



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:38 AM UTC

PDB ID : 4QQW / pdb_00004qqw
Title : Crystal structure of T. fusca Cas3
Authors : Ke, A.; Huo, Y.; Nam, K.H.
Deposited on : 2014-06-30
Resolution : 2.66 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:

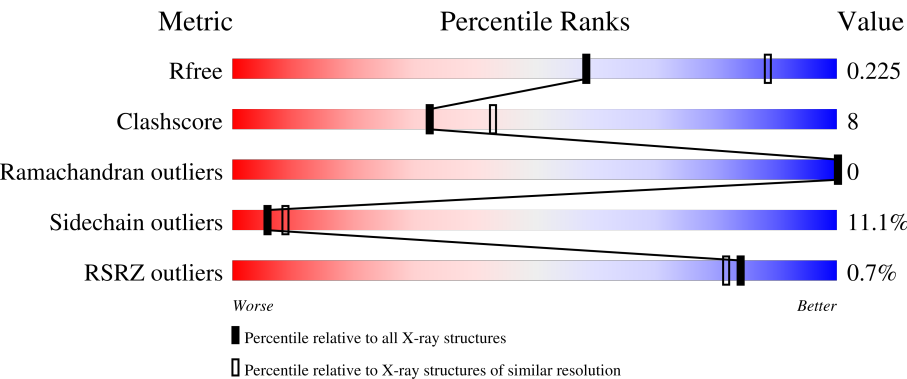
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	964	% 74%16%• 5%
1	C	964	71%18%• 6%
1	E	964	% 71%18%• 7%
1	G	964	% 72%18%• 7%
2	B	12	50%25%17%8%

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Mol	Chain	Length	Quality of chain
2	D	12	8%25%42%25%8%
2	F	12	42%42%8%8%
2	H	12	8%50%33%8%8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29038 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 CRISPR-associated helicase, Cas3 family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	911	Total	C	N	O	S	0	0	0
			7082	4496	1260	1299	27			
1	C	902	Total	C	N	O	S	0	0	0
			7001	4441	1243	1290	27			
1	E	897	Total	C	N	O	S	0	0	0
			6971	4424	1241	1279	27			
1	G	898	Total	C	N	O	S	0	0	0
			6973	4426	1239	1281	27			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q47PJ0
A	-18	GLY	-	expression tag	UNP Q47PJ0
A	-17	SER	-	expression tag	UNP Q47PJ0
A	-16	SER	-	expression tag	UNP Q47PJ0
A	-15	HIS	-	expression tag	UNP Q47PJ0
A	-14	HIS	-	expression tag	UNP Q47PJ0
A	-13	HIS	-	expression tag	UNP Q47PJ0
A	-12	HIS	-	expression tag	UNP Q47PJ0
A	-11	HIS	-	expression tag	UNP Q47PJ0
A	-10	HIS	-	expression tag	UNP Q47PJ0
A	-9	SER	-	expression tag	UNP Q47PJ0
A	-8	SER	-	expression tag	UNP Q47PJ0
A	-7	GLY	-	expression tag	UNP Q47PJ0
A	-6	LEU	-	expression tag	UNP Q47PJ0
A	-5	VAL	-	expression tag	UNP Q47PJ0
A	-4	PRO	-	expression tag	UNP Q47PJ0
A	-3	ARG	-	expression tag	UNP Q47PJ0
A	-2	GLY	-	expression tag	UNP Q47PJ0
A	-1	SER	-	expression tag	UNP Q47PJ0
A	0	HIS	-	expression tag	UNP Q47PJ0
C	-19	MET	-	initiating methionine	UNP Q47PJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	GLY	-	expression tag	UNP Q47PJ0
C	-17	SER	-	expression tag	UNP Q47PJ0
C	-16	SER	-	expression tag	UNP Q47PJ0
C	-15	HIS	-	expression tag	UNP Q47PJ0
C	-14	HIS	-	expression tag	UNP Q47PJ0
C	-13	HIS	-	expression tag	UNP Q47PJ0
C	-12	HIS	-	expression tag	UNP Q47PJ0
C	-11	HIS	-	expression tag	UNP Q47PJ0
C	-10	HIS	-	expression tag	UNP Q47PJ0
C	-9	SER	-	expression tag	UNP Q47PJ0
C	-8	SER	-	expression tag	UNP Q47PJ0
C	-7	GLY	-	expression tag	UNP Q47PJ0
C	-6	LEU	-	expression tag	UNP Q47PJ0
C	-5	VAL	-	expression tag	UNP Q47PJ0
C	-4	PRO	-	expression tag	UNP Q47PJ0
C	-3	ARG	-	expression tag	UNP Q47PJ0
C	-2	GLY	-	expression tag	UNP Q47PJ0
C	-1	SER	-	expression tag	UNP Q47PJ0
C	0	HIS	-	expression tag	UNP Q47PJ0
E	-19	MET	-	initiating methionine	UNP Q47PJ0
E	-18	GLY	-	expression tag	UNP Q47PJ0
E	-17	SER	-	expression tag	UNP Q47PJ0
E	-16	SER	-	expression tag	UNP Q47PJ0
E	-15	HIS	-	expression tag	UNP Q47PJ0
E	-14	HIS	-	expression tag	UNP Q47PJ0
E	-13	HIS	-	expression tag	UNP Q47PJ0
E	-12	HIS	-	expression tag	UNP Q47PJ0
E	-11	HIS	-	expression tag	UNP Q47PJ0
E	-10	HIS	-	expression tag	UNP Q47PJ0
E	-9	SER	-	expression tag	UNP Q47PJ0
E	-8	SER	-	expression tag	UNP Q47PJ0
E	-7	GLY	-	expression tag	UNP Q47PJ0
E	-6	LEU	-	expression tag	UNP Q47PJ0
E	-5	VAL	-	expression tag	UNP Q47PJ0
E	-4	PRO	-	expression tag	UNP Q47PJ0
E	-3	ARG	-	expression tag	UNP Q47PJ0
E	-2	GLY	-	expression tag	UNP Q47PJ0
E	-1	SER	-	expression tag	UNP Q47PJ0
E	0	HIS	-	expression tag	UNP Q47PJ0
G	-19	MET	-	initiating methionine	UNP Q47PJ0
G	-18	GLY	-	expression tag	UNP Q47PJ0
G	-17	SER	-	expression tag	UNP Q47PJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	SER	-	expression tag	UNP Q47PJ0
G	-15	HIS	-	expression tag	UNP Q47PJ0
G	-14	HIS	-	expression tag	UNP Q47PJ0
G	-13	HIS	-	expression tag	UNP Q47PJ0
G	-12	HIS	-	expression tag	UNP Q47PJ0
G	-11	HIS	-	expression tag	UNP Q47PJ0
G	-10	HIS	-	expression tag	UNP Q47PJ0
G	-9	SER	-	expression tag	UNP Q47PJ0
G	-8	SER	-	expression tag	UNP Q47PJ0
G	-7	GLY	-	expression tag	UNP Q47PJ0
G	-6	LEU	-	expression tag	UNP Q47PJ0
G	-5	VAL	-	expression tag	UNP Q47PJ0
G	-4	PRO	-	expression tag	UNP Q47PJ0
G	-3	ARG	-	expression tag	UNP Q47PJ0
G	-2	GLY	-	expression tag	UNP Q47PJ0
G	-1	SER	-	expression tag	UNP Q47PJ0
G	0	HIS	-	expression tag	UNP Q47PJ0

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	0	0
			197	90	45	51	11			
2	D	11	Total	C	N	O	P	0	0	0
			197	90	45	51	11			
2	F	11	Total	C	N	O	P	0	0	0
			197	90	45	51	11			
2	H	11	Total	C	N	O	P	0	0	0
			197	90	45	51	11			

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Fe	0	0
			2	2		
3	C	2	Total	Fe	0	0
			2	2		
3	E	2	Total	Fe	0	0
			2	2		
3	G	2	Total	Fe	0	0
			2	2		

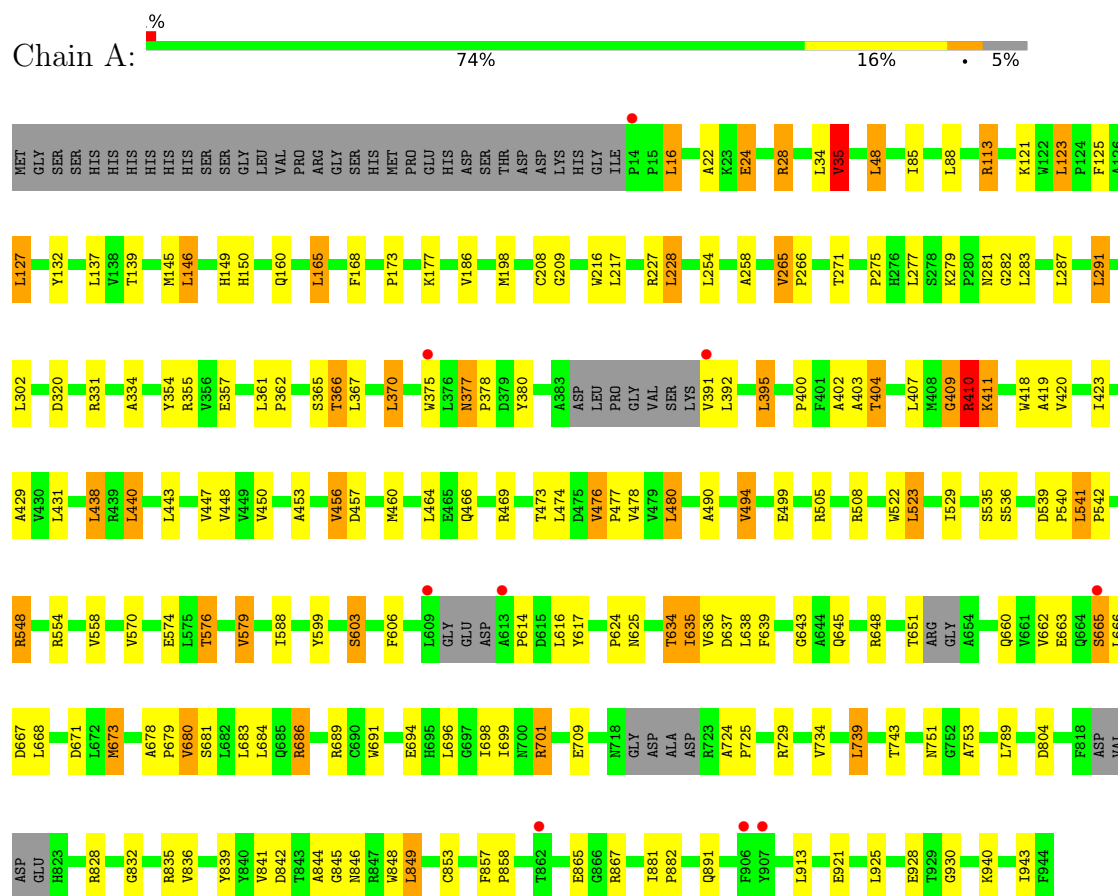
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total 61	O 61	0	0
4	B	3	Total 3	O 3	0	0
4	C	62	Total 62	O 62	0	0
4	D	1	Total 1	O 1	0	0
4	E	51	Total 51	O 51	0	0
4	G	37	Total 37	O 37	0	0

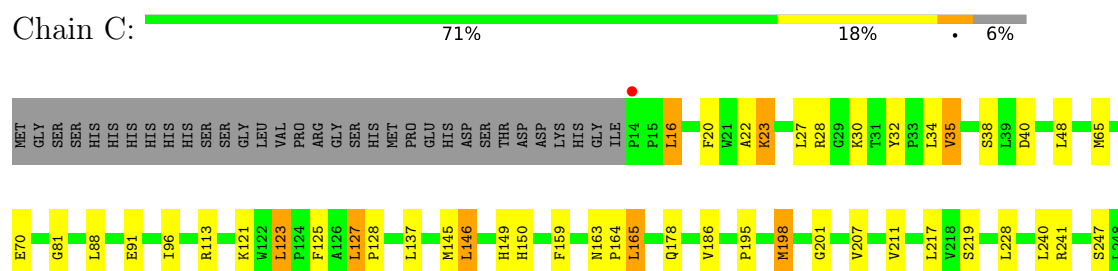
3 Residue-property plots

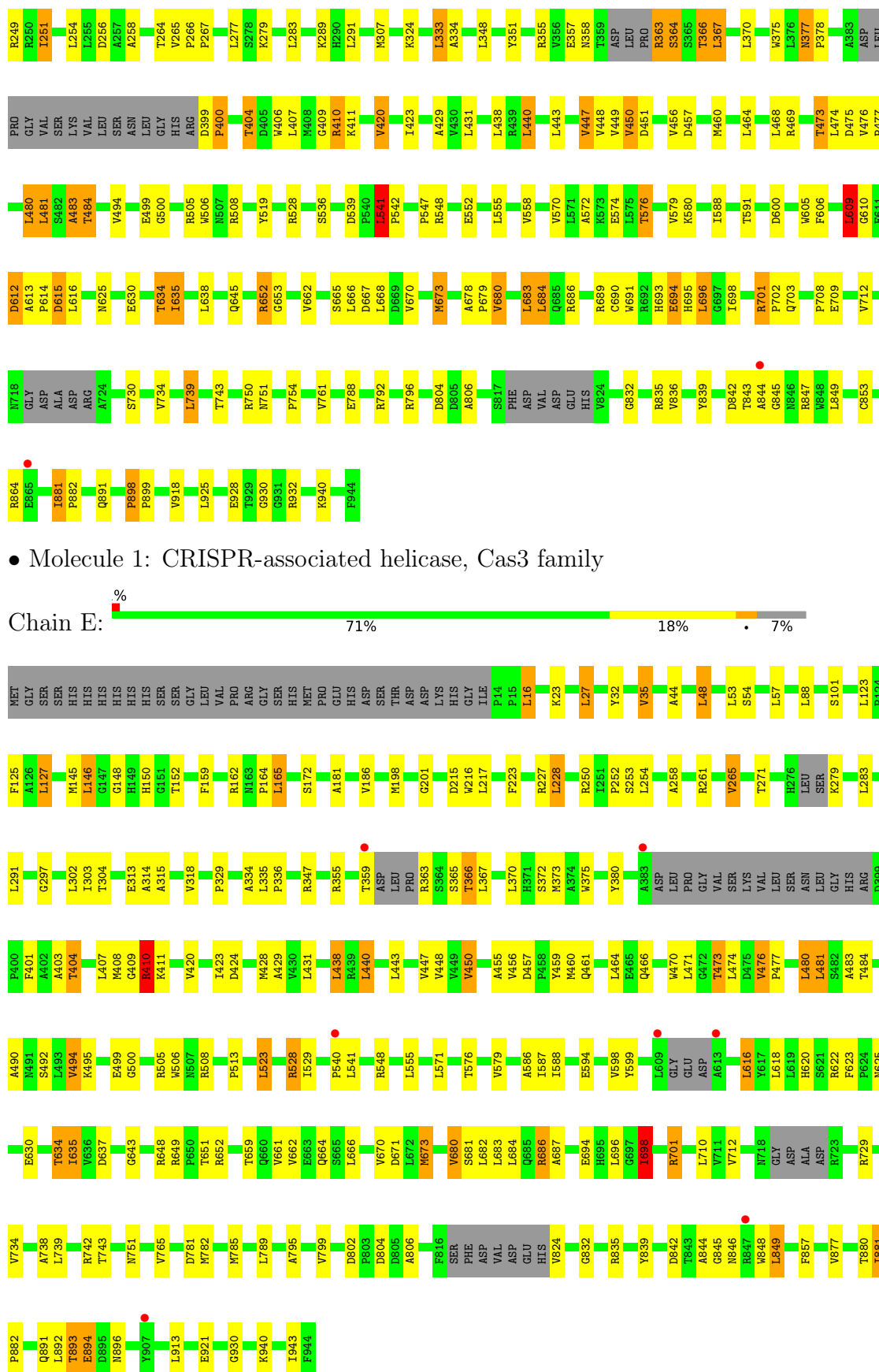
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CRISPR-associated helicase, Cas3 family

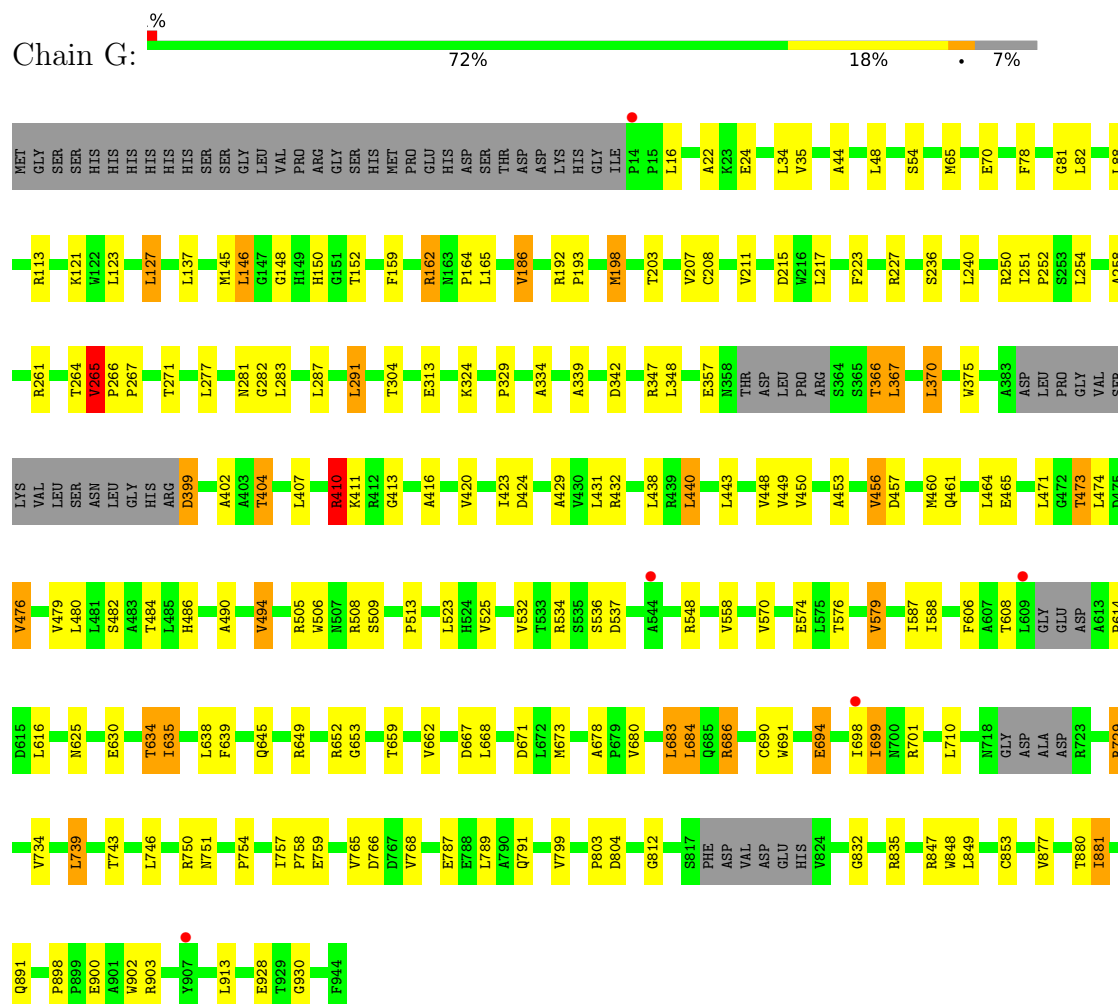


- Molecule 1: CRISPR-associated helicase, Cas3 family

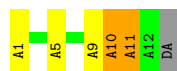




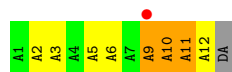
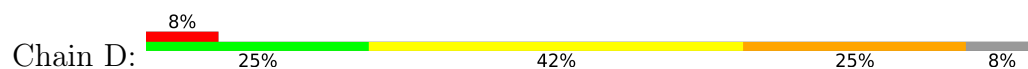
- Molecule 1: CRISPR-associated helicase, Cas3 family



- Molecule 2: DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



- Molecule 2: DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

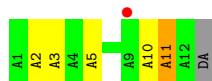


- Molecule 2: DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')





- Molecule 2: DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.79Å 218.54Å 123.75Å 90.00° 105.00° 90.00°	Depositor
Resolution (Å)	30.21 – 2.66 30.21 – 2.66	Depositor EDS
% Data completeness (in resolution range)	92.1 (30.21-2.66) 89.4 (30.21-2.66)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.173 , 0.226 0.176 , 0.225	Depositor DCC
R_{free} test set	2000 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	29038	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	0.65	3/7260 (0.0%)	0.97	18/9904 (0.2%)
1	C	0.68	7/7176 (0.1%)	0.99	32/9790 (0.3%)
1	E	0.62	2/7144 (0.0%)	0.94	21/9743 (0.2%)
1	G	0.57	2/7147 (0.0%)	0.91	7/9749 (0.1%)
2	B	0.60	0/222	1.44	3/339 (0.9%)
2	D	0.54	0/222	1.31	3/339 (0.9%)
2	F	0.46	0/222	1.21	1/339 (0.3%)
2	H	0.45	0/222	1.24	2/339 (0.6%)
All	All	0.63	14/29615 (0.0%)	0.97	87/40542 (0.2%)

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	C	0	2
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	701	ARG	C-N	6.16	1.41	1.33
1	C	613	ALA	C-N	5.87	1.40	1.33
1	A	541	LEU	C-N	5.77	1.40	1.33
1	E	649	ARG	C-N	5.65	1.40	1.33
1	C	541	LEU	C-N	5.51	1.40	1.33
1	C	127	LEU	C-N	5.41	1.40	1.34
1	A	701	ARG	C-N	5.32	1.40	1.33
1	C	400	PRO	N-CD	5.31	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	542	PRO	N-CD	5.24	1.55	1.47
1	G	192	ARG	C-N	5.17	1.40	1.33
1	C	702	PRO	N-CD	5.17	1.54	1.47
1	C	542	PRO	N-CD	5.12	1.54	1.47
1	C	701	ARG	C-N	5.12	1.40	1.33
1	G	193	PRO	N-CD	5.05	1.54	1.47

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	27	LEU	N-CA-C	8.76	123.27	112.59
1	C	35	VAL	CB-CA-C	-8.69	100.75	111.88
1	C	609	LEU	CA-C-N	8.06	128.93	119.98
1	C	609	LEU	C-N-CA	8.06	128.93	119.98
1	E	35	VAL	CB-CA-C	-7.96	101.39	112.14
1	A	410	ARG	CB-CA-C	-7.88	107.48	116.54
1	E	410	ARG	CB-CA-C	-7.70	107.70	116.63
2	B	11	DA	O4'-C1'-N9	7.60	119.80	108.40
1	C	123	LEU	CA-C-N	-7.52	112.05	119.87
1	C	123	LEU	C-N-CA	-7.52	112.05	119.87
1	C	613	ALA	CA-C-N	-7.17	113.28	120.31
1	C	613	ALA	C-N-CA	-7.17	113.28	120.31
1	A	701	ARG	CA-C-N	-7.15	113.34	120.21
1	A	701	ARG	C-N-CA	-7.15	113.34	120.21
1	C	483	ALA	N-CA-C	-6.97	99.41	109.31
1	G	265	VAL	CA-C-N	6.95	124.73	119.66
1	G	265	VAL	C-N-CA	6.95	124.73	119.66
1	E	649	ARG	CA-C-N	-6.91	112.64	119.90
1	E	649	ARG	C-N-CA	-6.91	112.64	119.90
1	C	400	PRO	N-CA-C	6.90	123.12	113.53
1	A	753	ALA	CA-C-N	6.88	126.84	120.03
1	A	753	ALA	C-N-CA	6.88	126.84	120.03
1	C	539	ASP	CA-C-N	6.88	126.34	118.85
1	C	539	ASP	C-N-CA	6.88	126.34	118.85
1	E	701	ARG	CA-C-N	-6.84	113.65	120.21
1	E	701	ARG	C-N-CA	-6.84	113.65	120.21
1	G	659	THR	CB-CA-C	-6.66	102.64	113.37
1	E	483	ALA	N-CA-C	-6.62	99.90	109.31
1	C	475	ASP	CA-C-N	-6.60	116.97	123.04
1	C	475	ASP	C-N-CA	-6.60	116.97	123.04
1	A	24	GLU	CB-CA-C	6.47	123.30	110.42
2	D	9	DA	O4'-C1'-N9	6.47	118.10	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	192	ARG	CA-C-N	-6.45	113.31	119.76
1	G	192	ARG	C-N-CA	-6.45	113.31	119.76
1	A	377	ASN	CA-C-N	6.43	126.01	119.19
1	A	377	ASN	C-N-CA	6.43	126.01	119.19
1	A	541	LEU	CA-C-N	-6.40	113.69	120.03
1	A	541	LEU	C-N-CA	-6.40	113.69	120.03
1	C	541	LEU	CA-C-N	-6.38	113.38	119.76
1	C	541	LEU	C-N-CA	-6.38	113.38	119.76
2	H	11	DA	O5'-C5'-C4'	-6.30	101.34	110.80
1	A	409	GLY	N-CA-C	6.30	119.17	111.93
2	B	10	DA	C1'-O4'-C4'	-6.02	100.67	109.70
1	A	35	VAL	CB-CA-C	-6.00	104.04	112.14
1	C	163	ASN	CA-C-N	6.00	125.20	118.97
1	C	163	ASN	C-N-CA	6.00	125.20	118.97
1	E	127	LEU	CA-C-N	-5.98	113.46	119.56
1	E	127	LEU	C-N-CA	-5.98	113.46	119.56
1	G	410	ARG	CB-CA-C	-5.97	109.11	117.23
2	B	11	DA	O4'-C4'-C3'	5.86	114.19	105.40
1	C	701	ARG	CA-C-N	-5.83	113.69	119.92
1	C	701	ARG	C-N-CA	-5.83	113.69	119.92
1	C	610	GLY	N-CA-C	-5.79	105.78	112.73
2	D	10	DA	C1'-O4'-C4'	-5.76	101.06	109.70
1	C	377	ASN	CA-C-N	5.75	125.29	119.19
1	C	377	ASN	C-N-CA	5.75	125.29	119.19
2	D	11	DA	C3'-C2'-C1'	5.72	110.18	101.60
1	A	476	VAL	CA-C-N	5.70	125.61	119.85
1	A	476	VAL	C-N-CA	5.70	125.61	119.85
1	E	680	VAL	CB-CA-C	-5.70	104.58	112.04
1	E	698	ILE	N-CA-C	5.66	115.85	110.53
2	H	11	DA	C5'-C4'-O4'	-5.62	100.98	109.40
1	E	172	SER	CA-C-N	5.51	125.17	119.05
1	E	172	SER	C-N-CA	5.51	125.17	119.05
1	C	128	PRO	CA-N-CD	-5.51	104.28	112.00
1	E	470	TRP	N-CA-C	5.46	117.31	111.36
1	C	898	PRO	O-C-N	5.45	123.81	121.31
1	C	447	VAL	CA-C-N	-5.44	116.44	123.19
1	C	447	VAL	C-N-CA	-5.44	116.44	123.19
1	C	195	PRO	O-C-N	5.33	123.65	121.15
1	A	410	ARG	N-CA-C	5.24	116.27	108.31
1	A	539	ASP	CA-C-N	-5.21	113.27	119.05
1	A	539	ASP	C-N-CA	-5.21	113.27	119.05
1	C	127	LEU	CA-C-N	-5.20	114.46	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	127	LEU	C-N-CA	-5.20	114.46	119.87
1	C	358	ASN	N-CA-C	5.19	116.63	110.97
1	E	297	GLY	CA-C-N	5.19	125.48	119.93
1	E	297	GLY	C-N-CA	5.19	125.48	119.93
1	C	16	LEU	CA-CB-CG	5.16	134.36	116.30
1	E	32	TYR	CA-C-N	5.15	125.09	119.78
1	E	32	TYR	C-N-CA	5.15	125.09	119.78
1	E	172	SER	N-CA-C	5.13	116.11	109.65
1	G	799	VAL	N-CA-C	5.08	116.55	109.80
1	E	410	ARG	N-CA-C	5.05	116.62	108.08
1	C	483	ALA	CB-CA-C	-5.04	102.51	114.16
1	A	209	GLY	N-CA-C	-5.03	106.69	112.73
2	F	10	DA	O4'-C1'-C2'	-5.02	98.86	106.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	409	GLY	Peptide
1	C	409	GLY	Peptide
1	C	609	LEU	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	7082	0	7030	117	0
1	C	7001	0	6944	122	0
1	E	6971	0	6921	109	0
1	G	6973	0	6923	99	0
2	B	197	0	99	9	0
2	D	197	0	99	10	0
2	F	197	0	99	10	0
2	H	197	0	99	9	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
3	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	2	0	0	0	0
4	A	61	0	0	0	0
4	B	3	0	0	0	0
4	C	62	0	0	3	0
4	D	1	0	0	0	0
4	E	51	0	0	3	0
4	G	37	0	0	1	0
All	All	29038	0	28214	448	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 8.

All (448) 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:844:ALA:H	1:C:845:GLY:HA2	1.29	0.95
1:C:694:GLU:HG2	1:C:701:ARG:HH21	1.33	0.93
1:C:256:ASP:HB3	1:C:363:ARG:HH22	1.33	0.93
1:A:665:SER:O	1:A:666:LEU:HD23	1.75	0.86
1:A:844:ALA:H	1:A:845:GLY:HA2	1.40	0.86
1:C:667:ASP:O	1:C:668:LEU:HD23	1.76	0.83
1:C:652:ARG:CB	1:C:652:ARG:HH11	1.93	0.81
1:C:150:HIS:CE1	2:D:11:DA:H5'	2.17	0.79
1:A:832:GLY:HA2	2:B:5:DA:H61	1.47	0.79
1:C:547:PRO:HG2	1:C:695:HIS:CE1	2.18	0.79
1:C:410:ARG:HD3	2:D:10:DA:H8	1.48	0.79
1:C:694:GLU:CG	1:C:701:ARG:HH21	1.97	0.78
1:E:429:ALA:HB1	1:E:440:LEU:HD13	1.66	0.77
1:A:848:TRP:CD1	1:A:853:CYS:SG	2.80	0.75
1:E:893:THR:OG1	1:E:894:GLU:N	2.17	0.75
1:G:832:GLY:HA2	2:H:5:DA:H61	1.50	0.75
1:E:150:HIS:CE1	2:F:11:DA:H5'	2.22	0.75
1:E:832:GLY:HA2	2:F:5:DA:H61	1.53	0.74
1:A:150:HIS:CE1	2:B:11:DA:H5'	2.23	0.73
1:A:848:TRP:CD1	1:A:853:CYS:HG	2.06	0.72
1:C:410:ARG:HD3	2:D:10:DA:C8	2.23	0.72
1:A:429:ALA:HB1	1:A:440:LEU:HD13	1.72	0.71
1:C:404:THR:HG22	1:C:407:LEU:H	1.54	0.71
1:C:266:PRO:O	1:C:355:ARG:NH2	2.23	0.71
1:C:541:LEU:HD13	1:C:541:LEU:C	2.16	0.70
1:E:313:GLU:OE2	1:E:347:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:404:THR:HG22	1:G:407:LEU:H	1.54	0.69
1:A:844:ALA:N	1:A:845:GLY:HA2	2.02	0.69
1:E:359:THR:HG22	1:E:363:ARG:HH11	1.56	0.69
1:A:410:ARG:HD3	2:B:10:DA:H8	1.58	0.68
1:G:699:ILE:HD11	1:G:701:ARG:HG2	1.76	0.68
1:A:410:ARG:HD3	2:B:10:DA:C8	2.28	0.68
1:C:832:GLY:HA2	2:D:5:DA:H61	1.59	0.68
1:C:457:ASP:H	1:C:460:MET:HE3	1.58	0.68
1:E:844:ALA:H	1:E:845:GLY:HA2	1.59	0.67
1:A:844:ALA:H	1:A:845:GLY:CA	2.07	0.67
1:E:302:LEU:HB3	1:E:523:LEU:HD22	1.76	0.67
1:G:150:HIS:HD1	2:H:11:DA:H5'	1.60	0.66
1:E:404:THR:HG22	1:E:407:LEU:H	1.59	0.66
1:G:150:HIS:CE1	2:H:11:DA:H5'	2.31	0.66
1:G:410:ARG:HD3	2:H:10:DA:H8	1.61	0.65
1:A:258:ALA:O	1:A:404:THR:HG21	1.97	0.65
1:C:844:ALA:N	1:C:845:GLY:HA2	1.97	0.65
1:G:150:HIS:ND1	2:H:11:DA:H5'	2.10	0.65
1:A:404:THR:CG2	1:A:407:LEU:H	2.10	0.65
1:G:645:GLN:HG2	1:G:698:ILE:HD13	1.79	0.65
1:E:844:ALA:H	1:E:845:GLY:CA	2.10	0.64
1:A:404:THR:HG22	1:A:407:LEU:HB2	1.79	0.64
1:C:679:PRO:HG3	1:C:739:LEU:HD13	1.80	0.63
1:G:678:ALA:HB3	1:G:683:LEU:HD13	1.80	0.63
1:C:429:ALA:HB1	1:C:440:LEU:HD13	1.80	0.63
1:C:652:ARG:HH11	1:C:652:ARG:HB3	1.64	0.63
1:E:893:THR:HG23	1:E:896:ASN:OD1	1.99	0.63
1:C:652:ARG:CG	1:C:653:GLY:H	2.12	0.62
1:C:447:VAL:HG22	1:C:477:PRO:HG2	1.81	0.62
1:E:844:ALA:N	1:E:845:GLY:HA2	2.12	0.62
1:G:410:ARG:HD3	2:H:10:DA:C8	2.34	0.62
1:C:404:THR:CG2	1:C:407:LEU:H	2.12	0.62
1:C:680:VAL:HG13	1:C:743:THR:HG23	1.81	0.62
1:A:366:THR:HB	1:A:402:ALA:O	2.00	0.61
1:E:842:ASP:OD1	1:E:846:ASN:N	2.31	0.61
1:A:540:PRO:HG2	1:A:541:LEU:HD22	1.82	0.61
1:C:591:THR:HG21	1:C:730:SER:HB2	1.83	0.61
1:G:404:THR:CG2	1:G:407:LEU:H	2.13	0.61
1:A:457:ASP:H	1:A:460:MET:HE3	1.65	0.61
1:G:366:THR:HG21	1:G:404:THR:HB	1.81	0.61
1:G:258:ALA:O	1:G:404:THR:HG21	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:THR:HG21	1:A:404:THR:HB	1.83	0.60
1:C:864:ARG:NH1	4:C:1123:HOH:O	2.33	0.60
1:G:22:ALA:HB2	1:G:34:LEU:HA	1.83	0.60
1:C:665:SER:O	1:C:666:LEU:HD23	2.02	0.60
1:A:645:GLN:HA	1:A:698:ILE:HD13	1.84	0.60
1:A:150:HIS:ND1	2:B:11:DA:H5'	2.17	0.60
1:A:22:ALA:HB2	1:A:34:LEU:HA	1.82	0.60
1:G:900:GLU:HG3	1:G:903:ARG:HH12	1.66	0.60
1:G:162:ARG:H	1:G:162:ARG:NH1	2.00	0.59
1:C:125:PHE:HB2	1:C:165:LEU:HD13	1.85	0.59
1:G:614:PRO:HB3	1:G:653:GLY:HA3	1.85	0.59
1:G:848:TRP:CD1	1:G:853:CYS:HG	2.21	0.59
1:C:891:GLN:O	1:C:930:GLY:HA2	2.03	0.58
1:C:366:THR:HG21	1:C:404:THR:HB	1.85	0.58
1:C:600:ASP:OD2	1:C:940:LYS:NZ	2.35	0.58
1:A:404:THR:HG22	1:A:407:LEU:H	1.69	0.57
1:C:23:LYS:NZ	1:C:219:SER:OG	2.37	0.57
1:C:22:ALA:HB2	1:C:34:LEU:HA	1.87	0.57
1:A:835:ARG:NH2	1:A:882:PRO:HD3	2.20	0.57
1:A:576:THR:O	1:A:579:VAL:HG22	2.04	0.57
1:A:828:ARG:HB2	2:B:5:DA:C2	2.40	0.57
1:C:150:HIS:ND1	2:D:11:DA:H5'	2.19	0.57
1:C:541:LEU:HD13	1:C:541:LEU:O	2.05	0.56
1:C:667:ASP:C	1:C:668:LEU:HD23	2.31	0.56
1:E:145:MET:HE3	1:E:146:LEU:HD13	1.88	0.56
1:E:457:ASP:H	1:E:460:MET:HE3	1.71	0.56
1:E:125:PHE:HB2	1:E:165:LEU:HD13	1.87	0.56
1:E:846:ASN:HB2	1:E:848:TRP:HE1	1.71	0.56
1:E:846:ASN:HB2	1:E:848:TRP:NE1	2.20	0.56
1:G:558:VAL:HG22	1:G:570:VAL:HG21	1.86	0.56
1:A:625:ASN:OD1	1:A:835:ARG:NH2	2.38	0.56
1:E:252:PRO:HB3	1:E:261:ARG:HH22	1.70	0.56
1:A:113:ARG:NH2	1:A:168:PHE:O	2.32	0.56
1:C:333:LEU:HD22	1:C:449:VAL:HB	1.87	0.56
1:E:844:ALA:HB3	1:E:845:GLY:HA2	1.88	0.55
1:G:313:GLU:OE2	1:G:347:ARG:NH2	2.37	0.55
1:C:247:SER:O	1:C:251:ILE:HD13	2.06	0.55
1:E:366:THR:HG21	1:E:404:THR:HB	1.87	0.55
1:A:691:TRP:HE3	1:A:694:GLU:HG3	1.71	0.55
1:A:696:LEU:N	1:A:696:LEU:HD12	2.22	0.55
1:C:258:ALA:O	1:C:404:THR:HG21	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:932:ARG:NH2	4:C:1133:HOH:O	2.26	0.55
1:G:457:ASP:H	1:G:460:MET:HE3	1.72	0.55
1:G:691:TRP:CE3	1:G:694:GLU:HG3	2.42	0.55
1:A:281:ASN:OD1	1:A:282:GLY:N	2.39	0.55
1:A:361:LEU:HD13	1:A:400:PRO:HG3	1.89	0.55
1:C:348:LEU:HD23	1:C:367:LEU:HD11	1.89	0.55
1:E:315:ALA:HB2	1:E:481:LEU:HD21	1.88	0.55
1:G:750:ARG:NH2	1:G:754:PRO:O	2.41	0.54
1:C:588:ILE:HD12	1:C:662:VAL:HG11	1.89	0.54
1:A:848:TRP:HD1	1:A:853:CYS:HG	1.51	0.54
1:E:404:THR:CG2	1:E:407:LEU:H	2.19	0.54
1:G:159:PHE:CE2	1:G:164:PRO:HG3	2.43	0.54
1:G:287:LEU:O	1:G:291:LEU:HB2	2.08	0.54
1:C:678:ALA:HB3	1:C:683:LEU:HD13	1.90	0.54
1:E:250:ARG:NH1	1:E:253:SER:OG	2.40	0.54
1:G:399:ASP:N	1:G:399:ASP:OD1	2.41	0.53
1:E:410:ARG:NH1	2:F:9:DA:H8	2.06	0.53
1:A:844:ALA:HB3	1:A:845:GLY:HA2	1.89	0.53
1:A:698:ILE:HG12	1:A:698:ILE:O	2.08	0.53
1:G:366:THR:HB	1:G:402:ALA:O	2.08	0.53
1:C:615:ASP:OD1	1:C:615:ASP:N	2.42	0.53
1:C:652:ARG:HG3	1:C:653:GLY:H	1.74	0.53
1:G:429:ALA:HB1	1:G:440:LEU:HD13	1.89	0.53
1:A:132:TYR:HB3	1:A:139:THR:OG1	2.09	0.53
1:A:671:ASP:OD1	1:A:701:ARG:NH1	2.42	0.53
1:A:921:GLU:N	1:A:921:GLU:OE1	2.40	0.53
1:C:363:ARG:N	1:C:400:PRO:HA	2.24	0.53
1:E:586:ALA:HB2	1:E:670:VAL:HG11	1.91	0.53
1:E:630:GLU:O	1:E:634:THR:HG23	2.09	0.53
1:G:639:PHE:HB2	1:G:668:LEU:HD22	1.92	0.52
1:C:20:PHE:HE2	1:C:178:GLN:HG3	1.74	0.52
1:C:23:LYS:NZ	2:D:12:DA:OP2	2.41	0.52
1:C:652:ARG:CG	1:C:653:GLY:N	2.73	0.52
1:E:506:TRP:CH2	1:E:513:PRO:HD3	2.43	0.52
1:G:630:GLU:O	1:G:634:THR:HG23	2.09	0.52
1:C:842:ASP:O	1:C:845:GLY:HA2	2.09	0.52
1:C:844:ALA:H	1:C:845:GLY:CA	2.12	0.52
1:G:404:THR:HG22	1:G:407:LEU:HB2	1.92	0.52
1:A:639:PHE:HB2	1:A:668:LEU:HD22	1.92	0.52
1:A:665:SER:O	1:A:665:SER:OG	2.21	0.52
1:A:691:TRP:CE3	1:A:694:GLU:HG3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:VAL:HG22	1:C:570:VAL:HG21	1.92	0.52
1:E:637:ASP:O	1:E:643:GLY:HA3	2.09	0.52
1:G:634:THR:O	1:G:638:LEU:HG	2.09	0.52
1:G:645:GLN:HG2	1:G:698:ILE:CD1	2.40	0.51
1:G:680:VAL:HG13	1:G:743:THR:HG23	1.92	0.51
1:E:258:ALA:O	1:E:404:THR:HG21	2.10	0.51
1:E:659:THR:C	1:E:661:VAL:H	2.19	0.51
1:A:370:LEU:HD22	1:A:419:ALA:HB1	1.93	0.51
1:A:123:LEU:O	1:A:127:LEU:HB2	2.10	0.51
1:A:28:ARG:HH11	1:A:28:ARG:CG	2.24	0.51
1:A:678:ALA:HB3	1:A:683:LEU:HD13	1.93	0.51
1:A:696:LEU:N	1:A:696:LEU:CD1	2.73	0.51
1:G:506:TRP:CH2	1:G:513:PRO:HD3	2.46	0.51
1:A:848:TRP:CD1	1:A:853:CYS:CB	2.94	0.51
1:C:38:SER:HB3	1:C:81:GLY:O	2.11	0.51
1:A:606:PHE:CD2	1:A:614:PRO:HD2	2.46	0.50
1:C:839:TYR:CE2	1:C:847:ARG:HD2	2.46	0.50
1:E:265:VAL:HG13	1:E:355:ARG:CZ	2.40	0.50
1:A:145:MET:HG3	1:A:208:CYS:HB2	1.93	0.50
1:A:865:GLU:HB3	1:A:867:ARG:HH21	1.77	0.50
1:C:450:VAL:HG13	1:C:480:LEU:HD12	1.93	0.50
1:E:372:SER:O	1:E:373:MET:HE2	2.12	0.50
1:E:891:GLN:O	1:E:930:GLY:HA2	2.11	0.50
1:E:495:LYS:O	1:E:499:GLU:HG3	2.11	0.50
1:E:410:ARG:HD3	2:F:10:DA:C8	2.47	0.50
1:E:201:GLY:HA3	1:E:806:ALA:O	2.12	0.50
1:A:667:ASP:O	1:A:668:LEU:HD23	2.11	0.49
1:C:469:ARG:O	1:C:500:GLY:HA3	2.11	0.49
1:C:201:GLY:HA3	1:C:806:ALA:O	2.13	0.49
1:E:694:GLU:HG2	1:E:701:ARG:HH21	1.78	0.49
1:A:558:VAL:HG22	1:A:570:VAL:HG21	1.94	0.49
1:E:159:PHE:CE2	1:E:164:PRO:HG3	2.47	0.49
1:E:314:ALA:O	1:E:318:VAL:HG23	2.12	0.49
1:G:694:GLU:HG2	1:G:701:ARG:HH21	1.77	0.49
1:E:540:PRO:HG2	1:E:541:LEU:HD22	1.95	0.49
1:G:832:GLY:CA	2:H:5:DA:H61	2.23	0.49
1:A:522:TRP:CE2	1:A:535:SER:HB3	2.47	0.49
1:C:351:TYR:CZ	1:C:355:ARG:HD3	2.48	0.49
1:C:835:ARG:NH2	1:C:882:PRO:HD3	2.27	0.49
1:E:44:ALA:O	1:E:48:LEU:HB2	2.12	0.49
1:G:215:ASP:OD2	2:H:11:DA:H3'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:848:TRP:CG	1:A:853:CYS:HA	2.48	0.49
1:G:680:VAL:HG11	1:G:746:LEU:HD23	1.93	0.49
1:G:691:TRP:HE3	1:G:694:GLU:HG3	1.75	0.49
1:A:410:ARG:NH1	2:B:9:DA:H8	2.10	0.49
1:E:150:HIS:ND1	2:F:11:DA:H5'	2.26	0.49
1:C:679:PRO:CG	1:C:739:LEU:HD13	2.42	0.49
1:E:101:SER:O	1:G:729:ARG:NH2	2.43	0.49
1:E:459:TYR:CD1	1:E:795:ALA:HB2	2.47	0.49
1:G:78:PHE:CZ	1:G:82:LEU:HD11	2.47	0.49
1:E:618:LEU:HD23	1:E:940:LYS:HA	1.94	0.49
1:C:241:ARG:NH2	4:C:1161:HOH:O	2.44	0.48
1:A:844:ALA:HB3	1:A:845:GLY:CA	2.43	0.48
1:C:606:PHE:CD2	1:C:614:PRO:HD2	2.47	0.48
1:C:684:LEU:HD23	1:C:761:VAL:HG13	1.95	0.48
1:E:682:LEU:O	1:E:686:ARG:HD3	2.13	0.48
1:E:742:ARG:NH1	1:E:781:ASP:OD1	2.46	0.48
1:C:576:THR:O	1:C:580:LYS:HG2	2.14	0.48
1:G:281:ASN:OD1	1:G:282:GLY:N	2.46	0.48
1:C:334:ALA:HB1	1:C:423:ILE:HA	1.96	0.48
1:E:455:ALA:O	4:E:1137:HOH:O	2.20	0.48
1:G:576:THR:O	1:G:579:VAL:HG22	2.14	0.48
1:G:625:ASN:OD1	1:G:835:ARG:NH2	2.47	0.48
1:C:363:ARG:HB2	1:C:364:SER:HB3	1.96	0.48
1:A:835:ARG:HH22	1:A:882:PRO:HD3	1.79	0.47
1:A:679:PRO:HG3	1:A:739:LEU:HD13	1.96	0.47
1:G:348:LEU:HD23	1:G:367:LEU:HD11	1.96	0.47
1:G:490:ALA:O	1:G:494:VAL:HG13	2.14	0.47
1:A:940:LYS:HE3	1:A:943:ILE:HD11	1.96	0.47
1:C:552:GLU:HB2	1:C:709:GLU:HG3	1.96	0.47
1:E:620:HIS:CE1	1:E:622:ARG:HB2	2.49	0.47
1:E:659:THR:O	1:E:661:VAL:N	2.47	0.47
1:G:898:PRO:HB2	1:G:902:TRP:HB2	1.95	0.47
1:A:680:VAL:HG13	1:A:743:THR:HG23	1.97	0.47
1:A:466:GLN:OE1	1:A:469:ARG:NH1	2.42	0.47
1:A:367:LEU:HD13	1:A:418:TRP:HB3	1.95	0.47
1:C:23:LYS:CE	2:D:12:DA:OP2	2.63	0.47
1:E:410:ARG:HD3	2:F:10:DA:H8	1.79	0.47
1:G:461:GLN:O	1:G:465:GLU:HG3	2.14	0.47
1:G:649:ARG:NH2	1:G:671:ASP:OD1	2.48	0.47
1:A:275:PRO:HG3	1:A:354:TYR:CZ	2.50	0.47
1:C:630:GLU:O	1:C:634:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:TYR:CE1	1:E:403:ALA:HB2	2.49	0.47
1:A:320:ASP:HA	1:A:331:ARG:NH2	2.30	0.47
2:D:5:DA:H2''	2:D:6:DA:O5'	2.15	0.47
1:C:377:ASN:HA	1:C:378:PRO:HD3	1.77	0.46
1:A:145:MET:HE3	1:A:146:LEU:HD13	1.98	0.46
1:C:451:ASP:HA	1:C:481:LEU:HB2	1.97	0.46
1:C:625:ASN:OD1	1:C:835:ARG:NH2	2.48	0.46
1:E:380:TYR:CE2	1:E:408:MET:HE1	2.50	0.46
1:G:370:LEU:HD21	1:G:413:GLY:C	2.40	0.46
1:G:486:HIS:CD2	1:G:766:ASP:HA	2.51	0.46
1:A:832:GLY:HA2	2:B:5:DA:N6	2.23	0.46
1:E:680:VAL:HG13	1:E:743:THR:HG23	1.98	0.46
1:G:252:PRO:HB3	1:G:261:ARG:HH22	1.80	0.46
1:A:265:VAL:HG13	1:A:355:ARG:NH1	2.31	0.46
1:C:652:ARG:HH11	1:C:652:ARG:HB2	1.75	0.46
1:E:250:ARG:O	1:E:250:ARG:HD3	2.15	0.46
1:G:207:VAL:O	1:G:211:VAL:HG23	2.14	0.46
1:C:541:LEU:C	1:C:541:LEU:CD1	2.85	0.46
1:C:691:TRP:CG	1:C:708:PRO:HB3	2.50	0.46
1:C:853:CYS:SG	1:C:918:VAL:HG11	2.55	0.46
1:G:449:VAL:HG22	1:G:479:VAL:HB	1.97	0.46
1:A:848:TRP:CD1	1:A:853:CYS:HB3	2.50	0.46
1:G:673:MET:HE1	1:G:686:ARG:HB3	1.97	0.46
1:C:499:GLU:HG2	1:C:506:TRP:HD1	1.80	0.46
1:E:148:GLY:HA2	1:E:152:THR:O	2.16	0.46
1:C:652:ARG:CB	1:C:652:ARG:NH1	2.73	0.46
1:C:145:MET:HE3	1:C:146:LEU:HD13	1.98	0.46
1:G:54:SER:OG	1:G:329:PRO:HD2	2.16	0.46
1:G:635:ILE:HA	1:G:635:ILE:HD13	1.66	0.46
1:C:267:PRO:HA	1:C:324:LYS:NZ	2.31	0.46
1:G:453:ALA:HB3	1:G:482:SER:HB2	1.98	0.46
1:G:678:ALA:O	1:G:743:THR:HG21	2.16	0.46
1:G:44:ALA:HA	1:G:251:ILE:HD13	1.98	0.45
1:G:757:ILE:HA	1:G:758:PRO:HA	1.75	0.45
1:A:149:HIS:CD2	1:A:150:HIS:CD2	3.04	0.45
1:A:453:ALA:O	1:A:456:VAL:HG13	2.17	0.45
1:A:617:TYR:CG	1:A:635:ILE:HD11	2.52	0.45
1:C:670:VAL:HG21	1:C:673:MET:HG3	1.97	0.45
1:G:267:PRO:HA	1:G:324:LYS:HE2	1.97	0.45
1:A:635:ILE:HD13	1:A:635:ILE:HA	1.74	0.45
1:C:468:LEU:HA	1:C:468:LEU:HD23	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ALA:O	1:A:494:VAL:HG13	2.17	0.45
1:A:842:ASP:OD1	1:A:846:ASN:N	2.49	0.45
1:E:782:MET:HA	1:E:785:MET:HE3	1.98	0.45
1:G:877:VAL:HA	1:G:880:THR:HG23	1.99	0.45
1:E:842:ASP:OD1	1:E:845:GLY:HA2	2.17	0.45
1:G:65:MET:HA	1:G:198:MET:O	2.16	0.45
1:G:198:MET:HE3	1:G:198:MET:HB2	1.76	0.45
1:G:227:ARG:HD3	1:G:250:ARG:HD2	1.99	0.45
1:C:65:MET:HA	1:C:198:MET:O	2.17	0.45
1:C:609:LEU:HD13	1:C:609:LEU:HA	1.72	0.45
1:G:236:SER:O	1:G:240:LEU:HG	2.16	0.45
1:C:652:ARG:HB3	1:C:652:ARG:NH1	2.31	0.45
1:E:839:TYR:CE1	1:E:913:LEU:HB3	2.52	0.45
1:A:160:GLN:OE1	1:C:796:ARG:HD2	2.17	0.44
1:E:16:LEU:HB3	1:E:181:ALA:HB1	1.98	0.44
1:E:303:ILE:HB	1:E:481:LEU:HD13	1.99	0.44
1:E:409:GLY:HA3	1:E:410:ARG:HE	1.81	0.44
1:E:447:VAL:HG22	1:E:477:PRO:HG2	1.99	0.44
1:E:671:ASP:OD1	1:E:701:ARG:NH1	2.50	0.44
1:E:473:THR:HG22	1:E:500:GLY:CA	2.47	0.44
1:C:635:ILE:HD13	1:C:635:ILE:HA	1.73	0.44
1:G:81:GLY:HA3	1:G:186:VAL:HG21	1.99	0.44
1:G:127:LEU:HD12	1:G:127:LEU:HA	1.87	0.44
1:G:203:THR:O	1:G:207:VAL:HG23	2.17	0.44
1:A:554:ARG:NH2	1:A:709:GLU:OE2	2.36	0.44
1:A:839:TYR:CE1	1:A:913:LEU:HB3	2.52	0.44
1:C:410:ARG:NH1	2:D:9:DA:H8	2.16	0.44
1:G:900:GLU:HG3	1:G:903:ARG:NH1	2.31	0.44
1:A:28:ARG:CG	1:A:28:ARG:NH1	2.79	0.44
1:E:490:ALA:O	1:E:494:VAL:HG13	2.18	0.44
1:E:505:ARG:HD2	1:E:802:ASP:OD2	2.18	0.44
1:A:377:ASN:HA	1:A:378:PRO:HD3	1.70	0.44
1:A:694:GLU:HG2	1:A:701:ARG:HH21	1.83	0.44
1:C:473:THR:HG22	1:C:500:GLY:CA	2.48	0.44
1:C:483:ALA:O	1:C:484:THR:C	2.60	0.44
2:H:2:DA:H2''	2:H:3:DA:O5'	2.17	0.44
1:A:302:LEU:HB3	1:A:523:LEU:HD22	1.99	0.44
1:A:380:TYR:CE1	1:A:403:ALA:HB2	2.53	0.44
1:C:159:PHE:CE2	1:C:164:PRO:HG3	2.53	0.44
1:E:424:ASP:O	1:E:428:MET:HG3	2.18	0.44
1:E:844:ALA:CB	1:E:845:GLY:HA2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:THR:O	1:A:638:LEU:HG	2.18	0.44
1:G:145:MET:HG3	1:G:208:CYS:HB2	1.98	0.44
1:G:339:ALA:O	1:G:342:ASP:HB2	2.18	0.44
1:C:666:LEU:O	1:C:689:ARG:NH1	2.51	0.43
1:E:466:GLN:HG2	1:E:799:VAL:HB	2.00	0.43
1:E:696:LEU:HD23	1:E:698:ILE:HD11	2.01	0.43
1:G:891:GLN:O	1:G:930:GLY:HA2	2.17	0.43
1:A:362:PRO:HB2	1:A:365:SER:HB2	1.99	0.43
1:E:27:LEU:HD13	1:E:228:LEU:HD21	2.01	0.43
1:E:849:LEU:HD13	1:E:857:PHE:HA	2.00	0.43
1:E:460:MET:HE1	4:E:1137:HOH:O	2.17	0.43
1:G:145:MET:HE3	1:G:146:LEU:HD13	2.00	0.43
1:G:787:GLU:O	1:G:791:GLN:HG3	2.19	0.43
1:A:729:ARG:HG2	2:B:1:DA:N6	2.34	0.43
1:E:594:GLU:O	1:E:598:VAL:HG23	2.18	0.43
1:G:223:PHE:O	1:G:227:ARG:HG2	2.19	0.43
1:G:898:PRO:HA	1:G:913:LEU:HD11	2.01	0.43
1:C:333:LEU:HB2	1:C:420:VAL:HB	2.01	0.43
1:E:198:MET:HB2	1:E:198:MET:HE3	1.73	0.43
1:E:265:VAL:HG13	1:E:355:ARG:NH1	2.33	0.43
1:E:410:ARG:HG2	2:F:10:DA:H5"	2.01	0.43
1:E:738:ALA:O	1:E:742:ARG:HG3	2.19	0.43
1:A:548:ARG:HE	1:A:548:ARG:HB3	1.53	0.43
1:E:54:SER:OG	1:E:329:PRO:HD2	2.19	0.43
1:E:635:ILE:HD13	1:E:635:ILE:HA	1.68	0.43
1:G:432:ARG:NH1	1:G:812:GLY:O	2.52	0.43
1:A:125:PHE:HB2	1:A:165:LEU:HD13	2.01	0.43
1:E:571:LEU:HD11	1:E:598:VAL:HG13	2.00	0.43
1:E:555:LEU:HD23	1:E:712:VAL:HB	2.01	0.43
1:E:216:TRP:CZ3	1:E:438:LEU:HD11	2.54	0.42
1:A:848:TRP:NE1	1:A:853:CYS:HB3	2.34	0.42
1:C:572:ALA:HA	1:C:605:TRP:CH2	2.54	0.42
1:C:665:SER:O	1:C:665:SER:OG	2.29	0.42
1:E:48:LEU:HD12	1:E:48:LEU:HA	1.76	0.42
1:E:687:ALA:HB2	1:E:710:LEU:HD22	2.01	0.42
1:A:173:PRO:O	1:A:177:LYS:HG3	2.19	0.42
1:A:599:TYR:O	1:A:603:SER:HB2	2.19	0.42
1:C:410:ARG:HG3	1:C:410:ARG:HH11	1.84	0.42
1:C:673:MET:HE2	1:C:673:MET:HB3	1.66	0.42
1:A:624:PRO:HA	1:A:881:ILE:HG12	2.02	0.42
1:A:660:GLN:O	1:A:663:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:PHE:CE2	1:C:614:PRO:HD2	2.55	0.42
1:C:691:TRP:HA	1:C:701:ARG:NH2	2.35	0.42
1:E:23:LYS:NZ	2:F:12:DA:OP2	2.51	0.42
1:E:877:VAL:HA	1:E:880:THR:HG23	2.01	0.42
1:A:673:MET:HE1	1:A:686:ARG:HB3	2.01	0.42
1:C:149:HIS:NE2	1:C:150:HIS:CD2	2.86	0.42
1:C:207:VAL:O	1:C:211:VAL:HG23	2.19	0.42
1:C:612:ASP:OD2	1:C:652:ARG:NE	2.52	0.42
1:C:693:HIS:O	1:C:696:LEU:HB2	2.19	0.42
1:E:471:LEU:HB3	1:E:476:VAL:HG22	2.02	0.42
1:G:471:LEU:HD22	1:G:476:VAL:HG21	2.01	0.42
1:A:844:ALA:CB	1:A:845:GLY:HA2	2.47	0.42
1:E:335:LEU:HB3	1:E:336:PRO:HD2	2.02	0.42
1:E:523:LEU:C	1:E:523:LEU:HD23	2.45	0.42
1:E:588:ILE:HD12	1:E:662:VAL:HG11	2.01	0.42
1:G:606:PHE:C	1:G:608:THR:H	2.28	0.42
1:A:228:LEU:HD12	1:A:228:LEU:HA	1.91	0.42
1:A:334:ALA:HB1	1:A:423:ILE:HA	2.01	0.42
1:A:540:PRO:HG2	1:A:541:LEU:CD2	2.47	0.42
1:A:836:VAL:HG22	1:A:881:ILE:O	2.20	0.42
1:C:279:LYS:HD2	1:C:279:LYS:HA	1.89	0.42
1:C:844:ALA:N	1:C:845:GLY:CA	2.73	0.42
1:G:588:ILE:HD12	1:G:662:VAL:HG11	2.00	0.42
1:A:216:TRP:CZ3	1:A:438:LEU:HD11	2.55	0.42
1:A:637:ASP:O	1:A:643:GLY:HA3	2.20	0.42
1:C:576:THR:O	1:C:579:VAL:HG22	2.20	0.42
1:E:450:VAL:HG13	1:E:480:LEU:HD12	2.02	0.42
1:E:528:ARG:NE	4:E:1142:HOH:O	2.39	0.42
1:C:750:ARG:NH2	1:C:754:PRO:O	2.53	0.42
1:E:53:LEU:HG	1:E:57:LEU:HD23	2.01	0.42
1:A:265:VAL:HA	1:A:266:PRO:HD3	1.84	0.42
2:D:2:DA:H2''	2:D:3:DA:O5'	2.19	0.42
1:G:673:MET:HB2	1:G:690:CYS:SG	2.60	0.42
1:A:857:PHE:HA	1:A:858:PRO:HD2	1.95	0.41
1:C:836:VAL:HG22	1:C:881:ILE:O	2.20	0.41
1:E:599:TYR:CD1	1:E:616:LEU:HD13	2.54	0.41
1:E:940:LYS:HE3	1:E:943:ILE:HD11	2.02	0.41
1:G:673:MET:HE2	1:G:710:LEU:CD1	2.50	0.41
1:C:634:THR:O	1:C:638:LEU:HG	2.19	0.41
1:C:694:GLU:HG2	1:C:701:ARG:NH2	2.16	0.41
1:G:684:LEU:HD12	1:G:684:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:ILE:HD12	1:A:662:VAL:HG11	2.01	0.41
1:A:849:LEU:HD13	1:A:857:PHE:HA	2.02	0.41
1:E:146:LEU:HD12	1:E:146:LEU:HA	1.89	0.41
1:G:881:ILE:HD13	1:G:881:ILE:HG21	1.81	0.41
1:C:27:LEU:HD23	1:C:27:LEU:HA	1.85	0.41
1:C:240:LEU:HD23	1:C:240:LEU:HA	1.87	0.41
1:E:215:ASP:OD2	2:F:11:DA:H3'	2.21	0.41
1:G:148:GLY:HA2	1:G:152:THR:O	2.20	0.41
1:G:667:ASP:O	1:G:668:LEU:HD23	2.20	0.41
1:C:484:THR:HG22	1:C:519:TYR:CZ	2.55	0.41
1:G:525:VAL:HG22	1:G:532:VAL:HG22	2.01	0.41
1:G:534:ARG:NH2	1:G:537:ASP:OD1	2.53	0.41
1:G:739:LEU:HA	1:G:739:LEU:HD23	1.75	0.41
1:A:686:ARG:O	1:A:689:ARG:HG2	2.21	0.41
1:E:334:ALA:HB1	1:E:423:ILE:HA	2.02	0.41
1:A:410:ARG:HB3	1:A:411:LYS:H	1.47	0.41
1:C:404:THR:HG23	1:C:406:TRP:N	2.36	0.41
1:C:606:PHE:HA	1:C:609:LEU:HD23	2.03	0.41
1:C:696:LEU:HD12	1:C:696:LEU:HA	1.83	0.41
1:G:765:VAL:O	1:G:768:VAL:HG12	2.20	0.41
1:C:32:TYR:OH	1:C:40:ASP:OD2	2.27	0.41
1:C:645:GLN:HA	1:C:698:ILE:HD11	2.02	0.41
1:C:673:MET:HB2	1:C:690:CYS:SG	2.61	0.41
1:C:898:PRO:HA	1:C:899:PRO:HD3	1.90	0.41
1:A:48:LEU:HD12	1:A:48:LEU:HA	1.93	0.41
1:A:395:LEU:HD23	1:A:395:LEU:HA	1.88	0.41
1:A:478:VAL:HG12	1:A:480:LEU:HD13	2.03	0.41
1:E:673:MET:HE2	1:E:673:MET:HB3	1.90	0.41
1:A:499:GLU:HG2	1:A:505:ARG:HA	2.03	0.41
1:E:365:SER:O	1:E:401:PHE:HA	2.21	0.41
1:E:625:ASN:OD1	1:E:835:ARG:NH2	2.54	0.41
1:E:223:PHE:O	1:E:227:ARG:HG2	2.21	0.40
1:E:729:ARG:HG2	2:F:1:DA:N6	2.36	0.40
1:E:835:ARG:NH2	1:E:882:PRO:HD3	2.36	0.40
1:A:848:TRP:CB	1:A:853:CYS:HA	2.52	0.40
1:G:456:VAL:HA	1:G:460:MET:HE3	2.03	0.40
1:A:891:GLN:O	1:A:930:GLY:HA2	2.21	0.40
1:C:691:TRP:HA	1:C:701:ARG:HH22	1.86	0.40
1:G:407:LEU:HD13	1:G:416:ALA:HB2	2.04	0.40
1:G:473:THR:HG21	1:G:803:PRO:HG2	2.02	0.40
1:G:625:ASN:HA	4:G:1128:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LEU:O	1:A:291:LEU:HB2	2.20	0.40
1:A:447:VAL:HG22	1:A:477:PRO:HG2	2.04	0.40
1:A:724:ALA:HA	1:A:725:PRO:HD3	1.91	0.40
1:C:788:GLU:HG2	1:C:792:ARG:NH2	2.37	0.40
1:E:623:PHE:O	1:E:881:ILE:HB	2.22	0.40
1:G:265:VAL:HA	1:G:266:PRO:HD3	1.87	0.40
1:G:334:ALA:HB1	1:G:423:ILE:HA	2.02	0.40
1:A:16:LEU:HD11	1:A:35:VAL:HG21	2.04	0.40
1:A:227:ARG:HA	1:A:227:ARG:HD2	1.88	0.40
1:A:698:ILE:O	1:A:698:ILE:CG1	2.70	0.40
1:C:555:LEU:HD23	1:C:712:VAL:HB	2.04	0.40
1:E:265:VAL:HG22	1:E:355:ARG:HB3	2.04	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	899/964 (93%)	867 (96%)	32 (4%)	0	100	100
1	C	892/964 (92%)	861 (96%)	31 (4%)	0	100	100
1	E	883/964 (92%)	855 (97%)	28 (3%)	0	100	100
1	G	886/964 (92%)	852 (96%)	34 (4%)	0	100	100
All	All	3560/3856 (92%)	3435 (96%)	125 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	752/796 (94%)	672 (89%)	80 (11%)	6	10
1	C	742/796 (93%)	651 (88%)	91 (12%)	4	7
1	E	738/796 (93%)	659 (89%)	79 (11%)	6	9
1	G	739/796 (93%)	660 (89%)	79 (11%)	6	9
All	All	2971/3184 (93%)	2642 (89%)	329 (11%)	6	9

All (329) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	24	GLU
1	A	28	ARG
1	A	35	VAL
1	A	48	LEU
1	A	85	ILE
1	A	88	LEU
1	A	113	ARG
1	A	121	LYS
1	A	123	LEU
1	A	127	LEU
1	A	137	LEU
1	A	146	LEU
1	A	165	LEU
1	A	186	VAL
1	A	198	MET
1	A	217	LEU
1	A	228	LEU
1	A	254	LEU
1	A	265	VAL
1	A	271	THR
1	A	277	LEU
1	A	279	LYS
1	A	283	LEU
1	A	291	LEU
1	A	357	GLU
1	A	366	THR
1	A	370	LEU

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Mol	Chain	Res	Type
1	A	375	TRP
1	A	391	VAL
1	A	392	LEU
1	A	395	LEU
1	A	404	THR
1	A	410	ARG
1	A	411	LYS
1	A	420	VAL
1	A	431	LEU
1	A	438	LEU
1	A	440	LEU
1	A	443	LEU
1	A	448	VAL
1	A	450	VAL
1	A	456	VAL
1	A	464	LEU
1	A	473	THR
1	A	474	LEU
1	A	476	VAL
1	A	480	LEU
1	A	494	VAL
1	A	508	ARG
1	A	523	LEU
1	A	529	ILE
1	A	536	SER
1	A	548	ARG
1	A	574	GLU
1	A	576	THR
1	A	579	VAL
1	A	603	SER
1	A	616	LEU
1	A	634	THR
1	A	635	ILE
1	A	636	VAL
1	A	648	ARG
1	A	651	THR
1	A	665	SER
1	A	673	MET
1	A	680	VAL
1	A	681	SER
1	A	684	LEU
1	A	686	ARG

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Mol	Chain	Res	Type
1	A	699	ILE
1	A	734	VAL
1	A	739	LEU
1	A	751	ASN
1	A	789	LEU
1	A	804	ASP
1	A	841	VAL
1	A	849	LEU
1	A	925	LEU
1	A	928	GLU
1	C	16	LEU
1	C	23	LYS
1	C	28	ARG
1	C	30	LYS
1	C	35	VAL
1	C	48	LEU
1	C	70	GLU
1	C	88	LEU
1	C	91	GLU
1	C	96	ILE
1	C	113	ARG
1	C	121	LYS
1	C	123	LEU
1	C	127	LEU
1	C	137	LEU
1	C	146	LEU
1	C	165	LEU
1	C	186	VAL
1	C	198	MET
1	C	217	LEU
1	C	228	LEU
1	C	249	ARG
1	C	251	ILE
1	C	254	LEU
1	C	264	THR
1	C	265	VAL
1	C	277	LEU
1	C	283	LEU
1	C	289	LYS
1	C	291	LEU
1	C	307	MET
1	C	333	LEU

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Mol	Chain	Res	Type
1	C	357	GLU
1	C	363	ARG
1	C	364	SER
1	C	366	THR
1	C	367	LEU
1	C	370	LEU
1	C	375	TRP
1	C	399	ASP
1	C	404	THR
1	C	410	ARG
1	C	411	LYS
1	C	420	VAL
1	C	431	LEU
1	C	438	LEU
1	C	440	LEU
1	C	443	LEU
1	C	448	VAL
1	C	450	VAL
1	C	456	VAL
1	C	464	LEU
1	C	473	THR
1	C	474	LEU
1	C	476	VAL
1	C	480	LEU
1	C	481	LEU
1	C	484	THR
1	C	494	VAL
1	C	505	ARG
1	C	508	ARG
1	C	528	ARG
1	C	536	SER
1	C	541	LEU
1	C	548	ARG
1	C	574	GLU
1	C	576	THR
1	C	609	LEU
1	C	612	ASP
1	C	615	ASP
1	C	616	LEU
1	C	634	THR
1	C	635	ILE
1	C	652	ARG

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Mol	Chain	Res	Type
1	C	673	MET
1	C	680	VAL
1	C	683	LEU
1	C	684	LEU
1	C	686	ARG
1	C	694	GLU
1	C	696	LEU
1	C	703	GLN
1	C	734	VAL
1	C	739	LEU
1	C	751	ASN
1	C	804	ASP
1	C	843	THR
1	C	849	LEU
1	C	881	ILE
1	C	925	LEU
1	C	928	GLU
1	E	16	LEU
1	E	35	VAL
1	E	48	LEU
1	E	88	LEU
1	E	123	LEU
1	E	127	LEU
1	E	146	LEU
1	E	162	ARG
1	E	165	LEU
1	E	186	VAL
1	E	217	LEU
1	E	228	LEU
1	E	254	LEU
1	E	265	VAL
1	E	271	THR
1	E	279	LYS
1	E	283	LEU
1	E	291	LEU
1	E	304	THR
1	E	366	THR
1	E	367	LEU
1	E	370	LEU
1	E	375	TRP
1	E	404	THR
1	E	410	ARG

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Mol	Chain	Res	Type
1	E	411	LYS
1	E	420	VAL
1	E	431	LEU
1	E	438	LEU
1	E	440	LEU
1	E	443	LEU
1	E	448	VAL
1	E	450	VAL
1	E	456	VAL
1	E	461	GLN
1	E	464	LEU
1	E	473	THR
1	E	474	LEU
1	E	476	VAL
1	E	480	LEU
1	E	481	LEU
1	E	484	THR
1	E	492	SER
1	E	494	VAL
1	E	508	ARG
1	E	523	LEU
1	E	528	ARG
1	E	529	ILE
1	E	548	ARG
1	E	576	THR
1	E	579	VAL
1	E	587	ILE
1	E	616	LEU
1	E	634	THR
1	E	635	ILE
1	E	648	ARG
1	E	651	THR
1	E	652	ARG
1	E	664	GLN
1	E	666	LEU
1	E	673	MET
1	E	681	SER
1	E	683	LEU
1	E	684	LEU
1	E	686	ARG
1	E	698	ILE
1	E	734	VAL

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Mol	Chain	Res	Type
1	E	739	LEU
1	E	751	ASN
1	E	765	VAL
1	E	789	LEU
1	E	804	ASP
1	E	824	VAL
1	E	849	LEU
1	E	881	ILE
1	E	892	LEU
1	E	893	THR
1	E	894	GLU
1	E	921	GLU
1	G	16	LEU
1	G	24	GLU
1	G	35	VAL
1	G	48	LEU
1	G	70	GLU
1	G	88	LEU
1	G	113	ARG
1	G	121	LYS
1	G	123	LEU
1	G	127	LEU
1	G	137	LEU
1	G	146	LEU
1	G	162	ARG
1	G	165	LEU
1	G	186	VAL
1	G	198	MET
1	G	217	LEU
1	G	254	LEU
1	G	264	THR
1	G	265	VAL
1	G	271	THR
1	G	277	LEU
1	G	283	LEU
1	G	291	LEU
1	G	304	THR
1	G	357	GLU
1	G	366	THR
1	G	367	LEU
1	G	370	LEU
1	G	375	TRP

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Mol	Chain	Res	Type
1	G	399	ASP
1	G	404	THR
1	G	410	ARG
1	G	411	LYS
1	G	420	VAL
1	G	424	ASP
1	G	431	LEU
1	G	438	LEU
1	G	440	LEU
1	G	443	LEU
1	G	448	VAL
1	G	450	VAL
1	G	456	VAL
1	G	464	LEU
1	G	473	THR
1	G	474	LEU
1	G	476	VAL
1	G	480	LEU
1	G	484	THR
1	G	494	VAL
1	G	505	ARG
1	G	508	ARG
1	G	509	SER
1	G	523	LEU
1	G	536	SER
1	G	548	ARG
1	G	574	GLU
1	G	579	VAL
1	G	587	ILE
1	G	616	LEU
1	G	634	THR
1	G	635	ILE
1	G	652	ARG
1	G	683	LEU
1	G	684	LEU
1	G	686	ARG
1	G	694	GLU
1	G	699	ILE
1	G	729	ARG
1	G	734	VAL
1	G	739	LEU
1	G	751	ASN

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Mol	Chain	Res	Type
1	G	759	GLU
1	G	789	LEU
1	G	804	ASP
1	G	847	ARG
1	G	849	LEU
1	G	881	ILE
1	G	928	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	HIS
1	A	220	GLN
1	A	317	HIS
1	A	394	ASN
1	A	860	GLN
1	C	695	HIS
1	C	811	ASN
1	E	154	HIS
1	E	317	HIS
1	E	507	ASN
1	E	846	ASN
1	G	507	ASN
1	G	811	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	911/964 (94%)	-0.37	9 (0%) 79 76	31, 52, 90, 115	0
1	C	902/964 (93%)	-0.41	3 (0%) 90 89	31, 50, 79, 107	0
1	E	897/964 (93%)	-0.28	7 (0%) 82 79	31, 55, 94, 134	0
1	G	898/964 (93%)	-0.23	5 (0%) 85 83	37, 58, 88, 127	0
2	B	11/12 (91%)	-0.13	0 100 100	39, 55, 87, 107	0
2	D	11/12 (91%)	-0.16	1 (9%) 15 11	42, 54, 83, 96	0
2	F	11/12 (91%)	-0.09	0 100 100	45, 61, 97, 108	0
2	H	11/12 (91%)	-0.01	1 (9%) 15 11	49, 64, 98, 110	0
All	All	3652/3904 (93%)	-0.32	26 (0%) 84 82	31, 54, 90, 134	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	665	SER	3.9
1	E	613	ALA	3.7
1	C	865	GLU	3.3
1	E	383	ALA	3.1
1	G	544	ALA	2.9
1	A	391	VAL	2.7
1	E	609	LEU	2.6
1	C	14	PRO	2.6
1	A	375	TRP	2.6
1	G	609	LEU	2.6
1	A	906	PHE	2.6
1	E	359	THR	2.5
1	A	609	LEU	2.4
1	E	907	TYR	2.3
1	E	847	ARG	2.3
1	G	907	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	9	DA	2.2
1	A	14	PRO	2.2
1	C	844	ALA	2.1
1	A	862	THR	2.1
1	G	698	ILE	2.1
1	G	14	PRO	2.0
2	H	9	DA	2.0
1	A	613	ALA	2.0
1	E	540	PRO	2.0
1	A	907	TYR	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 [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, 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($\text{\AA}^2$)	Q<0.9
3	FE	G	1001	1/1	0.96	0.07	44,44,44,44	0
3	FE	A	1002	1/1	0.99	0.05	35,35,35,35	0
3	FE	C	1001	1/1	0.99	0.05	34,34,34,34	0
3	FE	C	1002	1/1	0.99	0.04	35,35,35,35	0
3	FE	E	1001	1/1	0.99	0.04	38,38,38,38	0
3	FE	E	1002	1/1	0.99	0.03	35,35,35,35	0
3	FE	A	1001	1/1	0.99	0.05	34,34,34,34	0
3	FE	G	1002	1/1	0.99	0.02	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.