



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:03 PM GMT

PDB ID : 4QQY  
Title : Crystal structure of T. fusca Cas3-ADP  
Authors : Ke, A.; Huo, Y.; Nam, K.H.  
Deposited on : 2014-06-30  
Resolution : 3.12 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

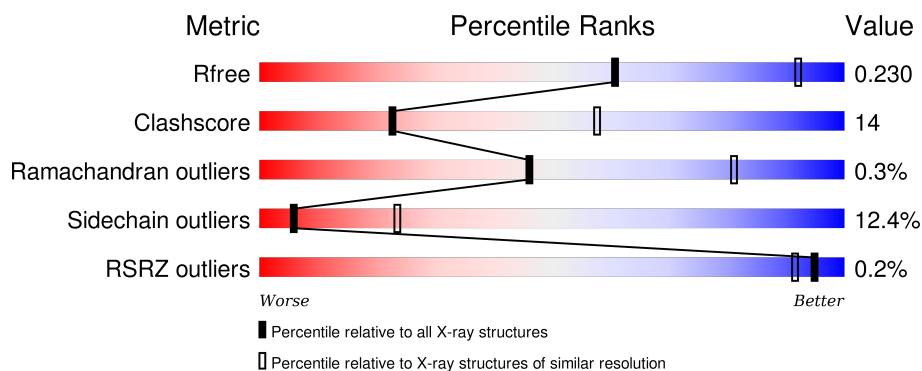
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





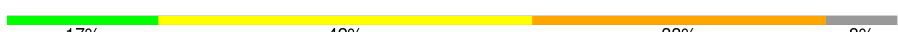
The reported resolution of this entry is 3.12 Å.

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))
$R_{free}$	91344	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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. 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	 64% 25% • 7%
1	C	964	 62% 26% 5% 6%
1	E	964	 64% 25% • 6%
1	G	964	 59% 29% • 7%
2	B	12	 17% 42% 33% 8%

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Mol	Chain	Length	Quality of chain
2	D	12	<div><div></div><div></div><div></div><div></div></div> <div>17%17%58%8%</div>
2	F	12	<div><div></div><div></div><div></div><div></div></div> <div>8%42%33%17%8%</div>
2	H	12	<div><div></div><div></div><div></div><div></div></div> <div>50%25%17%8%</div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28826 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	896	Total	C	N	O	S	0	0	0
			6973	4430	1240	1276	27			
1	C	902	Total	C	N	O	S	0	0	0
			7001	4441	1243	1290	27			
1	E	902	Total	C	N	O	S	0	0	0
			7006	4444	1246	1289	27			
1	G	894	Total	C	N	O	S	0	0	0
			6942	4408	1235	1272	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

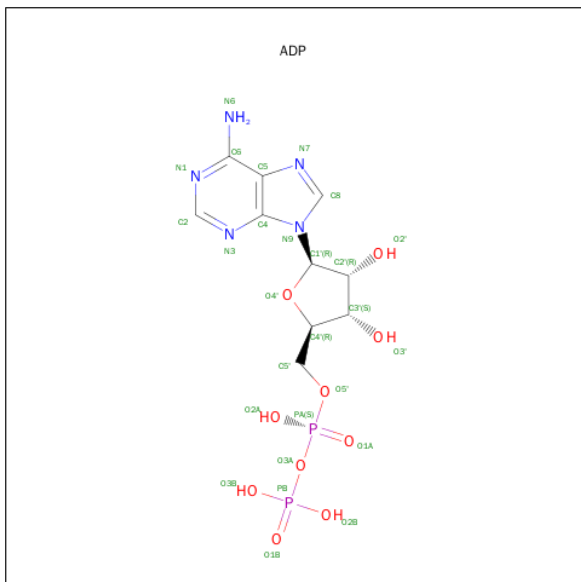
- Molecule 2 is a DNA chain called HD nuclease.

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 (three-letter code: FE) (formula: Fe).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).

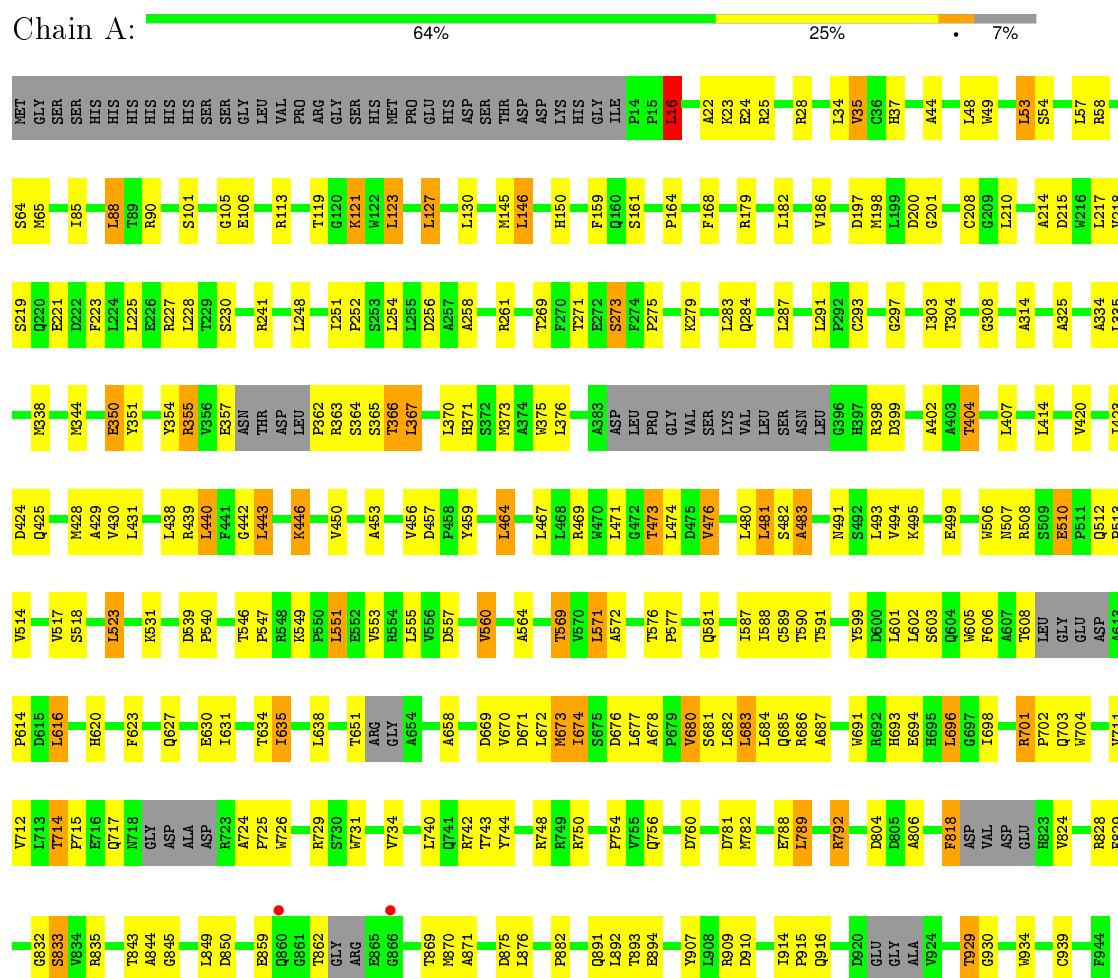


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	G	1	Total 27	C 10	N 5	O 10	P 2	0	0

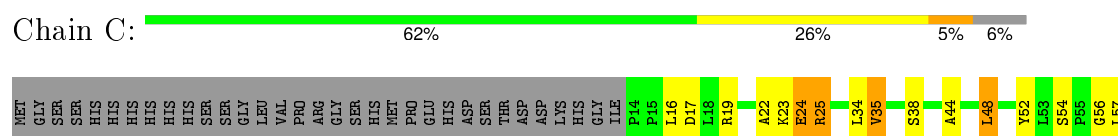
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

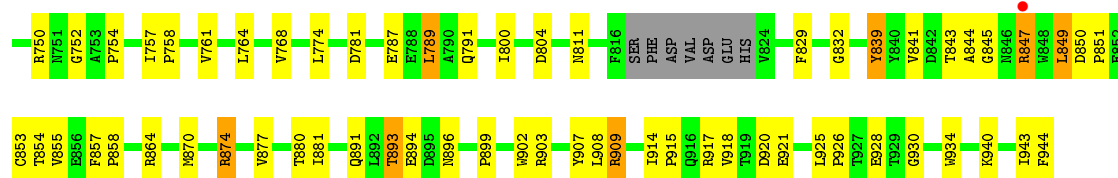


- Molecule 1: CRISPR-associated helicase, Cas3 family



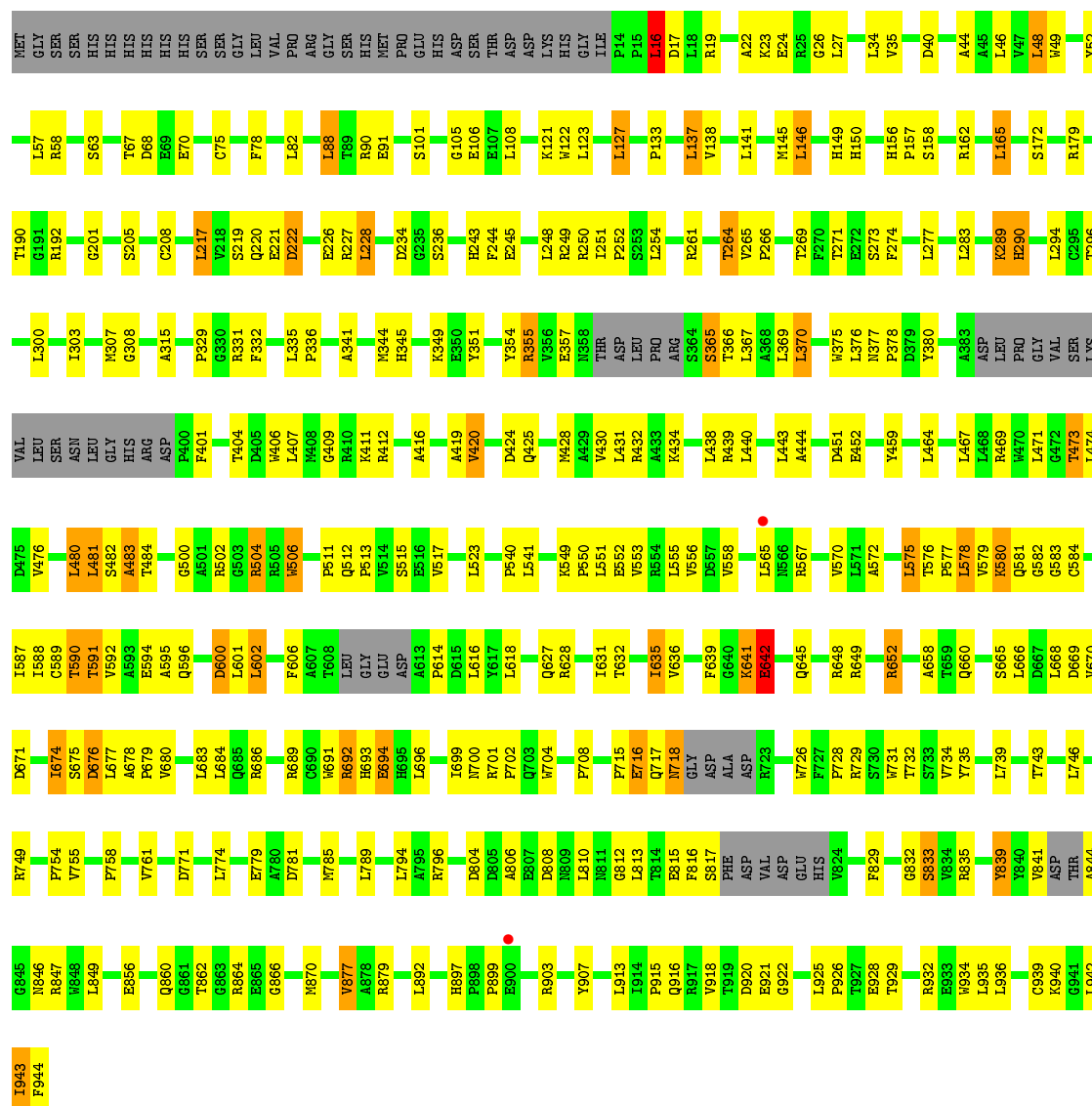






• Molecule 1: CRISPR-associated helicase, Cas3 family

Chain G: 59% 29% 7%



• Molecule 2: HD nuclease

Chain B: 17% 42% 33% 8%



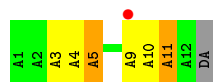
• Molecule 2: HD nuclease

Chain D:  17% 17% 58% 8%



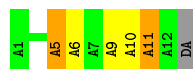
- Molecule 2: HD nuclease

Chain F:  8% 42% 33% 17% 8%



- Molecule 2: HD nuclease

Chain H:  50% 25% 17% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.21Å 222.61Å 124.85Å 90.00° 104.07° 90.00°	Depositor
Resolution (Å)	47.84 – 3.12 47.84 – 2.91	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.84-3.12) 90.9 (47.84-2.91)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.170 , 0.236 0.166 , 0.230	Depositor DCC
$R_{free}$ test set	1563 reflections (2.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.5	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 58.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 99041 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	28826	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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, ADP

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	0.51	0/7148	0.67	7/9746 (0.1%)
1	C	0.53	1/7176 (0.0%)	0.68	10/9790 (0.1%)
1	E	0.52	0/7181	0.66	3/9796 (0.0%)
1	G	0.47	0/7115	0.65	3/9702 (0.0%)
2	B	1.10	1/222 (0.5%)	2.09	11/339 (3.2%)
2	D	1.65	6/222 (2.7%)	2.56	25/339 (7.4%)
2	F	1.24	0/222	2.62	21/339 (6.2%)
2	H	0.90	0/222	1.90	10/339 (2.9%)
All	All	0.54	8/29508 (0.0%)	0.78	90/40390 (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	E	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	10	DA	P-O5'	11.51	1.71	1.59
2	D	10	DA	P-OP1	7.39	1.61	1.49
2	D	9	DA	C3'-C2'	5.56	1.58	1.52
2	D	9	DA	C5'-C4'	-5.31	1.45	1.51
2	D	10	DA	C3'-O3'	5.21	1.50	1.44
1	C	754	PRO	N-CD	5.20	1.55	1.47
2	B	3	DA	C3'-O3'	-5.15	1.37	1.44
2	D	10	DA	N9-C4	-5.04	1.34	1.37

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	10	DA	C1'-O4'-C4'	-13.80	96.30	110.10
2	D	9	DA	O4'-C1'-N9	13.19	117.23	108.00
2	F	11	DA	O4'-C4'-C3'	11.95	113.17	106.00
2	H	11	DA	C1'-O4'-C4'	-11.54	98.56	110.10
1	C	410	ARG	NE-CZ-NH1	-11.34	114.63	120.30
2	H	10	DA	C1'-O4'-C4'	-10.88	99.22	110.10
2	F	10	DA	O4'-C1'-N9	10.49	115.34	108.00
2	F	11	DA	O4'-C1'-N9	10.37	115.26	108.00
2	D	10	DA	C5'-C4'-C3'	10.24	132.53	114.10
2	B	4	DA	O4'-C4'-C3'	-9.70	100.18	106.00
2	B	2	DA	O4'-C1'-N9	-9.32	101.47	108.00
2	D	9	DA	O4'-C4'-C3'	9.20	111.52	106.00
2	B	11	DA	O4'-C4'-C3'	9.02	111.41	106.00
2	D	4	DA	O4'-C1'-N9	8.99	114.30	108.00
2	H	11	DA	C4'-C3'-C2'	-8.77	95.21	103.10
2	D	10	DA	O4'-C4'-C3'	8.62	111.17	106.00
2	F	11	DA	C4'-C3'-C2'	-8.62	95.35	103.10
2	F	4	DA	O4'-C4'-C3'	-8.32	101.01	106.00
2	D	11	DA	O4'-C4'-C3'	8.18	110.91	106.00
2	F	5	DA	O4'-C1'-N9	-8.11	102.32	108.00
2	D	10	DA	O5'-C5'-C4'	-8.02	90.95	111.00
2	F	10	DA	OP1-P-OP2	8.01	131.62	119.60
2	D	9	DA	OP1-P-O3'	-7.86	87.91	105.20
2	D	9	DA	C5'-C4'-O4'	-7.73	94.62	109.30
2	H	11	DA	O4'-C1'-C2'	-7.38	100.00	105.90
2	B	4	DA	C4'-C3'-C2'	-7.36	96.48	103.10
2	F	10	DA	O4'-C1'-C2'	-7.31	100.05	105.90
2	B	10	DA	C1'-O4'-C4'	-7.28	102.82	110.10
2	F	4	DA	C1'-O4'-C4'	-7.26	102.84	110.10
2	D	3	DA	O4'-C1'-N9	7.25	113.07	108.00
2	F	9	DA	C3'-C2'-C1'	-7.16	93.91	102.50
2	D	11	DA	C4'-C3'-C2'	-7.04	96.76	103.10
2	H	11	DA	O5'-P-OP2	-7.01	99.39	105.70
2	D	10	DA	O4'-C1'-N9	-6.92	103.16	108.00
2	D	1	DA	O4'-C4'-C3'	-6.91	101.74	104.50
2	D	11	DA	O4'-C1'-N9	6.87	112.81	108.00
2	D	5	DA	O4'-C1'-N9	-6.74	103.28	108.00
2	F	11	DA	C1'-O4'-C4'	-6.70	103.40	110.10
2	F	9	DA	C1'-O4'-C4'	-6.69	103.41	110.10
2	F	10	DA	C4'-C3'-C2'	-6.64	97.13	103.10
1	A	16	LEU	CA-CB-CG	6.50	130.26	115.30
1	A	367	LEU	CA-CB-CG	6.44	130.11	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	DA	C1'-O4'-C4'	-6.40	103.70	110.10
1	C	483	ALA	N-CA-C	-6.31	93.97	111.00
2	F	10	DA	O4'-C4'-C3'	6.29	109.78	106.00
1	C	541	LEU	C-N-CD	6.05	141.10	128.40
2	F	11	DA	OP1-P-O3'	6.03	118.46	105.20
1	E	539	ASP	C-N-CD	6.02	141.04	128.40
2	H	9	DA	O4'-C1'-N9	5.98	112.19	108.00
1	C	163	ASN	C-N-CD	5.97	140.95	128.40
2	F	10	DA	P-O5'-C5'	-5.96	111.37	120.90
2	D	1	DA	O4'-C1'-N9	-5.94	103.84	108.00
2	D	11	DA	O5'-P-OP2	-5.87	100.41	105.70
1	A	701	ARG	C-N-CD	5.87	140.72	128.40
1	A	523	LEU	CA-CB-CG	5.86	128.78	115.30
2	D	10	DA	C8-N9-C4	5.86	108.14	105.80
2	D	10	DA	C4'-C3'-C2'	-5.84	97.84	103.10
2	F	4	DA	O4'-C1'-N9	5.83	112.08	108.00
2	B	6	DA	N1-C6-N6	5.81	122.09	118.60
1	A	54	SER	C-N-CD	5.80	140.59	128.40
1	G	192	ARG	C-N-CD	5.78	140.53	128.40
1	C	367	LEU	CA-CB-CG	5.78	128.59	115.30
1	C	753	ALA	C-N-CD	5.76	140.50	128.40
1	C	613	ALA	C-N-CD	5.76	140.50	128.40
1	C	410	ARG	CB-CG-CD	5.75	126.54	111.60
2	D	10	DA	C1'-O4'-C4'	-5.66	104.44	110.10
2	B	9	DA	C3'-C2'-C1'	-5.64	95.73	102.50
2	B	10	DA	O4'-C1'-C2'	-5.62	101.41	105.90
2	F	10	DA	N3-C4-C5	5.61	130.73	126.80
1	A	443	LEU	CA-CB-CG	5.60	128.19	115.30
1	C	483	ALA	CB-CA-C	-5.60	101.70	110.10
2	H	5	DA	N1-C6-N6	5.56	121.94	118.60
1	G	16	LEU	CA-CB-CG	5.54	128.05	115.30
2	B	9	DA	O4'-C1'-N9	5.53	111.87	108.00
2	B	11	DA	C4'-C3'-C2'	-5.45	98.20	103.10
1	A	483	ALA	N-CA-C	-5.44	96.32	111.00
2	D	10	DA	OP1-P-OP2	5.40	127.70	119.60
2	D	11	DA	O4'-C1'-C2'	-5.35	101.62	105.90
2	F	3	DA	O4'-C1'-N9	5.31	111.72	108.00
2	H	9	DA	C3'-C2'-C1'	-5.21	96.24	102.50
2	H	10	DA	O4'-C1'-N9	5.17	111.62	108.00
2	F	9	DA	O4'-C1'-N9	5.16	111.61	108.00
1	E	680	VAL	CB-CA-C	-5.16	101.59	111.40
2	D	10	DA	N1-C6-N6	5.16	121.69	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	410	ARG	CD-NE-CZ	5.13	130.78	123.60
2	D	9	DA	N1-C2-N3	-5.08	126.76	129.30
1	E	16	LEU	CA-CB-CG	5.07	126.96	115.30
2	H	11	DA	O5'-P-OP1	5.06	116.77	110.70
1	G	483	ALA	N-CA-C	-5.04	97.38	111.00
2	D	9	DA	C8-N9-C4	-5.03	103.79	105.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	355	ARG	Sidechain
1	E	355	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6973	0	6917	156	0
1	C	7001	0	6944	217	0
1	E	7006	0	6952	178	0
1	G	6942	0	6897	228	0
2	B	197	0	99	8	0
2	D	197	0	99	14	0
2	F	197	0	99	4	0
2	H	197	0	99	7	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
3	E	2	0	0	0	0
3	G	2	0	0	0	0
4	A	27	0	12	3	0
4	C	27	0	12	3	0
4	E	27	0	12	0	0
4	G	27	0	12	6	0
All	All	28826	0	28154	773	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 14.

All (773) 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:G:575:LEU:O	1:G:579:VAL:HG13	1.41	1.18
1:G:576:THR:O	1:G:579:VAL:HG22	1.46	1.13
1:C:612:ASP:HA	1:C:613:ALA:HB3	1.25	1.12
1:C:610:GLY:O	1:C:613:ALA:HB2	1.57	1.04
1:G:576:THR:OG1	1:G:577:PRO:HD3	1.64	0.96
1:G:579:VAL:CG2	1:G:580:LYS:HD2	1.97	0.95
1:G:580:LYS:HD2	1:G:580:LYS:H	1.32	0.93
1:C:281:ASN:HB2	1:C:284:GLN:CD	1.89	0.93
1:G:150:HIS:CE1	2:H:11:DA:H5'	2.05	0.92
1:E:909:ARG:HG3	1:E:909:ARG:HH11	1.34	0.90
1:E:375:TRP:HB2	1:E:907:TYR:OH	1.73	0.89
1:C:833:SER:H	2:D:6:DA:H61	1.19	0.89
1:A:482:SER:OG	1:A:483:ALA:O	1.93	0.86
1:C:694:GLU:HG2	1:C:701:ARG:HH21	1.40	0.85
1:E:903:ARG:HD2	1:E:909:ARG:HG3	1.57	0.85
1:G:579:VAL:HG22	1:G:580:LYS:HD2	1.59	0.84
1:A:308:GLY:N	4:A:1003:ADP:O1B	2.12	0.83
1:C:610:GLY:O	1:C:613:ALA:CB	2.26	0.82
1:A:832:GLY:HA2	2:B:5:DA:H61	1.43	0.82
1:G:308:GLY:CA	4:G:1003:ADP:O1B	2.28	0.82
1:G:833:SER:H	2:H:6:DA:H61	1.23	0.82
1:A:572:ALA:HA	1:A:605:TRP:HH2	1.46	0.81
1:C:832:GLY:HA2	2:D:5:DA:H61	1.44	0.81
1:G:308:GLY:HA2	4:G:1003:ADP:PB	2.20	0.81
1:A:572:ALA:HA	1:A:605:TRP:CH2	2.17	0.80
1:C:263:ILE:HD11	1:C:365:SER:OG	1.81	0.80
1:C:692:ARG:NH1	4:C:1003:ADP:O1B	2.15	0.80
1:G:579:VAL:HG23	1:G:580:LYS:HD2	1.64	0.80
1:C:612:ASP:HA	1:C:613:ALA:CB	2.08	0.79
1:G:482:SER:OG	1:G:483:ALA:O	2.00	0.79
1:C:694:GLU:CG	1:C:701:ARG:HH21	1.96	0.78
1:C:23:LYS:NZ	1:C:219:SER:CB	2.47	0.78
1:G:308:GLY:HA2	4:G:1003:ADP:O1B	1.84	0.77
1:G:580:LYS:HG2	1:G:581:GLN:H	1.49	0.77
1:C:23:LYS:NZ	1:C:219:SER:HB3	2.01	0.75
1:E:832:GLY:HA2	2:F:5:DA:N6	2.01	0.75
1:A:572:ALA:CA	1:A:605:TRP:HH2	1.99	0.75
1:C:113:ARG:NH2	1:C:168:PHE:O	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1003:ADP:N3	4:A:1003:ADP:H2'	2.02	0.75
1:A:571:LEU:HD22	1:A:602:LEU:HD21	1.68	0.74
1:G:832:GLY:HA2	2:H:5:DA:H61	1.51	0.74
2:D:10:DA:OP1	2:D:10:DA:H4'	1.87	0.73
1:G:576:THR:OG1	1:G:577:PRO:CD	2.36	0.73
1:C:678:ALA:HB3	1:C:683:LEU:HD13	1.70	0.73
1:G:576:THR:CB	1:G:577:PRO:HD3	2.18	0.73
1:C:161:SER:HB3	1:C:167:GLU:OE1	1.87	0.73
1:G:579:VAL:CG2	1:G:580:LYS:CD	2.66	0.73
1:E:909:ARG:HG3	1:E:909:ARG:NH1	2.02	0.73
1:A:429:ALA:HB1	1:A:440:LEU:HD13	1.71	0.72
1:A:404:THR:HG22	1:A:407:LEU:H	1.54	0.72
1:C:680:VAL:HG13	1:C:743:THR:HG23	1.69	0.72
1:E:188:ASP:OD1	1:E:192:ARG:NH1	2.22	0.72
1:G:266:PRO:O	1:G:355:ARG:NH2	2.21	0.72
1:E:150:HIS:CE1	2:F:11:DA:H5'	2.24	0.72
1:C:612:ASP:OD2	1:C:652:ARG:HG2	1.90	0.71
1:G:694:GLU:HG2	1:G:701:ARG:HH21	1.56	0.71
1:A:23:LYS:NZ	1:A:219:SER:OG	2.24	0.71
1:C:22:ALA:HB2	1:C:34:LEU:HA	1.71	0.71
1:E:558:VAL:HB	1:E:565:LEU:HD13	1.72	0.71
1:G:504:ARG:HG2	1:G:504:ARG:HH11	1.55	0.71
1:C:263:ILE:CD1	1:C:365:SER:OG	2.39	0.70
1:G:432:ARG:NH1	1:G:812:GLY:O	2.25	0.70
1:G:579:VAL:CG2	1:G:580:LYS:CE	2.71	0.69
1:C:150:HIS:CE1	2:D:11:DA:H5'	2.27	0.69
1:G:22:ALA:HB2	1:G:34:LEU:HA	1.73	0.69
1:A:150:HIS:CE1	2:B:11:DA:H5'	2.28	0.69
1:C:439:ARG:O	1:C:443:LEU:HD22	1.93	0.68
1:C:266:PRO:O	1:C:355:ARG:NH2	2.26	0.68
1:E:832:GLY:HA2	2:F:5:DA:H61	1.59	0.68
1:G:580:LYS:HD2	1:G:580:LYS:N	2.06	0.68
1:G:106:GLU:OE2	1:G:179:ARG:NH2	2.26	0.68
1:G:575:LEU:O	1:G:579:VAL:CG1	2.29	0.68
1:G:579:VAL:HG23	1:G:580:LYS:CE	2.23	0.68
1:A:750:ARG:NH2	1:A:754:PRO:O	2.27	0.68
1:G:190:THR:HG22	1:G:190:THR:O	1.91	0.67
1:C:674:ILE:HG22	1:C:713:LEU:HD11	1.75	0.67
1:G:579:VAL:HG23	1:G:580:LYS:CD	2.24	0.67
1:A:469:ARG:O	1:A:473:THR:HG22	1.93	0.67
1:E:644:ALA:HB1	1:E:698:ILE:HD12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:935:LEU:HD23	1:G:943:ILE:HD11	1.76	0.67
1:C:589:CYS:HB2	1:C:595:ALA:HB2	1.75	0.67
1:G:591:THR:OG1	1:G:592:VAL:N	2.28	0.67
1:C:815:GLU:O	1:C:815:GLU:HG3	1.94	0.66
1:A:915:PRO:HD2	1:A:929:THR:HG21	1.78	0.66
1:C:34:LEU:HD23	1:C:88:LEU:HD22	1.78	0.66
1:G:506:TRP:HH2	1:G:511:PRO:O	1.79	0.66
1:C:164:PRO:O	1:C:165:LEU:C	2.32	0.66
1:E:841:VAL:HB	1:E:847:ARG:CZ	2.26	0.65
1:G:579:VAL:CG2	1:G:580:LYS:HE3	2.26	0.65
1:A:572:ALA:CB	1:A:605:TRP:HH2	2.08	0.65
1:E:471:LEU:HB3	1:E:476:VAL:HG22	1.78	0.65
1:E:358:ASN:N	1:E:358:ASN:OD1	2.24	0.65
1:E:558:VAL:HG22	1:E:570:VAL:HG21	1.78	0.65
1:C:663:GLU:OE2	1:C:686:ARG:NH1	2.30	0.65
1:G:600:ASP:OD1	1:G:940:LYS:NZ	2.29	0.65
1:G:833:SER:N	2:H:6:DA:H61	1.94	0.65
1:C:694:GLU:O	1:C:697:GLY:N	2.29	0.65
1:E:565:LEU:HD21	1:E:715:PRO:HG3	1.79	0.64
1:E:376:LEU:HG	1:E:907:TYR:CE2	2.33	0.64
1:C:303:ILE:HD12	1:C:481:LEU:HD11	1.79	0.64
1:E:27:LEU:HD13	1:E:228:LEU:HD21	1.80	0.64
1:C:750:ARG:NH2	1:C:755:VAL:HG22	2.12	0.64
1:E:20:PHE:HE2	1:E:178:GLN:HG3	1.62	0.64
1:C:106:GLU:HG3	1:C:172:SER:HB2	1.78	0.64
1:G:578:LEU:HA	1:G:704:TRP:CZ2	2.32	0.64
1:C:351:TYR:CZ	1:C:355:ARG:HD3	2.33	0.64
1:E:698:ILE:HG13	1:E:699:ILE:N	2.10	0.64
1:C:929:THR:HG22	1:C:934:TRP:NE1	2.13	0.64
1:A:678:ALA:HB3	1:A:683:LEU:HD13	1.80	0.64
1:A:832:GLY:HA2	2:B:5:DA:N6	2.13	0.63
1:C:281:ASN:HB2	1:C:284:GLN:NE2	2.12	0.63
1:C:71:HIS:NE2	1:C:194:THR:O	2.31	0.63
1:A:442:GLY:O	1:A:446:LYS:HD3	1.98	0.63
1:A:430:VAL:HG11	1:A:467:LEU:HA	1.80	0.63
1:G:245:GLU:HA	1:G:248:LEU:HD12	1.81	0.63
1:G:407:LEU:HD22	1:G:416:ALA:HB2	1.81	0.63
1:G:506:TRP:CH2	1:G:512:GLN:HA	2.34	0.63
1:A:197:ASP:OD2	1:E:528:ARG:NH2	2.27	0.63
1:A:742:ARG:NH1	1:A:781:ASP:OD1	2.32	0.62
1:C:410:ARG:HE	2:D:9:DA:H3'	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:729:ARG:NH2	1:G:101:SER:O	2.32	0.62
1:C:333:LEU:HD11	1:C:348:LEU:HD13	1.82	0.62
1:A:788:GLU:OE2	1:A:792:ARG:NH1	2.32	0.62
1:A:53:LEU:HG	1:A:57:LEU:HD23	1.82	0.62
1:E:921:GLU:OE1	1:E:921:GLU:N	2.32	0.62
1:C:591:THR:HG21	1:C:730:SER:HB2	1.81	0.62
1:A:671:ASP:OD1	1:A:701:ARG:NH1	2.33	0.61
1:A:850:ASP:N	1:A:850:ASP:OD1	2.33	0.61
1:C:554:ARG:NH2	1:C:574:GLU:OE2	2.24	0.61
1:C:839:TYR:CE1	1:C:847:ARG:HD2	2.36	0.61
1:E:22:ALA:HB2	1:E:34:LEU:HA	1.81	0.61
1:E:899:PRO:HG2	1:E:902:TRP:CD1	2.35	0.61
1:C:290:HIS:NE2	1:C:539:ASP:OD1	2.33	0.61
1:C:528:ARG:HD2	1:C:529:ILE:HG13	1.83	0.61
1:G:580:LYS:HG2	1:G:581:GLN:N	2.15	0.61
1:C:519:TYR:HB3	1:C:762:GLN:HB2	1.82	0.61
1:E:375:TRP:CB	1:E:907:TYR:OH	2.48	0.61
1:E:270:PHE:CE2	1:E:280:PRO:HB3	2.36	0.60
1:G:841:VAL:O	1:G:918:VAL:N	2.34	0.60
1:E:261:ARG:O	1:E:365:SER:HB2	2.01	0.60
1:A:338:MET:HG2	1:A:371:HIS:CG	2.37	0.60
1:A:507:ASN:HB2	1:A:510:GLU:HB2	1.84	0.60
1:A:789:LEU:HD22	1:C:167:GLU:HG3	1.83	0.60
1:E:430:VAL:HG11	1:E:467:LEU:HA	1.84	0.60
1:E:541:LEU:HD13	1:E:542:PRO:HD2	1.84	0.59
1:G:589:CYS:HB2	1:G:595:ALA:HB2	1.84	0.59
1:A:22:ALA:HB2	1:A:34:LEU:HA	1.84	0.59
1:E:315:ALA:HB2	1:E:481:LEU:HD21	1.83	0.59
1:A:90:ARG:NH2	1:A:105:GLY:O	2.26	0.59
1:C:164:PRO:O	1:C:166:ALA:N	2.36	0.59
1:C:884:ARG:HH12	2:D:1:DA:H5'	1.68	0.59
1:G:300:LEU:HD11	1:G:480:LEU:HD22	1.83	0.59
1:C:639:PHE:HB2	1:C:668:LEU:HD22	1.83	0.59
1:G:78:PHE:HB2	1:G:190:THR:HG21	1.85	0.59
1:C:608:THR:OG1	1:C:609:LEU:HD23	2.01	0.59
1:G:222:ASP:N	1:G:222:ASP:OD1	2.36	0.59
1:C:159:PHE:CD2	1:C:164:PRO:HB3	2.38	0.58
1:G:680:VAL:HG13	1:G:743:THR:HG23	1.86	0.58
1:C:457:ASP:H	1:C:460:MET:HE3	1.67	0.58
1:G:226:GLU:OE1	1:G:250:ARG:HD3	2.04	0.58
1:G:44:ALA:HA	1:G:251:ILE:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:MET:HG3	1:A:208:CYS:HB2	1.86	0.58
1:C:281:ASN:ND2	1:C:309:GLU:O	2.37	0.58
1:C:60:THR:OG1	1:C:475:ASP:OD2	2.21	0.57
1:G:627:GLN:O	1:G:631:ILE:HG13	2.04	0.57
1:G:665:SER:HA	1:G:689:ARG:HH22	1.69	0.57
1:C:371:HIS:HB3	1:C:422:THR:HG23	1.86	0.57
1:C:90:ARG:NH2	1:C:105:GLY:O	2.27	0.57
1:E:137:LEU:HD21	1:E:199:LEU:O	2.04	0.57
1:E:137:LEU:HD23	1:E:138:VAL:N	2.18	0.57
1:G:370:LEU:HB3	1:G:425:GLN:HG3	1.86	0.57
1:A:453:ALA:O	1:A:456:VAL:HG13	2.04	0.57
1:C:606:PHE:N	1:C:606:PHE:CD1	2.73	0.57
1:C:612:ASP:CA	1:C:613:ALA:HB3	2.16	0.57
1:C:833:SER:N	2:D:6:DA:H61	1.99	0.57
1:C:23:LYS:HZ1	1:C:219:SER:CB	2.15	0.57
1:A:916:GLN:NE2	1:A:934:TRP:O	2.34	0.57
1:E:266:PRO:O	1:E:355:ARG:NH2	2.38	0.57
1:G:579:VAL:HG22	1:G:580:LYS:CD	2.29	0.57
1:G:106:GLU:HG3	1:G:172:SER:H	1.70	0.57
1:G:190:THR:CG2	1:G:190:THR:O	2.53	0.57
1:G:579:VAL:HG23	1:G:580:LYS:N	2.20	0.56
1:E:903:ARG:HD2	1:E:909:ARG:CG	2.31	0.56
1:E:376:LEU:HD11	1:E:907:TYR:CD2	2.40	0.56
1:E:644:ALA:CB	1:E:698:ILE:HD12	2.35	0.56
1:E:917:ARG:CZ	1:E:925:LEU:HD11	2.35	0.56
1:C:665:SER:O	1:C:665:SER:OG	2.18	0.56
1:A:789:LEU:HD11	1:C:161:SER:OG	2.05	0.56
1:C:44:ALA:HA	1:C:251:ILE:HG12	1.87	0.56
1:E:429:ALA:HB1	1:E:440:LEU:HD13	1.86	0.56
1:E:315:ALA:CB	1:E:481:LEU:HD21	2.35	0.56
1:A:674:ILE:HG23	1:A:711:VAL:HB	1.86	0.56
1:G:549:LYS:HD2	1:G:550:PRO:HD2	1.88	0.56
1:C:611:GLU:HA	1:C:613:ALA:HB3	1.88	0.56
1:C:308:GLY:HA2	4:C:1003:ADP:O3A	2.05	0.56
1:G:841:VAL:HG23	1:G:846:ASN:HB3	1.88	0.56
1:G:376:LEU:HD23	1:G:877:VAL:HG11	1.87	0.56
1:E:424:ASP:O	1:E:428:MET:HG3	2.06	0.56
1:G:691:TRP:CE3	1:G:694:GLU:HG3	2.40	0.56
1:A:549:LYS:NZ	1:A:694:GLU:OE2	2.39	0.56
1:E:664:GLN:O	1:E:689:ARG:NH2	2.39	0.56
1:C:256:ASP:OD1	1:C:261:ARG:NE	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:PHE:HB2	1:C:167:GLU:OE1	2.06	0.56
1:E:123:LEU:O	1:E:127:LEU:HB2	2.05	0.56
1:G:584:CYS:N	1:G:671:ASP:OD2	2.35	0.55
1:A:101:SER:O	1:C:729:ARG:NH2	2.28	0.55
1:G:150:HIS:HE1	2:H:11:DA:H5'	1.65	0.55
1:C:23:LYS:HE2	2:D:12:DA:OP2	2.07	0.55
1:A:375:TRP:HB2	1:A:907:TYR:OH	2.06	0.55
1:G:430:VAL:HG11	1:G:467:LEU:HA	1.89	0.55
1:A:669:ASP:OD2	1:A:693:HIS:N	2.29	0.55
1:G:576:THR:CB	1:G:577:PRO:CD	2.84	0.55
1:A:37:HIS:CE1	1:A:215:ASP:OD1	2.60	0.55
1:G:145:MET:HG3	1:G:208:CYS:HB2	1.87	0.55
1:E:49:TRP:HA	1:E:53:LEU:HD13	1.89	0.55
1:E:491:ASN:OD1	1:E:513:PRO:HD2	2.07	0.55
1:C:159:PHE:N	1:C:159:PHE:CD1	2.72	0.55
1:G:844:ALA:N	1:G:918:VAL:O	2.40	0.55
1:C:486:HIS:CE1	1:C:487:HIS:CD2	2.95	0.55
1:C:137:LEU:HD11	1:C:808:ASP:HB3	1.88	0.55
1:E:332:PHE:HA	1:E:419:ALA:O	2.07	0.55
1:E:125:PHE:HB2	1:E:165:LEU:HD13	1.88	0.55
1:G:669:ASP:HB2	1:G:693:HIS:CD2	2.42	0.55
1:E:287:LEU:O	1:E:291:LEU:HB2	2.06	0.55
1:C:198:MET:HG3	1:C:199:LEU:N	2.20	0.55
1:E:839:TYR:H	1:E:839:TYR:HD1	1.55	0.54
1:E:111:GLU:HB2	1:G:794:LEU:HD11	1.89	0.54
1:C:265:VAL:HG13	1:C:355:ARG:NH2	2.21	0.54
1:E:844:ALA:N	1:E:845:GLY:HA2	2.22	0.54
1:C:471:LEU:HB3	1:C:476:VAL:HG22	1.88	0.54
1:C:581:GLN:OE1	1:C:703:GLN:HB3	2.06	0.54
1:E:644:ALA:HB1	1:E:698:ILE:CD1	2.37	0.54
1:E:847:ARG:HB3	1:E:857:PHE:CB	2.38	0.54
1:E:300:LEU:HD21	1:E:480:LEU:HD22	1.90	0.54
1:C:687:ALA:HB2	1:C:710:LEU:HD22	1.89	0.54
1:G:345:HIS:CD2	1:G:369:LEU:HB2	2.43	0.54
1:A:85:ILE:HG13	1:A:182:LEU:HD23	1.88	0.54
1:G:26:GLY:C	1:G:27:LEU:HD23	2.27	0.54
1:C:621:SER:HB3	2:D:3:DA:P	2.48	0.54
1:G:315:ALA:HB2	1:G:481:LEU:HD21	1.89	0.54
1:G:642:GLU:HA	1:G:645:GLN:HG3	1.89	0.54
1:C:335:LEU:HD13	1:C:341:ALA:HA	1.90	0.54
1:C:23:LYS:HZ2	1:C:219:SER:CB	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD11	1:A:210:LEU:HD12	1.89	0.54
1:G:540:PRO:HG2	1:G:541:LEU:HD22	1.90	0.54
1:G:34:LEU:HD23	1:G:88:LEU:HD22	1.89	0.53
1:E:847:ARG:HB3	1:E:857:PHE:HB3	1.90	0.53
1:A:334:ALA:HB1	1:A:423:ILE:HA	1.90	0.53
1:G:587:ILE:HD12	1:G:674:ILE:HG12	1.90	0.53
1:C:471:LEU:HD22	1:C:476:VAL:HG21	1.89	0.53
1:C:852:GLU:O	1:C:854:THR:HG23	2.09	0.53
1:E:750:ARG:NH2	1:E:754:PRO:O	2.41	0.53
1:C:215:ASP:O	1:C:219:SER:OG	2.20	0.53
1:C:24:GLU:HG3	1:C:25:ARG:H	1.73	0.53
1:A:569:THR:O	1:A:572:ALA:N	2.41	0.53
1:A:572:ALA:HB2	1:A:605:TRP:HH2	1.72	0.53
1:A:34:LEU:HD23	1:A:88:LEU:HD22	1.90	0.53
1:G:27:LEU:HD13	1:G:228:LEU:CD2	2.38	0.53
1:E:893:THR:OG1	1:E:894:GLU:N	2.38	0.53
1:E:150:HIS:ND1	2:F:11:DA:H5'	2.23	0.53
1:G:506:TRP:CZ2	1:G:513:PRO:HD3	2.44	0.53
1:A:376:LEU:HD13	1:A:907:TYR:CZ	2.43	0.53
1:G:137:LEU:HD12	1:G:808:ASP:HB3	1.91	0.53
1:E:619:LEU:HG	1:E:661:VAL:HG21	1.91	0.53
1:G:849:LEU:HD23	1:G:879:ARG:NH1	2.23	0.53
1:G:642:GLU:O	1:G:648:ARG:NH2	2.42	0.53
1:G:336:PRO:HG3	1:G:452:GLU:HG3	1.90	0.53
1:G:366:THR:HG21	1:G:404:THR:HG23	1.90	0.53
1:G:916:GLN:OE1	1:G:936:LEU:N	2.39	0.53
1:G:702:PRO:HB2	1:G:704:TRP:CD1	2.44	0.53
1:C:605:TRP:CE3	1:C:606:PHE:HE1	2.27	0.53
1:G:265:VAL:HG13	1:G:355:ARG:NH2	2.24	0.53
1:G:718:ASN:N	1:G:718:ASN:OD1	2.38	0.53
1:E:451:ASP:OD1	1:E:452:GLU:N	2.42	0.53
1:G:502:ARG:HG3	1:G:504:ARG:HG3	1.91	0.52
1:A:424:ASP:O	1:A:428:MET:HG3	2.09	0.52
1:G:580:LYS:CD	1:G:580:LYS:H	2.04	0.52
1:G:576:THR:O	1:G:580:LYS:CD	2.57	0.52
1:C:450:VAL:HG13	1:C:480:LEU:HD12	1.90	0.52
1:C:630:GLU:O	1:C:634:THR:HG23	2.10	0.52
1:G:678:ALA:HB3	1:G:683:LEU:HD13	1.92	0.52
1:C:261:ARG:O	1:C:365:SER:HB3	2.09	0.52
1:C:106:GLU:HG3	1:C:172:SER:CB	2.39	0.52
1:E:90:ARG:NH2	1:E:105:GLY:O	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:ARG:O	1:G:365:SER:HB3	2.10	0.52
1:G:349:LYS:HE3	1:G:401:PHE:HB2	1.90	0.52
1:A:414:LEU:HD12	1:A:439:ARG:HB3	1.91	0.52
1:G:572:ALA:O	1:G:576:THR:HG23	2.10	0.52
1:C:281:ASN:HB2	1:C:284:GLN:CG	2.39	0.52
1:C:680:VAL:HG11	1:C:746:LEU:HD23	1.91	0.52
1:G:249:ARG:O	1:G:252:PRO:HD2	2.09	0.52
1:E:693:HIS:HB3	1:E:696:LEU:HD22	1.91	0.52
1:E:453:ALA:O	1:E:456:VAL:HG13	2.10	0.52
1:G:122:TRP:CE2	1:G:179:ARG:HD2	2.45	0.52
1:C:849:LEU:HD21	1:C:858:PRO:HD3	1.91	0.52
1:G:693:HIS:HB3	1:G:696:LEU:HD13	1.92	0.52
1:A:121:LYS:HE2	1:A:168:PHE:CE1	2.44	0.52
1:G:590:THR:HG21	1:G:731:TRP:HA	1.92	0.52
1:C:842:ASP:O	1:C:845:GLY:N	2.35	0.52
1:C:483:ALA:O	1:C:484:THR:C	2.48	0.52
1:A:702:PRO:CG	1:A:704:TRP:NE1	2.73	0.51
1:C:742:ARG:NH1	1:C:781:ASP:OD2	2.42	0.51
1:A:287:LEU:HD12	1:A:314:ALA:HB1	1.92	0.51
1:G:929:THR:HB	1:G:934:TRP:CD1	2.45	0.51
1:A:366:THR:HB	1:A:402:ALA:O	2.09	0.51
1:E:638:LEU:HD22	1:E:650:PRO:HD3	1.92	0.51
1:A:49:TRP:CZ2	1:A:58:ARG:HG2	2.45	0.51
1:C:606:PHE:N	1:C:606:PHE:HD1	2.06	0.51
1:C:35:VAL:O	1:C:38:SER:OG	2.28	0.51
1:A:284:GLN:NE2	4:A:1003:ADP:N1	2.58	0.51
1:A:630:GLU:O	1:A:634:THR:HG23	2.10	0.51
1:A:590:THR:HG22	1:A:591:THR:HG23	1.92	0.51
1:A:338:MET:HG2	1:A:371:HIS:ND1	2.26	0.51
1:C:54:SER:OG	1:C:329:PRO:HD2	2.10	0.51
1:E:678:ALA:H	1:E:683:LEU:HD13	1.75	0.51
1:G:576:THR:O	1:G:580:LYS:HD2	2.11	0.51
1:A:16:LEU:HD11	1:A:35:VAL:HG21	1.91	0.51
1:A:64:SER:HB3	1:A:200:ASP:OD1	2.09	0.51
1:A:113:ARG:NH2	1:A:168:PHE:O	2.29	0.51
1:C:289:LYS:HB3	1:C:290:HIS:CD2	2.46	0.51
1:E:696:LEU:N	1:E:696:LEU:CD1	2.73	0.51
1:E:522:TRP:HE3	1:E:523:LEU:N	2.09	0.51
1:E:132:TYR:HB3	1:E:139:THR:OG1	2.11	0.51
1:C:816:PHE:CD1	1:C:817:SER:N	2.79	0.51
1:C:209:GLY:HA3	1:C:441:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:244:PHE:CE2	1:G:248:LEU:HD11	2.46	0.50
1:A:506:TRP:CZ2	1:A:513:PRO:HG3	2.46	0.50
1:E:65:MET:HA	1:E:198:MET:O	2.11	0.50
1:G:308:GLY:CA	4:G:1003:ADP:PB	2.95	0.50
1:C:164:PRO:C	1:C:166:ALA:N	2.65	0.50
1:A:495:LYS:O	1:A:499:GLU:HG3	2.12	0.50
1:E:632:THR:O	1:E:636:VAL:HG13	2.10	0.50
1:A:258:ALA:O	1:A:404:THR:HG21	2.11	0.50
1:A:491:ASN:OD1	1:A:513:PRO:HD2	2.11	0.50
1:E:850:ASP:HB2	1:E:851:PRO:HD2	1.94	0.50
1:C:17:ASP:OD2	1:C:19:ARG:NE	2.41	0.50
1:E:521:GLY:HA2	1:E:543:ILE:HD12	1.93	0.50
1:E:853:CYS:SG	1:E:918:VAL:HG11	2.52	0.50
1:E:738:ALA:O	1:E:742:ARG:HG3	2.11	0.50
1:G:332:PHE:HA	1:G:419:ALA:O	2.11	0.50
1:C:261:ARG:O	1:C:365:SER:CB	2.60	0.50
2:D:9:DA:H2''	2:D:10:DA:O5'	2.11	0.50
1:G:335:LEU:HD11	1:G:344:MET:HG2	1.94	0.50
1:E:87:LYS:HG2	1:E:92:PHE:CZ	2.47	0.49
1:E:893:THR:HG23	1:E:896:ASN:OD1	2.12	0.49
1:A:531:LYS:HD2	1:E:133:PRO:HB3	1.93	0.49
1:G:734:VAL:HG23	1:G:735:TYR:CD2	2.48	0.49
1:G:23:LYS:NZ	1:G:219:SER:OG	2.39	0.49
1:C:506:TRP:CH2	1:C:513:PRO:HD3	2.48	0.49
1:A:844:ALA:H	1:A:845:GLY:HA2	1.77	0.49
1:G:929:THR:HB	1:G:934:TRP:NE1	2.27	0.49
1:A:159:PHE:CD2	1:A:164:PRO:HB3	2.47	0.49
1:A:682:LEU:O	1:A:686:ARG:HD3	2.12	0.49
1:E:594:GLU:O	1:E:598:VAL:HG23	2.13	0.49
1:E:160:GLN:OE1	1:G:796:ARG:HD2	2.13	0.49
1:G:856:GLU:OE1	1:G:856:GLU:N	2.45	0.49
1:G:578:LEU:HB2	1:G:704:TRP:CH2	2.48	0.49
1:A:261:ARG:O	1:A:365:SER:OG	2.20	0.49
1:A:119:THR:HG23	1:A:123:LEU:HD22	1.95	0.49
1:G:771:ASP:HB3	1:G:774:LEU:HG	1.95	0.49
1:C:164:PRO:O	1:C:167:GLU:N	2.45	0.49
1:A:197:ASP:CG	1:E:528:ARG:HH22	2.14	0.49
1:E:917:ARG:NE	1:E:925:LEU:HD11	2.28	0.49
1:E:600:ASP:O	1:E:604:GLN:HG3	2.12	0.49
1:G:219:SER:CB	2:H:11:DA:H2'	2.42	0.49
1:G:351:TYR:CZ	1:G:355:ARG:HD3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:584:CYS:HB3	1:G:639:PHE:CE2	2.47	0.49
1:C:473:THR:HG22	1:C:500:GLY:O	2.12	0.49
2:B:1:DA:C8	2:B:1:DA:H5"	2.48	0.49
1:C:56:GLY:HA3	1:C:326:THR:O	2.12	0.49
1:G:308:GLY:HA2	4:G:1003:ADP:O3A	2.13	0.49
1:C:149:HIS:CD2	1:C:150:HIS:CD2	3.01	0.49
1:C:505:ARG:HD3	1:C:802:ASP:OD2	2.13	0.49
1:G:67:THR:OG1	1:G:68:ASP:N	2.45	0.49
1:A:223:PHE:O	1:A:227:ARG:HG2	2.12	0.49
1:C:571:LEU:HD11	1:C:598:VAL:HG13	1.95	0.49
1:C:605:TRP:HE3	1:C:606:PHE:HE1	1.60	0.49
1:G:839:TYR:HE1	1:G:915:PRO:HG3	1.78	0.49
1:E:691:TRP:CD2	1:E:708:PRO:HG3	2.48	0.49
1:G:345:HIS:HA	1:G:420:VAL:HG11	1.95	0.49
1:C:461:GLN:O	1:C:465:GLU:HG3	2.13	0.49
1:G:234:ASP:OD2	1:G:236:SER:HB3	2.12	0.49
1:A:828:ARG:HB2	2:B:5:DA:C2	2.48	0.48
1:C:24:GLU:HG3	1:C:25:ARG:N	2.27	0.48
1:E:940:LYS:HE3	1:E:943:ILE:HD11	1.94	0.48
1:G:679:PRO:HG3	1:G:739:LEU:HD23	1.95	0.48
1:G:226:GLU:OE2	1:G:250:ARG:NH1	2.46	0.48
1:E:680:VAL:HG13	1:E:743:THR:HG23	1.95	0.48
1:C:227:ARG:NH2	1:C:246:THR:HG23	2.27	0.48
1:C:453:ALA:O	1:C:456:VAL:HG22	2.13	0.48
1:A:303:ILE:HB	1:A:481:LEU:HD12	1.95	0.48
1:G:506:TRP:HH2	1:G:511:PRO:C	2.16	0.48
1:C:482:SER:OG	1:C:483:ALA:O	2.26	0.48
1:G:565:LEU:HD21	1:G:715:PRO:HG3	1.95	0.48
1:C:906:PHE:C	1:C:906:PHE:CD1	2.85	0.48
1:G:639:PHE:HB2	1:G:668:LEU:HD22	1.95	0.48
1:C:409:GLY:HA3	1:C:412:ARG:HD2	1.95	0.48
1:C:332:PHE:HA	1:C:419:ALA:O	2.12	0.48
1:C:23:LYS:HZ2	1:C:219:SER:HB3	1.73	0.48
1:G:717:GLN:OE1	1:G:726:TRP:N	2.37	0.48
1:G:329:PRO:O	1:G:331:ARG:NH1	2.45	0.48
1:C:284:GLN:HE22	4:C:1003:ADP:HN61	1.62	0.48
1:C:149:HIS:NE2	1:C:150:HIS:CD2	2.81	0.48
1:C:259:GLY:HA3	1:C:366:THR:HG23	1.96	0.48
1:C:258:ALA:O	1:C:404:THR:HG21	2.13	0.48
1:E:345:HIS:CD2	1:E:369:LEU:HB2	2.48	0.48
1:E:269:THR:O	1:E:273:SER:OG	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:584:CYS:SG	1:G:649:ARG:NH2	2.87	0.48
1:G:810:LEU:O	1:G:813:LEU:HB2	2.14	0.48
1:G:551:LEU:O	1:G:755:VAL:N	2.32	0.48
1:C:506:TRP:HH2	1:C:511:PRO:O	1.97	0.48
1:A:606:PHE:CE2	1:A:614:PRO:HD2	2.49	0.48
1:E:145:MET:HE2	1:E:146:LEU:HD13	1.94	0.48
1:C:363:ARG:HA	1:C:364:SER:HA	1.52	0.48
1:A:145:MET:CE	1:A:146:LEU:HD13	2.44	0.48
1:A:182:LEU:O	1:A:186:VAL:HG13	2.13	0.48
1:E:122:TRP:HE3	1:E:123:LEU:HD13	1.78	0.47
1:A:744:TYR:OH	1:A:748:ARG:NH1	2.47	0.47
1:E:351:TYR:CZ	1:E:355:ARG:HD3	2.49	0.47
1:E:696:LEU:HD13	1:E:696:LEU:H	1.78	0.47
1:E:483:ALA:O	1:E:484:THR:C	2.51	0.47
1:G:289:LYS:HB3	1:G:290:HIS:CD2	2.49	0.47
1:C:303:ILE:HD12	1:C:481:LEU:CD1	2.43	0.47
1:G:217:LEU:O	1:G:220:GLN:HG3	2.13	0.47
1:G:578:LEU:HD12	1:G:583:GLY:C	2.35	0.47
1:E:300:LEU:HD12	1:E:478:VAL:HB	1.96	0.47
1:A:44:ALA:HA	1:A:251:ILE:HD13	1.95	0.47
1:E:64:SER:OG	1:E:200:ASP:OD1	2.29	0.47
1:G:596:GLN:NE2	1:G:943:ILE:HG23	2.30	0.47
1:G:578:LEU:HB2	1:G:704:TRP:CZ2	2.50	0.47
1:C:226:GLU:OE1	1:C:250:ARG:NE	2.32	0.47
1:G:40:ASP:OD1	1:G:243:HIS:NE2	2.45	0.47
1:A:572:ALA:HB2	1:A:605:TRP:CH2	2.49	0.47
1:G:354:TYR:CD2	1:G:355:ARG:HG2	2.49	0.47
1:G:451:ASP:OD1	1:G:452:GLU:N	2.46	0.47
1:C:637:ASP:O	1:C:643:GLY:HA3	2.15	0.47
1:A:756:GLN:O	1:A:760:ASP:HB2	2.14	0.47
1:E:891:GLN:O	1:E:930:GLY:HA2	2.13	0.47
1:G:504:ARG:HG2	1:G:504:ARG:NH1	2.28	0.47
1:A:789:LEU:HD11	1:C:161:SER:HG	1.78	0.47
1:C:303:ILE:HB	1:C:481:LEU:CD1	2.45	0.47
1:G:335:LEU:HD13	1:G:341:ALA:HA	1.96	0.47
1:A:581:GLN:OE1	1:A:703:GLN:HB3	2.15	0.47
1:G:91:GLU:HG3	1:G:108:LEU:HD22	1.96	0.47
1:C:686:ARG:O	1:C:689:ARG:HG2	2.15	0.47
1:G:264:THR:HG23	1:G:329:PRO:HB3	1.97	0.47
1:G:269:THR:O	1:G:273:SER:OG	2.27	0.47
1:E:849:LEU:HD21	1:E:858:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:GLY:HA3	1:C:806:ALA:O	2.15	0.47
1:E:742:ARG:NH1	1:E:781:ASP:OD1	2.47	0.46
1:E:459:TYR:CG	1:E:829:PHE:HB2	2.50	0.46
1:A:560:VAL:HA	1:A:564:ALA:O	2.14	0.46
1:G:691:TRP:CG	1:G:708:PRO:HB3	2.51	0.46
1:E:632:THR:HG23	1:E:666:LEU:HD11	1.98	0.46
1:G:781:ASP:O	1:G:785:MET:HG3	2.16	0.46
1:C:219:SER:OG	2:D:11:DA:H2''	2.15	0.46
1:G:122:TRP:CZ2	1:G:179:ARG:HB3	2.50	0.46
1:E:87:LYS:HE2	1:E:92:PHE:CZ	2.50	0.46
1:C:320:ASP:HA	1:C:331:ARG:HH21	1.80	0.46
1:A:627:GLN:O	1:A:631:ILE:HG13	2.15	0.46
1:E:787:GLU:O	1:E:791:GLN:HG3	2.16	0.46
1:A:670:VAL:HG21	1:A:673:MET:HG3	1.98	0.46
1:E:539:ASP:OD1	1:E:540:PRO:HD2	2.15	0.46
1:C:742:ARG:NH2	1:C:769:TYR:O	2.48	0.46
1:A:494:VAL:HG21	1:A:514:VAL:HG23	1.97	0.46
1:E:375:TRP:CH2	1:E:408:MET:HG2	2.50	0.46
1:A:150:HIS:ND1	2:B:11:DA:H5'	2.29	0.46
1:E:145:MET:HG3	1:E:208:CYS:HB2	1.96	0.46
1:E:877:VAL:HA	1:E:880:THR:HG23	1.98	0.46
1:G:227:ARG:HD2	1:G:250:ARG:HH11	1.81	0.46
1:C:366:THR:HG22	1:C:402:ALA:O	2.16	0.46
1:E:679:PRO:CG	1:E:739:LEU:HD13	2.45	0.46
1:E:854:THR:OG1	1:E:855:VAL:N	2.48	0.46
1:E:430:VAL:HA	1:E:800:ILE:HD13	1.97	0.46
1:G:471:LEU:HD22	1:G:476:VAL:HG21	1.98	0.46
1:A:471:LEU:HD22	1:A:476:VAL:HG21	1.97	0.46
1:C:825:LEU:HD23	1:C:825:LEU:HA	1.63	0.46
1:C:252:PRO:HB3	1:C:261:ARG:HH22	1.81	0.46
1:A:65:MET:HA	1:A:198:MET:O	2.15	0.46
1:A:221:GLU:O	1:A:225:LEU:HD13	2.16	0.46
1:E:149:HIS:CD2	1:E:150:HIS:CD2	3.04	0.46
1:A:693:HIS:HB3	1:A:696:LEU:HD22	1.98	0.46
1:E:84:ASP:O	1:E:87:LYS:HB2	2.16	0.46
1:A:891:GLN:O	1:A:930:GLY:HA2	2.16	0.46
1:A:909:ARG:HG3	1:A:910:ASP:N	2.30	0.46
1:A:677:LEU:HD21	1:A:740:LEU:O	2.16	0.46
1:E:251:ILE:HA	1:E:254:LEU:HD22	1.98	0.46
1:E:789:LEU:HD23	1:E:789:LEU:HA	1.77	0.46
1:E:261:ARG:HB2	1:E:365:SER:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:GLU:CG	1:C:25:ARG:N	2.79	0.45
1:A:201:GLY:HA3	1:A:806:ALA:O	2.16	0.45
1:C:604:GLN:O	1:C:607:ALA:HB3	2.16	0.45
1:C:451:ASP:OD1	1:C:452:GLU:N	2.50	0.45
1:A:835:ARG:HH21	1:A:882:PRO:HD3	1.81	0.45
1:C:828:ARG:HB2	2:D:5:DA:C2	2.51	0.45
1:E:16:LEU:HB2	1:E:178:GLN:HE22	1.81	0.45
1:C:788:GLU:O	1:C:792:ARG:HG3	2.15	0.45
1:E:644:ALA:CB	1:E:698:ILE:CD1	2.95	0.45
1:G:596:GLN:HE22	1:G:943:ILE:HG23	1.82	0.45
1:G:376:LEU:HD13	1:G:907:TYR:CZ	2.51	0.45
1:E:506:TRP:CH2	1:E:513:PRO:HD3	2.51	0.45
1:E:691:TRP:HB3	1:E:694:GLU:HG2	1.97	0.45
1:G:221:GLU:OE1	1:G:221:GLU:N	2.49	0.45
1:A:248:LEU:HA	1:A:248:LEU:HD23	1.80	0.45
1:C:457:ASP:HB2	1:C:458:PRO:HD2	1.98	0.45
1:G:692:ARG:HB3	1:G:693:HIS:CE1	2.51	0.45
1:A:891:GLN:HB2	1:A:930:GLY:O	2.16	0.45
1:A:683:LEU:HA	1:A:683:LEU:HD12	1.67	0.45
1:E:109:SER:HB2	1:G:794:LEU:HD22	1.99	0.45
1:C:223:PHE:O	1:C:227:ARG:HG2	2.17	0.45
1:E:525:VAL:HG22	1:E:532:VAL:HG22	1.99	0.45
1:E:23:LYS:HD3	1:E:224:LEU:HD11	1.98	0.45
1:C:611:GLU:HA	1:C:612:ASP:HA	1.77	0.45
1:E:698:ILE:CG1	1:E:699:ILE:N	2.79	0.45
1:G:578:LEU:CA	1:G:704:TRP:CZ2	2.98	0.45
1:C:836:VAL:HB	1:C:914:ILE:HG12	1.99	0.45
1:G:377:ASN:HA	1:G:378:PRO:HD3	1.83	0.45
1:C:683:LEU:HA	1:C:683:LEU:HD12	1.64	0.45
1:C:351:TYR:O	1:C:355:ARG:HG3	2.17	0.45
1:C:526:ASP:O	1:C:530:GLY:HA2	2.16	0.45
1:G:578:LEU:HD12	1:G:583:GLY:CA	2.47	0.45
1:C:526:ASP:OD2	1:C:529:ILE:HD12	2.16	0.45
1:G:674:ILE:HG13	1:G:674:ILE:O	2.16	0.45
1:G:632:THR:O	1:G:635:ILE:HG22	2.15	0.45
1:G:579:VAL:CG2	1:G:580:LYS:N	2.80	0.45
1:E:16:LEU:HD11	1:E:35:VAL:HG21	1.99	0.45
1:A:338:MET:SD	1:A:373:MET:HG3	2.57	0.45
1:A:788:GLU:O	1:A:792:ARG:HG3	2.18	0.44
1:G:641:LYS:O	1:G:645:GLN:HG2	2.18	0.44
1:G:588:ILE:HA	1:G:658:ALA:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:308:GLY:N	4:G:1003:ADP:O1B	2.49	0.44
1:G:78:PHE:CZ	1:G:82:LEU:HD11	2.53	0.44
1:G:926:PRO:N	1:G:935:LEU:HD13	2.33	0.44
1:E:300:LEU:HD13	1:E:497:TYR:CG	2.53	0.44
1:C:366:THR:HG21	1:C:404:THR:HG22	1.98	0.44
1:G:606:PHE:CE2	1:G:614:PRO:HG2	2.52	0.44
1:G:201:GLY:HA3	1:G:806:ALA:O	2.17	0.44
1:C:337:THR:HG22	2:D:4:DA:H4'	2.00	0.44
1:G:90:ARG:NH2	1:G:105:GLY:O	2.46	0.44
1:C:921:GLU:OE1	1:C:921:GLU:N	2.49	0.44
1:C:161:SER:CB	1:C:167:GLU:OE1	2.60	0.44
1:C:934:TRP:N	1:C:934:TRP:CD1	2.86	0.44
1:A:252:PRO:HB3	1:A:261:ARG:HH22	1.83	0.44
1:E:289:LYS:HD3	1:E:290:HIS:CE1	2.52	0.44
1:A:214:ALA:O	1:A:218:VAL:HG22	2.17	0.44
1:G:274:PHE:HB3	1:G:277:LEU:HD13	2.00	0.44
1:A:680:VAL:HG13	1:A:743:THR:HG23	1.99	0.44
1:A:127:LEU:HD12	1:A:127:LEU:HA	1.85	0.44
1:C:303:ILE:HB	1:C:481:LEU:HD12	1.98	0.44
1:A:678:ALA:O	1:A:683:LEU:HD22	2.18	0.44
1:E:914:ILE:HA	1:E:915:PRO:HD2	1.87	0.44
1:C:906:PHE:O	1:C:906:PHE:CD1	2.70	0.44
1:C:632:THR:O	1:C:636:VAL:HG22	2.17	0.44
1:C:217:LEU:HD12	1:C:217:LEU:HA	1.82	0.44
1:C:424:ASP:OD1	1:C:424:ASP:N	2.48	0.44
1:C:283:LEU:CD2	1:C:283:LEU:C	2.86	0.44
1:C:926:PRO:HG3	1:C:935:LEU:HD22	1.99	0.44
1:C:305:ALA:O	1:C:483:ALA:HA	2.18	0.44
1:E:47:VAL:HG11	1:E:251:ILE:HG22	1.99	0.44
1:E:324:LYS:HG3	1:E:325:ALA:N	2.32	0.44
1:G:675:SER:OG	1:G:676:ASP:O	2.35	0.44
1:A:818:PHE:HD1	1:A:818:PHE:HA	1.69	0.44
1:G:601:LEU:HG	1:G:602:LEU:HD23	2.00	0.44
1:G:578:LEU:O	1:G:582:GLY:N	2.47	0.44
1:C:320:ASP:HA	1:C:331:ARG:NH2	2.33	0.44
1:G:424:ASP:O	1:G:428:MET:HG3	2.18	0.44
1:G:156:HIS:HA	1:G:157:PRO:HD3	1.86	0.44
1:C:84:ASP:HB3	1:C:87:LYS:HD2	2.00	0.44
1:G:141:LEU:HD23	1:G:141:LEU:HA	1.82	0.44
1:G:439:ARG:HG3	1:G:439:ARG:HH11	1.82	0.44
1:A:635:ILE:HD13	1:A:635:ILE:HA	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:918:VAL:HG22	1:G:922:GLY:HA2	1.99	0.43
1:G:205:SER:O	1:G:208:CYS:HB3	2.18	0.43
1:A:275:PRO:HG3	1:A:354:TYR:CE2	2.53	0.43
1:E:14:PRO:HG3	1:E:177:LYS:HD2	2.00	0.43
1:C:150:HIS:ND1	2:D:11:DA:H5'	2.32	0.43
1:G:504:ARG:CG	1:G:504:ARG:NH1	2.81	0.43
1:C:929:THR:HG22	1:C:934:TRP:CD1	2.54	0.43
1:G:294:LEU:O	1:G:296:THR:HG23	2.18	0.43
1:E:268:ALA:HB2	1:E:355:ARG:NH2	2.33	0.43
1:G:145:MET:HE2	1:G:146:LEU:HD13	2.01	0.43
1:G:149:HIS:NE2	1:G:150:HIS:CD2	2.86	0.43
1:G:588:ILE:HD13	1:G:686:ARG:NE	2.33	0.43
1:G:558:VAL:O	1:G:716:GLU:HG2	2.19	0.43
1:G:406:TRP:O	1:G:412:ARG:HD2	2.19	0.43
1:G:935:LEU:HB3	1:G:943:ILE:HG13	2.01	0.43
1:G:683:LEU:HA	1:G:683:LEU:HD12	1.87	0.43
1:A:275:PRO:HG3	1:A:354:TYR:CZ	2.53	0.43
1:E:155:PRO:HG3	1:E:811:ASN:ND2	2.34	0.43
1:G:434:LYS:HE2	1:G:434:LYS:HB3	1.78	0.43
1:C:281:ASN:ND2	1:C:309:GLU:C	2.72	0.43
1:C:159:PHE:N	1:C:159:PHE:HD1	2.15	0.43
1:G:227:ARG:HA	1:G:227:ARG:HD2	1.88	0.43
1:E:839:TYR:HE1	1:E:915:PRO:N	2.16	0.43
1:E:84:ASP:HB3	1:E:87:LYS:HD2	2.01	0.43
1:C:243:HIS:HA	1:C:246:THR:HG22	2.01	0.43
1:A:833:SER:N	2:B:6:DA:H61	2.17	0.43
1:G:228:LEU:HA	1:G:228:LEU:HD12	1.75	0.43
1:A:634:THR:O	1:A:638:LEU:HD13	2.19	0.43
1:E:482:SER:OG	1:E:483:ALA:N	2.52	0.43
1:C:541:LEU:HB3	1:C:542:PRO:CD	2.48	0.43
1:C:848:TRP:CD1	1:C:853:CYS:SG	3.09	0.43
1:E:16:LEU:HB3	1:E:181:ALA:HB1	2.01	0.43
1:C:583:GLY:H	1:C:653:GLY:HA2	1.83	0.43
1:C:696:LEU:HD23	1:C:696:LEU:N	2.34	0.43
1:E:580:LYS:HA	1:E:580:LYS:HD3	1.82	0.43
1:C:165:LEU:HA	1:C:165:LEU:HD12	1.75	0.43
1:G:137:LEU:HD23	1:G:138:VAL:N	2.33	0.43
1:A:557:ASP:HA	1:A:714:THR:O	2.19	0.43
1:C:48:LEU:HD12	1:C:52:TYR:HB3	2.01	0.43
1:E:375:TRP:HB2	1:E:907:TYR:HH	1.79	0.43
1:A:671:ASP:OD2	1:A:702:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:ARG:HD2	1:C:529:ILE:CG1	2.49	0.43
1:G:746:LEU:O	1:G:749:ARG:HB3	2.18	0.43
1:E:56:GLY:HA3	1:E:326:THR:O	2.19	0.43
1:E:189:ALA:HA	1:E:241:ARG:NH2	2.34	0.43
1:E:217:LEU:HA	1:E:217:LEU:HD12	1.81	0.43
1:C:164:PRO:HA	1:C:167:GLU:HB2	2.01	0.42
1:E:358:ASN:HB2	1:E:359:THR:HG23	1.99	0.42
1:E:294:LEU:HD21	1:E:533:THR:HG21	2.00	0.42
1:G:57:LEU:HD11	1:G:444:ALA:HB1	2.01	0.42
1:G:46:LEU:O	1:G:49:TRP:HB3	2.19	0.42
1:G:618:LEU:HD23	1:G:940:LYS:HA	2.00	0.42
1:A:49:TRP:CE3	1:A:53:LEU:HD22	2.54	0.42
1:A:914:ILE:HD12	1:A:934:TRP:CD2	2.54	0.42
1:E:522:TRP:CE3	1:E:523:LEU:N	2.86	0.42
1:G:48:LEU:HD12	1:G:52:TYR:CB	2.48	0.42
1:A:123:LEU:HD12	1:A:123:LEU:HA	1.77	0.42
1:A:351:TYR:CZ	1:A:355:ARG:HG3	2.54	0.42
1:C:432:ARG:NE	1:C:799:VAL:O	2.52	0.42
1:C:900:GLU:HG2	1:C:903:ARG:NH1	2.33	0.42
1:C:241:ARG:HD3	1:C:241:ARG:HA	1.86	0.42
2:H:11:DA:OP1	2:H:11:DA:H4'	2.18	0.42
1:E:228:LEU:HA	1:E:231:LEU:HD21	2.01	0.42
1:C:57:LEU:O	1:C:60:THR:N	2.52	0.42
1:E:925:LEU:HA	1:E:926:PRO:HD3	1.93	0.42
1:C:486:HIS:HD2	1:C:769:TYR:HD2	1.67	0.42
1:A:287:LEU:O	1:A:291:LEU:HB2	2.19	0.42
1:C:223:PHE:CD1	1:C:254:LEU:HD21	2.53	0.42
1:A:362:PRO:HB2	1:A:363:ARG:H	1.57	0.42
1:G:552:GLU:HA	1:G:754:PRO:HA	2.01	0.42
1:A:297:GLY:N	1:A:325:ALA:HB1	2.35	0.42
1:A:844:ALA:N	1:A:845:GLY:HA2	2.34	0.42
1:A:682:LEU:HD23	1:A:682:LEU:HA	1.88	0.42
1:A:717:GLN:OE1	1:A:726:TRP:N	2.47	0.42
1:A:555:LEU:HD23	1:A:712:VAL:HB	2.01	0.42
1:G:932:ARG:HD2	1:G:932:ARG:HA	1.78	0.42
1:C:429:ALA:HB1	1:C:440:LEU:HD13	2.02	0.42
1:E:250:ARG:HD3	1:E:250:ARG:O	2.20	0.42
1:E:696:LEU:H	1:E:696:LEU:CD1	2.32	0.42
1:G:16:LEU:HD12	1:G:17:ASP:O	2.20	0.42
1:A:256:ASP:HA	1:A:364:SER:OG	2.19	0.42
1:E:870:MET:O	1:E:874:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:DA:H2''	2:B:3:DA:O5'	2.19	0.42
1:G:942:LEU:HA	1:G:942:LEU:HD12	1.84	0.42
1:E:447:VAL:HG22	1:E:477:PRO:HG2	2.01	0.42
1:E:44:ALA:O	1:E:48:LEU:HB2	2.19	0.42
1:A:691:TRP:CZ2	1:A:701:ARG:HD2	2.54	0.42
1:A:491:ASN:HD21	1:A:512:GLN:HB3	1.85	0.42
1:E:370:LEU:HD21	1:E:413:GLY:C	2.40	0.42
1:G:459:TYR:CG	1:G:829:PHE:HB2	2.55	0.42
1:C:130:LEU:HD23	1:C:130:LEU:HA	1.80	0.42
1:A:789:LEU:HD21	1:C:161:SER:HB2	2.02	0.42
1:G:504:ARG:CG	1:G:504:ARG:HH11	2.24	0.42
1:E:83:HIS:CG	1:E:84:ASP:N	2.88	0.42
1:A:715:PRO:HG2	1:A:717:GLN:NE2	2.35	0.42
1:E:745:THR:HG22	1:E:774:LEU:HD23	2.02	0.42
1:G:691:TRP:HB2	1:G:708:PRO:HB3	2.01	0.41
1:E:334:ALA:HB1	1:E:423:ILE:HA	2.02	0.41
1:A:588:ILE:HA	1:A:658:ALA:O	2.20	0.41
1:G:357:GLU:N	1:G:357:GLU:OE1	2.53	0.41
1:G:691:TRP:CE3	1:G:708:PRO:HD3	2.54	0.41
1:C:486:HIS:CD2	1:C:769:TYR:HD2	2.37	0.41
1:E:165:LEU:HA	1:E:165:LEU:HD12	1.75	0.41
1:C:404:THR:HG23	1:C:407:LEU:H	1.85	0.41
1:C:848:TRP:CG	1:C:853:CYS:HA	2.55	0.41
1:A:620:HIS:CE1	1:A:623:PHE:CE2	3.08	0.41
1:G:165:LEU:HA	1:G:165:LEU:HD12	1.79	0.41
1:G:473:THR:HG22	1:G:500:GLY:O	2.19	0.41
1:G:354:TYR:HD2	1:G:355:ARG:HG2	1.84	0.41
1:A:702:PRO:CG	1:A:704:TRP:CE2	3.03	0.41
1:G:369:LEU:HB3	1:G:380:TYR:CE1	2.56	0.41
1:C:335:LEU:HB3	1:C:336:PRO:HD2	2.01	0.41
1:E:484:THR:HG21	1:E:761:VAL:HG12	2.02	0.41
1:A:724:ALA:HA	1:A:725:PRO:HD3	1.87	0.41
1:A:459:TYR:CB	1:A:829:PHE:HB2	2.50	0.41
1:E:141:LEU:HD23	1:E:141:LEU:HA	1.74	0.41
1:E:290:HIS:CD2	1:E:538:VAL:HB	2.56	0.41
1:E:701:ARG:HA	1:E:702:PRO:HD2	1.89	0.41
1:C:132:TYR:CD1	1:C:195:PRO:HG3	2.55	0.41
1:E:258:ALA:O	1:E:404:THR:HG21	2.21	0.41
1:C:146:LEU:HD12	1:C:146:LEU:HA	1.89	0.41
1:E:864:ARG:HA	1:E:864:ARG:HD3	1.89	0.41
1:G:580:LYS:HB3	1:G:580:LYS:HE2	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:909:ARG:CG	1:E:909:ARG:NH1	2.73	0.41
1:C:263:ILE:HB	1:C:418:TRP:NE1	2.35	0.41
1:G:578:LEU:CD1	1:G:583:GLY:C	2.89	0.41
1:G:251:ILE:O	1:G:254:LEU:HB2	2.20	0.41
1:C:571:LEU:O	1:C:575:LEU:HB2	2.20	0.41
1:G:469:ARG:O	1:G:500:GLY:HA3	2.21	0.41
1:A:546:THR:HG22	1:A:547:PRO:O	2.20	0.41
1:A:464:LEU:HD13	1:A:493:LEU:HD22	2.01	0.41
1:C:269:THR:OG1	1:C:272:GLU:HB2	2.20	0.41
1:G:652:ARG:HE	1:G:652:ARG:HB2	1.45	0.41
1:A:145:MET:HE3	1:A:146:LEU:HD13	2.03	0.41
1:E:450:VAL:HG13	1:E:480:LEU:HD12	2.03	0.41
1:C:54:SER:OG	1:C:328:ARG:HA	2.21	0.41
1:E:156:HIS:HA	1:E:157:PRO:HD3	1.88	0.41
1:A:676:ASP:HB3	1:A:731:TRP:CZ2	2.56	0.41
1:A:350:GLU:H	1:A:350:GLU:HG2	1.62	0.41
1:E:375:TRP:CZ2	1:E:408:MET:HG2	2.55	0.41
1:C:694:GLU:HG2	1:C:701:ARG:NH2	2.22	0.41
1:G:432:ARG:HD3	1:G:815:GLU:O	2.20	0.41
1:E:20:PHE:CE2	1:E:178:GLN:HG3	2.49	0.41
1:C:914:ILE:HD12	1:C:929:THR:HG21	2.03	0.41
1:C:286:SER:O	1:C:290:HIS:HD2	2.03	0.41
1:G:145:MET:CE	1:G:146:LEU:HD13	2.51	0.41
1:C:871:ALA:HA	1:C:874:ARG:NH2	2.35	0.41
1:A:576:THR:HB	1:A:577:PRO:HD3	2.01	0.41
1:E:934:TRP:N	1:E:934:TRP:CD1	2.88	0.41
1:E:123:LEU:HA	1:E:123:LEU:HD12	1.89	0.41
1:G:48:LEU:HD12	1:G:52:TYR:HB3	2.02	0.41
1:E:404:THR:HG22	1:E:407:LEU:H	1.86	0.41
1:C:438:LEU:HA	1:C:438:LEU:HD23	1.62	0.41
1:G:618:LEU:HD22	1:G:940:LYS:HG2	2.03	0.41
1:C:106:GLU:OE2	1:C:179:ARG:NH2	2.47	0.41
1:C:482:SER:OG	1:C:483:ALA:N	2.54	0.41
1:C:469:ARG:O	1:C:473:THR:HG23	2.20	0.41
1:C:363:ARG:HE	1:C:363:ARG:HB2	1.72	0.41
1:A:269:THR:O	1:A:273:SER:OG	2.32	0.41
1:A:539:ASP:HA	1:A:540:PRO:HD2	1.95	0.41
1:A:106:GLU:OE2	1:A:179:ARG:NH2	2.44	0.41
1:G:127:LEU:HD12	1:G:127:LEU:HA	1.78	0.41
1:E:537:ASP:OD1	1:E:537:ASP:N	2.52	0.41
1:E:495:LYS:O	1:E:499:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:O	1:A:425:GLN:HG3	2.20	0.41
1:E:333:LEU:HD12	1:E:344:MET:HG3	2.03	0.41
1:E:410:ARG:HG3	1:E:411:LYS:HG3	2.03	0.41
1:C:141:LEU:HA	1:C:141:LEU:HD23	1.84	0.41
1:G:484:THR:HG23	1:G:484:THR:O	2.20	0.41
1:C:652:ARG:HD3	1:C:652:ARG:HA	1.79	0.40
1:E:291:LEU:HA	1:E:291:LEU:HD12	1.88	0.40
1:A:363:ARG:O	1:A:398:ARG:NH2	2.54	0.40
1:C:128:PRO:HA	1:C:132:TYR:O	2.21	0.40
1:E:71:HIS:NE2	1:E:194:THR:O	2.54	0.40
1:E:757:ILE:HA	1:E:758:PRO:HA	1.87	0.40
1:G:728:PRO:O	1:G:732:THR:HG23	2.20	0.40
1:C:576:THR:O	1:C:579:VAL:HG22	2.20	0.40
1:A:430:VAL:HG11	1:A:467:LEU:CA	2.47	0.40
1:E:138:VAL:HG22	1:E:199:LEU:HB3	2.03	0.40
1:G:669:ASP:OD1	1:G:670:VAL:N	2.54	0.40
1:G:303:ILE:HD12	1:G:481:LEU:HD11	2.02	0.40
1:C:138:VAL:HG11	1:C:196:PRO:HG2	2.02	0.40
1:E:684:LEU:HD21	1:E:764:LEU:HD13	2.02	0.40
1:E:412:ARG:O	1:E:415:LEU:HB2	2.21	0.40
1:A:876:LEU:HA	1:A:876:LEU:HD23	1.86	0.40
1:A:870:MET:HG3	1:A:871:ALA:N	2.36	0.40
1:C:839:TYR:CZ	1:C:915:PRO:HB3	2.56	0.40
1:G:677:LEU:HD11	1:G:743:THR:HG22	2.04	0.40
1:C:491:ASN:OD1	1:C:513:PRO:HD2	2.21	0.40
1:G:49:TRP:CH2	1:G:58:ARG:HG2	2.56	0.40
1:G:567:ARG:NH2	1:G:594:GLU:OE2	2.44	0.40
1:C:546:THR:HA	1:C:547:PRO:HD3	1.98	0.40
1:A:672:LEU:HD11	1:A:711:VAL:HG23	2.03	0.40
1:E:839:TYR:CE1	1:E:915:PRO:HA	2.57	0.40
1:G:849:LEU:HD23	1:G:879:ARG:HH12	1.86	0.40
1:G:860:GLN:NE2	1:G:866:GLY:O	2.55	0.40
1:G:27:LEU:HD13	1:G:228:LEU:HD21	2.04	0.40
1:A:512:GLN:HA	1:A:513:PRO:HD3	1.93	0.40
1:A:557:ASP:N	1:A:557:ASP:OD1	2.55	0.40
1:G:17:ASP:OD2	1:G:19:ARG:NE	2.51	0.40
1:A:599:TYR:CD2	1:A:616:LEU:HD13	2.55	0.40
1:A:551:LEU:HD11	1:A:687:ALA:HB1	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	878/964 (91%)	819 (93%)	58 (7%)	1 (0%)	56	88
1	C	892/964 (92%)	834 (94%)	57 (6%)	1 (0%)	56	88
1	E	892/964 (92%)	831 (93%)	60 (7%)	1 (0%)	56	88
1	G	880/964 (91%)	823 (94%)	51 (6%)	6 (1%)	26	67
All	All	3542/3856 (92%)	3307 (93%)	226 (6%)	9 (0%)	46	81

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	660	GLN
1	A	698	ILE
1	E	752	GLY
1	G	409	GLY
1	G	642	GLU
1	G	133	PRO
1	C	680	VAL
1	G	899	PRO
1	G	758	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	740/796 (93%)	646 (87%)	94 (13%)	5	22
1	C	742/796 (93%)	651 (88%)	91 (12%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	742/796 (93%)	660 (89%)	82 (11%)	8	30
1	G	735/796 (92%)	635 (86%)	100 (14%)	5	20
All	All	2959/3184 (93%)	2592 (88%)	367 (12%)	6	23

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

Mol	Chain	Res	Type
1	A	16	LEU
1	A	24	GLU
1	A	25	ARG
1	A	28	ARG
1	A	35	VAL
1	A	48	LEU
1	A	53	LEU
1	A	88	LEU
1	A	121	LYS
1	A	123	LEU
1	A	127	LEU
1	A	130	LEU
1	A	146	LEU
1	A	161	SER
1	A	217	LEU
1	A	228	LEU
1	A	230	SER
1	A	241	ARG
1	A	254	LEU
1	A	271	THR
1	A	273	SER
1	A	279	LYS
1	A	283	LEU
1	A	293	CYS
1	A	304	THR
1	A	335	LEU
1	A	344	MET
1	A	350	GLU
1	A	357	GLU
1	A	366	THR
1	A	367	LEU
1	A	399	ASP
1	A	404	THR
1	A	420	VAL

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Mol	Chain	Res	Type
1	A	431	LEU
1	A	438	LEU
1	A	440	LEU
1	A	443	LEU
1	A	446	LYS
1	A	450	VAL
1	A	457	ASP
1	A	464	LEU
1	A	473	THR
1	A	474	LEU
1	A	476	VAL
1	A	480	LEU
1	A	481	LEU
1	A	508	ARG
1	A	510	GLU
1	A	517	VAL
1	A	518	SER
1	A	523	LEU
1	A	551	LEU
1	A	553	VAL
1	A	560	VAL
1	A	569	THR
1	A	571	LEU
1	A	587	ILE
1	A	589	CYS
1	A	601	LEU
1	A	603	SER
1	A	608	THR
1	A	616	LEU
1	A	635	ILE
1	A	651	THR
1	A	673	MET
1	A	674	ILE
1	A	680	VAL
1	A	681	SER
1	A	683	LEU
1	A	684	LEU
1	A	685	GLN
1	A	696	LEU
1	A	714	THR
1	A	729	ARG
1	A	734	VAL

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Mol	Chain	Res	Type
1	A	782	MET
1	A	789	LEU
1	A	792	ARG
1	A	804	ASP
1	A	818	PHE
1	A	824	VAL
1	A	833	SER
1	A	843	THR
1	A	849	LEU
1	A	859	GLU
1	A	862	THR
1	A	869	THR
1	A	875	ASP
1	A	892	LEU
1	A	893	THR
1	A	894	GLU
1	A	929	THR
1	A	939	CYS
1	C	16	LEU
1	C	24	GLU
1	C	25	ARG
1	C	35	VAL
1	C	48	LEU
1	C	60	THR
1	C	88	LEU
1	C	91	GLU
1	C	113	ARG
1	C	121	LYS
1	C	123	LEU
1	C	127	LEU
1	C	129	SER
1	C	137	LEU
1	C	139	THR
1	C	146	LEU
1	C	152	THR
1	C	159	PHE
1	C	165	LEU
1	C	194	THR
1	C	217	LEU
1	C	226	GLU
1	C	241	ARG
1	C	253	SER

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Mol	Chain	Res	Type
1	C	254	LEU
1	C	279	LYS
1	C	283	LEU
1	C	291	LEU
1	C	296	THR
1	C	304	THR
1	C	324	LYS
1	C	356	VAL
1	C	357	GLU
1	C	364	SER
1	C	367	LEU
1	C	410	ARG
1	C	420	VAL
1	C	424	ASP
1	C	431	LEU
1	C	438	LEU
1	C	440	LEU
1	C	443	LEU
1	C	450	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	492	SER
1	C	516	GLU
1	C	518	SER
1	C	528	ARG
1	C	529	ILE
1	C	531	LYS
1	C	541	LEU
1	C	546	THR
1	C	551	LEU
1	C	568	SER
1	C	569	THR
1	C	574	GLU
1	C	578	LEU
1	C	615	ASP
1	C	616	LEU
1	C	621	SER

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Mol	Chain	Res	Type
1	C	634	THR
1	C	641	LYS
1	C	642	GLU
1	C	680	VAL
1	C	683	LEU
1	C	684	LEU
1	C	692	ARG
1	C	694	GLU
1	C	696	LEU
1	C	700	ASN
1	C	734	VAL
1	C	739	LEU
1	C	748	ARG
1	C	782	MET
1	C	804	ASP
1	C	807	GLU
1	C	833	SER
1	C	849	LEU
1	C	867	ARG
1	C	884	ARG
1	C	905	SER
1	C	906	PHE
1	C	925	LEU
1	C	929	THR
1	C	944	PHE
1	E	16	LEU
1	E	23	LYS
1	E	48	LEU
1	E	70	GLU
1	E	101	SER
1	E	113	ARG
1	E	123	LEU
1	E	127	LEU
1	E	145	MET
1	E	146	LEU
1	E	158	SER
1	E	162	ARG
1	E	165	LEU
1	E	186	VAL
1	E	194	THR
1	E	217	LEU
1	E	228	LEU

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Mol	Chain	Res	Type
1	E	230	SER
1	E	238	SER
1	E	248	LEU
1	E	250	ARG
1	E	254	LEU
1	E	271	THR
1	E	273	SER
1	E	283	LEU
1	E	286	SER
1	E	291	LEU
1	E	293	CYS
1	E	300	LEU
1	E	304	THR
1	E	356	VAL
1	E	357	GLU
1	E	358	ASN
1	E	359	THR
1	E	366	THR
1	E	367	LEU
1	E	375	TRP
1	E	431	LEU
1	E	438	LEU
1	E	440	LEU
1	E	443	LEU
1	E	450	VAL
1	E	464	LEU
1	E	474	LEU
1	E	476	VAL
1	E	480	LEU
1	E	481	LEU
1	E	484	THR
1	E	494	VAL
1	E	504	ARG
1	E	508	ARG
1	E	510	GLU
1	E	537	ASP
1	E	540	PRO
1	E	541	LEU
1	E	548	ARG
1	E	565	LEU
1	E	569	THR
1	E	601	LEU

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Mol	Chain	Res	Type
1	E	603	SER
1	E	608	THR
1	E	612	ASP
1	E	635	ILE
1	E	680	VAL
1	E	684	LEU
1	E	696	LEU
1	E	739	LEU
1	E	768	VAL
1	E	789	LEU
1	E	804	ASP
1	E	839	TYR
1	E	843	THR
1	E	847	ARG
1	E	849	LEU
1	E	874	ARG
1	E	881	ILE
1	E	893	THR
1	E	908	LEU
1	E	909	ARG
1	E	920	ASP
1	E	928	GLU
1	E	944	PHE
1	G	16	LEU
1	G	24	GLU
1	G	35	VAL
1	G	48	LEU
1	G	63	SER
1	G	70	GLU
1	G	75	CYS
1	G	88	LEU
1	G	121	LYS
1	G	123	LEU
1	G	127	LEU
1	G	137	LEU
1	G	146	LEU
1	G	158	SER
1	G	162	ARG
1	G	165	LEU
1	G	217	LEU
1	G	222	ASP
1	G	228	LEU

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Mol	Chain	Res	Type
1	G	264	THR
1	G	271	THR
1	G	283	LEU
1	G	289	LYS
1	G	290	HIS
1	G	307	MET
1	G	355	ARG
1	G	365	SER
1	G	367	LEU
1	G	370	LEU
1	G	375	TRP
1	G	411	LYS
1	G	420	VAL
1	G	431	LEU
1	G	438	LEU
1	G	440	LEU
1	G	443	LEU
1	G	464	LEU
1	G	473	THR
1	G	474	LEU
1	G	480	LEU
1	G	481	LEU
1	G	504	ARG
1	G	506	TRP
1	G	515	SER
1	G	517	VAL
1	G	523	LEU
1	G	553	VAL
1	G	555	LEU
1	G	556	VAL
1	G	570	VAL
1	G	575	LEU
1	G	578	LEU
1	G	580	LYS
1	G	590	THR
1	G	591	THR
1	G	600	ASP
1	G	602	LEU
1	G	616	LEU
1	G	628	ARG
1	G	635	ILE
1	G	636	VAL

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Mol	Chain	Res	Type
1	G	641	LYS
1	G	642	GLU
1	G	652	ARG
1	G	666	LEU
1	G	674	ILE
1	G	676	ASP
1	G	684	LEU
1	G	692	ARG
1	G	694	GLU
1	G	699	ILE
1	G	700	ASN
1	G	716	GLU
1	G	718	ASN
1	G	729	ARG
1	G	761	VAL
1	G	779	GLU
1	G	789	LEU
1	G	804	ASP
1	G	816	PHE
1	G	817	SER
1	G	833	SER
1	G	835	ARG
1	G	839	TYR
1	G	847	ARG
1	G	862	THR
1	G	864	ARG
1	G	870	MET
1	G	877	VAL
1	G	892	LEU
1	G	897	HIS
1	G	903	ARG
1	G	913	LEU
1	G	920	ASP
1	G	921	GLU
1	G	925	LEU
1	G	928	GLU
1	G	939	CYS
1	G	943	ILE
1	G	944	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	220	GLN
1	C	345	HIS
1	G	160	GLN
1	G	290	HIS
1	G	693	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	ADP	A	1003	-	22,29,29	1.18	1 (4%)	27,45,45	2.00	6 (22%)
4	ADP	C	1003	-	22,29,29	1.01	2 (9%)	27,45,45	2.03	6 (22%)
4	ADP	E	1003	-	22,29,29	0.99	0	27,45,45	2.33	10 (37%)
4	ADP	G	1003	-	22,29,29	1.02	2 (9%)	27,45,45	1.88	7 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	1003	-	-	0/12/32/32	0/3/3/3
4	ADP	C	1003	-	-	0/12/32/32	0/3/3/3
4	ADP	E	1003	-	-	0/12/32/32	0/3/3/3
4	ADP	G	1003	-	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1003	ADP	C5-N7	-2.05	1.32	1.39
4	C	1003	ADP	C5-N7	-2.00	1.32	1.39
4	C	1003	ADP	C5-C4	2.04	1.45	1.40
4	G	1003	ADP	C5-C4	2.13	1.45	1.40
4	A	1003	ADP	C5-C4	2.37	1.45	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1003	ADP	N3-C2-N1	-7.64	123.04	128.89
4	C	1003	ADP	N3-C2-N1	-7.27	123.33	128.89
4	A	1003	ADP	N3-C2-N1	-6.41	123.98	128.89
4	G	1003	ADP	N3-C2-N1	-5.83	124.43	128.89
4	E	1003	ADP	PA-O3A-PB	-4.51	117.56	132.67
4	E	1003	ADP	C4-C5-N7	-3.57	106.20	109.48
4	A	1003	ADP	O3'-C3'-C2'	-3.54	100.31	111.83
4	G	1003	ADP	PA-O3A-PB	-3.52	120.86	132.67
4	C	1003	ADP	PA-O3A-PB	-3.31	121.57	132.67
4	C	1003	ADP	C4-C5-N7	-3.14	106.59	109.48
4	A	1003	ADP	PA-O3A-PB	-2.89	122.96	132.67
4	A	1003	ADP	O2'-C2'-C3'	-2.78	102.79	111.83
4	G	1003	ADP	C4-C5-N7	-2.77	106.93	109.48
4	E	1003	ADP	C1'-N9-C4	-2.72	122.84	126.94
4	G	1003	ADP	O2'-C2'-C3'	-2.62	103.32	111.83
4	E	1003	ADP	C2'-C1'-N9	-2.56	110.38	114.29
4	E	1003	ADP	O3'-C3'-C2'	-2.52	103.64	111.83
4	C	1003	ADP	O2'-C2'-C3'	-2.48	103.75	111.83
4	G	1003	ADP	O3'-C3'-C2'	-2.35	104.17	111.83
4	G	1003	ADP	C2'-C1'-N9	-2.25	110.85	114.29
4	C	1003	ADP	C1'-N9-C4	-2.20	123.62	126.94
4	E	1003	ADP	O2'-C2'-C3'	-2.08	105.07	111.83
4	A	1003	ADP	N6-C6-N1	2.03	123.56	119.20
4	C	1003	ADP	O3B-PB-O2B	2.03	115.11	107.38
4	E	1003	ADP	O2B-PB-O1B	2.07	117.23	110.58
4	E	1003	ADP	C4'-O4'-C1'	2.07	112.00	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	1003	ADP	C2'-C3'-C4'	2.37	107.49	102.61
4	G	1003	ADP	O3B-PB-O2B	2.54	117.05	107.38
4	E	1003	ADP	C2'-C3'-C4'	2.56	107.87	102.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	ADP	3	0
4	C	1003	ADP	3	0
4	G	1003	ADP	6	0

## 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	896/964 (92%)	-0.48	2 (0%) 95 91	42, 69, 111, 131	0
1	C	902/964 (93%)	-0.51	0 100 100	47, 73, 103, 126	0
1	E	902/964 (93%)	-0.47	1 (0%) 95 92	40, 65, 102, 128	0
1	G	894/964 (92%)	-0.40	2 (0%) 95 91	46, 82, 122, 137	0
2	B	11/12 (91%)	0.14	0 100 100	64, 69, 115, 132	0
2	D	11/12 (91%)	0.11	0 100 100	63, 75, 121, 126	0
2	F	11/12 (91%)	0.45	1 (9%) 11 4	56, 66, 128, 128	0
2	H	11/12 (91%)	0.25	0 100 100	64, 89, 132, 149	0
All	All	3638/3904 (93%)	-0.46	6 (0%) 95 91	40, 72, 113, 149	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	860	GLN	3.1
2	F	9	DA	2.5
1	E	847	ARG	2.5
1	G	565	LEU	2.2
1	A	866	GLY	2.1
1	G	900	GLU	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FE	A	1001	1/1	0.98	0.20	1.69	55,55,55,55	0
3	FE	G	1001	1/1	0.99	0.17	1.31	55,55,55,55	0
3	FE	C	1001	1/1	0.99	0.17	1.07	52,52,52,52	0
3	FE	C	1002	1/1	0.99	0.16	1.02	60,60,60,60	0
3	FE	A	1002	1/1	0.99	0.18	0.81	50,50,50,50	0
3	FE	E	1002	1/1	1.00	0.16	0.74	49,49,49,49	0
3	FE	G	1002	1/1	0.99	0.15	0.32	57,57,57,57	0
3	FE	E	1001	1/1	0.99	0.16	0.32	54,54,54,54	0
4	ADP	E	1003	27/27	0.90	0.19	0.18	67,84,102,120	0
4	ADP	G	1003	27/27	0.81	0.20	0.08	95,108,134,138	0
4	ADP	A	1003	27/27	0.92	0.12	-0.98	74,84,99,105	0
4	ADP	C	1003	27/27	0.92	0.12	-2.30	87,98,115,123	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.