



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4GX5 / pdb_00004gx5
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

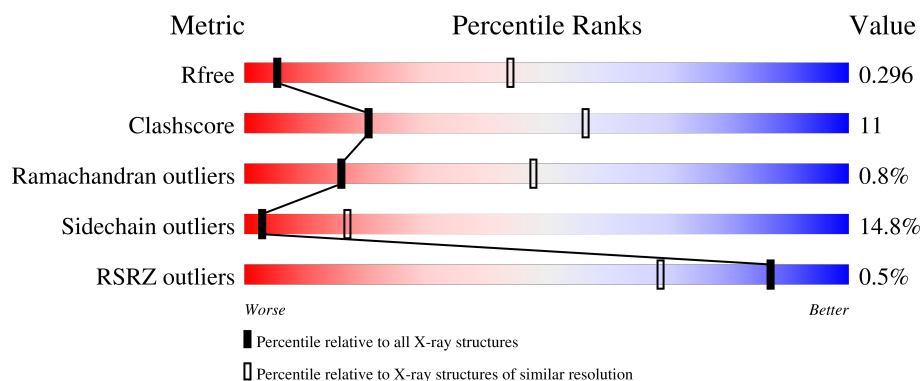
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	565	
1	B	565	
1	C	565	
1	D	565	

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 (CCD ID: 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 (CCD ID: ZN) (formula: Zn).

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

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

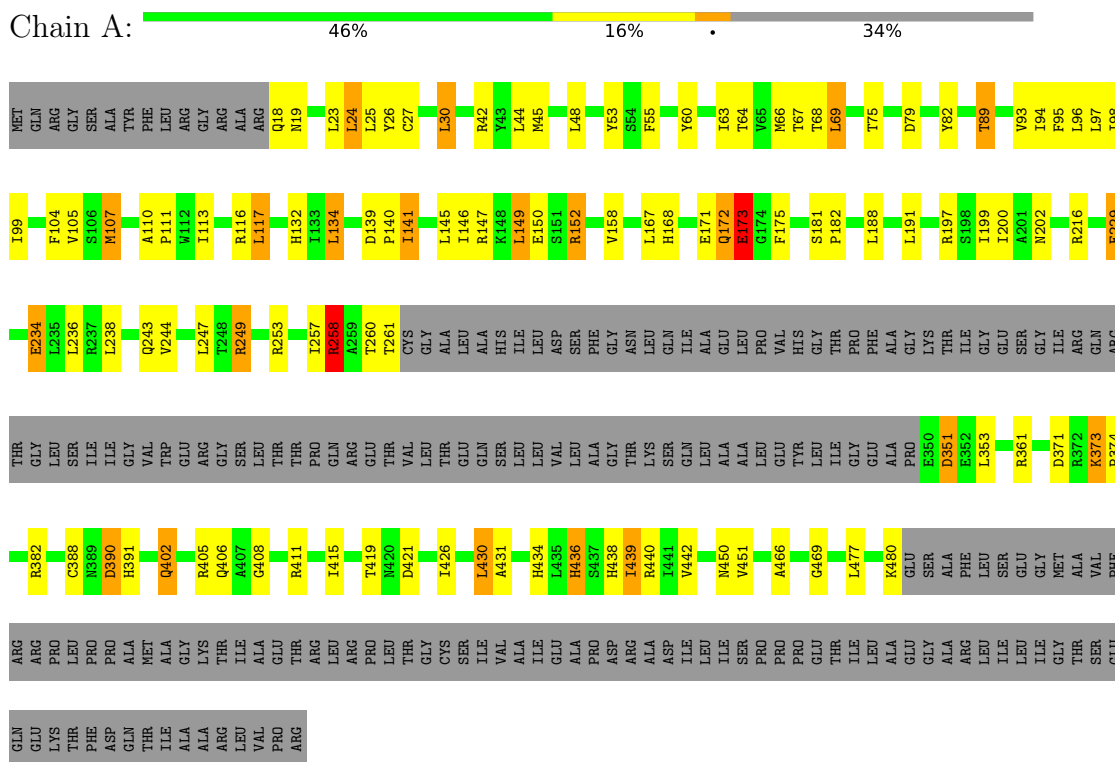
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

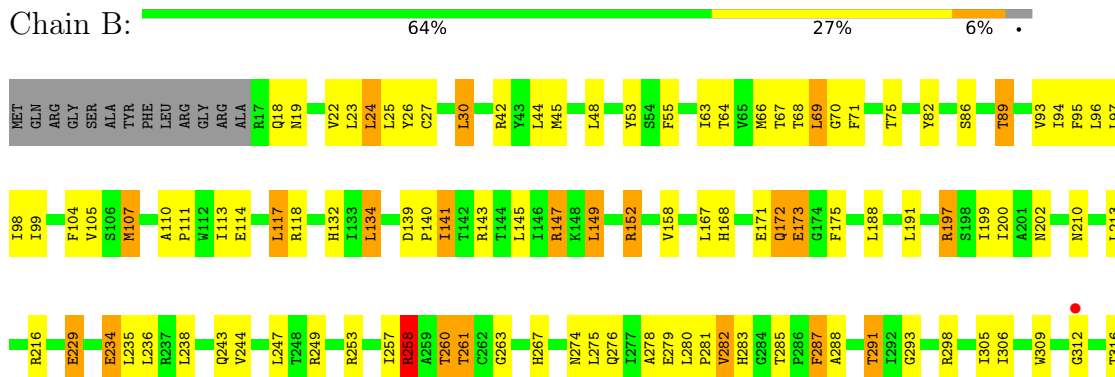
3 Residue-property plots

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: TrkA domain protein



- Molecule 1: TrkA domain protein





R361		SER	ILE
		GLU	LEU
D371		GLY	ILE
R372		MET	GLY
K373		ALA	THR
P374		VAL	SER
		PHE	GLU
R382		ARG	GLN
		ARG	GLU
C388		PRO	LYS
N389		LEU	THR
D390		PRO	PHE
H391		PRO	ASP
		ALA	GLN
Q402		MET	THR
		ALA	ILE
R405		GLY	ALA
Q406		LYS	ALA
M407		THR	ARG
G408		ILE	LEU
		ALA	VAL
R411		GLU	PRO
		THR	ARG
I415		ARG	
I416		LEU	
V417		ARG	
I418		PRO	
I419		LEU	
N420		THR	
D421		GLY	
		CYS	
I426		SER	
		ILE	
L430		VAL	
		ALA	
R433		ILE	
H434		GLU	
L435		ALA	
H436		PRO	
S437		ASP	
H438		ARG	
I439		ALA	
R440		ASP	
		ILE	
V451		LEU	
		ILE	
F461		SER	
		PRO	
A466		PRO	
		PRO	
G469		GLU	
		THR	
L477		ILE	
		LEU	
K480		ALA	
E481		GLU	
S482		GLY	
		ALA	
		PHE	
		ARG	
		LEU	

ILE
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GLU
LYS
THR
PHE
ASP
GLN
THR
ILE
ALA
ALA
ARG
LEU
VAL
PRO
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	234.98Å 108.36Å 165.79Å 90.00° 134.96° 90.00°	Depositor
Resolution (Å)	45.39 – 3.70 45.39 – 3.70	Depositor EDS
% Data completeness (in resolution range)	86.8 (45.39-3.70) 86.5 (45.39-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.261 , 0.293 0.262 , 0.296	Depositor DCC
R_{free} test set	1383 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	153.1	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 265.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	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	0.94	EDS
Total number of atoms	14266	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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

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	0.43	0/2982	0.96	19/4060 (0.5%)
1	B	0.42	0/4291	0.94	22/5843 (0.4%)
1	C	0.42	0/4271	0.93	18/5817 (0.3%)
1	D	0.44	0/2988	0.99	26/4068 (0.6%)
All	All	0.43	0/14532	0.95	85/19788 (0.4%)

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 (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ARG	NE-CZ-NH2	8.54	126.88	119.20
1	A	249	ARG	NE-CZ-NH2	8.35	126.72	119.20
1	C	249	ARG	NE-CZ-NH2	8.34	126.71	119.20
1	B	258	ARG	NE-CZ-NH2	8.20	126.58	119.20
1	C	382	ARG	NE-CZ-NH2	8.03	126.43	119.20
1	B	147	ARG	NE-CZ-NH2	7.99	126.39	119.20
1	D	147	ARG	NE-CZ-NH2	7.96	126.37	119.20
1	B	197	ARG	NE-CZ-NH2	7.82	126.24	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	197	ARG	NE-CZ-NH2	7.76	126.19	119.20
1	D	258	ARG	NE-CZ-NH2	7.67	126.10	119.20
1	B	258	ARG	NE-CZ-NH1	-7.67	113.83	121.50
1	A	382	ARG	NE-CZ-NH1	-7.57	113.93	121.50
1	A	249	ARG	NE-CZ-NH1	-7.53	113.97	121.50
1	C	249	ARG	NE-CZ-NH1	-7.50	114.00	121.50
1	B	147	ARG	NE-CZ-NH1	-7.38	114.12	121.50
1	B	197	ARG	NE-CZ-NH1	-7.36	114.14	121.50
1	D	197	ARG	NE-CZ-NH1	-7.34	114.16	121.50
1	D	258	ARG	NE-CZ-NH1	-7.33	114.17	121.50
1	D	147	ARG	NE-CZ-NH1	-7.32	114.18	121.50
1	D	373	LYS	CA-C-N	7.27	128.93	119.84
1	D	373	LYS	C-N-CA	7.27	128.93	119.84
1	B	373	LYS	CA-C-N	7.25	128.91	119.84
1	B	373	LYS	C-N-CA	7.25	128.91	119.84
1	C	382	ARG	NE-CZ-NH1	-7.24	114.26	121.50
1	C	373	LYS	CA-C-N	7.17	128.80	119.84
1	C	373	LYS	C-N-CA	7.17	128.80	119.84
1	A	373	LYS	CA-C-N	7.06	128.66	119.84
1	A	373	LYS	C-N-CA	7.06	128.66	119.84
1	D	372	ARG	NE-CZ-NH2	7.02	125.52	119.20
1	B	372	ARG	NE-CZ-NH2	6.82	125.33	119.20
1	D	481	GLU	N-CA-C	-6.45	105.71	113.97
1	D	372	ARG	NE-CZ-NH1	-6.36	115.14	121.50
1	B	372	ARG	NE-CZ-NH1	-6.35	115.15	121.50
1	A	382	ARG	CD-NE-CZ	6.00	132.80	124.40
1	D	173	GLU	N-CA-C	5.94	115.94	108.45
1	B	258	ARG	CD-NE-CZ	5.92	132.69	124.40
1	A	249	ARG	CD-NE-CZ	5.90	132.66	124.40
1	C	173	GLU	N-CA-C	5.88	115.86	108.45
1	A	173	GLU	N-CA-C	5.87	115.84	108.45
1	C	249	ARG	CD-NE-CZ	5.86	132.61	124.40
1	A	260	THR	N-CA-C	-5.85	104.50	111.69
1	C	382	ARG	CD-NE-CZ	5.82	132.55	124.40
1	C	258	ARG	NE-CZ-NH2	-5.77	114.00	119.20
1	C	258	ARG	CD-NE-CZ	5.74	132.44	124.40
1	A	258	ARG	NE-CZ-NH2	-5.71	114.06	119.20
1	D	147	ARG	CD-NE-CZ	5.67	132.34	124.40
1	C	147	ARG	NE-CZ-NH2	-5.66	114.10	119.20
1	B	147	ARG	CD-NE-CZ	5.65	132.31	124.40
1	B	382	ARG	NE-CZ-NH2	-5.64	114.12	119.20
1	D	382	ARG	NE-CZ-NH2	-5.64	114.12	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	382	ARG	CD-NE-CZ	5.64	132.29	124.40
1	A	147	ARG	NE-CZ-NH2	-5.63	114.14	119.20
1	D	258	ARG	CD-NE-CZ	5.61	132.26	124.40
1	A	229	GLU	CA-C-N	5.58	126.82	119.84
1	A	229	GLU	C-N-CA	5.58	126.82	119.84
1	B	382	ARG	CD-NE-CZ	5.56	132.19	124.40
1	A	258	ARG	CD-NE-CZ	5.49	132.08	124.40
1	D	229	GLU	CA-C-N	5.46	126.67	119.84
1	D	229	GLU	C-N-CA	5.46	126.67	119.84
1	D	197	ARG	CD-NE-CZ	5.44	132.01	124.40
1	C	197	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	B	497	PRO	CA-C-N	5.41	125.08	119.56
1	B	497	PRO	C-N-CA	5.41	125.08	119.56
1	B	197	ARG	CD-NE-CZ	5.39	131.94	124.40
1	B	229	GLU	CA-C-N	5.36	126.54	119.84
1	B	229	GLU	C-N-CA	5.36	126.54	119.84
1	A	197	ARG	NE-CZ-NH2	-5.33	114.41	119.20
1	C	229	GLU	CA-C-N	5.31	126.47	119.84
1	C	229	GLU	C-N-CA	5.31	126.47	119.84
1	C	147	ARG	CD-NE-CZ	5.29	131.80	124.40
1	D	237	ARG	N-CA-C	-5.24	105.69	111.71
1	D	260	THR	CB-CA-C	-5.24	102.22	110.86
1	A	147	ARG	CD-NE-CZ	5.20	131.67	124.40
1	D	249	ARG	NE-CZ-NH2	-5.18	114.53	119.20
1	B	141	ILE	CB-CA-C	-5.15	105.22	111.87
1	D	141	ILE	CB-CA-C	-5.13	105.25	111.87
1	D	417	VAL	CB-CA-C	5.12	117.76	111.25
1	A	141	ILE	CB-CA-C	-5.09	105.30	111.87
1	A	150	GLU	N-CA-C	-5.08	106.67	112.92
1	D	150	GLU	N-CA-C	-5.07	106.68	112.92
1	D	249	ARG	CD-NE-CZ	5.06	131.49	124.40
1	B	249	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	B	249	ARG	CD-NE-CZ	5.01	131.41	124.40
1	C	523	ALA	CA-C-N	5.00	126.09	119.84
1	C	523	ALA	C-N-CA	5.00	126.09	119.84

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

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

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	2922	0	2964	65	0
1	B	4208	0	4288	113	0
1	C	4188	0	4268	101	0
1	D	2928	0	2969	64	0
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	323	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 (323) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:200:ILE:HD11	1:D:477:LEU:HD11	1.84	0.59
1:D:402:GLN:OE1	1:D:405:ARG:NH2	2.34	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: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:O	1:C:172:GLN:NE2	2.37	0.57
1:D:93:VAL:O	1:D:97:LEU:HB3	2.05	0.57
1:D:141:ILE:HD12	1:D:469:GLY:HA3	1.86	0.57
1:C:93:VAL:O	1:C:97:LEU:HB3	2.05	0.57
1:D:480:LYS:HZ2	1:D:481:GLU:HB2	1.69	0.57
1:B:149:LEU:HD22	1:B:152:ARG:HD3	1.86	0.56
1:B:172:GLN:O	1:B:172:GLN:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:94:ILE:O	1:C:99:ILE:HG12	2.06	0.56
1:C:97:LEU:O	1:C:97:LEU:HD22	2.06	0.56
1:A:94:ILE:O	1:A:99:ILE:HG12	2.06	0.55
1:A:351:ASP:N	1:A:351:ASP:OD1	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:HD22	1:B:97:LEU:O	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
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:HD22	1:A:97:LEU:O	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:C:66:MET:C	1:C:68:THR:H	2.18	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:67:THR:HG21	1:D:89:THR:HG21	1.91	0.51
1:C:351:ASP:OD1	1:C:351:ASP:N	2.43	0.51
1:C:479:HIS:HB3	1:C:483:ALA:HB2	1.92	0.51
1:C:258:ARG:O	1:C:440:ARG:HD3	2.10	0.51
1:B:282:VAL:O	1:B:285:THR:OG1	2.25	0.51
1:B:504:THR:HB	1:B:507:GLU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:ASP:N	1:D:351:ASP:OD1	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:B:66:MET:C	1:B:68:THR:H	2.17	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
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:67:THR:HG21	1:B:89:THR:HG21	1.94	0.49
1:A:258:ARG:O	1:A:440:ARG:HD3	2.12	0.49
1:B:390:ASP:OD2	1:B:390:ASP:N	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:N	1:A:390:ASP:OD2	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:OD2	1:D:390:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:93:VAL:O	1:D:98:ILE:HG12	2.13	0.48
1:D:141:ILE:HD13	1:D:466:ALA:HA	1.95	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: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: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:A:67:THR:HG21	1:B:89:THR:CG2	2.46	0.46
1:B:258:ARG:HG2	1:B:461:PHE:CD1	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:63:ILE:O	1:C:67:THR:HG22	2.15	0.46
1:C:139:ASP:HB2	1:C:140:PRO:HD2	1.97	0.46
1:B:274:ASN:ND2	1:B:554:GLU:OE2	2.49	0.46
1:B:436:HIS:HB3	1:B:439:ILE:HG23	1.97	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:44:LEU:O	1:B:48:LEU:N	2.47	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
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:HA	1:C:216:ARG:HD3	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:HA	1:D:216:ARG:HD3	1.71	0.45
1:C:292:ILE:HD13	1:C:527:ALA:HB1	1.98	0.44
1:C:388:CYS:SG	1:C:391:HIS:HB2	2.57	0.44
1:D:172:GLN:HE21	1:D:172:GLN:C	2.25	0.44
1:A:66:MET:C	1:A:68:THR:H	2.24	0.44
1:B:45:MET:HG3	1:B:53:TYR:CD2	2.52	0.44
1:B:172:GLN:HE21	1:B:172:GLN:C	2.25	0.44
1:C:348:ALA:HA	1:C:349:PRO:HD3	1.89	0.44
1:D:234:GLU:H	1:D:234:GLU:HG3	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:HE3	1:B:335:LYS:HB2	1.74	0.44
1:C:258:ARG:O	1:C:440:ARG:NH1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:26:TYR:OH	1:B:95:PHE:O	2.34	0.43
1:B:216:ARG:HA	1:B:216:ARG:HD3	1.74	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
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:A:172:GLN:C	1:A:172:GLN:HE21	2.26	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:HD12	1:A:30:LEU:HA	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:63:ILE:O	1:B:67:THR:HG22	2.19	0.42
1:B:213:LEU:HD23	1:B:213:LEU:HA	1.87	0.42
1:C:24:LEU:HA	1:C:27:CYS:HB2	2.01	0.42
1:C:234:GLU:H	1:C:234:GLU:HG3	1.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:C:30:LEU:HA	1.93	0.42
1:C:172:GLN:HE21	1:C:172:GLN:C	2.27	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:69:LEU:HD11	1:B:71:PHE:CZ	2.55	0.41
1:B:426:ILE:O	1:B:430:LEU:HB2	2.20	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:OD1	1:B:528:ASP:N	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:B:260:THR:O	1:B:261:THR:C	2.64	0.41
1:D:419:THR:HG22	1:D:421:ASP:H	1.84	0.41
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:HD12	1:D:134:LEU:HA	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:B:408:GLY:C	1:B:410:ASP:H	2.29	0.41
1:D:402:GLN:H	1:D:402:GLN:HG2	1.72	0.41
1:A:60:TYR:HB2	1:B:82:TYR:HB3	2.03	0.41
1:B:514:THR:HG21	1:B:557:PHE:HD1	1.85	0.41
1:C:324:THR:C	1:C:326:GLN:H	2.29	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:141:ILE:HG23	1:C:469:GLY:HA3	2.02	0.41
1:C:303:LEU:HD23	1:C:333:GLY:HA3	2.03	0.41
1:A:44:LEU:O	1:A:48:LEU:N	2.45	0.41
1:A:450:ASN:OD1	1:B:210:ASN:ND2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:TYR:OH	1:B:99:ILE:HB	2.20	0.41
1:B:114:GLU:HA	1:B:117:LEU:HD23	2.03	0.41
1:B:134:LEU:HD12	1:B:134:LEU:HA	1.91	0.41
1:B:141:ILE:HG23	1:B:469:GLY:HA3	2.02	0.41
1:C:26:TYR:OH	1:C:99:ILE:HB	2.21	0.41
1:C:45:MET:HG3	1:C:53:TYR:CD2	2.55	0.41
1:D:480:LYS:HZ2	1:D:480:LYS:HB3	1.86	0.41
1:D:30:LEU:HD11	1:D:95:PHE:HB3	2.02	0.41
1:D:138:ILE:HG13	1:D:143:ARG:HG3	2.03	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:66:MET:C	1:B:68:THR:N	2.80	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:423:SER:O	1:D:206:PRO:HB3	2.21	0.40
1:C:479:HIS:O	1:C:483:ALA:N	2.42	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
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%)	24	56
1	B	546/565 (97%)	509 (93%)	33 (6%)	4 (1%)	18	50
1	C	544/565 (96%)	498 (92%)	40 (7%)	6 (1%)	11	42
1	D	372/565 (66%)	345 (93%)	25 (7%)	2 (0%)	24	56
All	All	1833/2260 (81%)	1698 (93%)	121 (7%)	14 (1%)	16	48

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/463 (68%)	267 (85%)	46 (15%)	3	17
1	B	449/463 (97%)	386 (86%)	63 (14%)	3	18
1	C	447/463 (96%)	380 (85%)	67 (15%)	3	16
1	D	314/463 (68%)	265 (84%)	49 (16%)	2	15
All	All	1523/1852 (82%)	1298 (85%)	225 (15%)	3	17

All (225) 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	64	THR
1	A	69	LEU
1	A	75	THR
1	A	89	THR
1	A	96	LEU
1	A	104	PHE
1	A	105	VAL
1	A	107	MET
1	A	117	LEU
1	A	132	HIS
1	A	134	LEU
1	A	145	LEU
1	A	149	LEU
1	A	152	ARG
1	A	158	VAL
1	A	167	LEU
1	A	168	HIS
1	A	171	GLU
1	A	172	GLN
1	A	234	GLU
1	A	236	LEU
1	A	238	LEU
1	A	243	GLN
1	A	244	VAL
1	A	247	LEU
1	A	249	ARG
1	A	258	ARG
1	A	261	THR
1	A	351	ASP
1	A	353	LEU
1	A	371	ASP
1	A	390	ASP
1	A	406	GLN
1	A	430	LEU
1	A	434	HIS
1	A	436	HIS
1	A	438	HIS

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Mol	Chain	Res	Type
1	A	439	ILE
1	A	442	VAL
1	A	451	VAL
1	A	480	LYS
1	B	23	LEU
1	B	24	LEU
1	B	25	LEU
1	B	30	LEU
1	B	64	THR
1	B	69	LEU
1	B	75	THR
1	B	89	THR
1	B	96	LEU
1	B	104	PHE
1	B	105	VAL
1	B	107	MET
1	B	117	LEU
1	B	132	HIS
1	B	134	LEU
1	B	145	LEU
1	B	149	LEU
1	B	152	ARG
1	B	158	VAL
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	236	LEU
1	B	238	LEU
1	B	243	GLN
1	B	244	VAL
1	B	247	LEU
1	B	258	ARG
1	B	260	THR
1	B	275	LEU
1	B	282	VAL
1	B	287	PHE
1	B	291	THR
1	B	306	ILE
1	B	316	THR

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Mol	Chain	Res	Type
1	B	330	VAL
1	B	334	THR
1	B	347	GLU
1	B	351	ASP
1	B	353	LEU
1	B	364	CYS
1	B	371	ASP
1	B	372	ARG
1	B	382	ARG
1	B	390	ASP
1	B	406	GLN
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	451	VAL
1	B	480	LYS
1	B	481	GLU
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	64	THR
1	C	75	THR
1	C	89	THR
1	C	96	LEU
1	C	97	LEU
1	C	104	PHE
1	C	105	VAL
1	C	107	MET
1	C	117	LEU
1	C	132	HIS
1	C	134	LEU
1	C	145	LEU
1	C	149	LEU

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Mol	Chain	Res	Type
1	C	152	ARG
1	C	158	VAL
1	C	167	LEU
1	C	168	HIS
1	C	171	GLU
1	C	172	GLN
1	C	234	GLU
1	C	236	LEU
1	C	238	LEU
1	C	244	VAL
1	C	247	LEU
1	C	249	ARG
1	C	258	ARG
1	C	260	THR
1	C	262	CYS
1	C	292	ILE
1	C	300	ARG
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	350	GLU
1	C	351	ASP
1	C	353	LEU
1	C	371	ASP
1	C	390	ASP
1	C	406	GLN
1	C	430	LEU
1	C	434	HIS
1	C	436	HIS
1	C	438	HIS
1	C	439	ILE
1	C	451	VAL
1	C	480	LYS
1	C	484	PHE
1	C	485	LEU
1	C	491	VAL
1	C	500	MET
1	C	504	THR
1	C	508	THR

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Mol	Chain	Res	Type
1	C	510	LEU
1	C	518	ILE
1	C	522	GLU
1	C	539	LEU
1	C	551	SER
1	C	554	GLU
1	C	555	LYS
1	C	561	ILE
1	D	23	LEU
1	D	24	LEU
1	D	25	LEU
1	D	30	LEU
1	D	64	THR
1	D	69	LEU
1	D	75	THR
1	D	89	THR
1	D	96	LEU
1	D	97	LEU
1	D	104	PHE
1	D	105	VAL
1	D	107	MET
1	D	117	LEU
1	D	132	HIS
1	D	134	LEU
1	D	145	LEU
1	D	149	LEU
1	D	152	ARG
1	D	158	VAL
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	236	LEU
1	D	238	LEU
1	D	243	GLN
1	D	244	VAL
1	D	247	LEU
1	D	258	ARG
1	D	351	ASP
1	D	353	LEU

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Mol	Chain	Res	Type
1	D	371	ASP
1	D	372	ARG
1	D	382	ARG
1	D	390	ASP
1	D	406	GLN
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	451	VAL
1	D	480	LYS
1	D	481	GLU
1	D	482	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	391	HIS
1	B	267	HIS
1	B	276	GLN
1	B	337	GLN
1	B	391	HIS
1	C	220	GLN
1	C	391	HIS
1	C	479	HIS
1	D	18	GLN
1	D	391	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 oligosaccharides 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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	375/565 (66%)	-0.79	0 100 100	126, 189, 324, 425	0
1	B	548/565 (96%)	-0.49	2 (0%) 88 72	135, 230, 370, 487	0
1	C	546/565 (96%)	-0.52	7 (1%) 75 50	124, 223, 381, 519	0
1	D	376/565 (66%)	-0.73	0 100 100	124, 187, 332, 475	0
All	All	1845/2260 (81%)	-0.61	9 (0%) 87 69	124, 205, 368, 519	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	438	HIS	5.9
1	C	516	CYS	3.6
1	B	498	PRO	3.5
1	C	437	SER	3.0
1	C	313	SER	2.8
1	C	172	GLN	2.6
1	C	517	SER	2.1
1	C	113	ILE	2.0
1	B	312	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 oligosaccharides in this entry.

6.4 Ligands

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, 95th 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 ²)	Q<0.9
2	K	A	608	1/1	0.92	0.26	225,225,225,225	1
2	K	A	607	1/1	0.96	0.11	199,199,199,199	1
2	K	C	601	1/1	0.97	0.07	207,207,207,207	1
2	K	C	608	1/1	0.97	0.15	241,241,241,241	1
2	K	C	602	1/1	0.99	0.05	153,153,153,153	1
2	K	A	601	1/1	0.99	0.02	166,166,166,166	1
2	K	C	609	1/1	0.99	0.14	200,200,200,200	1
3	ZN	A	605	1/1	0.99	0.03	160,160,160,160	0
4	CA	A	606	1/1	0.99	0.04	173,173,173,173	0
4	CA	C	606	1/1	0.99	0.04	185,185,185,185	0
4	CA	C	607	1/1	0.99	0.05	138,138,138,138	0
2	K	A	604	1/1	1.00	0.02	186,186,186,186	1
2	K	A	602	1/1	1.00	0.03	154,154,154,154	1
3	ZN	B	601	1/1	1.00	0.01	134,134,134,134	0
3	ZN	C	605	1/1	1.00	0.02	152,152,152,152	0
3	ZN	D	601	1/1	1.00	0.02	149,149,149,149	0
2	K	C	603	1/1	1.00	0.02	160,160,160,160	1
4	CA	B	602	1/1	1.00	0.02	175,175,175,175	0
2	K	C	604	1/1	1.00	0.02	143,143,143,143	1
2	K	A	603	1/1	1.00	0.02	169,169,169,169	1

6.5 Other polymers

There are no such residues in this entry.