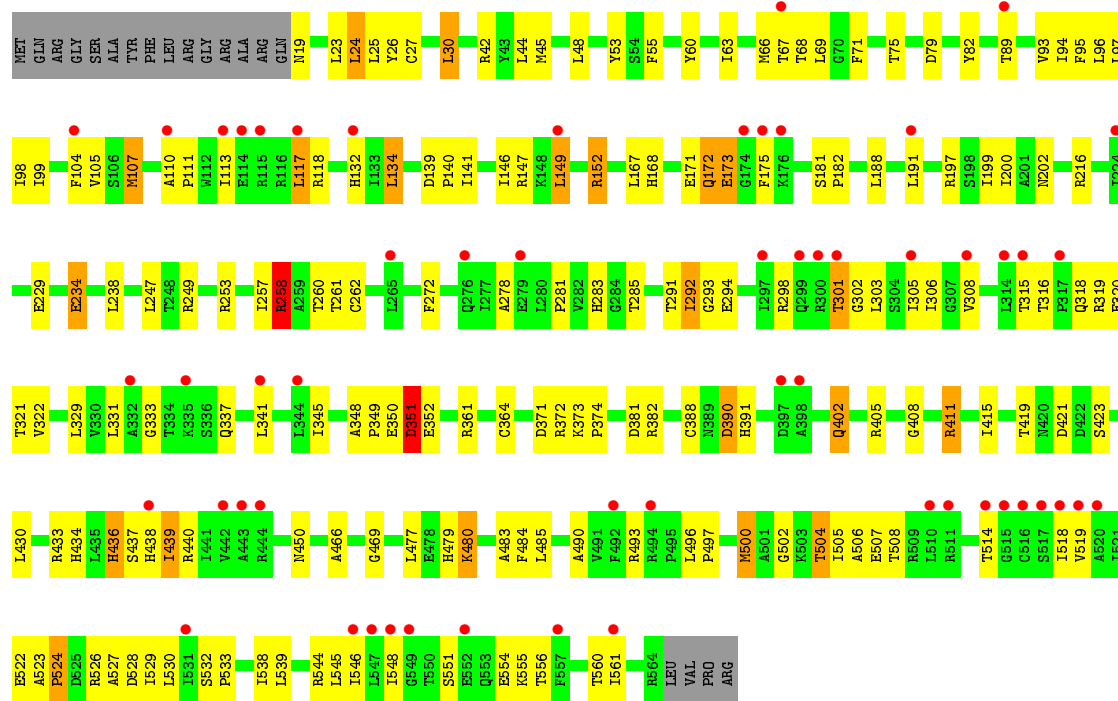
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	C	2	Total	Ca	0	0
			2	2		

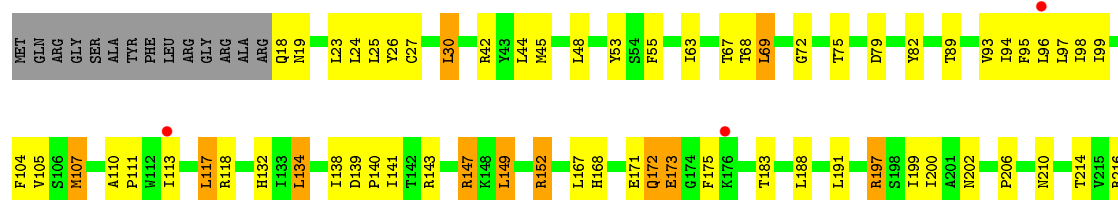




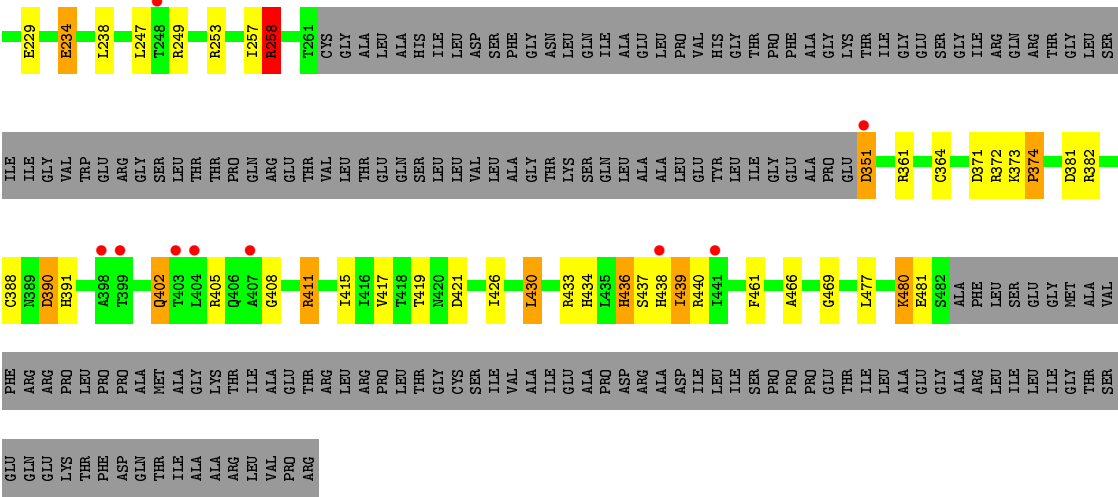
• Molecule 1: TrkA domain protein



• Molecule 1: TrkA domain protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	234.98Å 108.36Å 165.79Å 90.00° 134.96° 90.00°	Depositor
Resolution (Å)	45.39 – 3.70 49.34 – 3.70	Depositor EDS
% Data completeness (in resolution range)	86.8 (45.39-3.70) 86.5 (49.34-3.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.261 , 0.293 0.259 , 0.291	Depositor DCC
$R_{free}$ test set	1383 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	153.1	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 187.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.287 for -h-2*k,h+1 0.045 for -h,-k,h+1 0.044 for -h-2*k,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14266	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	229.0	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 38.05 % 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 3.9078e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: K, ZN, CA

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	0.33	0/2982	0.86	18/4060 (0.4%)
1	B	0.30	0/4291	0.76	17/5843 (0.3%)
1	C	0.31	0/4271	0.76	17/5817 (0.3%)
1	D	0.33	0/2988	0.86	17/4068 (0.4%)
All	All	0.32	0/14532	0.80	69/19788 (0.3%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ARG	NE-CZ-NH2	13.17	126.88	120.30
1	B	258	ARG	NE-CZ-NH1	-12.93	113.83	120.30
1	A	249	ARG	NE-CZ-NH2	12.84	126.72	120.30
1	C	249	ARG	NE-CZ-NH2	12.81	126.71	120.30
1	A	382	ARG	NE-CZ-NH1	-12.74	113.93	120.30
1	A	249	ARG	NE-CZ-NH1	-12.65	113.97	120.30
1	C	249	ARG	NE-CZ-NH1	-12.60	114.00	120.30
1	C	258	ARG	NE-CZ-NH2	-12.59	114.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	ARG	NE-CZ-NH2	12.56	126.58	120.30
1	A	258	ARG	NE-CZ-NH2	-12.47	114.06	120.30
1	C	147	ARG	NE-CZ-NH2	-12.39	114.10	120.30
1	B	382	ARG	NE-CZ-NH2	-12.36	114.12	120.30
1	C	258	ARG	NE-CZ-NH1	12.36	126.48	120.30
1	B	147	ARG	NE-CZ-NH1	-12.36	114.12	120.30
1	D	382	ARG	NE-CZ-NH2	-12.36	114.12	120.30
1	A	147	ARG	NE-CZ-NH2	-12.33	114.14	120.30
1	B	197	ARG	NE-CZ-NH1	-12.31	114.14	120.30
1	D	197	ARG	NE-CZ-NH1	-12.27	114.16	120.30
1	D	258	ARG	NE-CZ-NH1	-12.26	114.17	120.30
1	C	382	ARG	NE-CZ-NH2	12.26	126.43	120.30
1	D	147	ARG	NE-CZ-NH1	-12.25	114.18	120.30
1	B	147	ARG	NE-CZ-NH2	12.19	126.39	120.30
1	A	258	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	D	147	ARG	NE-CZ-NH2	12.14	126.37	120.30
1	D	382	ARG	NE-CZ-NH1	12.11	126.36	120.30
1	C	382	ARG	NE-CZ-NH1	-12.09	114.26	120.30
1	B	382	ARG	NE-CZ-NH1	11.98	126.29	120.30
1	C	197	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	C	147	ARG	NE-CZ-NH1	11.93	126.27	120.30
1	B	197	ARG	NE-CZ-NH2	11.87	126.24	120.30
1	A	197	ARG	NE-CZ-NH2	-11.79	114.41	120.30
1	D	197	ARG	NE-CZ-NH2	11.77	126.19	120.30
1	A	147	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	D	258	ARG	NE-CZ-NH2	11.61	126.10	120.30
1	D	249	ARG	NE-CZ-NH2	-11.53	114.53	120.30
1	D	249	ARG	NE-CZ-NH1	11.47	126.04	120.30
1	B	249	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	B	249	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	A	197	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	C	197	ARG	NE-CZ-NH1	10.79	125.70	120.30
1	A	372	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	A	372	ARG	NE-CZ-NH2	-10.48	115.06	120.30
1	C	372	ARG	NE-CZ-NH2	-10.45	115.08	120.30
1	D	372	ARG	NE-CZ-NH2	10.44	125.52	120.30
1	D	372	ARG	NE-CZ-NH1	-10.32	115.14	120.30
1	B	372	ARG	NE-CZ-NH1	-10.29	115.15	120.30
1	B	372	ARG	NE-CZ-NH2	10.07	125.33	120.30
1	C	372	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	A	382	ARG	CD-NE-CZ	6.57	132.80	123.60
1	B	258	ARG	CD-NE-CZ	6.49	132.69	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ARG	CD-NE-CZ	6.47	132.66	123.60
1	C	249	ARG	CD-NE-CZ	6.43	132.61	123.60
1	C	382	ARG	CD-NE-CZ	6.39	132.55	123.60
1	C	258	ARG	CD-NE-CZ	6.31	132.44	123.60
1	D	147	ARG	CD-NE-CZ	6.25	132.34	123.60
1	B	147	ARG	CD-NE-CZ	6.22	132.31	123.60
1	D	382	ARG	CD-NE-CZ	6.21	132.29	123.60
1	D	258	ARG	CD-NE-CZ	6.19	132.26	123.60
1	B	382	ARG	CD-NE-CZ	6.13	132.19	123.60
1	A	258	ARG	CD-NE-CZ	6.06	132.08	123.60
1	D	197	ARG	CD-NE-CZ	6.01	132.01	123.60
1	B	197	ARG	CD-NE-CZ	5.96	131.94	123.60
1	C	147	ARG	CD-NE-CZ	5.86	131.80	123.60
1	A	147	ARG	CD-NE-CZ	5.77	131.67	123.60
1	D	249	ARG	CD-NE-CZ	5.63	131.49	123.60
1	B	249	ARG	CD-NE-CZ	5.58	131.41	123.60
1	C	197	ARG	CD-NE-CZ	5.52	131.33	123.60
1	A	197	ARG	CD-NE-CZ	5.49	131.29	123.60
1	A	372	ARG	CD-NE-CZ	5.03	130.64	123.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	GLU	Peptide
1	B	173	GLU	Peptide
1	C	173	GLU	Peptide
1	D	173	GLU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2922	0	2964	63	0
1	B	4208	0	4288	108	0
1	C	4188	0	4268	99	0
1	D	2928	0	2969	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6	0	0	0	0
2	C	6	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
All	All	14266	0	14489	312	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 11.

All (312) 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:C:117:LEU:HB2	1:D:117:LEU:HD11	1.43	1.00
1:A:117:LEU:HB2	1:B:117:LEU:HD11	1.49	0.95
1:C:523:ALA:HB3	1:C:526:ARG:HD3	1.64	0.78
1:D:19:ASN:HB3	1:D:107:MET:HG3	1.66	0.77
1:B:19:ASN:HB3	1:B:107:MET:HG3	1.67	0.76
1:C:19:ASN:HB3	1:C:107:MET:HG3	1.67	0.75
1:A:19:ASN:HB3	1:A:107:MET:HG3	1.68	0.74
1:C:139:ASP:OD2	1:C:202:ASN:ND2	2.24	0.71
1:A:139:ASP:OD2	1:A:202:ASN:ND2	2.24	0.71
1:B:258:ARG:HH12	1:B:328:LEU:HB2	1.55	0.70
1:B:139:ASP:OD2	1:B:202:ASN:ND2	2.24	0.70
1:D:139:ASP:OD2	1:D:202:ASN:ND2	2.25	0.69
1:B:505:ILE:HD11	1:B:521:ILE:HD11	1.80	0.64
1:D:415:ILE:HG13	1:D:439:ILE:HD11	1.79	0.64
1:C:415:ILE:HG13	1:C:439:ILE:HD11	1.79	0.64
1:C:200:ILE:HD11	1:C:477:LEU:HD11	1.81	0.62
1:B:200:ILE:HD11	1:B:477:LEU:HD11	1.81	0.62
1:C:257:ILE:HG22	1:C:281:PRO:HG3	1.81	0.62
1:B:559:GLN:O	1:B:562:ALA:N	2.33	0.62
1:A:402:GLN:OE1	1:A:405:ARG:NH2	2.33	0.61
1:B:402:GLN:OE1	1:B:405:ARG:NH2	2.33	0.61
1:A:415:ILE:HG13	1:A:439:ILE:HD11	1.82	0.61
1:C:505:ILE:HD13	1:C:518:ILE:HG21	1.82	0.61
1:B:415:ILE:HG13	1:B:439:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:GLN:OE1	1:C:405:ARG:NH2	2.34	0.61
1:C:318:GLN:HB2	1:C:321:THR:HG23	1.82	0.60
1:C:526:ARG:NE	1:C:528:ASP:OD1	2.35	0.60
1:C:292:ILE:HD11	1:C:305:ILE:HD13	1.83	0.60
1:A:200:ILE:HD11	1:A:477:LEU:HD11	1.84	0.60
1:B:523:ALA:HB3	1:B:526:ARG:HB2	1.84	0.59
1:D:402:GLN:OE1	1:D:405:ARG:NH2	2.34	0.59
1:D:200:ILE:HD11	1:D:477:LEU:HD11	1.84	0.59
1:A:69:LEU:CD2	1:B:70:GLY:HA3	2.33	0.59
1:C:298:ARG:NH1	1:C:523:ALA:O	2.36	0.59
1:C:149:LEU:HD22	1:C:152:ARG:HD3	1.85	0.58
1:A:149:LEU:HD22	1:A:152:ARG:HD3	1.85	0.58
1:B:496:LEU:HD23	1:B:545:LEU:HD11	1.85	0.58
1:D:172:GLN:O	1:D:172:GLN:NE2	2.36	0.58
1:D:480:LYS:HZ2	1:D:481:GLU:HB2	1.68	0.58
1:A:93:VAL:O	1:A:97:LEU:HB3	2.04	0.58
1:B:93:VAL:O	1:B:97:LEU:HB3	2.04	0.58
1:C:293:GLY:HA3	1:C:319:ARG:HG3	1.85	0.58
1:A:172:GLN:O	1:A:172:GLN:NE2	2.37	0.58
1:C:172:GLN:NE2	1:C:172:GLN:O	2.37	0.57
1:D:141:ILE:HD12	1:D:469:GLY:HA3	1.86	0.57
1:D:93:VAL:O	1:D:97:LEU:HB3	2.05	0.57
1:C:93:VAL:O	1:C:97:LEU:HB3	2.05	0.57
1:B:149:LEU:HD22	1:B:152:ARG:HD3	1.86	0.56
1:B:172:GLN:NE2	1:B:172:GLN:O	2.38	0.56
1:B:258:ARG:NH1	1:B:328:LEU:HB2	2.21	0.56
1:C:493:ARG:HD2	1:C:544:ARG:HD3	1.87	0.56
1:B:267:HIS:HE1	1:B:276:GLN:HB3	1.69	0.56
1:B:267:HIS:CE1	1:B:276:GLN:HB3	2.40	0.56
1:D:149:LEU:HD22	1:D:152:ARG:HD3	1.86	0.56
1:C:97:LEU:O	1:C:97:LEU:HD22	2.06	0.56
1:C:94:ILE:O	1:C:99:ILE:HG12	2.06	0.56
1:A:94:ILE:O	1:A:99:ILE:HG12	2.06	0.55
1:A:351:ASP:OD1	1:A:351:ASP:N	2.39	0.55
1:C:504:THR:HG22	1:C:507:GLU:H	1.71	0.55
1:B:551:SER:O	1:B:555:LYS:HG2	2.07	0.55
1:B:97:LEU:O	1:B:97:LEU:HD22	2.07	0.55
1:C:69:LEU:HD23	1:D:68:THR:HA	1.89	0.54
1:B:141:ILE:HD12	1:B:469:GLY:HA3	1.89	0.54
1:A:141:ILE:HD12	1:A:469:GLY:HA3	1.89	0.54
1:B:94:ILE:O	1:B:99:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:ILE:O	1:D:99:ILE:HG12	2.07	0.54
1:C:67:THR:HG23	1:C:69:LEU:H	1.71	0.54
1:D:97:LEU:HD22	1:D:97:LEU:O	2.08	0.54
1:B:67:THR:HG23	1:B:69:LEU:H	1.72	0.54
1:C:529:ILE:HG12	1:C:530:LEU:H	1.73	0.53
1:A:44:LEU:HB3	1:A:48:LEU:HD12	1.91	0.53
1:C:496:LEU:HD23	1:C:545:LEU:HD11	1.91	0.53
1:B:298:ARG:NH2	1:B:526:ARG:O	2.42	0.53
1:C:522:GLU:HG3	1:C:544:ARG:HB3	1.89	0.53
1:A:97:LEU:O	1:A:97:LEU:HD22	2.09	0.53
1:B:44:LEU:HB3	1:B:48:LEU:HD12	1.90	0.53
1:C:350:GLU:O	1:C:352:GLU:N	2.39	0.52
1:D:44:LEU:HB3	1:D:48:LEU:HD12	1.91	0.52
1:C:141:ILE:HD12	1:C:469:GLY:HA3	1.91	0.52
1:C:44:LEU:HB3	1:C:48:LEU:HD12	1.92	0.52
1:B:351:ASP:OD1	1:B:351:ASP:N	2.43	0.52
1:C:504:THR:HG23	1:C:506:ALA:H	1.74	0.52
1:D:408:GLY:HA3	1:D:411:ARG:CZ	2.41	0.52
1:C:351:ASP:N	1:C:351:ASP:OD1	2.43	0.51
1:C:479:HIS:HB3	1:C:483:ALA:HB2	1.92	0.51
1:C:67:THR:HG21	1:D:89:THR:HG21	1.91	0.51
1:C:258:ARG:O	1:C:440:ARG:HD3	2.10	0.51
1:B:504:THR:HB	1:B:507:GLU:H	1.76	0.51
1:D:351:ASP:OD1	1:D:351:ASP:N	2.44	0.51
1:C:134:LEU:HB2	1:C:199:ILE:HG12	1.93	0.51
1:B:253:ARG:HG2	1:B:257:ILE:HD11	1.92	0.51
1:B:291:THR:HA	1:B:322:VAL:HA	1.93	0.51
1:B:305:ILE:HD12	1:B:527:ALA:HB1	1.91	0.51
1:C:291:THR:HG22	1:C:322:VAL:HG22	1.93	0.51
1:D:258:ARG:O	1:D:440:ARG:HD3	2.11	0.51
1:C:253:ARG:O	1:C:257:ILE:HG13	2.11	0.50
1:D:253:ARG:O	1:D:257:ILE:HG13	2.11	0.50
1:B:323:LEU:HD22	1:B:329:LEU:HD21	1.93	0.50
1:C:390:ASP:OD2	1:C:390:ASP:N	2.45	0.50
1:C:522:GLU:HB3	1:C:529:ILE:HG13	1.92	0.50
1:D:67:THR:HG23	1:D:69:LEU:H	1.76	0.50
1:A:253:ARG:O	1:A:257:ILE:HG13	2.12	0.50
1:A:408:GLY:HA3	1:A:411:ARG:CZ	2.42	0.50
1:C:258:ARG:HH11	1:C:281:PRO:HB3	1.77	0.50
1:A:67:THR:OG1	1:B:93:VAL:HG21	2.12	0.50
1:A:134:LEU:HB2	1:A:199:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ARG:O	1:B:440:ARG:HD3	2.11	0.50
1:B:279:GLU:OE1	1:B:328:LEU:HD21	2.12	0.50
1:B:496:LEU:HD22	1:B:497:PRO:HD2	1.92	0.50
1:D:480:LYS:NZ	1:D:481:GLU:HB2	2.26	0.50
1:B:305:ILE:O	1:B:317:PRO:HG3	2.11	0.50
1:B:408:GLY:HA3	1:B:411:ARG:CZ	2.42	0.50
1:A:258:ARG:O	1:A:440:ARG:HD3	2.12	0.49
1:A:67:THR:HG21	1:B:89:THR:HG21	1.94	0.49
1:B:390:ASP:N	1:B:390:ASP:OD2	2.45	0.49
1:B:489:MET:HG2	1:B:550:THR:HA	1.93	0.49
1:C:305:ILE:H	1:C:305:ILE:HD12	1.77	0.49
1:B:113:ILE:O	1:B:117:LEU:HB3	2.12	0.49
1:B:134:LEU:HB2	1:B:199:ILE:HG12	1.93	0.49
1:A:431:ALA:HA	1:B:235:LEU:HD21	1.93	0.49
1:A:390:ASP:OD2	1:A:390:ASP:N	2.46	0.49
1:C:253:ARG:HG2	1:C:257:ILE:HD11	1.94	0.49
1:C:308:VAL:HG22	1:C:329:LEU:HD23	1.94	0.49
1:C:281:PRO:HB2	1:C:283:HIS:ND1	2.28	0.49
1:C:408:GLY:HA3	1:C:411:ARG:CZ	2.43	0.49
1:D:390:ASP:N	1:D:390:ASP:OD2	2.46	0.49
1:A:253:ARG:HG2	1:A:257:ILE:HD11	1.95	0.49
1:D:253:ARG:HG2	1:D:257:ILE:HD11	1.94	0.48
1:A:93:VAL:O	1:A:98:ILE:HG12	2.13	0.48
1:B:293:GLY:HA3	1:B:319:ARG:HG2	1.95	0.48
1:B:93:VAL:O	1:B:98:ILE:HG12	2.13	0.48
1:C:229:GLU:HB2	1:C:361:ARG:HH21	1.79	0.48
1:B:139:ASP:HB2	1:B:140:PRO:HD2	1.96	0.48
1:B:253:ARG:O	1:B:257:ILE:HG13	2.13	0.48
1:D:134:LEU:HB2	1:D:199:ILE:HG12	1.95	0.48
1:C:93:VAL:O	1:C:98:ILE:HG12	2.13	0.48
1:D:139:ASP:HB2	1:D:140:PRO:HD2	1.96	0.48
1:D:141:ILE:HD13	1:D:466:ALA:HA	1.95	0.48
1:D:93:VAL:O	1:D:98:ILE:HG12	2.13	0.48
1:A:436:HIS:HB3	1:A:439:ILE:HG23	1.96	0.48
1:A:63:ILE:HD12	1:B:86:SER:HB3	1.94	0.48
1:A:116:ARG:O	1:B:118:ARG:HG2	2.14	0.48
1:C:66:MET:C	1:C:68:THR:H	2.18	0.47
1:A:42:ARG:HD2	1:A:55:PHE:HA	1.95	0.47
1:C:298:ARG:NH1	1:C:524:PRO:O	2.47	0.47
1:B:229:GLU:HB2	1:B:361:ARG:HH21	1.78	0.47
1:B:66:MET:C	1:B:68:THR:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:ASN:OD1	1:D:210:ASN:ND2	2.44	0.47
1:D:44:LEU:O	1:D:48:LEU:N	2.44	0.47
1:C:113:ILE:O	1:C:117:LEU:HB3	2.15	0.47
1:C:278:ALA:O	1:C:331:LEU:N	2.47	0.47
1:C:436:HIS:HB3	1:C:439:ILE:HG23	1.97	0.47
1:C:496:LEU:HD22	1:C:497:PRO:HD2	1.96	0.47
1:C:291:THR:OG1	1:C:294:GLU:HB2	2.14	0.47
1:A:67:THR:HG23	1:A:69:LEU:H	1.79	0.47
1:B:522:GLU:HB3	1:B:529:ILE:HG13	1.97	0.47
1:A:229:GLU:HB2	1:A:361:ARG:HH21	1.80	0.47
1:B:141:ILE:HD13	1:B:466:ALA:HA	1.96	0.47
1:A:141:ILE:HD13	1:A:466:ALA:HA	1.97	0.46
1:C:419:THR:HG22	1:C:421:ASP:H	1.79	0.46
1:B:337:GLN:HE22	1:B:493:ARG:HH22	1.63	0.46
1:A:419:THR:HG22	1:A:421:ASP:H	1.80	0.46
1:C:42:ARG:HD2	1:C:55:PHE:HA	1.96	0.46
1:A:216:ARG:HA	1:A:216:ARG:HD3	1.72	0.46
1:B:258:ARG:HG2	1:B:461:PHE:CD1	2.51	0.46
1:A:67:THR:HG21	1:B:89:THR:CG2	2.46	0.46
1:C:141:ILE:HD13	1:C:466:ALA:HA	1.97	0.46
1:D:258:ARG:HG2	1:D:461:PHE:CD1	2.51	0.46
1:A:188:LEU:HA	1:A:191:LEU:HD12	1.97	0.46
1:B:42:ARG:HD2	1:B:55:PHE:HA	1.97	0.46
1:B:278:ALA:O	1:B:331:LEU:N	2.46	0.46
1:C:301:THR:HG21	1:C:337:GLN:O	2.16	0.46
1:C:519:VAL:HG21	1:C:548:ILE:HD12	1.97	0.46
1:D:436:HIS:HB3	1:D:439:ILE:HG23	1.96	0.46
1:C:139:ASP:HB2	1:C:140:PRO:HD2	1.97	0.46
1:C:63:ILE:O	1:C:67:THR:HG22	2.15	0.46
1:B:436:HIS:HB3	1:B:439:ILE:HG23	1.97	0.46
1:B:274:ASN:ND2	1:B:554:GLU:OE2	2.49	0.46
1:C:173:GLU:HB2	1:C:175:PHE:H	1.81	0.46
1:D:42:ARG:HD2	1:D:55:PHE:HA	1.96	0.45
1:B:309:TRP:CZ2	1:B:312:GLY:HA2	2.52	0.45
1:D:188:LEU:HA	1:D:191:LEU:HD12	1.98	0.45
1:B:173:GLU:HB2	1:B:175:PHE:H	1.81	0.45
1:B:234:GLU:H	1:B:234:GLU:HG3	1.41	0.45
1:B:281:PRO:HB2	1:B:283:HIS:CD2	2.52	0.45
1:A:113:ILE:O	1:A:117:LEU:HB3	2.17	0.45
1:B:188:LEU:HA	1:B:191:LEU:HD12	1.98	0.45
1:B:282:VAL:O	1:B:288:ALA:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LEU:O	1:B:48:LEU:N	2.47	0.45
1:C:60:TYR:HB2	1:D:82:TYR:HB3	1.99	0.45
1:A:139:ASP:HB2	1:A:140:PRO:HD2	1.98	0.45
1:C:188:LEU:HA	1:C:191:LEU:HD12	1.99	0.45
1:C:216:ARG:HD3	1:C:216:ARG:HA	1.74	0.45
1:A:173:GLU:HB2	1:A:175:PHE:H	1.82	0.45
1:D:173:GLU:HB2	1:D:175:PHE:H	1.82	0.45
1:A:45:MET:HG3	1:A:53:TYR:CD2	2.51	0.45
1:B:18:GLN:O	1:B:22:VAL:HG23	2.16	0.45
1:B:521:ILE:HG13	1:B:533:PRO:HG2	1.99	0.45
1:D:216:ARG:HD3	1:D:216:ARG:HA	1.71	0.45
1:C:388:CYS:SG	1:C:391:HIS:HB2	2.57	0.44
1:C:292:ILE:HD13	1:C:527:ALA:HB1	1.98	0.44
1:B:45:MET:HG3	1:B:53:TYR:CD2	2.52	0.44
1:C:348:ALA:HA	1:C:349:PRO:HD3	1.89	0.44
1:D:234:GLU:HG3	1:D:234:GLU:H	1.40	0.44
1:D:433:ARG:HD3	1:D:437:SER:HA	2.00	0.44
1:A:69:LEU:CD2	1:B:70:GLY:CA	2.95	0.44
1:A:63:ILE:O	1:A:67:THR:HG22	2.17	0.44
1:B:335:LYS:HB2	1:B:335:LYS:HE3	1.74	0.44
1:C:258:ARG:O	1:C:440:ARG:NH1	2.47	0.44
1:B:24:LEU:HA	1:B:27:CYS:HB2	2.00	0.44
1:C:373:LYS:HE3	1:C:373:LYS:HB2	1.87	0.44
1:C:89:THR:O	1:C:93:VAL:HG23	2.18	0.44
1:B:279:GLU:HA	1:B:329:LEU:O	2.18	0.43
1:B:291:THR:HG22	1:B:322:VAL:HG22	1.99	0.43
1:D:89:THR:O	1:D:93:VAL:HG23	2.18	0.43
1:D:24:LEU:HA	1:D:27:CYS:HB2	2.00	0.43
1:D:258:ARG:O	1:D:440:ARG:NH1	2.48	0.43
1:A:69:LEU:HD12	1:B:89:THR:OG1	2.17	0.43
1:B:263:GLY:HA3	1:B:281:PRO:O	2.18	0.43
1:B:283:HIS:HB3	1:B:325:GLU:O	2.19	0.43
1:D:45:MET:HG3	1:D:53:TYR:CD2	2.53	0.43
1:A:89:THR:O	1:A:93:VAL:HG23	2.18	0.43
1:B:216:ARG:HA	1:B:216:ARG:HD3	1.74	0.43
1:B:26:TYR:OH	1:B:95:PHE:O	2.34	0.43
1:C:285:THR:HG22	1:C:345:ILE:HG23	1.99	0.43
1:C:303:LEU:HG	1:C:337:GLN:HB3	1.99	0.43
1:A:234:GLU:H	1:A:234:GLU:HG3	1.40	0.43
1:B:258:ARG:O	1:B:440:ARG:NH1	2.48	0.43
1:D:113:ILE:O	1:D:117:LEU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:LYS:NZ	1:B:480:LYS:HB3	2.33	0.43
1:B:433:ARG:HD3	1:B:437:SER:HA	2.01	0.43
1:C:433:ARG:HD3	1:C:437:SER:HA	2.00	0.43
1:C:496:LEU:HD21	1:C:500:MET:HB3	2.00	0.43
1:A:30:LEU:HA	1:A:30:LEU:HD12	1.92	0.43
1:A:79:ASP:O	1:A:82:TYR:HB2	2.19	0.43
1:C:79:ASP:O	1:C:82:TYR:HB2	2.19	0.43
1:D:63:ILE:O	1:D:67:THR:HG22	2.18	0.43
1:A:373:LYS:HE3	1:A:373:LYS:HB2	1.89	0.42
1:B:419:THR:HG22	1:B:421:ASP:H	1.83	0.42
1:D:143:ARG:O	1:D:147:ARG:HG3	2.19	0.42
1:A:426:ILE:O	1:A:430:LEU:HB2	2.19	0.42
1:B:89:THR:O	1:B:93:VAL:HG23	2.19	0.42
1:C:480:LYS:NZ	1:C:480:LYS:HB3	2.33	0.42
1:C:496:LEU:HA	1:C:497:PRO:HD2	1.91	0.42
1:C:514:THR:HG22	1:C:560:THR:HB	2.01	0.42
1:B:213:LEU:HA	1:B:213:LEU:HD23	1.87	0.42
1:B:63:ILE:O	1:B:67:THR:HG22	2.19	0.42
1:C:234:GLU:H	1:C:234:GLU:HG3	1.40	0.42
1:C:24:LEU:HA	1:C:27:CYS:HB2	2.01	0.42
1:C:181:SER:HA	1:C:182:PRO:HD3	1.89	0.42
1:C:302:GLY:O	1:C:544:ARG:NH1	2.52	0.42
1:A:26:TYR:OH	1:A:99:ILE:HB	2.20	0.42
1:A:69:LEU:HD22	1:B:70:GLY:HA3	2.01	0.42
1:C:71:PHE:O	1:D:72:GLY:HA3	2.20	0.42
1:C:30:LEU:HD11	1:C:95:PHE:HB3	2.01	0.42
1:D:426:ILE:O	1:D:430:LEU:HB2	2.19	0.42
1:B:143:ARG:O	1:B:147:ARG:HG3	2.20	0.42
1:C:532:SER:N	1:C:533:PRO:HD3	2.35	0.42
1:C:30:LEU:HA	1:C:30:LEU:HD12	1.93	0.42
1:C:272:PHE:CE1	1:C:490:ALA:HB2	2.55	0.42
1:D:79:ASP:O	1:D:82:TYR:HB2	2.19	0.42
1:B:388:CYS:SG	1:B:391:HIS:HB2	2.60	0.41
1:B:426:ILE:O	1:B:430:LEU:HB2	2.20	0.41
1:B:69:LEU:HD11	1:B:71:PHE:CZ	2.55	0.41
1:D:26:TYR:OH	1:D:99:ILE:HB	2.20	0.41
1:A:141:ILE:HG23	1:A:469:GLY:HA3	2.01	0.41
1:B:528:ASP:N	1:B:528:ASP:OD1	2.52	0.41
1:D:388:CYS:SG	1:D:391:HIS:HB2	2.60	0.41
1:A:388:CYS:SG	1:A:391:HIS:HB2	2.61	0.41
1:D:419:THR:HG22	1:D:421:ASP:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:HIS:O	1:B:283:HIS:ND1	2.54	0.41
1:B:287:PHE:CE1	1:B:345:ILE:HG12	2.56	0.41
1:D:134:LEU:HA	1:D:134:LEU:HD12	1.90	0.41
1:D:229:GLU:HB2	1:D:361:ARG:HH21	1.84	0.41
1:A:30:LEU:HD11	1:A:95:PHE:HB3	2.02	0.41
1:D:402:GLN:H	1:D:402:GLN:HG2	1.72	0.41
1:B:514:THR:HG21	1:B:557:PHE:HD1	1.85	0.41
1:A:60:TYR:HB2	1:B:82:TYR:HB3	2.03	0.41
1:C:493:ARG:HG3	1:C:546:ILE:HG12	2.03	0.41
1:D:110:ALA:N	1:D:111:PRO:HD2	2.36	0.41
1:A:24:LEU:HA	1:A:27:CYS:HB2	2.02	0.41
1:B:30:LEU:HD11	1:B:95:PHE:HB3	2.02	0.41
1:C:303:LEU:HD23	1:C:333:GLY:HA3	2.03	0.41
1:C:141:ILE:HG23	1:C:469:GLY:HA3	2.02	0.41
1:A:450:ASN:OD1	1:B:210:ASN:ND2	2.52	0.41
1:B:134:LEU:HD12	1:B:134:LEU:HA	1.91	0.41
1:B:26:TYR:OH	1:B:99:ILE:HB	2.20	0.41
1:C:26:TYR:OH	1:C:99:ILE:HB	2.21	0.41
1:A:44:LEU:O	1:A:48:LEU:N	2.45	0.41
1:B:114:GLU:HA	1:B:117:LEU:HD23	2.03	0.41
1:B:141:ILE:HG23	1:B:469:GLY:HA3	2.02	0.41
1:C:45:MET:HG3	1:C:53:TYR:CD2	2.55	0.41
1:D:138:ILE:HG13	1:D:143:ARG:HG3	2.03	0.41
1:D:30:LEU:HD11	1:D:95:PHE:HB3	2.02	0.41
1:D:408:GLY:HA3	1:D:411:ARG:NH1	2.36	0.41
1:A:258:ARG:O	1:A:440:ARG:NH1	2.49	0.40
1:B:110:ALA:N	1:B:111:PRO:HD2	2.36	0.40
1:B:402:GLN:H	1:B:402:GLN:HG2	1.74	0.40
1:C:479:HIS:O	1:C:483:ALA:N	2.42	0.40
1:C:423:SER:O	1:D:206:PRO:HB3	2.21	0.40
1:A:181:SER:HA	1:A:182:PRO:HD3	1.90	0.40
1:A:408:GLY:HA3	1:A:411:ARG:NH1	2.37	0.40
1:B:280:LEU:HA	1:B:281:PRO:HD2	1.96	0.40
1:C:146:ILE:HG21	1:C:175:PHE:CD2	2.57	0.40
1:B:415:ILE:HD13	1:B:432:CYS:SG	2.61	0.40
1:C:502:GLY:O	1:C:538:ILE:HG23	2.20	0.40
1:A:146:ILE:HG21	1:A:175:PHE:CD2	2.57	0.40
1:C:110:ALA:N	1:C:111:PRO:HD2	2.36	0.40
1:A:110:ALA:N	1:A:111:PRO:HD2	2.36	0.40
1:B:373:LYS:HA	1:B:374:PRO:HD2	1.76	0.40
1:D:183:THR:O	1:D:214:THR:HG21	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:LYS:HA	1:D:374:PRO:HD2	1.76	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	371/565 (66%)	346 (93%)	23 (6%)	2 (0%)	29	66
1	B	546/565 (97%)	509 (93%)	33 (6%)	4 (1%)	22	59
1	C	544/565 (96%)	498 (92%)	40 (7%)	6 (1%)	14	50
1	D	372/565 (66%)	345 (93%)	25 (7%)	2 (0%)	29	66
All	All	1833/2260 (81%)	1698 (93%)	121 (7%)	14 (1%)	19	56

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	351	ASP
1	A	374	PRO
1	B	374	PRO
1	C	374	PRO
1	D	374	PRO
1	B	261	THR
1	C	261	THR
1	C	556	THR
1	A	402	GLN
1	C	402	GLN
1	D	402	GLN
1	B	402	GLN
1	B	346	GLY
1	C	524	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/463 (68%)	275 (88%)	38 (12%)	5	24
1	B	449/463 (97%)	398 (89%)	51 (11%)	5	27
1	C	447/463 (96%)	393 (88%)	54 (12%)	5	24
1	D	314/463 (68%)	276 (88%)	38 (12%)	5	24
All	All	1523/1852 (82%)	1342 (88%)	181 (12%)	5	25

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	23	LEU
1	A	24	LEU
1	A	25	LEU
1	A	30	LEU
1	A	69	LEU
1	A	75	THR
1	A	96	LEU
1	A	104	PHE
1	A	105	VAL
1	A	107	MET
1	A	117	LEU
1	A	118	ARG
1	A	132	HIS
1	A	134	LEU
1	A	149	LEU
1	A	152	ARG
1	A	167	LEU
1	A	168	HIS
1	A	171	GLU
1	A	172	GLN
1	A	234	GLU
1	A	238	LEU
1	A	247	LEU

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Mol	Chain	Res	Type
1	A	258	ARG
1	A	261	THR
1	A	351	ASP
1	A	364	CYS
1	A	371	ASP
1	A	381	ASP
1	A	390	ASP
1	A	411	ARG
1	A	430	LEU
1	A	434	HIS
1	A	436	HIS
1	A	438	HIS
1	A	439	ILE
1	A	480	LYS
1	B	23	LEU
1	B	25	LEU
1	B	30	LEU
1	B	69	LEU
1	B	75	THR
1	B	96	LEU
1	B	104	PHE
1	B	105	VAL
1	B	107	MET
1	B	117	LEU
1	B	118	ARG
1	B	132	HIS
1	B	134	LEU
1	B	149	LEU
1	B	152	ARG
1	B	167	LEU
1	B	168	HIS
1	B	171	GLU
1	B	172	GLN
1	B	197	ARG
1	B	234	GLU
1	B	238	LEU
1	B	247	LEU
1	B	258	ARG
1	B	260	THR
1	B	275	LEU
1	B	287	PHE
1	B	291	THR

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Mol	Chain	Res	Type
1	B	334	THR
1	B	347	GLU
1	B	351	ASP
1	B	364	CYS
1	B	371	ASP
1	B	381	ASP
1	B	390	ASP
1	B	411	ARG
1	B	417	VAL
1	B	430	LEU
1	B	434	HIS
1	B	436	HIS
1	B	438	HIS
1	B	439	ILE
1	B	480	LYS
1	B	481	GLU
1	B	509	ARG
1	B	528	ASP
1	B	536	GLU
1	B	539	LEU
1	B	550	THR
1	B	552	GLU
1	B	560	THR
1	C	23	LEU
1	C	24	LEU
1	C	25	LEU
1	C	30	LEU
1	C	75	THR
1	C	96	LEU
1	C	104	PHE
1	C	105	VAL
1	C	107	MET
1	C	117	LEU
1	C	118	ARG
1	C	132	HIS
1	C	134	LEU
1	C	149	LEU
1	C	152	ARG
1	C	167	LEU
1	C	168	HIS
1	C	171	GLU
1	C	172	GLN

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Mol	Chain	Res	Type
1	C	234	GLU
1	C	238	LEU
1	C	247	LEU
1	C	258	ARG
1	C	260	THR
1	C	262	CYS
1	C	292	ILE
1	C	301	THR
1	C	306	ILE
1	C	315	THR
1	C	316	THR
1	C	320	GLU
1	C	341	LEU
1	C	351	ASP
1	C	364	CYS
1	C	371	ASP
1	C	381	ASP
1	C	390	ASP
1	C	411	ARG
1	C	430	LEU
1	C	434	HIS
1	C	436	HIS
1	C	438	HIS
1	C	439	ILE
1	C	480	LYS
1	C	484	PHE
1	C	485	LEU
1	C	500	MET
1	C	504	THR
1	C	508	THR
1	C	539	LEU
1	C	551	SER
1	C	554	GLU
1	C	555	LYS
1	C	561	ILE
1	D	18	GLN
1	D	23	LEU
1	D	25	LEU
1	D	30	LEU
1	D	69	LEU
1	D	75	THR
1	D	96	LEU

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Mol	Chain	Res	Type
1	D	104	PHE
1	D	105	VAL
1	D	107	MET
1	D	117	LEU
1	D	118	ARG
1	D	132	HIS
1	D	134	LEU
1	D	149	LEU
1	D	152	ARG
1	D	167	LEU
1	D	168	HIS
1	D	171	GLU
1	D	172	GLN
1	D	197	ARG
1	D	234	GLU
1	D	238	LEU
1	D	247	LEU
1	D	258	ARG
1	D	351	ASP
1	D	364	CYS
1	D	371	ASP
1	D	381	ASP
1	D	390	ASP
1	D	411	ARG
1	D	417	VAL
1	D	430	LEU
1	D	434	HIS
1	D	436	HIS
1	D	438	HIS
1	D	439	ILE
1	D	480	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	267	HIS
1	B	276	GLN
1	B	337	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](#)

Of 20 ligands modelled in this entry, 20 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	375/565 (66%)	0.20	20 (5%) 26 20	126, 189, 324, 425	0
1	B	548/565 (96%)	0.52	61 (11%) 5 4	135, 230, 370, 487	0
1	C	546/565 (96%)	0.52	56 (10%) 6 5	124, 223, 381, 519	0
1	D	376/565 (66%)	0.24	12 (3%) 47 35	124, 187, 332, 475	0
All	All	1845/2260 (81%)	0.40	149 (8%) 12 9	124, 205, 368, 519	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	516	CYS	16.3
1	B	307	GLY	12.3
1	D	398	ALA	10.3
1	C	519	VAL	8.7
1	C	518	ILE	8.6
1	C	114	GLU	8.5
1	B	308	VAL	8.1
1	A	398	ALA	7.2
1	C	517	SER	6.4
1	C	175	PHE	6.3
1	D	403	THR	5.8
1	C	315	THR	5.6
1	C	531	ILE	5.6
1	B	341	LEU	5.4
1	C	510	LEU	5.4
1	B	297	ILE	5.2
1	C	520	ALA	5.1
1	B	516	CYS	4.9
1	B	561	ILE	4.8
1	D	399	THR	4.6
1	A	114	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	511	ARG	4.4
1	B	332	ALA	4.4
1	C	299	GLN	4.3
1	B	306	ILE	4.3
1	A	404	LEU	4.3
1	C	113	ILE	4.2
1	C	265	LEU	4.1
1	B	494	ARG	4.1
1	A	399	THR	4.0
1	B	542	GLY	4.0
1	B	301	THR	4.0
1	A	113	ILE	3.9
1	C	308	VAL	3.9
1	B	300	ARG	3.8
1	B	511	ARG	3.8
1	A	397	ASP	3.8
1	C	191	LEU	3.8
1	B	505	ILE	3.7
1	B	329	LEU	3.6
1	B	256	GLY	3.6
1	C	514	THR	3.6
1	C	557	PHE	3.5
1	C	276	GLN	3.5
1	C	149	LEU	3.5
1	C	332	ALA	3.4
1	C	305	ILE	3.4
1	C	443	ALA	3.4
1	A	104	PHE	3.4
1	C	438	HIS	3.3
1	B	518	ILE	3.3
1	B	224	ILE	3.3
1	B	344	LEU	3.3
1	B	331	LEU	3.3
1	B	519	VAL	3.3
1	B	517	SER	3.1
1	C	552	GLU	3.1
1	C	297	ILE	3.1
1	B	497	PRO	3.1
1	D	113	ILE	3.1
1	B	399	THR	3.1
1	B	345	ILE	3.1
1	C	115	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	317	PRO	3.0
1	B	547	LEU	3.0
1	B	305	ILE	3.0
1	B	498	PRO	3.0
1	B	176	LYS	3.0
1	C	548	ILE	3.0
1	C	110	ALA	3.0
1	B	191	LEU	3.0
1	C	314	LEU	3.0
1	B	149	LEU	2.9
1	B	492	PHE	2.9
1	C	301	THR	2.9
1	D	404	LEU	2.9
1	C	547	LEU	2.9
1	C	546	ILE	2.8
1	C	174	GLY	2.8
1	A	71	PHE	2.8
1	B	135	ILE	2.8
1	B	134	LEU	2.8
1	B	564	ARG	2.8
1	B	398	ALA	2.7
1	A	191	LEU	2.7
1	D	351	ASP	2.7
1	B	546	ILE	2.7
1	B	198	SER	2.7
1	C	67	THR	2.7
1	D	438	HIS	2.7
1	C	300	ARG	2.7
1	B	159	VAL	2.7
1	C	515	GLY	2.7
1	A	438	HIS	2.6
1	A	373	LYS	2.6
1	B	318	GLN	2.6
1	C	494	ARG	2.6
1	B	510	LEU	2.5
1	C	104	PHE	2.5
1	D	441	ILE	2.5
1	B	541	GLU	2.5
1	A	254	TYR	2.4
1	C	398	ALA	2.4
1	B	373	LYS	2.4
1	B	348	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	133	ILE	2.4
1	B	125	LEU	2.4
1	D	248	THR	2.4
1	C	279	GLU	2.4
1	C	176	LYS	2.4
1	A	110	ALA	2.4
1	B	370	LEU	2.3
1	C	397	ASP	2.3
1	D	407	ALA	2.3
1	C	117	LEU	2.3
1	B	531	ILE	2.3
1	C	492	PHE	2.3
1	B	251	LEU	2.2
1	C	89	THR	2.2
1	B	343	TYR	2.2
1	A	175	PHE	2.2
1	C	549	GLY	2.2
1	A	225	ALA	2.2
1	B	175	PHE	2.2
1	B	352	GLU	2.2
1	B	438	HIS	2.2
1	C	335	LYS	2.2
1	A	403	THR	2.2
1	A	409	ILE	2.2
1	C	132	HIS	2.2
1	C	444	ARG	2.2
1	C	561	ILE	2.2
1	C	442	VAL	2.2
1	A	136	PHE	2.2
1	C	341	LEU	2.1
1	B	274	ASN	2.1
1	C	224	ILE	2.1
1	B	330	VAL	2.1
1	B	465	ASN	2.1
1	D	176	LYS	2.1
1	A	188	LEU	2.1
1	B	320	GLU	2.1
1	C	344	LEU	2.1
1	D	96	LEU	2.0
1	B	273	GLY	2.0
1	B	200	ILE	2.0
1	A	96	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	481	GLU	2.0
1	B	156	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	K	C	602	1/1	0.53	0.15	153,153,153,153	1
2	K	C	603	1/1	0.68	0.14	160,160,160,160	1
2	K	C	608	1/1	0.72	0.50	241,241,241,241	1
2	K	A	608	1/1	0.74	0.19	225,225,225,225	1
2	K	A	603	1/1	0.82	0.21	169,169,169,169	1
2	K	C	609	1/1	0.83	0.78	200,200,200,200	1
4	CA	C	606	1/1	0.85	0.10	185,185,185,185	0
4	CA	B	602	1/1	0.90	0.20	175,175,175,175	0
2	K	A	607	1/1	0.90	0.81	199,199,199,199	1
4	CA	A	606	1/1	0.93	0.17	173,173,173,173	0
4	CA	C	607	1/1	0.93	0.27	138,138,138,138	0
2	K	A	602	1/1	0.93	0.19	154,154,154,154	1
3	ZN	C	605	1/1	0.98	0.28	152,152,152,152	0
3	ZN	B	601	1/1	0.98	0.28	134,134,134,134	0
3	ZN	A	605	1/1	0.98	0.25	160,160,160,160	0
3	ZN	D	601	1/1	0.99	0.24	149,149,149,149	0
2	K	A	601	1/1	0.99	0.12	166,166,166,166	1
2	K	A	604	1/1	0.99	0.12	186,186,186,186	1
2	K	C	601	1/1	0.99	0.12	207,207,207,207	1
2	K	C	604	1/1	0.99	0.07	143,143,143,143	1

## 6.5 Other polymers

There are no such residues in this entry.