



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 5, 2017 – 06:20 PM EDT

PDB ID : 5NG6  
Title : Crystal structure of FnCas12a bound to a crRNA  
Authors : Swarts, D.C.; van der Oost, J.; Jinek, M.  
Deposited on : 2017-03-16  
Resolution : 3.34 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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029077

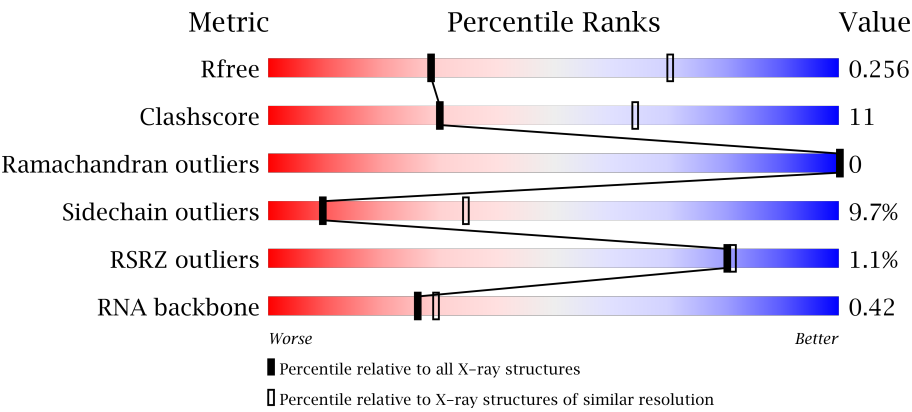
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.34 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))
$R_{free}$	100719	1167 (3.40-3.28)
Clashscore	112137	1239 (3.40-3.28)
Ramachandran outliers	110173	1219 (3.40-3.28)
Sidechain outliers	110143	1218 (3.40-3.28)
RSRZ outliers	101464	1176 (3.40-3.28)
RNA backbone	2435	1121 (3.88-2.80)

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	1302	<div><div>67%</div><div>26%</div><div>.</div><div>.</div></div>
1	C	1302	<div><div>2%</div><div>69%</div><div>25%</div><div>.</div><div>.</div></div>
1	E	1302	<div><div>2%</div><div>66%</div><div>27%</div><div>.</div><div>.</div></div>
1	G	1302	<div><div>2%</div><div>65%</div><div>27%</div><div>.</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
2	B	43	
2	D	43	
2	F	43	
2	H	43	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	C	1401	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 43813 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 endonuclease Cpf1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1268	Total	C	N	O	S	0	0	0
			10476	6737	1729	1989	21			
1	C	1268	Total	C	N	O	S	0	0	0
			10476	6737	1729	1989	21			
1	E	1262	Total	C	N	O	S	0	0	0
			10425	6708	1721	1976	20			
1	G	1253	Total	C	N	O	S	0	0	0
			10355	6665	1705	1964	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A0Q7Q2
A	0	ASN	-	expression tag	UNP A0Q7Q2
A	1	ALA	-	expression tag	UNP A0Q7Q2
C	-1	SER	-	expression tag	UNP A0Q7Q2
C	0	ASN	-	expression tag	UNP A0Q7Q2
C	1	ALA	-	expression tag	UNP A0Q7Q2
E	-1	SER	-	expression tag	UNP A0Q7Q2
E	0	ASN	-	expression tag	UNP A0Q7Q2
E	1	ALA	-	expression tag	UNP A0Q7Q2
G	-1	SER	-	expression tag	UNP A0Q7Q2
G	0	ASN	-	expression tag	UNP A0Q7Q2
G	1	ALA	-	expression tag	UNP A0Q7Q2

- Molecule 2 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	25	Total	C	N	O	P	0	0	0
			507	227	83	173	24			
2	D	25	Total	C	N	O	P	0	0	0
			507	227	83	173	24			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	25	Total	C	N	O	P	0	0	0
			507	227	83	173	24			
2	H	25	Total	C	N	O	P	0	0	0
			507	227	83	173	24			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

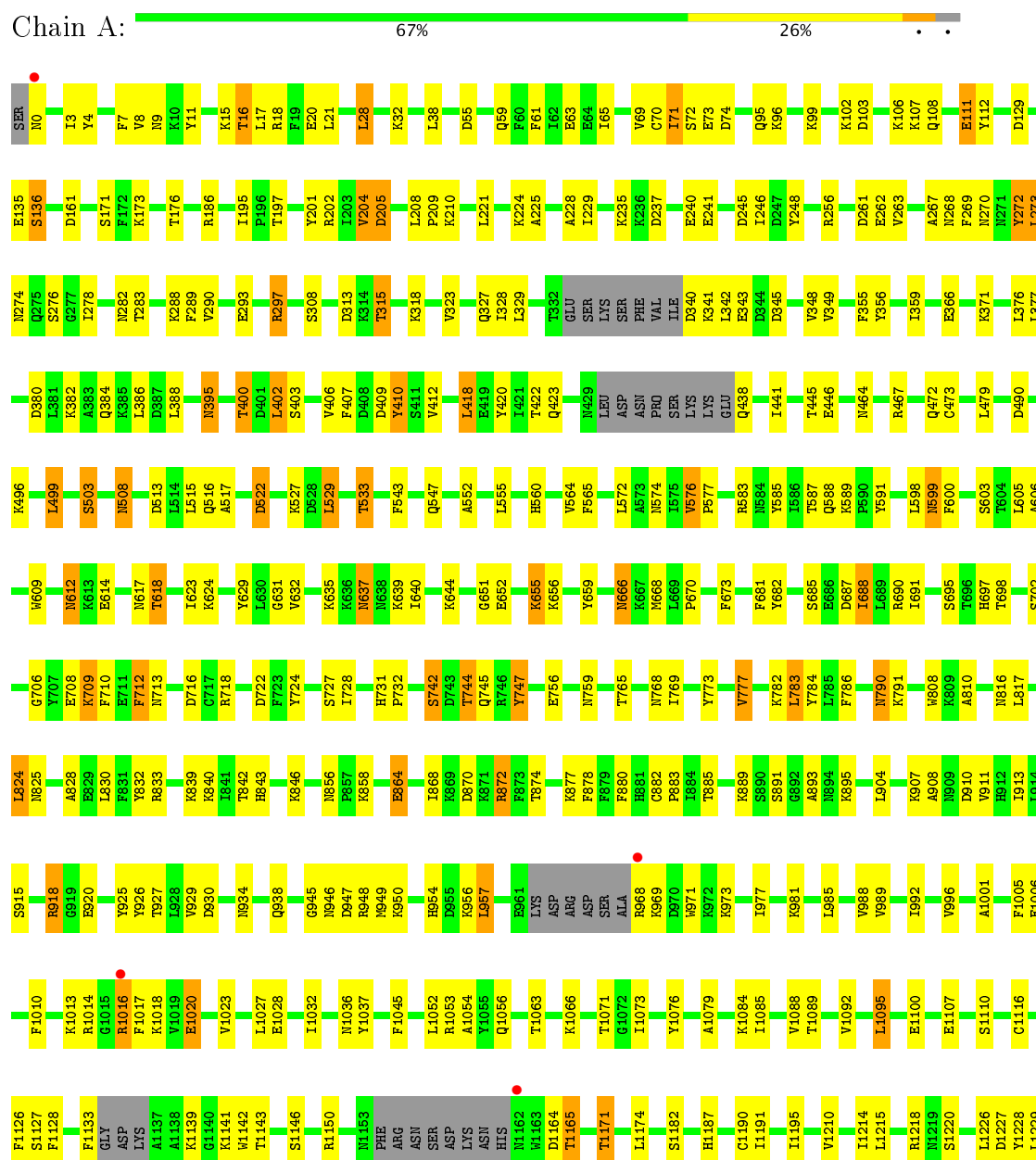
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	10	Total	O	0	0
			10	10		
4	D	6	Total	O	0	0
			6	6		
4	E	5	Total	O	0	0
			5	5		
4	F	10	Total	O	0	0
			10	10		
4	G	3	Total	O	0	0
			3	3		
4	H	6	Total	O	0	0
			6	6		

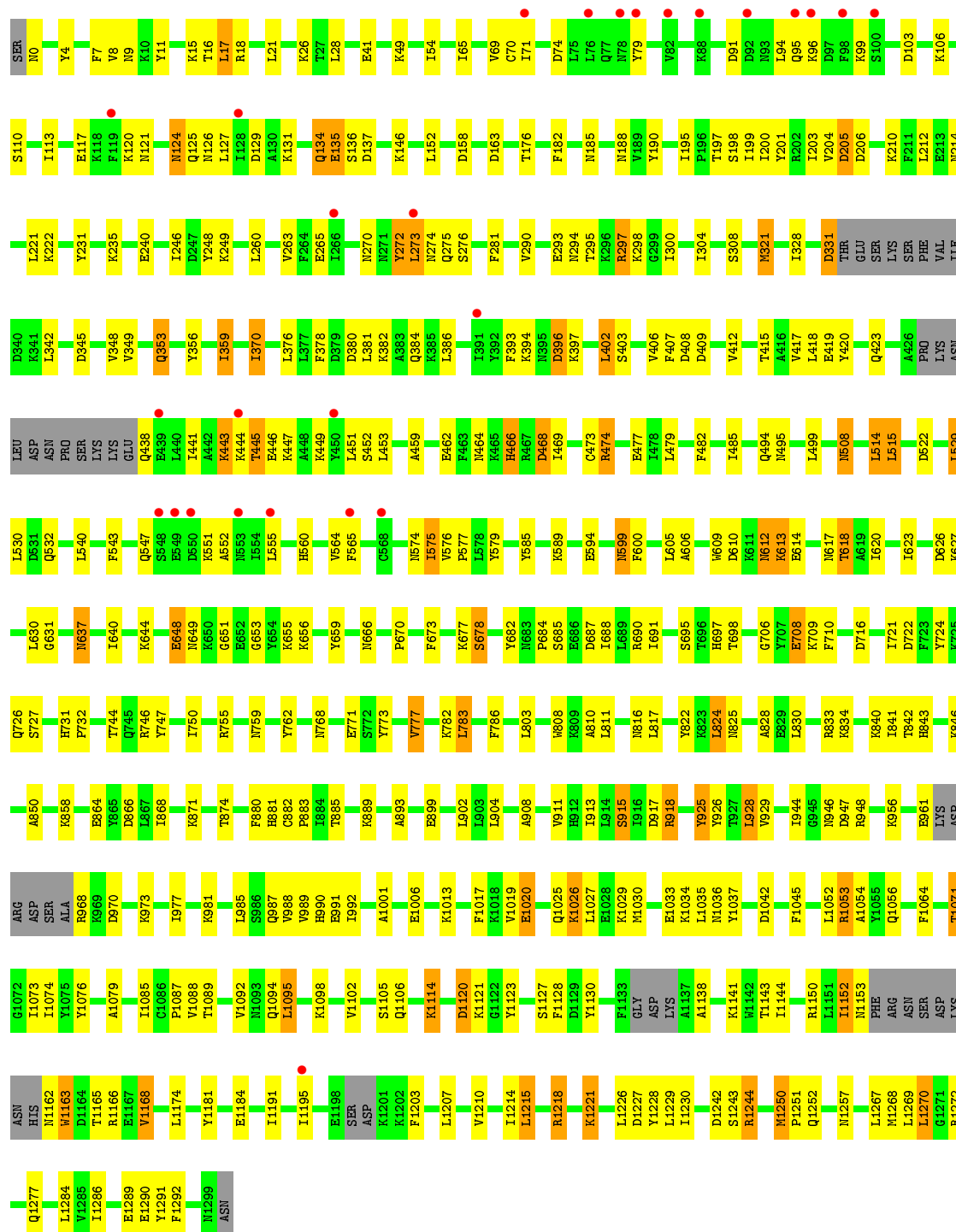
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: CRISPR-associated endonuclease Cpf1



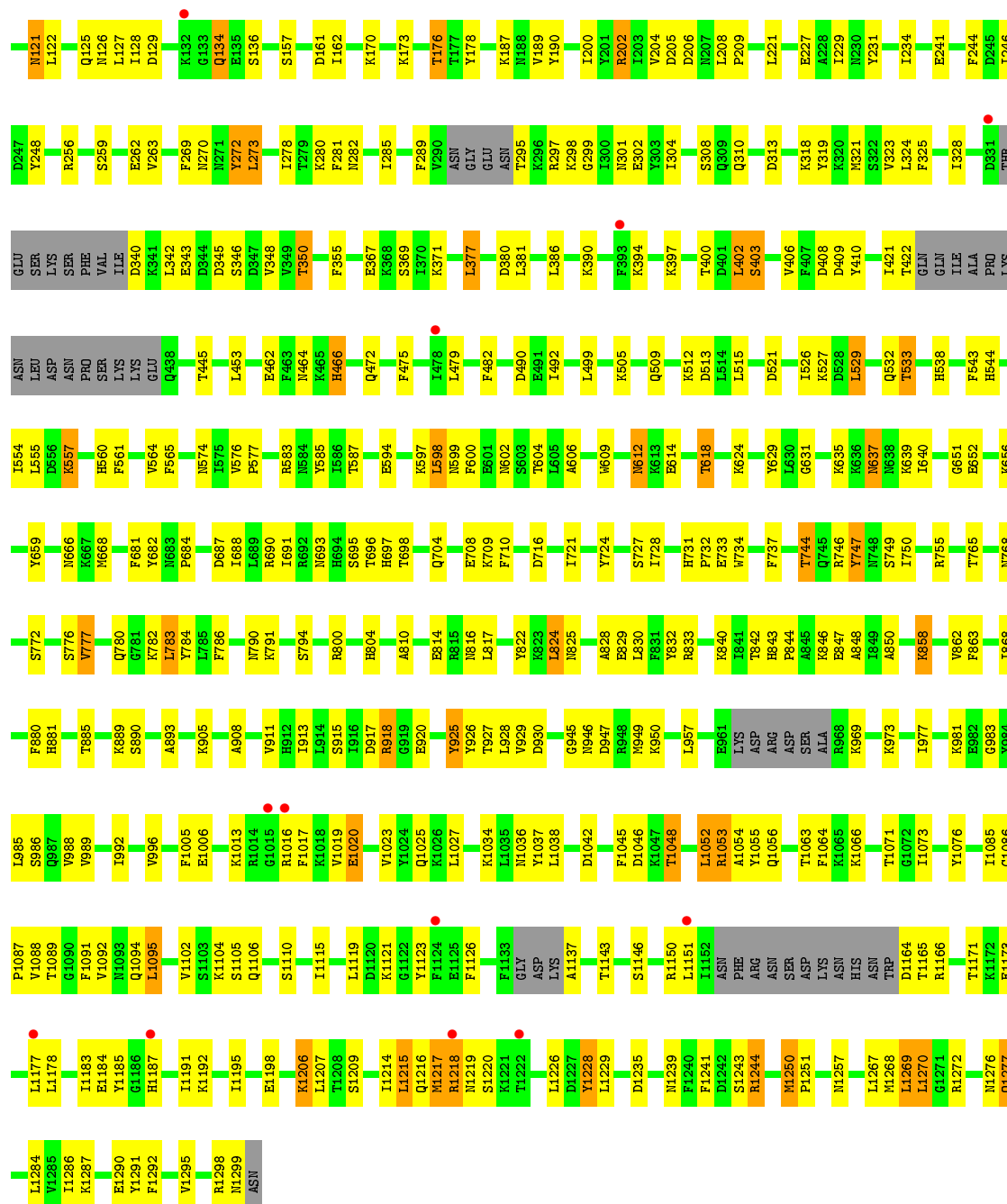




• Molecule 1: CRISPR-associated endonuclease Cpf1

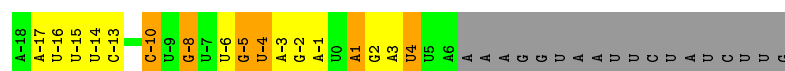






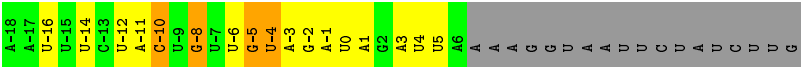
- Molecule 2: crRNA

Chain B:  19% 26% 14% 42%

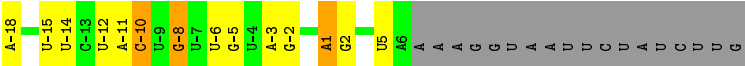
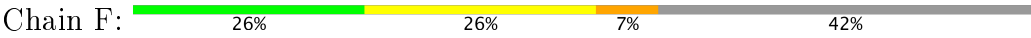


- Molecule 2: crRNA

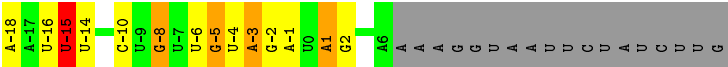
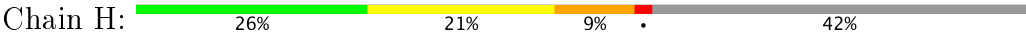
Chain D:  19% 30% 9% 42%



● Molecule 2: crRNA



● Molecule 2: crRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.68Å 277.06Å 135.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 3.34 49.24 – 3.34	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.24-3.34) 99.8 (49.24-3.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, $R_{free}$	0.239 , 0.258 0.236 , 0.256	Depositor DCC
$R_{free}$ test set	5695 reflections (4.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	85.7	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	43813	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.74% 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, 0.333 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: MG

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	0.41	0/10683	0.48	2/14342 (0.0%)
1	C	0.38	0/10683	0.47	2/14342 (0.0%)
1	E	0.38	0/10630	0.47	2/14267 (0.0%)
1	G	0.38	0/10558	0.48	2/14169 (0.0%)
2	B	1.03	0/565	0.95	0/878
2	D	0.86	0/565	0.88	0/878
2	F	1.02	0/565	0.88	0/878
2	H	0.93	0/565	0.95	2/878 (0.2%)
All	All	0.44	0/44814	0.51	10/60632 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	H	-15	U	C2-N1-C1'	7.35	126.52	117.70
1	A	1095	LEU	CA-CB-CG	6.77	130.88	115.30
1	G	1095	LEU	CA-CB-CG	6.24	129.66	115.30
1	E	1095	LEU	CA-CB-CG	6.17	129.49	115.30
1	C	1095	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	273	LEU	CA-CB-CG	5.82	128.69	115.30
2	H	-15	U	C6-N1-C1'	-5.82	113.06	121.20
1	C	273	LEU	CA-CB-CG	5.78	128.59	115.30
1	E	515	LEU	CA-CB-CG	5.29	127.47	115.30
1	G	273	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	10476	0	10455	222	1
1	C	10476	0	10455	216	0
1	E	10425	0	10402	241	0
1	G	10355	0	10344	226	0
2	B	507	0	254	16	0
2	D	507	0	254	11	0
2	F	507	0	254	10	0
2	H	507	0	254	10	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	5	0	0	1	0
4	B	10	0	0	3	0
4	D	6	0	0	0	0
4	E	5	0	0	0	0
4	F	10	0	0	0	0
4	G	3	0	0	0	0
4	H	6	0	0	0	0
All	All	43813	0	42672	919	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (919) 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:A:293:GLU:OE2	1:A:297:ARG:NH1	2.09	0.85
1:A:872:ARG:NH1	2:B:-13:C:OP2	2.11	0.84
1:G:1272:ARG:NH2	1:G:1290:GLU:OE2	2.11	0.82
2:B:-17:A:OP1	4:B:301:HOH:O	1.98	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:920:GLU:O	1:A:1016:ARG:NH2	2.11	0.82
1:C:913:ILE:HB	1:C:929:VAL:HG22	1.62	0.80
1:A:870:ASP:OD1	4:B:301:HOH:O	2.00	0.80
1:E:41:GLU:OE1	1:E:834:LYS:NZ	2.15	0.80
1:C:293:GLU:OE2	1:C:297:ARG:NH1	2.16	0.79
1:G:913:ILE:HB	1:G:929:VAL:HG22	1.65	0.78
1:E:1153:ASN:HA	1:E:1163:TRP:HE1	1.48	0.78
1:E:913:ILE:HB	1:E:929:VAL:HG22	1.64	0.78
1:E:15:LYS:HG3	2:F:1:A:H5"	1.65	0.77
1:E:944:ILE:HG21	1:E:987:GLN:HB3	1.66	0.77
1:A:913:ILE:HB	1:A:929:VAL:HG22	1.65	0.77
1:G:499:LEU:HD22	1:G:529:LEU:HD12	1.67	0.77
1:C:985:LEU:HD13	1:C:1027:LEU:HB2	1.67	0.77
1:G:15:LYS:HG3	2:H:1:A:H5"	1.67	0.77
1:C:602:ASN:ND2	1:C:604:THR:O	2.17	0.76
1:A:467:ARG:NH1	1:A:1100:GLU:OE2	2.19	0.76
1:A:15:LYS:NZ	2:B:1:A:OP2	2.18	0.76
1:C:491:GLU:O	1:C:495:ASN:ND2	2.19	0.75
1:E:331:ASP:OD2	1:E:331:ASP:N	2.19	0.75
1:G:527:LYS:NZ	1:G:969:LYS:O	2.19	0.75
1:E:4:TYR:CZ	1:E:1073:ILE:HD11	2.22	0.75
1:C:689:LEU:O	1:C:693:ASN:ND2	2.20	0.75
1:G:985:LEU:HD13	1:G:1027:LEU:HB2	1.69	0.74
1:C:10:LYS:NZ	1:C:899:GLU:OE1	2.19	0.74
1:E:918:ARG:NH1	1:E:1006:GLU:OE1	2.21	0.73
1:A:624:LYS:HB3	1:A:629:TYR:HE2	1.52	0.73
1:G:755:ARG:NH2	1:G:889:LYS:O	2.20	0.73
1:C:693:ASN:HB3	1:C:707:TYR:HD1	1.53	0.73
1:E:499:LEU:HD12	1:E:529:LEU:HD12	1.70	0.73
1:G:91:ASP:HB2	1:G:94:LEU:HB2	1.71	0.73
1:G:74:ASP:OD2	1:G:74:ASP:N	2.21	0.72
1:G:833:ARG:NH2	2:H:-14:U:OP1	2.22	0.72
1:A:637:ASN:OD1	1:A:637:ASN:N	2.21	0.72
1:A:1293:GLU:O	1:A:1297:ASN:ND2	2.23	0.72
1:E:106:LYS:HG2	1:E:204:VAL:HG11	1.72	0.71
1:G:400:THR:HG23	1:G:410:TYR:HB2	1.71	0.71
1:E:1165:THR:HG21	1:E:1221:LYS:HA	1.71	0.71
1:G:918:ARG:NH1	1:G:1006:GLU:OE1	2.23	0.71
1:A:833:ARG:NH2	2:B:-14:U:OP1	2.20	0.71
1:A:918:ARG:NH1	1:A:1006:GLU:OE1	2.24	0.70
1:E:95:GLN:OE1	1:E:552:ALA:N	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:482:PHE:HA	1:E:485:ILE:HG12	1.72	0.70
1:G:308:SER:OG	1:G:313:ASP:O	2.09	0.69
1:E:1218:ARG:NH2	1:E:1227:ASP:OD1	2.26	0.69
1:A:95:GLN:OE1	1:A:552:ALA:N	2.22	0.69
1:A:589:LYS:NZ	4:A:1501:HOH:O	2.25	0.69
1:E:690:ARG:NH1	1:E:716:ASP:OD2	2.25	0.68
1:A:400:THR:HG22	1:A:410:TYR:HB2	1.75	0.68
1:E:210:LYS:O	1:E:214:ASN:ND2	2.27	0.68
1:C:310:GLN:OE1	1:G:746:ARG:NH2	2.24	0.68
1:A:1272:ARG:NH2	1:A:1290:GLU:OE2	2.27	0.68
1:A:547:GLN:NE2	1:A:552:ALA:O	2.26	0.68
1:G:346:SER:O	1:G:350:THR:OG1	2.09	0.67
1:C:4:TYR:CZ	1:C:1073:ILE:HD11	2.29	0.67
1:C:1271:GLY:HA2	1:C:1274:LYS:HD3	1.76	0.67
1:G:1177:LEU:HD13	1:G:1206:LYS:HG2	1.76	0.67
1:A:985:LEU:HD13	1:A:1027:LEU:HB2	1.77	0.67
1:E:185:ASN:OD1	2:F:5:U:O2'	2.13	0.67
1:C:1253:ASP:OD1	1:C:1253:ASP:N	2.26	0.67
1:E:864:GLU:N	1:E:864:GLU:OE2	2.25	0.67
1:G:421:ILE:HG13	1:G:445:THR:HG21	1.76	0.67
1:G:1071:THR:HG22	1:G:1076:TYR:HE2	1.57	0.67
1:G:263:VAL:O	1:G:272:TYR:OH	2.12	0.67
1:A:0:ASN:ND2	1:A:910:ASP:OD2	2.28	0.67
1:A:1220:SER:HB3	1:A:1227:ASP:HB3	1.75	0.67
1:A:872:ARG:HG3	2:B:-16:U:OP2	1.95	0.67
1:C:345:ASP:OD1	1:C:585:TYR:OH	2.11	0.67
1:G:1219:ASN:HB2	1:G:1228:TYR:HE2	1.60	0.67
1:E:961:GLU:OE1	1:E:968:ARG:NH2	2.27	0.66
1:G:1086:CYS:HG	1:G:1089:THR:HG1	1.37	0.66
1:E:956:LYS:NZ	2:F:-10:C:OP1	2.26	0.66
1:G:282:ASN:OD1	1:G:324:LEU:N	2.26	0.66
1:C:947:ASP:OD1	1:C:947:ASP:N	2.27	0.66
1:E:382:LYS:HA	1:E:479:LEU:HD13	1.78	0.66
1:G:403:SER:OG	1:G:409:ASP:O	2.14	0.66
1:E:1127:SER:HA	1:E:1143:THR:HA	1.77	0.66
1:C:692:ARG:NH2	1:C:704:GLN:OE1	2.29	0.66
1:E:614:GLU:OE2	1:E:656:LYS:NZ	2.29	0.66
1:E:777:VAL:HG22	1:E:782:LYS:HB2	1.76	0.66
1:A:106:LYS:HG2	1:A:204:VAL:HG11	1.78	0.66
2:B:-17:A:OP2	2:B:-10:C:N4	2.25	0.66
1:E:345:ASP:OD1	1:E:585:TYR:OH	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:VAL:O	1:A:272:TYR:OH	2.14	0.65
1:A:4:TYR:OH	1:A:1001:ALA:O	2.14	0.65
1:G:1085:ILE:HG12	1:G:1092:VAL:HG12	1.78	0.65
1:A:9:ASN:HD21	1:A:1053:ARG:HE	1.43	0.65
1:C:693:ASN:HB3	1:C:707:TYR:CD1	2.31	0.65
1:A:99:LYS:NZ	1:A:103:ASP:OD2	2.29	0.64
1:C:704:GLN:HA	1:C:704:GLN:HE21	1.63	0.64
1:G:1164:ASP:OD1	1:G:1165:THR:N	2.29	0.64
1:A:1088:VAL:HG23	1:A:1089:THR:HG23	1.79	0.64
1:A:4:TYR:CZ	1:A:1073:ILE:HD11	2.32	0.64
1:C:527:LYS:NZ	1:C:969:LYS:O	2.24	0.64
1:A:690:ARG:NH1	1:A:716:ASP:OD2	2.31	0.64
2:B:-4:U:OP2	4:B:302:HOH:O	2.15	0.63
1:E:1085:ILE:HG12	1:E:1092:VAL:HG12	1.80	0.63
1:C:637:ASN:OD1	1:C:637:ASN:N	2.31	0.63
1:E:1120:ASP:N	1:E:1120:ASP:OD2	2.31	0.63
1:G:905:LYS:NZ	1:G:1276:ASN:O	2.25	0.63
1:C:1088:VAL:HG23	1:C:1089:THR:HG23	1.81	0.63
1:C:791:LYS:NZ	2:D:-16:U:O2	2.26	0.63
1:A:1164:ASP:OD1	1:A:1165:THR:N	2.32	0.62
1:E:124:ASN:OD1	1:E:126:ASN:N	2.19	0.62
1:A:1191:ILE:HG22	1:A:1195:ILE:HG13	1.80	0.62
1:A:283:THR:HG23	1:A:288:LYS:HB3	1.80	0.62
1:E:842:THR:HG22	1:E:843:HIS:HD2	1.63	0.62
1:G:981:LYS:NZ	1:G:1020:GLU:OE2	2.24	0.62
1:E:1162:ASN:OD1	1:E:1163:TRP:N	2.31	0.62
1:E:468:ASP:OD1	1:E:468:ASP:N	2.32	0.62
1:C:1272:ARG:NH2	1:C:1290:GLU:OE2	2.31	0.62
1:E:623:ILE:O	1:E:655:LYS:HG2	1.99	0.62
1:G:915:SER:OG	1:G:927:THR:OG1	2.18	0.62
1:C:825:ASN:OD1	1:C:885:THR:OG1	2.14	0.62
1:G:278:ILE:O	1:G:282:ASN:ND2	2.33	0.62
1:G:791:LYS:NZ	2:H:-16:U:O2	2.33	0.62
1:C:944:ILE:HD13	1:C:987:GLN:HB2	1.82	0.61
1:G:466:HIS:HB3	1:G:1104:LYS:HE3	1.83	0.61
1:G:637:ASN:N	1:G:637:ASN:OD1	2.33	0.61
1:C:925:TYR:HE1	1:C:1256:ALA:HB2	1.65	0.61
1:E:1228:TYR:HB2	1:E:1243:SER:HB3	1.82	0.61
1:C:63:GLU:OE1	1:C:274:ASN:ND2	2.32	0.61
1:E:1152:ILE:HD12	1:E:1168:VAL:HG21	1.83	0.61
1:C:340:ASP:OD1	1:C:340:ASP:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:ARG:NH2	1:G:262:GLU:OE1	2.32	0.61
1:E:612:ASN:N	1:E:612:ASN:OD1	2.32	0.61
1:C:1174:LEU:HG	1:C:1210:VAL:HG11	1.83	0.61
1:E:124:ASN:OD1	1:E:125:GLN:N	2.34	0.60
1:A:945:GLY:HA3	1:A:950:LYS:HD3	1.83	0.60
1:E:842:THR:HG22	1:E:843:HIS:CD2	2.36	0.60
1:A:499:LEU:O	1:A:503:SER:OG	2.19	0.60
1:C:11:TYR:CG	1:C:893:ALA:HB2	2.36	0.60
1:A:1085:ILE:HG12	1:A:1092:VAL:HG12	1.82	0.60
1:A:349:VAL:HG13	1:A:503:SER:HB3	1.83	0.60
1:A:790:ASN:N	1:A:790:ASN:OD1	2.32	0.60
1:A:1290:GLU:HA	1:C:1277:GLN:HG2	1.81	0.60
1:C:106:LYS:HG2	1:C:204:VAL:HG11	1.83	0.60
1:C:235:LYS:NZ	1:E:706:GLY:O	2.22	0.60
1:C:71:ILE:HG22	1:C:270:ASN:OD1	2.01	0.60
1:C:617:ASN:O	1:C:618:THR:HG22	2.02	0.60
1:E:135:GLU:OE2	1:E:136:SER:N	2.31	0.60
1:A:16:THR:HA	1:A:883:PRO:HA	1.84	0.60
1:C:403:SER:OG	1:C:409:ASP:O	2.18	0.60
1:C:1243:SER:OG	1:C:1252:GLN:O	2.19	0.60
1:E:1029:LYS:NZ	1:E:1033:GLU:OE2	2.34	0.60
1:G:1088:VAL:HG23	1:G:1089:THR:HG23	1.84	0.60
1:E:121:ASN:ND2	1:E:137:ASP:OD2	2.32	0.60
1:E:925:TYR:HD2	1:E:926:TYR:H	1.50	0.60
1:A:1150:ARG:NH1	1:A:1214:ILE:O	2.35	0.59
1:C:1183:ILE:HG21	1:C:1191:ILE:HG23	1.82	0.59
1:C:600:PHE:HE2	1:C:830:LEU:HD12	1.65	0.59
1:G:342:LEU:HD23	1:G:348:VAL:HG22	1.84	0.59
1:G:91:ASP:N	1:G:91:ASP:OD1	2.33	0.59
1:G:946:ASN:OD1	1:G:947:ASP:N	2.35	0.59
1:C:135:GLU:OE2	1:C:136:SER:N	2.34	0.59
1:E:777:VAL:HG13	1:E:783:LEU:HB3	1.84	0.59
1:A:55:ASP:OD1	1:A:186:ARG:NH1	2.35	0.59
1:C:342:LEU:HD23	1:C:348:VAL:HG22	1.85	0.59
1:A:210:LYS:NZ	1:A:323:VAL:O	2.31	0.59
1:C:691:ILE:HD12	1:C:716:ASP:HB3	1.85	0.59
1:G:1150:ARG:NH1	1:G:1214:ILE:O	2.34	0.59
1:A:278:ILE:O	1:A:282:ASN:ND2	2.36	0.59
2:F:-10:C:O2'	2:F:-8:G:N7	2.32	0.59
1:A:1013:LYS:HD3	1:A:1017:PHE:CZ	2.37	0.59
1:A:267:ALA:O	1:A:270:ASN:ND2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:589:LYS:NZ	2:F:-12:U:OP1	2.36	0.59
1:C:833:ARG:NH2	2:D:-14:U:OP1	2.27	0.58
1:G:659:TYR:HE1	1:G:824:LEU:HB3	1.68	0.58
1:C:464:ASN:ND2	1:C:473:CYS:O	2.33	0.58
1:E:11:TYR:CG	1:E:893:ALA:HB2	2.38	0.58
1:E:576:VAL:HG12	1:E:577:PRO:HD3	1.85	0.58
1:G:1219:ASN:HB2	1:G:1228:TYR:CE2	2.37	0.58
1:G:602:ASN:ND2	1:G:604:THR:O	2.36	0.58
1:A:576:VAL:HG13	1:A:577:PRO:HD3	1.85	0.58
1:E:99:LYS:NZ	1:E:103:ASP:OD2	2.37	0.58
1:G:1119:LEU:HD13	1:G:1187:HIS:HB3	1.85	0.58
1:C:1143:THR:OG1	1:C:1143:THR:O	2.17	0.58
1:E:1153:ASN:CA	1:E:1163:TRP:HE1	2.17	0.58
1:G:161:ASP:OD1	1:G:162:ILE:N	2.37	0.58
1:G:848:ALA:HA	1:G:862:VAL:HG22	1.85	0.58
1:G:731:HIS:CD2	1:G:732:PRO:HD2	2.38	0.58
1:G:913:ILE:HD11	1:G:1270:LEU:HD12	1.86	0.58
1:A:464:ASN:O	1:A:472:GLN:NE2	2.37	0.58
1:E:850:ALA:O	2:F:-18:A:N6	2.37	0.57
1:G:1094:GLN:HE22	1:G:1137:ALA:HB3	1.69	0.57
1:E:146:LYS:NZ	1:E:163:ASP:OD1	2.34	0.57
1:E:610:ASP:HB2	1:E:613:LYS:HG3	1.87	0.57
1:G:1298:ARG:O	1:G:1299:ASN:HB2	2.04	0.57
1:G:464:ASN:O	1:G:472:GLN:NE2	2.36	0.57
1:A:403:SER:OG	1:A:409:ASP:O	2.22	0.57
1:G:106:LYS:HG2	1:G:204:VAL:HG11	1.85	0.57
1:A:599:ASN:HA	1:A:605:LEU:HD22	1.86	0.57
1:E:1243:SER:OG	1:E:1252:GLN:O	2.22	0.57
1:G:380:ASP:HB3	1:G:386:LEU:HD13	1.86	0.57
1:G:600:PHE:HE2	1:G:830:LEU:HD12	1.69	0.57
1:A:527:LYS:NZ	1:A:969:LYS:O	2.31	0.57
1:E:810:ALA:O	1:E:816:ASN:ND2	2.37	0.57
1:G:1046:ASP:OD2	1:G:1053:ARG:NH1	2.38	0.57
1:A:409:ASP:HB3	1:A:412:VAL:HG23	1.87	0.57
1:A:687:ASP:OD1	1:A:690:ARG:NH2	2.38	0.57
1:E:117:GLU:HA	1:E:120:LYS:HE3	1.86	0.57
1:E:441:ILE:O	1:E:445:THR:HG22	2.05	0.57
1:C:1191:ILE:HG22	1:C:1195:ILE:HG13	1.86	0.57
1:E:380:ASP:HB3	1:E:386:LEU:HD13	1.87	0.57
1:A:842:THR:HG22	1:A:843:HIS:HD2	1.71	0.56
1:G:1269:LEU:HD13	1:G:1286:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:SER:OG	1:A:756:GLU:OE2	2.22	0.56
1:E:1150:ARG:NH1	1:E:1214:ILE:O	2.38	0.56
1:E:575:ILE:O	1:E:579:TYR:N	2.23	0.56
1:E:249:LYS:HD3	1:E:265:GLU:HG2	1.86	0.56
1:C:985:LEU:HD11	1:C:1023:VAL:HG12	1.88	0.56
1:E:203:ILE:HG21	1:E:273:LEU:HD12	1.88	0.56
1:G:79:TYR:HB2	1:G:105:ILE:HD11	1.88	0.56
1:A:981:LYS:HE3	1:A:1020:GLU:OE2	2.05	0.56
1:G:576:VAL:HG12	1:G:577:PRO:HD3	1.87	0.56
1:G:917:ASP:OD2	1:G:1013:LYS:NZ	2.39	0.56
1:A:810:ALA:O	1:A:816:ASN:ND2	2.39	0.56
1:E:637:ASN:O	1:E:640:ILE:HG13	2.06	0.56
1:A:709:LYS:NZ	1:A:710:PHE:O	2.35	0.56
1:C:697:HIS:CD2	1:C:698:THR:HG23	2.41	0.56
1:E:637:ASN:N	1:E:637:ASN:OD1	2.39	0.56
1:E:637:ASN:HD22	1:E:782:LYS:HG2	1.70	0.56
1:G:666:ASN:N	1:G:666:ASN:OD1	2.39	0.55
1:G:690:ARG:NH1	1:G:716:ASP:OD2	2.39	0.55
1:G:925:TYR:HD2	1:G:926:TYR:H	1.53	0.55
1:G:1216:GLN:NE2	1:G:1219:ASN:OD1	2.28	0.55
1:E:697:HIS:CD2	1:E:698:THR:HG23	2.41	0.55
1:A:308:SER:OG	1:A:313:ASP:O	2.24	0.55
1:C:1114:LYS:HG2	1:C:1127:SER:HB2	1.86	0.55
1:E:1269:LEU:HD13	1:E:1286:ILE:HD11	1.88	0.55
1:E:687:ASP:OD1	1:E:690:ARG:NH2	2.39	0.55
1:A:4:TYR:CE1	1:A:1073:ILE:HD11	2.42	0.55
1:A:445:THR:OG1	1:A:446:GLU:N	2.39	0.55
1:C:1150:ARG:NH1	1:C:1214:ILE:O	2.39	0.55
1:C:313:ASP:OD1	1:C:315:THR:OG1	2.24	0.55
1:G:70:CYS:HB2	1:G:248:TYR:HE1	1.71	0.55
1:A:65:ILE:O	1:A:69:VAL:HG23	2.07	0.55
1:A:915:SER:OG	1:A:927:THR:OG1	2.23	0.55
2:B:-10:C:O2'	2:B:-8:G:N7	2.35	0.55
1:E:70:CYS:HB3	1:E:248:TYR:HE1	1.72	0.55
1:C:54:ILE:HD11	1:C:128:ILE:HD11	1.89	0.55
1:C:65:ILE:O	1:C:69:VAL:HG23	2.07	0.55
1:E:4:TYR:OH	1:E:1001:ALA:O	2.23	0.55
1:E:197:THR:HG23	1:E:328:ILE:HD11	1.89	0.55
1:A:1174:LEU:HG	1:A:1210:VAL:HG11	1.88	0.55
1:A:71:ILE:HG23	1:A:270:ASN:OD1	2.07	0.55
1:E:985:LEU:HA	1:E:988:VAL:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:221:LEU:HD23	1:G:229:ILE:HD11	1.89	0.55
1:G:945:GLY:HA3	1:G:950:LYS:HA	1.89	0.55
1:E:1163:TRP:HH2	1:E:1166:ARG:HD2	1.72	0.55
1:C:708:GLU:OE2	1:E:231:TYR:HB3	2.07	0.55
1:E:407:PHE:CD1	1:E:473:CYS:HB3	2.42	0.55
1:E:70:CYS:HB3	1:E:248:TYR:CE1	2.41	0.55
1:A:617:ASN:O	1:A:618:THR:HG22	2.07	0.54
1:E:560:HIS:O	1:E:564:VAL:HG22	2.08	0.54
1:C:17:LEU:HD23	1:C:808:TRP:HB2	1.90	0.54
1:C:195:ILE:HG22	1:C:197:THR:H	1.71	0.54
1:A:600:PHE:HE2	1:A:830:LEU:HD12	1.71	0.54
1:E:617:ASN:O	1:E:618:THR:HG22	2.08	0.54
1:E:1153:ASN:HA	1:E:1163:TRP:NE1	2.20	0.54
1:G:1048:THR:HA	1:G:1053:ARG:HB3	1.89	0.54
1:C:599:ASN:HA	1:C:605:LEU:HD22	1.90	0.54
2:D:-10:C:O2'	2:D:-8:G:N7	2.30	0.54
1:G:612:ASN:ND2	1:G:733:GLU:OE2	2.41	0.54
1:G:1086:CYS:HB3	1:G:1091:PHE:H	1.72	0.54
1:A:1036:ASN:O	1:A:1056:GLN:HG2	2.08	0.54
1:C:712:PHE:HD2	1:C:713:ASN:N	2.05	0.54
1:E:1242:ASP:OD2	1:E:1244:ARG:HD2	2.07	0.54
1:A:1269:LEU:HD13	1:A:1286:ILE:HD11	1.90	0.54
1:C:599:ASN:OD1	1:C:599:ASN:N	2.40	0.54
1:A:17:LEU:HD23	1:A:808:TRP:HB2	1.89	0.53
1:G:1038:LEU:HB3	1:G:1055:TYR:HB2	1.90	0.53
1:C:915:SER:OG	1:C:927:THR:OG1	2.26	0.53
1:E:944:ILE:HD12	1:E:991:GLU:HG3	1.88	0.53
1:G:842:THR:HG22	1:G:843:HIS:CD2	2.43	0.53
1:A:70:CYS:HB2	1:A:248:TYR:HE1	1.74	0.53
1:A:618:THR:HG23	1:A:632:VAL:HG13	1.89	0.53
1:C:543:PHE:HB2	1:C:565:PHE:CZ	2.43	0.53
1:E:11:TYR:O	1:E:1056:GLN:NE2	2.40	0.53
1:G:340:ASP:OD1	1:G:340:ASP:N	2.40	0.53
1:C:402:LEU:O	1:C:406:VAL:HG12	2.09	0.53
1:G:421:ILE:HG13	1:G:445:THR:CG2	2.39	0.53
1:E:1174:LEU:HG	1:E:1210:VAL:HG11	1.90	0.53
1:E:547:GLN:NE2	1:E:552:ALA:O	2.41	0.53
1:G:915:SER:O	1:G:926:TYR:HA	2.08	0.53
1:C:18:ARG:HG2	1:C:881:HIS:CD2	2.43	0.53
1:G:825:ASN:OD1	1:G:885:THR:OG1	2.18	0.53
1:C:1036:ASN:O	1:C:1056:GLN:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:VAL:HG13	1:G:328:ILE:HD13	1.90	0.53
1:A:1006:GLU:HB2	1:A:1079:ALA:HB2	1.91	0.53
1:A:1218:ARG:NH2	1:A:1255:ASP:OD1	2.42	0.53
1:A:687:ASP:O	1:A:691:ILE:HG12	2.09	0.53
1:A:791:LYS:NZ	2:B:-16:U:O2	2.39	0.53
1:C:918:ARG:NH1	1:C:1006:GLU:OE1	2.36	0.53
1:E:403:SER:OG	1:E:409:ASP:O	2.25	0.53
1:C:259:SER:HB2	1:E:708:GLU:OE1	2.08	0.53
1:G:1228:TYR:HD1	1:G:1244:ARG:HG2	1.73	0.53
1:A:8:VAL:HG21	1:A:1053:ARG:HB3	1.91	0.52
1:E:199:ILE:HG22	1:E:328:ILE:HG21	1.90	0.52
1:A:382:LYS:HA	1:A:479:LEU:HD13	1.91	0.52
1:A:842:THR:HG22	1:A:843:HIS:CD2	2.43	0.52
1:E:447:LYS:O	1:E:551:LYS:NZ	2.27	0.52
1:A:599:ASN:OD1	1:A:599:ASN:N	2.41	0.52
1:C:985:LEU:HA	1:C:988:VAL:HG12	1.91	0.52
1:E:443:LYS:HA	1:E:447:LYS:HB2	1.91	0.52
1:G:1287:LYS:HB2	1:G:1290:GLU:OE1	2.08	0.52
1:A:135:GLU:OE2	1:A:136:SER:N	2.34	0.52
1:E:206:ASP:O	1:E:210:LYS:HG3	2.09	0.52
1:G:687:ASP:O	1:G:691:ILE:HG12	2.10	0.52
1:A:946:ASN:OD1	1:A:947:ASP:N	2.38	0.52
1:E:7:PHE:HZ	1:E:899:GLU:HG2	1.74	0.52
1:G:1268:MET:HE3	1:G:1286:ILE:HD13	1.92	0.52
1:G:597:LYS:HE3	1:G:829:GLU:HG2	1.92	0.52
1:A:624:LYS:HB3	1:A:629:TYR:CE2	2.38	0.52
1:C:342:LEU:HD21	1:C:582:ILE:HG12	1.92	0.52
1:E:409:ASP:HB3	1:E:412:VAL:HG23	1.92	0.52
1:G:640:ILE:HD11	1:G:782:LYS:HB3	1.91	0.52
1:C:221:LEU:HD23	1:C:229:ILE:HD11	1.90	0.52
1:E:721:ILE:HG12	1:E:750:ILE:HD12	1.92	0.52
1:G:925:TYR:HD2	1:G:926:TYR:N	2.08	0.52
1:A:102:LYS:HG3	1:A:204:VAL:HG21	1.92	0.52
1:A:73:GLU:HG3	1:A:267:ALA:HB2	1.92	0.52
1:G:612:ASN:N	1:G:612:ASN:OD1	2.41	0.52
1:A:985:LEU:HA	1:A:988:VAL:HG12	1.92	0.52
1:C:390:LYS:HB3	1:C:558:ASP:N	2.25	0.52
1:C:445:THR:OG1	1:C:446:GLU:N	2.43	0.52
1:E:445:THR:HG23	1:E:446:GLU:H	1.74	0.52
1:E:599:ASN:HA	1:E:605:LEU:HD22	1.92	0.52
1:E:659:TYR:HE1	1:E:824:LEU:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:576:VAL:HG13	1:C:577:PRO:HD3	1.92	0.51
1:E:825:ASN:OD1	1:E:885:THR:OG1	2.21	0.51
1:G:71:ILE:HG22	1:G:270:ASN:OD1	2.10	0.51
1:E:833:ARG:NH2	2:F:-14:U:OP1	2.39	0.51
1:A:278:ILE:HG22	1:A:282:ASN:HD21	1.75	0.51
1:E:71:ILE:HG22	1:E:270:ASN:OD1	2.10	0.51
1:G:983:GLY:O	1:G:986:SER:OG	2.17	0.51
1:G:709:LYS:NZ	1:G:710:PHE:O	2.33	0.51
1:G:11:TYR:CG	1:G:893:ALA:HB2	2.46	0.51
1:C:774:ILE:HA	1:C:777:VAL:HG12	1.93	0.51
1:E:1025:GLN:HG2	1:E:1064:PHE:CE1	2.46	0.51
1:C:706:GLY:O	1:E:235:LYS:HE3	2.11	0.51
1:E:985:LEU:O	1:E:989:VAL:HG13	2.10	0.51
1:G:390:LYS:O	1:G:557:LYS:HA	2.11	0.51
1:A:697:HIS:CE1	1:A:698:THR:HG23	2.45	0.51
1:A:21:LEU:HB3	1:A:786:PHE:HB3	1.93	0.51
1:G:11:TYR:O	1:G:1056:GLN:NE2	2.40	0.51
1:C:1195:ILE:HD13	1:C:1207:LEU:HD21	1.93	0.51
1:C:241:GLU:HG2	1:C:283:THR:HG21	1.93	0.51
1:C:452:SER:HG	1:C:455:THR:HG1	1.58	0.51
1:C:762:TYR:HD2	1:C:820:VAL:HG11	1.75	0.51
1:E:342:LEU:HD23	1:E:348:VAL:HG22	1.92	0.51
1:A:1063:THR:HG23	1:A:1066:LYS:H	1.76	0.51
1:A:256:ARG:HH22	1:A:262:GLU:CD	2.14	0.51
1:C:107:LYS:O	1:C:111:GLU:HB3	2.11	0.51
1:E:600:PHE:HE2	1:E:830:LEU:HD12	1.76	0.51
1:C:38:LEU:H	1:C:38:LEU:HD12	1.76	0.51
1:C:723:PHE:O	1:C:727:SER:OG	2.26	0.51
1:G:127:LEU:O	1:G:136:SER:HB3	2.11	0.51
1:G:598:LEU:HD12	1:G:832:TYR:HB2	1.93	0.51
1:A:825:ASN:OD1	1:A:885:THR:OG1	2.17	0.50
1:E:464:ASN:ND2	1:E:473:CYS:O	2.43	0.50
1:G:777:VAL:HG13	1:G:783:LEU:HB3	1.93	0.50
1:C:1087:PRO:HG3	1:C:1257:ASN:OD1	2.11	0.50
1:C:775:ASP:O	1:C:779:ASN:ND2	2.32	0.50
1:C:985:LEU:O	1:C:989:VAL:HG13	2.11	0.50
1:A:71:ILE:HA	1:A:108:GLN:NE2	2.26	0.50
1:A:659:TYR:HE1	1:A:824:LEU:HB3	1.75	0.50
1:C:7:PHE:HZ	1:C:899:GLU:HG2	1.76	0.50
1:A:195:ILE:HG22	1:A:197:THR:H	1.76	0.50
1:E:917:ASP:OD2	1:E:1013:LYS:NZ	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:GLN:HG2	1:A:517:ALA:H	1.76	0.50
1:C:1127:SER:HA	1:C:1143:THR:HA	1.93	0.50
1:C:688:ILE:HD12	1:C:723:PHE:CG	2.46	0.50
1:A:1092:VAL:HG11	1:A:1292:PHE:CE1	2.46	0.50
1:G:691:ILE:HD12	1:G:716:ASP:HB3	1.92	0.50
1:G:908:ALA:O	1:G:911:VAL:HG22	2.11	0.50
1:C:8:VAL:HG21	1:C:1053:ARG:HB3	1.93	0.50
1:E:1036:ASN:O	1:E:1056:GLN:HG2	2.12	0.50
1:G:301:ASN:HA	1:G:304:ILE:HD12	1.93	0.50
1:A:880:PHE:CE2	1:A:882:CYS:HB2	2.47	0.50
1:A:904:LEU:O	1:A:908:ALA:N	2.45	0.50
1:E:1268:MET:HE3	1:E:1291:TYR:HD1	1.75	0.50
1:G:18:ARG:HG2	1:G:881:HIS:CD2	2.47	0.50
1:A:380:ASP:HB3	1:A:386:LEU:HD13	1.93	0.49
1:A:977:ILE:HG22	1:A:981:LYS:HE2	1.92	0.49
1:E:274:ASN:OD1	1:E:275:GLN:N	2.45	0.49
1:G:377:LEU:HD11	1:G:561:PHE:CD1	2.47	0.49
1:C:659:TYR:HE1	1:C:824:LEU:HB3	1.77	0.49
1:E:1272:ARG:NH2	1:E:1290:GLU:OE2	2.46	0.49
1:E:200:ILE:O	1:E:204:VAL:HG12	2.12	0.49
1:E:356:TYR:CZ	1:E:529:LEU:HD22	2.46	0.49
1:G:842:THR:HG22	1:G:843:HIS:HD2	1.76	0.49
1:C:364:THR:OG1	1:C:368:LYS:O	2.30	0.49
1:C:708:GLU:OE1	1:C:708:GLU:N	2.45	0.49
1:C:956:LYS:NZ	2:D:-10:C:OP1	2.38	0.49
1:E:201:TYR:O	1:E:205:ASP:HB2	2.12	0.49
1:G:911:VAL:HG21	1:G:1270:LEU:HD21	1.94	0.49
1:A:420:TYR:O	1:A:423:GLN:HG3	2.11	0.49
1:G:1228:TYR:HE1	1:G:1244:ARG:CZ	2.25	0.49
1:G:1088:VAL:O	1:G:1299:ASN:ND2	2.46	0.49
1:G:318:LYS:HE3	1:G:319:TYR:CZ	2.47	0.49
1:G:72:SER:OG	1:G:108:GLN:OE1	2.29	0.49
1:C:256:ARG:HH22	1:C:262:GLU:CD	2.15	0.49
1:C:609:TRP:HB2	1:C:659:TYR:CG	2.47	0.49
1:E:925:TYR:HD2	1:E:926:TYR:N	2.10	0.49
1:G:822:TYR:HH	1:G:1037:TYR:HH	1.59	0.49
1:E:1128:PHE:HE2	1:E:1144:ILE:HG23	1.77	0.49
1:G:1071:THR:HG22	1:G:1076:TYR:CE2	2.44	0.49
1:G:1087:PRO:HG3	1:G:1257:ASN:OD1	2.12	0.49
1:G:65:ILE:O	1:G:69:VAL:HG23	2.12	0.49
1:G:810:ALA:O	1:G:816:ASN:ND2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:973:LYS:O	1:C:977:ILE:HG13	2.12	0.49
1:E:394:LYS:HG2	1:E:396:ASP:OD1	2.12	0.49
1:E:709:LYS:NZ	1:E:710:PHE:O	2.35	0.49
1:G:682:TYR:CD2	1:G:727:SER:HB3	2.48	0.49
1:C:1234:ALA:HB2	1:C:1240:PHE:CZ	2.48	0.49
1:C:666:ASN:OD1	1:C:666:ASN:N	2.45	0.49
1:A:543:PHE:HB2	1:A:565:PHE:CZ	2.47	0.49
1:C:685:SER:O	1:C:688:ILE:HG12	2.13	0.49
1:E:1088:VAL:HG23	1:E:1089:THR:HG23	1.95	0.49
1:A:1071:THR:HG22	1:A:1076:TYR:CE2	2.48	0.48
1:C:790:ASN:ND2	1:C:805:THR:OG1	2.37	0.48
1:E:651:GLY:O	1:E:768:ASN:HB3	2.12	0.48
1:A:985:LEU:O	1:A:989:VAL:HG13	2.13	0.48
1:C:371:LYS:NZ	1:C:490:ASP:OD1	2.41	0.48
1:G:1115:ILE:O	1:G:1191:ILE:N	2.33	0.48
1:G:202:ARG:HA	1:G:206:ASP:HB2	1.95	0.48
1:A:508:ASN:N	1:A:508:ASN:OD1	2.46	0.48
1:A:777:VAL:HG13	1:A:783:LEU:HB3	1.94	0.48
1:C:1093:ASN:HD22	1:C:1095:LEU:HD13	1.77	0.48
1:C:606:ALA:HB3	1:C:828:ALA:O	2.14	0.48
1:E:691:ILE:HD12	1:E:716:ASP:HB3	1.95	0.48
1:E:9:ASN:HD21	1:E:1053:ARG:HE	1.59	0.48
1:A:560:HIS:O	1:A:564:VAL:HG22	2.12	0.48
1:C:917:ASP:OD2	1:C:1013:LYS:NZ	2.47	0.48
1:C:742:SER:OG	1:C:756:GLU:OE2	2.32	0.48
1:C:944:ILE:HG21	1:C:987:GLN:HB3	1.96	0.48
2:D:-12:U:O4	2:D:-11:A:N6	2.46	0.48
1:A:340:ASP:N	1:A:340:ASP:OD1	2.46	0.48
1:A:589:LYS:HD3	1:A:591:TYR:CZ	2.49	0.48
1:C:61:PHE:O	1:C:65:ILE:HG22	2.12	0.48
1:G:281:PHE:O	1:G:285:ILE:HG12	2.13	0.48
1:G:985:LEU:HA	1:G:988:VAL:HG12	1.96	0.48
1:A:356:TYR:OH	1:A:533:THR:OG1	2.18	0.48
1:G:721:ILE:HG12	1:G:750:ILE:HD12	1.95	0.48
1:E:495:ASN:ND2	1:E:532:GLN:OE1	2.47	0.48
1:G:1228:TYR:HB2	1:G:1243:SER:HB3	1.94	0.48
1:G:83:TYR:CD1	1:G:554:ILE:HD13	2.49	0.48
1:A:237:ASP:HB3	1:A:297:ARG:HB3	1.96	0.48
1:A:957:LEU:HD21	1:A:981:LYS:HG2	1.95	0.48
1:C:394:LYS:HE3	1:C:396:ASP:OD1	2.14	0.48
1:E:1013:LYS:HD3	1:E:1017:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:475:PHE:HE2	1:G:479:LEU:HD13	1.79	0.48
1:G:977:ILE:HG22	1:G:981:LYS:HE3	1.96	0.48
1:G:985:LEU:HD11	1:G:1023:VAL:HG12	1.95	0.48
1:C:1035:LEU:HD12	1:C:1074:ILE:HD11	1.95	0.47
1:C:263:VAL:O	1:C:272:TYR:OH	2.22	0.47
1:E:609:TRP:HB2	1:E:659:TYR:CG	2.48	0.47
1:G:1191:ILE:HG22	1:G:1195:ILE:HG13	1.96	0.47
1:G:394:LYS:HE3	1:G:544:HIS:O	2.13	0.47
1:A:438:GLN:O	1:A:441:ILE:HG13	2.13	0.47
1:C:37:ILE:HD11	1:C:878:PHE:HZ	1.79	0.47
1:A:985:LEU:HD22	1:A:1027:LEU:HD22	1.97	0.47
1:A:355:PHE:CZ	1:A:359:ILE:HD11	2.49	0.47
1:C:1013:LYS:HD3	1:C:1017:PHE:CZ	2.49	0.47
1:C:1100:GLU:HB2	1:C:1104:LYS:HD3	1.97	0.47
1:E:1269:LEU:HG	1:E:1284:LEU:HD22	1.95	0.47
1:G:708:GLU:N	1:G:708:GLU:OE1	2.47	0.47
1:G:985:LEU:O	1:G:989:VAL:HG13	2.14	0.47
1:A:59:GLN:NE2	1:A:329:LEU:O	2.44	0.47
1:C:856:ASN:O	1:C:859:LYS:NZ	2.42	0.47
1:A:1242:ASP:OD2	1:A:1244:ARG:HG3	2.14	0.47
1:A:290:VAL:HB	1:A:293:GLU:HG3	1.95	0.47
1:A:609:TRP:HB2	1:A:659:TYR:CG	2.49	0.47
1:C:985:LEU:HD22	1:C:1027:LEU:HD22	1.97	0.47
1:C:18:ARG:HG2	1:C:881:HIS:HD2	1.79	0.47
1:C:990:HIS:ND1	2:D:-2:G:H4'	2.29	0.47
1:E:637:ASN:HD22	1:E:782:LYS:CG	2.27	0.47
1:E:65:ILE:O	1:E:69:VAL:HG23	2.15	0.47
1:A:973:LYS:O	1:A:977:ILE:HG13	2.15	0.47
1:C:678:SER:HB3	1:C:682:TYR:CE1	2.50	0.47
1:C:915:SER:O	1:C:926:TYR:HA	2.14	0.47
1:G:1146:SER:OG	1:G:1171:THR:HG22	2.14	0.47
1:A:407:PHE:CD1	1:A:473:CYS:HB3	2.50	0.47
1:A:640:ILE:O	1:A:773:TYR:OH	2.29	0.47
1:C:981:LYS:NZ	1:C:1020:GLU:OE2	2.33	0.47
1:C:1093:ASN:ND2	1:C:1095:LEU:HD13	2.30	0.47
2:H:-8:G:N3	2:H:-4:U:O2'	2.42	0.47
1:C:1052:LEU:HA	1:C:1052:LEU:HD12	1.75	0.47
1:E:911:VAL:HG21	1:E:1270:LEU:HD21	1.97	0.47
1:E:127:LEU:O	1:E:136:SER:OG	2.24	0.47
1:E:214:ASN:OD1	1:E:321:MET:HB2	2.15	0.47
1:E:687:ASP:O	1:E:691:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1086:CYS:SG	1:G:1089:THR:OG1	2.57	0.47
1:C:1139:LYS:HB2	1:C:1139:LYS:HE2	1.59	0.47
1:C:708:GLU:HG3	1:E:231:TYR:CD2	2.49	0.47
1:A:830:LEU:HD22	1:A:880:PHE:HD1	1.80	0.47
1:E:485:ILE:HG21	1:E:540:LEU:HD21	1.97	0.47
1:G:920:GLU:OE1	1:G:1218:ARG:NH1	2.48	0.47
1:G:583:ARG:O	1:G:587:THR:HG23	2.15	0.47
1:G:840:LYS:O	1:G:868:ILE:HG23	2.14	0.47
1:C:911:VAL:HG21	1:C:1270:LEU:HD21	1.96	0.47
1:G:1151:LEU:HB2	1:G:1219:ASN:HB3	1.97	0.47
1:G:574:ASN:O	1:G:577:PRO:HD2	2.15	0.47
1:A:1228:TYR:OH	1:A:1244:ARG:NH2	2.48	0.46
1:A:345:ASP:OD1	1:A:585:TYR:OH	2.32	0.46
1:A:744:THR:HA	1:A:747:TYR:HE1	1.80	0.46
1:C:454:GLU:HG3	1:C:458:LEU:HD13	1.95	0.46
1:E:1035:LEU:HD12	1:E:1074:ILE:HD11	1.96	0.46
1:E:759:ASN:HB3	1:E:889:LYS:HD2	1.98	0.46
1:E:988:VAL:O	1:E:992:ILE:HG13	2.15	0.46
1:G:259:SER:OG	1:G:262:GLU:N	2.42	0.46
1:G:693:ASN:HA	1:G:704:GLN:HB2	1.98	0.46
1:G:830:LEU:HD22	1:G:880:PHE:HD1	1.80	0.46
1:E:1087:PRO:HG3	1:E:1257:ASN:OD1	2.16	0.46
1:A:840:LYS:O	1:A:868:ILE:HG23	2.15	0.46
1:C:611:LYS:O	1:C:614:GLU:HB2	2.15	0.46
1:G:499:LEU:HD21	1:G:526:ILE:HA	1.97	0.46
1:A:666:ASN:OD1	1:A:666:ASN:N	2.31	0.46
1:A:69:VAL:HG22	1:A:112:TYR:CD2	2.51	0.46
1:E:673:PHE:CE2	1:E:727:SER:HB2	2.51	0.46
1:G:684:PRO:HA	1:G:688:ILE:HD11	1.98	0.46
1:C:326:LYS:NZ	1:C:331:ASP:O	2.49	0.46
1:C:992:ILE:O	1:C:996:VAL:HG23	2.15	0.46
1:A:614:GLU:OE2	1:A:656:LYS:NZ	2.48	0.46
1:G:1235:ASP:OD2	1:G:1239:ASN:N	2.47	0.46
1:G:1269:LEU:HG	1:G:1284:LEU:HD22	1.98	0.46
1:G:21:LEU:HB3	1:G:786:PHE:HB3	1.98	0.46
1:A:221:LEU:HD23	1:A:229:ILE:HD11	1.98	0.46
1:A:670:PRO:HG3	1:A:724:TYR:OH	2.15	0.46
1:E:21:LEU:HB3	1:E:786:PHE:HB3	1.98	0.46
1:E:453:LEU:HD23	1:E:453:LEU:HA	1.79	0.46
1:G:606:ALA:HB3	1:G:828:ALA:O	2.16	0.46
1:A:527:LYS:HG3	1:A:971:TRP:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1092:VAL:HG11	1:E:1292:PHE:CE1	2.50	0.46
1:E:880:PHE:CE2	1:E:882:CYS:HB2	2.51	0.46
1:G:355:PHE:HE1	1:G:574:ASN:HB2	1.81	0.46
1:G:543:PHE:HB2	1:G:565:PHE:CZ	2.51	0.46
1:G:744:THR:HA	1:G:747:TYR:CE1	2.50	0.46
1:A:583:ARG:O	1:A:587:THR:HG23	2.16	0.46
1:C:1269:LEU:HD13	1:C:1286:ILE:HD11	1.98	0.46
1:C:7:PHE:CZ	1:C:899:GLU:HG2	2.51	0.46
1:E:381:LEU:HD11	1:E:453:LEU:HD12	1.98	0.46
1:E:574:ASN:O	1:E:577:PRO:HD2	2.16	0.46
1:G:1036:ASN:O	1:G:1056:GLN:HG2	2.15	0.46
1:G:1126:PHE:O	1:G:1143:THR:HA	2.16	0.46
1:G:231:TYR:O	1:G:234:ILE:HG22	2.15	0.46
1:G:301:ASN:HD21	1:G:321:MET:H	1.64	0.46
1:G:651:GLY:O	1:G:768:ASN:HB3	2.16	0.46
1:C:1250:MET:HG3	1:C:1251:PRO:HD2	1.98	0.45
1:C:945:GLY:HA3	1:C:950:LYS:HA	1.97	0.45
2:D:-11:A:H2'	2:D:-10:C:O4'	2.16	0.45
1:E:1230:ILE:HG22	1:E:1242:ASP:HA	1.97	0.45
1:E:609:TRP:O	1:E:659:TYR:HB3	2.17	0.45
1:E:840:LYS:O	1:E:868:ILE:HG23	2.16	0.45
1:G:1025:GLN:HG2	1:G:1064:PHE:CE1	2.51	0.45
1:C:407:PHE:CD1	1:C:473:CYS:HB3	2.50	0.45
1:E:1181:TYR:CZ	1:E:1203:PHE:HB2	2.51	0.45
1:E:134:GLN:H	1:E:134:GLN:HG3	1.37	0.45
1:E:915:SER:O	1:E:926:TYR:HA	2.16	0.45
1:E:990:HIS:ND1	2:F:-2:G:H4'	2.30	0.45
1:A:402:LEU:O	1:A:406:VAL:HG12	2.16	0.45
1:C:27:THR:O	1:C:31:ILE:HG13	2.16	0.45
1:C:609:TRP:O	1:C:659:TYR:HB3	2.17	0.45
1:E:17:LEU:HD23	1:E:808:TRP:HB2	1.98	0.45
1:G:695:SER:OG	1:G:698:THR:OG1	2.32	0.45
1:A:1071:THR:HG22	1:A:1076:TYR:HE2	1.81	0.45
1:A:313:ASP:OD1	1:A:315:THR:OG1	2.35	0.45
1:A:612:ASN:OD1	1:A:612:ASN:N	2.45	0.45
1:A:856:ASN:ND2	1:A:858:LYS:O	2.50	0.45
1:C:731:HIS:CD2	1:C:732:PRO:HD2	2.50	0.45
1:E:1121:LYS:HB3	1:E:1123:TYR:CE1	2.52	0.45
1:E:263:VAL:O	1:E:272:TYR:OH	2.17	0.45
1:E:293:GLU:OE1	1:E:297:ARG:NH1	2.49	0.45
1:G:734:TRP:HA	1:G:737:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:GLY:O	1:A:768:ASN:HB3	2.16	0.45
2:B:-2:G:H2'	2:B:-1:A:O4'	2.16	0.45
1:E:928:LEU:HD22	1:E:928:LEU:HA	1.82	0.45
2:H:-4:U:C2'	2:H:-3:A:H5'	2.47	0.45
1:A:1142:TRP:O	1:A:1143:THR:OG1	2.34	0.45
1:A:673:PHE:CE2	1:A:727:SER:HB2	2.52	0.45
1:A:744:THR:HA	1:A:747:TYR:CE1	2.52	0.45
1:A:925:TYR:HE2	1:A:938:GLN:HB2	1.82	0.45
1:A:915:SER:O	1:A:926:TYR:HA	2.16	0.45
1:C:1217:MET:HE3	1:C:1217:MET:HB3	1.93	0.45
1:C:235:LYS:O	1:C:239:ALA:HB2	2.17	0.45
1:E:188:ASN:HB3	1:E:195:ILE:HD12	1.99	0.45
1:E:640:ILE:HD11	1:E:782:LYS:HB3	1.98	0.45
1:A:237:ASP:O	1:A:297:ARG:NH2	2.49	0.45
1:A:682:TYR:OH	1:A:731:HIS:HD2	1.99	0.45
1:C:802:ASN:HB3	2:D:0:U:O4	2.17	0.45
1:C:878:PHE:C	1:C:879:PHE:HD1	2.20	0.45
1:C:918:ARG:H	1:C:918:ARG:HG2	1.63	0.45
1:E:113:ILE:HD12	1:E:190:TYR:HD1	1.82	0.45
1:E:731:HIS:CD2	1:E:732:PRO:HD2	2.51	0.45
1:G:858:LYS:HG2	1:G:858:LYS:H	1.56	0.45
1:G:973:LYS:O	1:G:977:ILE:HG13	2.17	0.45
2:B:3:A:C2'	2:B:4:U:H5'	2.47	0.45
1:C:1218:ARG:NH2	1:C:1255:ASP:OD1	2.50	0.45
1:A:1268:MET:HE3	1:A:1291:TYR:HD1	1.81	0.45
1:A:208:LEU:HB3	1:A:209:PRO:HD3	1.99	0.45
1:A:202:ARG:HD2	1:A:327:GLN:HA	1.99	0.45
1:A:954:HIS:NE2	1:A:1018:LYS:HE3	2.32	0.45
1:C:71:ILE:CD1	1:C:105:ILE:HG23	2.46	0.45
1:C:50:ALA:O	1:C:54:ILE:HG13	2.17	0.45
1:E:121:ASN:O	1:E:127:LEU:HB2	2.17	0.45
1:E:946:ASN:OD1	1:E:947:ASP:N	2.48	0.45
1:A:712:PHE:HD2	1:A:713:ASN:N	2.15	0.45
1:A:731:HIS:CD2	1:A:732:PRO:HD2	2.52	0.45
1:C:244:PHE:CE1	1:C:280:LYS:HD3	2.51	0.45
1:E:300:ILE:O	1:E:304:ILE:HG13	2.16	0.45
1:E:417:VAL:HA	1:E:459:ALA:HB1	1.99	0.45
1:G:402:LEU:HD11	1:G:482:PHE:HE2	1.81	0.45
1:A:1250:MET:HG3	1:A:1251:PRO:HD2	1.98	0.44
1:C:639:LYS:HD2	1:C:639:LYS:HA	1.57	0.44
1:C:988:VAL:O	1:C:992:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:TYR:CE1	1:A:1054:ALA:HB3	2.52	0.44
1:A:1150:ARG:NE	1:A:1230:ILE:HD11	2.32	0.44
1:C:4:TYR:OH	1:C:1001:ALA:O	2.26	0.44
1:E:1114:LYS:HG3	1:E:1127:SER:HB2	2.00	0.44
1:E:606:ALA:HB3	1:E:828:ALA:O	2.17	0.44
1:G:1178:LEU:HD12	1:G:1185:TYR:HB3	1.99	0.44
1:G:1291:TYR:O	1:G:1295:VAL:HG12	2.17	0.44
1:E:474:ARG:HG2	1:E:477:GLU:HG2	1.99	0.44
1:E:981:LYS:HE3	1:E:1020:GLU:OE2	2.18	0.44
1:G:635:LYS:HD3	1:G:635:LYS:HA	1.85	0.44
1:A:11:TYR:CG	1:A:893:ALA:HB2	2.53	0.44
1:A:269:PHE:HA	1:A:272:TYR:CD2	2.52	0.44
1:C:1183:ILE:HG12	1:C:1194:ALA:HB1	2.00	0.44
1:E:1037:TYR:CE1	1:E:1054:ALA:HB3	2.52	0.44
1:E:1215:LEU:HA	1:E:1215:LEU:HD12	1.78	0.44
1:E:630:LEU:HG	1:E:631:GLY:N	2.31	0.44
1:E:670:PRO:HG3	1:E:724:TYR:OH	2.17	0.44
1:E:695:SER:HG	1:E:698:THR:HG1	1.63	0.44
1:G:682:TYR:HD2	1:G:727:SER:HB3	1.82	0.44
1:G:18:ARG:HD3	2:H:-15:U:O2	2.16	0.44
1:A:1028:GLU:O	1:A:1032:ILE:HG13	2.18	0.44
1:A:949:MET:HG3	2:B:-8:G:C5	2.52	0.44
1:C:880:PHE:CE2	1:C:882:CYS:HB2	2.52	0.44
1:E:677:LYS:HG3	1:E:678:SER:N	2.32	0.44
1:E:18:ARG:HG2	1:E:881:HIS:CD2	2.52	0.44
1:A:685:SER:OG	1:A:688:ILE:HG23	2.18	0.44
1:A:718:ARG:HD3	1:A:745:GLN:HA	1.99	0.44
1:C:1038:LEU:HB3	1:C:1055:TYR:HB2	1.99	0.44
1:C:441:ILE:HG13	1:C:442:ALA:N	2.33	0.44
1:E:973:LYS:O	1:E:977:ILE:HG13	2.18	0.44
1:G:1045:PHE:CE2	1:G:1052:LEU:HD13	2.53	0.44
1:G:560:HIS:O	1:G:564:VAL:HG22	2.18	0.44
1:G:981:LYS:O	1:G:985:LEU:HG	2.17	0.44
1:A:1146:SER:OG	1:A:1171:THR:HG23	2.18	0.44
1:A:697:HIS:ND1	1:A:698:THR:HG23	2.32	0.44
1:C:1006:GLU:HB2	1:C:1079:ALA:HB2	2.00	0.44
1:E:420:TYR:O	1:E:423:GLN:HG3	2.17	0.44
1:E:871:LYS:O	1:E:874:THR:OG1	2.28	0.44
1:G:110:SER:O	1:G:113:ILE:HG12	2.18	0.44
1:G:1183:ILE:HD11	1:G:1198:GLU:CG	2.48	0.44
1:A:1128:PHE:HB2	1:A:1133:PHE:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:ILE:HD11	1:A:782:LYS:HB3	1.99	0.44
1:C:1026:LYS:O	1:C:1030:MET:HG3	2.18	0.44
1:C:102:LYS:HG3	1:C:204:VAL:HG21	1.99	0.44
1:E:530:LEU:HB3	1:E:579:TYR:HD1	1.83	0.44
1:G:1102:VAL:O	1:G:1106:GLN:HG3	2.18	0.44
1:G:1121:LYS:HB3	1:G:1123:TYR:CE1	2.53	0.44
1:G:624:LYS:HB3	1:G:629:TYR:HE2	1.83	0.44
1:A:1116:CYS:HB3	1:A:1190:CYS:HA	2.00	0.44
1:A:598:LEU:HD11	1:A:832:TYR:HB2	2.00	0.44
1:A:722:ASP:OD2	1:A:744:THR:HG21	2.18	0.44
1:C:1045:PHE:CE2	1:C:1052:LEU:HD13	2.53	0.44
1:C:801:PRO:O	1:C:1041:LYS:NZ	2.27	0.44
1:G:121:ASN:HB3	1:G:126:ASN:HB2	2.00	0.44
1:A:20:GLU:OE2	1:A:877:LYS:HE3	2.17	0.43
1:E:609:TRP:HB2	1:E:659:TYR:CD2	2.53	0.43
2:F:-11:A:H2'	2:F:-10:C:O4'	2.18	0.43
1:A:631:GLY:HA2	1:A:784:TYR:O	2.18	0.43
1:C:127:LEU:O	1:C:136:SER:OG	2.27	0.43
1:C:21:LEU:HB3	1:C:786:PHE:HB3	2.00	0.43
1:C:234:ILE:HD13	1:C:260:LEU:HD21	1.99	0.43
1:G:15:LYS:HB2	1:G:15:LYS:HE2	1.85	0.43
1:G:688:ILE:HA	1:G:691:ILE:HG12	2.00	0.43
1:G:992:ILE:O	1:G:996:VAL:HG23	2.18	0.43
1:G:100:SER:O	1:G:104:THR:HG22	2.19	0.43
1:G:1087:PRO:HG2	1:G:1241:PHE:CE2	2.54	0.43
1:G:985:LEU:O	1:G:988:VAL:HG12	2.18	0.43
2:H:-2:G:H2'	2:H:-1:A:O4'	2.18	0.43
1:A:107:LYS:O	1:A:111:GLU:HB3	2.19	0.43
1:A:342:LEU:HD23	1:A:348:VAL:HG22	2.00	0.43
1:A:63:GLU:OE2	1:A:274:ASN:ND2	2.50	0.43
1:A:957:LEU:HD21	1:A:981:LYS:CG	2.48	0.43
1:C:1121:LYS:HB3	1:C:1123:TYR:CE1	2.53	0.43
1:C:281:PHE:O	1:C:285:ILE:HG12	2.19	0.43
1:G:1217:MET:H	1:G:1217:MET:HG2	1.42	0.43
1:G:128:ILE:HB	1:G:176:THR:HG23	1.99	0.43
1:A:356:TYR:CZ	1:A:529:LEU:HD22	2.54	0.43
1:A:839:LYS:HB2	1:A:874:THR:HB	2.01	0.43
1:A:992:ILE:O	1:A:996:VAL:HG23	2.19	0.43
1:C:643:ASP:O	1:C:646:ILE:HG12	2.18	0.43
1:C:670:PRO:HG3	1:C:724:TYR:OH	2.19	0.43
1:E:1195:ILE:HD13	1:E:1207:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:VAL:HG21	1:E:1053:ARG:HB3	2.01	0.43
1:G:285:ILE:HG23	1:G:321:MET:HB2	2.00	0.43
1:A:1234:ALA:HB2	1:A:1240:PHE:CE2	2.54	0.43
1:A:201:TYR:O	1:A:205:ASP:HB2	2.17	0.43
1:A:695:SER:OG	1:A:698:THR:OG1	2.21	0.43
2:B:1:A:H1'	2:B:2:G:C8	2.53	0.43
1:C:1071:THR:HG22	1:C:1076:TYR:HE2	1.84	0.43
1:C:1169:TYR:HD1	1:C:1169:TYR:N	2.17	0.43
1:C:313:ASP:CG	1:C:315:THR:HG1	2.21	0.43
1:G:822:TYR:OH	1:G:1037:TYR:OH	2.31	0.43
1:A:341:LYS:HG3	1:A:342:LEU:N	2.32	0.43
1:A:864:GLU:CD	1:A:864:GLU:H	2.15	0.43
1:A:18:ARG:HB3	2:B:-15:U:H1'	2.01	0.43
1:C:1087:PRO:HG2	1:C:1241:PHE:CE2	2.54	0.43
1:C:814:GLU:O	1:C:818:GLN:HG3	2.19	0.43
1:G:1013:LYS:HD3	1:G:1017:PHE:CZ	2.54	0.43
1:G:122:LEU:O	1:G:127:LEU:HD22	2.19	0.43
1:G:170:LYS:O	1:G:173:LYS:HB2	2.19	0.43
1:G:402:LEU:HD11	1:G:482:PHE:CE2	2.53	0.43
1:G:614:GLU:OE2	1:G:656:LYS:NZ	2.52	0.43
1:G:696:THR:HG22	1:G:710:PHE:HB2	2.00	0.43
1:C:1063:THR:HG23	1:C:1066:LYS:H	1.84	0.43
1:C:687:ASP:O	1:C:691:ILE:HG12	2.19	0.43
1:E:1006:GLU:HB2	1:E:1079:ALA:HB2	2.00	0.43
1:E:708:GLU:N	1:E:708:GLU:OE1	2.52	0.43
1:A:1107:GLU:O	1:A:1110:SER:OG	2.31	0.42
1:A:225:ALA:HB1	1:A:228:ALA:HB2	2.01	0.42
1:C:618:THR:HG23	1:C:618:THR:O	2.19	0.42
1:C:957:LEU:HD21	1:C:981:LYS:HE2	2.00	0.42
1:E:1094:GLN:OE1	1:E:1138:ALA:HB2	2.19	0.42
1:E:402:LEU:O	1:E:406:VAL:HG12	2.19	0.42
1:A:1045:PHE:CE2	1:A:1052:LEU:HD13	2.54	0.42
1:A:572:LEU:HA	1:A:572:LEU:HD23	1.77	0.42
1:A:623:ILE:O	1:A:655:LYS:HG2	2.19	0.42
1:A:985:LEU:O	1:A:988:VAL:HG12	2.18	0.42
2:B:-17:A:O2'	2:B:-5:G:N7	2.48	0.42
1:C:842:THR:HB	1:C:843:HIS:HD2	1.84	0.42
2:D:-5:G:HO2'	2:D:-4:U:P	2.42	0.42
1:E:803:LEU:HA	1:E:803:LEU:HD23	1.89	0.42
1:G:724:TYR:O	1:G:728:ILE:HG13	2.19	0.42
1:A:585:TYR:O	1:A:588:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:TYR:O	1:A:728:ILE:HG13	2.20	0.42
1:C:1071:THR:HG22	1:C:1076:TYR:CE2	2.54	0.42
1:C:125:GLN:HG3	1:C:125:GLN:H	1.40	0.42
1:C:31:ILE:HD13	1:C:600:PHE:HE1	1.84	0.42
1:C:482:PHE:HA	1:C:485:ILE:HG13	2.01	0.42
1:E:79:TYR:HD2	1:E:212:LEU:HD11	1.83	0.42
1:G:61:PHE:O	1:G:65:ILE:HG22	2.19	0.42
1:G:688:ILE:HA	1:G:691:ILE:CG1	2.49	0.42
1:E:349:VAL:O	1:E:353:GLN:HB3	2.19	0.42
1:E:438:GLN:O	1:E:441:ILE:HG13	2.20	0.42
1:E:508:ASN:OD1	1:E:508:ASN:N	2.50	0.42
1:E:684:PRO:CB	1:E:688:ILE:HD11	2.48	0.42
1:A:929:VAL:HA	1:A:934:ASN:O	2.20	0.42
1:C:110:SER:O	1:C:113:ILE:HG12	2.19	0.42
1:C:1169:TYR:CD1	1:C:1169:TYR:N	2.87	0.42
1:C:1228:TYR:HB2	1:C:1243:SER:HB3	2.01	0.42
1:C:524:LYS:HE3	1:C:970:ASP:HB3	2.02	0.42
1:E:1034:LYS:HD2	1:E:1034:LYS:HA	1.90	0.42
1:E:272:TYR:CD1	1:E:281:PHE:HB2	2.54	0.42
1:G:905:LYS:HZ1	1:G:1277:GLN:HG3	1.84	0.42
1:A:1210:VAL:O	1:A:1214:ILE:HG13	2.20	0.42
1:C:340:ASP:O	1:C:342:LEU:HD12	2.18	0.42
1:E:359:ILE:O	1:E:370:ILE:HD11	2.19	0.42
1:E:382:LYS:HE2	1:E:382:LYS:HB3	1.51	0.42
1:G:697:HIS:CE1	1:G:698:THR:HG23	2.54	0.42
1:G:844:PRO:HG2	1:G:847:GLU:HB2	2.02	0.42
1:A:395:ASN:O	1:A:395:ASN:ND2	2.36	0.42
1:C:231:TYR:O	1:C:234:ILE:HG22	2.18	0.42
1:C:691:ILE:HG23	1:C:696:THR:OG1	2.20	0.42
1:C:691:ILE:O	1:C:695:SER:N	2.53	0.42
1:C:87:LYS:HZ1	1:C:213:GLU:CD	2.22	0.42
1:E:648:GLU:HB3	1:E:649:ASN:OD1	2.20	0.42
1:A:985:LEU:HD11	1:A:1023:VAL:HG12	2.02	0.42
1:A:464:ASN:ND2	1:A:473:CYS:O	2.43	0.42
1:C:70:CYS:HB2	1:C:248:TYR:HE1	1.84	0.42
2:D:3:A:H2'	2:D:4:U:H5'	2.02	0.42
1:E:1174:LEU:HD23	1:E:1174:LEU:HA	1.91	0.42
1:E:49:LYS:HD3	1:E:158:ASP:HB3	2.02	0.42
1:E:682:TYR:CD2	1:E:727:SER:HB3	2.54	0.42
1:G:1037:TYR:CE1	1:G:1054:ALA:HB3	2.54	0.42
1:G:4:TYR:CZ	1:G:1073:ILE:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD22	1:A:32:LYS:HG3	2.01	0.42
1:A:759:ASN:HB3	1:A:889:LYS:HD2	2.02	0.42
1:C:109:ILE:O	1:C:113:ILE:HG23	2.19	0.42
1:C:197:THR:HG22	1:C:328:ILE:HD11	2.01	0.42
1:C:377:LEU:HG	1:C:564:VAL:HG21	2.02	0.42
1:C:499:LEU:HD13	1:C:502:ILE:HD12	2.02	0.42
1:C:985:LEU:O	1:C:988:VAL:HG12	2.20	0.42
1:E:345:ASP:OD2	1:E:514:LEU:N	2.52	0.42
1:E:406:VAL:HG13	1:E:407:PHE:CD2	2.54	0.42
1:E:443:LYS:HD2	1:E:447:LYS:HD2	2.01	0.42
1:E:466:HIS:N	1:E:466:HIS:ND1	2.68	0.42
1:E:378:PHE:HE2	1:E:543:PHE:CE1	2.38	0.42
1:E:543:PHE:HB2	1:E:565:PHE:CZ	2.55	0.42
1:G:609:TRP:CD1	1:G:824:LEU:HD13	2.54	0.42
1:A:371:LYS:NZ	1:A:490:ASP:OD1	2.52	0.42
1:A:606:ALA:HB3	1:A:828:ALA:O	2.19	0.42
1:C:352:MET:SD	1:C:526:ILE:HG23	2.60	0.42
1:E:418:LEU:HD12	1:E:445:THR:HG21	2.02	0.42
1:G:1063:THR:HG23	1:G:1066:LYS:H	1.85	0.42
1:G:687:ASP:O	1:G:690:ARG:HB3	2.19	0.42
1:G:70:CYS:SG	1:G:71:ILE:N	2.92	0.42
1:G:850:ALA:O	2:H:-18:A:N6	2.51	0.42
1:A:1126:PHE:O	1:A:1143:THR:HA	2.20	0.41
1:A:1174:LEU:HA	1:A:1174:LEU:HD23	1.81	0.41
1:A:366:GLU:OE1	1:A:560:HIS:NE2	2.30	0.41
1:A:38:LEU:H	1:A:38:LEU:HD12	1.85	0.41
1:C:378:PHE:CD2	1:C:482:PHE:HB3	2.55	0.41
1:C:693:ASN:HA	1:C:704:GLN:HB2	2.01	0.41
1:C:830:LEU:HD22	1:C:880:PHE:HD1	1.85	0.41
1:E:1130:TYR:HB3	1:E:1138:ALA:O	2.19	0.41
1:E:1250:MET:HG3	1:E:1251:PRO:HD2	2.02	0.41
1:G:1215:LEU:HD12	1:G:1215:LEU:HA	1.89	0.41
1:G:244:PHE:HE2	1:G:280:LYS:HD3	1.85	0.41
1:G:58:HIS:O	1:G:62:ILE:HG13	2.20	0.41
1:A:1127:SER:HA	1:A:1143:THR:HA	2.01	0.41
1:C:1087:PRO:O	1:C:1298:ARG:NH2	2.50	0.41
1:E:1045:PHE:CE2	1:E:1052:LEU:HD13	2.55	0.41
1:E:1102:VAL:O	1:E:1106:GLN:HG3	2.21	0.41
1:E:1191:ILE:HG22	1:E:1195:ILE:HG13	2.01	0.41
1:E:397:LYS:HE2	1:E:397:LYS:HB3	1.82	0.41
1:E:499:LEU:HA	1:E:499:LEU:HD23	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1250:MET:HG3	1:G:1251:PRO:HD2	2.02	0.41
1:G:631:GLY:HA2	1:G:784:TYR:O	2.21	0.41
1:A:355:PHE:HE1	1:A:574:ASN:HB2	1.85	0.41
1:A:908:ALA:O	1:A:911:VAL:HG22	2.20	0.41
1:E:290:VAL:HB	1:E:293:GLU:HG2	2.00	0.41
1:G:402:LEU:O	1:G:406:VAL:HG12	2.20	0.41
1:G:381:LEU:O	1:G:479:LEU:HD11	2.20	0.41
1:A:61:PHE:O	1:A:65:ILE:HG22	2.20	0.41
1:C:282:ASN:CG	1:C:323:VAL:HG12	2.40	0.41
1:E:131:LYS:HB2	1:E:134:GLN:NE2	2.35	0.41
1:E:659:TYR:CE1	1:E:762:TYR:HE1	2.38	0.41
1:E:91:ASP:HB2	1:E:94:LEU:HG	2.02	0.41
1:G:1110:SER:O	1:G:1192:LYS:NZ	2.47	0.41
1:G:371:LYS:NZ	1:G:490:ASP:OD1	2.40	0.41
1:A:11:TYR:CD1	1:A:893:ALA:HB2	2.56	0.41
1:A:872:ARG:H	1:A:872:ARG:HG3	1.66	0.41
1:C:1037:TYR:CE1	1:C:1054:ALA:HB3	2.55	0.41
1:C:463:PHE:CZ	1:C:467:ARG:HD2	2.55	0.41
1:C:780:GLN:OE1	1:C:782:LYS:HE3	2.21	0.41
2:D:-2:G:H2'	2:D:-1:A:O4'	2.19	0.41
1:G:1183:ILE:HD11	1:G:1198:GLU:HG3	2.03	0.41
1:G:200:ILE:O	1:G:204:VAL:HG12	2.21	0.41
1:G:618:THR:O	1:G:618:THR:HG23	2.21	0.41
1:A:1005:PHE:HB2	1:A:1076:TYR:CD1	2.55	0.41
1:E:393:PHE:CZ	1:E:453:LEU:HD21	2.56	0.41
1:E:722:ASP:O	1:E:726:GLN:HG3	2.19	0.41
1:G:1034:LYS:HA	1:G:1034:LYS:HD2	1.90	0.41
1:G:1094:GLN:NE2	1:G:1137:ALA:HB3	2.35	0.41
2:H:1:A:H1'	2:H:2:G:C8	2.55	0.41
1:A:418:LEU:O	1:A:422:THR:OG1	2.36	0.41
1:C:778:VAL:HB	1:C:783:LEU:HD23	2.03	0.41
1:E:222:LYS:HE2	1:E:222:LYS:HB3	1.83	0.41
1:E:904:LEU:O	1:E:908:ALA:N	2.53	0.41
1:E:970:ASP:OD1	1:E:973:LYS:HB2	2.21	0.41
1:G:1195:ILE:HD13	1:G:1207:LEU:HD21	2.03	0.41
1:G:1092:VAL:HG11	1:G:1292:PHE:CE1	2.55	0.41
1:G:299:GLY:H	1:G:302:GLU:HB3	1.86	0.41
1:A:1052:LEU:HD12	1:A:1052:LEU:HA	1.78	0.41
1:A:135:GLU:CD	1:A:136:SER:H	2.23	0.41
1:A:241:GLU:HG2	1:A:283:THR:HB	2.02	0.41
1:E:260:LEU:HD11	1:E:300:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:THR:O	1:E:419:GLU:HB3	2.21	0.41
1:G:1005:PHE:O	1:G:1076:TYR:HA	2.20	0.41
1:G:1216:GLN:HG3	1:G:1216:GLN:O	2.21	0.41
1:G:134:GLN:H	1:G:134:GLN:HG2	1.52	0.41
1:A:496:LYS:HD2	1:A:496:LYS:HA	1.86	0.41
1:C:1034:LYS:HD2	1:C:1034:LYS:HA	1.82	0.41
1:C:762:TYR:CD2	1:C:820:VAL:HG11	2.54	0.41
1:E:1026:LYS:O	1:E:1030:MET:HG3	2.21	0.41
1:E:402:LEU:HD11	1:E:482:PHE:CE2	2.56	0.41
1:E:576:VAL:CG1	1:E:577:PRO:HD3	2.50	0.41
1:E:640:ILE:HG23	1:E:773:TYR:OH	2.21	0.41
1:G:790:ASN:OD1	1:G:790:ASN:N	2.54	0.41
1:C:197:THR:CG2	1:C:328:ILE:HD11	2.51	0.41
1:C:409:ASP:HB3	1:C:412:VAL:HG23	2.03	0.41
1:C:740:ARG:HG2	1:C:740:ARG:H	1.74	0.41
1:E:575:ILE:HG13	1:E:575:ILE:H	1.54	0.41
1:A:4:TYR:OH	1:A:1073:ILE:HD11	2.20	0.41
1:E:653:GLY:HA3	1:E:771:GLU:HB2	2.03	0.41
1:E:16:THR:HA	1:E:883:PRO:HA	2.02	0.41
2:F:1:A:H1'	2:F:2:G:C8	2.55	0.41
1:G:113:ILE:HD12	1:G:190:TYR:HD1	1.86	0.41
1:G:84:PHE:O	1:G:87:LYS:HB2	2.21	0.41
1:A:224:LYS:O	1:A:224:LYS:HG3	2.20	0.40
1:A:21:LEU:O	1:A:878:PHE:HB2	2.22	0.40
1:C:231:TYR:HB3	1:E:708:GLU:OE2	2.21	0.40
1:C:981:LYS:O	1:C:985:LEU:HG	2.20	0.40
1:E:260:LEU:HD12	1:E:260:LEU:HA	1.91	0.40
1:E:396:ASP:OD1	1:E:396:ASP:N	2.54	0.40
1:E:841:ILE:HG23	1:E:866:ASP:HB3	2.03	0.40
1:G:208:LEU:HB3	1:G:209:PRO:HD3	2.04	0.40
1:G:776:SER:O	1:G:780:GLN:HG3	2.21	0.40
1:C:574:ASN:O	1:C:577:PRO:HD2	2.21	0.40
1:C:70:CYS:SG	1:C:71:ILE:N	2.94	0.40
1:C:840:LYS:O	1:C:868:ILE:HG23	2.21	0.40
1:E:1071:THR:HG22	1:E:1076:TYR:HE2	1.86	0.40
1:E:811:LEU:HD23	1:E:822:TYR:HB3	2.04	0.40
1:G:345:ASP:OD1	1:G:585:TYR:OH	2.27	0.40
1:G:492:ILE:HD13	1:G:533:THR:HG23	2.02	0.40
1:A:522:ASP:N	1:A:522:ASP:OD1	2.53	0.40
1:C:365:VAL:HG23	1:C:564:VAL:HG12	2.02	0.40
1:E:54:ILE:HG21	1:E:182:PHE:HE2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:800:ARG:NH1	1:G:1042:ASP:OD1	2.54	0.40
1:G:278:ILE:HG22	1:G:282:ASN:HD21	1.87	0.40
1:G:794:SER:OG	2:H:-5:G:OP1	2.20	0.40
1:A:278:ILE:HG22	1:A:282:ASN:ND2	2.36	0.40
2:B:-17:A:C8	2:B:-5:G:C6	3.10	0.40
1:C:948:ARG:HG2	1:C:949:MET:N	2.37	0.40
1:E:198:SER:HB3	1:E:201:TYR:HB3	2.04	0.40
1:E:618:THR:O	1:E:618:THR:HG23	2.21	0.40
1:E:7:PHE:CZ	1:E:899:GLU:HG2	2.56	0.40
1:G:269:PHE:HA	1:G:272:TYR:CD2	2.57	0.40
1:C:2:SER:HB3	1:C:5:GLN:HB2	2.02	0.40
1:C:722:ASP:OD2	1:C:744:THR:HG21	2.21	0.40
1:E:985:LEU:HD13	1:E:1027:LEU:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LYS:NZ	1:A:706:GLY:O[2_535]	2.15	0.05

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1256/1302 (96%)	1232 (98%)	24 (2%)	0	100	100
1	C	1256/1302 (96%)	1237 (98%)	19 (2%)	0	100	100
1	E	1248/1302 (96%)	1225 (98%)	23 (2%)	0	100	100
1	G	1239/1302 (95%)	1217 (98%)	22 (2%)	0	100	100
All	All	4999/5208 (96%)	4911 (98%)	88 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1153/1185 (97%)	1041 (90%)	112 (10%)	9	34
1	C	1153/1185 (97%)	1050 (91%)	103 (9%)	11	39
1	E	1146/1185 (97%)	1034 (90%)	112 (10%)	9	34
1	G	1140/1185 (96%)	1022 (90%)	118 (10%)	8	31
All	All	4592/4740 (97%)	4147 (90%)	445 (10%)	9	34

All (445) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	7	PHE
1	A	16	THR
1	A	28	LEU
1	A	71	ILE
1	A	72	SER
1	A	74	ASP
1	A	96	LYS
1	A	111	GLU
1	A	129	ASP
1	A	136	SER
1	A	161	ASP
1	A	171	SER
1	A	173	LYS
1	A	176	THR
1	A	204	VAL
1	A	205	ASP
1	A	240	GLU
1	A	245	ASP
1	A	246	ILE
1	A	261	ASP
1	A	268	ASN
1	A	272	TYR
1	A	273	LEU

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Mol	Chain	Res	Type
1	A	276	SER
1	A	289	PHE
1	A	297	ARG
1	A	315	THR
1	A	318	LYS
1	A	328	ILE
1	A	343	GLU
1	A	376	LEU
1	A	377	LEU
1	A	384	GLN
1	A	388	LEU
1	A	395	ASN
1	A	400	THR
1	A	402	LEU
1	A	410	TYR
1	A	418	LEU
1	A	499	LEU
1	A	503	SER
1	A	508	ASN
1	A	513	ASP
1	A	515	LEU
1	A	522	ASP
1	A	529	LEU
1	A	533	THR
1	A	555	LEU
1	A	576	VAL
1	A	599	ASN
1	A	603	SER
1	A	612	ASN
1	A	618	THR
1	A	635	LYS
1	A	637	ASN
1	A	639	LYS
1	A	644	LYS
1	A	652	GLU
1	A	655	LYS
1	A	666	ASN
1	A	668	MET
1	A	681	PHE
1	A	688	ILE
1	A	702	SER
1	A	708	GLU

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Mol	Chain	Res	Type
1	A	709	LYS
1	A	712	PHE
1	A	742	SER
1	A	744	THR
1	A	747	TYR
1	A	765	THR
1	A	769	ILE
1	A	777	VAL
1	A	783	LEU
1	A	790	ASN
1	A	817	LEU
1	A	824	LEU
1	A	846	LYS
1	A	864	GLU
1	A	872	ARG
1	A	891	SER
1	A	895	LYS
1	A	907	LYS
1	A	918	ARG
1	A	930	ASP
1	A	948	ARG
1	A	956	LYS
1	A	957	LEU
1	A	968	ARG
1	A	1010	PHE
1	A	1014	ARG
1	A	1016	ARG
1	A	1020	GLU
1	A	1084	LYS
1	A	1095	LEU
1	A	1139	LYS
1	A	1141	LYS
1	A	1165	THR
1	A	1171	THR
1	A	1182	SER
1	A	1187	HIS
1	A	1215	LEU
1	A	1226	LEU
1	A	1229	LEU
1	A	1243	SER
1	A	1244	ARG
1	A	1249	ASN

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Mol	Chain	Res	Type
1	A	1267	LEU
1	A	1270	LEU
1	A	1297	ASN
1	A	1298	ARG
1	C	0	ASN
1	C	3	ILE
1	C	17	LEU
1	C	28	LEU
1	C	34	ARG
1	C	48	LYS
1	C	70	CYS
1	C	74	ASP
1	C	91	ASP
1	C	111	GLU
1	C	120	LYS
1	C	125	GLN
1	C	129	ASP
1	C	135	GLU
1	C	136	SER
1	C	150	ILE
1	C	173	LYS
1	C	180	LYS
1	C	204	VAL
1	C	227	GLU
1	C	246	ILE
1	C	260	LEU
1	C	268	ASN
1	C	272	TYR
1	C	273	LEU
1	C	297	ARG
1	C	315	THR
1	C	318	LYS
1	C	323	VAL
1	C	340	ASP
1	C	365	VAL
1	C	377	LEU
1	C	384	GLN
1	C	397	LYS
1	C	402	LEU
1	C	428	LYS
1	C	439	GLU
1	C	440	LEU

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Mol	Chain	Res	Type
1	C	491	GLU
1	C	515	LEU
1	C	522	ASP
1	C	529	LEU
1	C	533	THR
1	C	535	ASN
1	C	555	LEU
1	C	575	ILE
1	C	576	VAL
1	C	594	GLU
1	C	598	LEU
1	C	599	ASN
1	C	610	ASP
1	C	612	ASN
1	C	634	ASN
1	C	637	ASN
1	C	639	LYS
1	C	644	LYS
1	C	666	ASN
1	C	704	GLN
1	C	712	PHE
1	C	736	ASP
1	C	740	ARG
1	C	742	SER
1	C	743	ASP
1	C	765	THR
1	C	783	LEU
1	C	794	SER
1	C	817	LEU
1	C	820	VAL
1	C	824	LEU
1	C	842	THR
1	C	846	LYS
1	C	895	LYS
1	C	918	ARG
1	C	922	HIS
1	C	925	TYR
1	C	943	ILE
1	C	947	ASP
1	C	957	LEU
1	C	968	ARG
1	C	995	LEU

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Mol	Chain	Res	Type
1	C	1020	GLU
1	C	1042	ASP
1	C	1071	THR
1	C	1084	LYS
1	C	1095	LEU
1	C	1119	LEU
1	C	1139	LYS
1	C	1143	THR
1	C	1152	ILE
1	C	1163	TRP
1	C	1169	TYR
1	C	1171	THR
1	C	1206	LYS
1	C	1215	LEU
1	C	1217	MET
1	C	1220	SER
1	C	1225	GLU
1	C	1226	LEU
1	C	1229	LEU
1	C	1250	MET
1	C	1253	ASP
1	C	1267	LEU
1	C	1270	LEU
1	E	0	ASN
1	E	17	LEU
1	E	26	LYS
1	E	28	LEU
1	E	74	ASP
1	E	96	LYS
1	E	110	SER
1	E	124	ASN
1	E	129	ASP
1	E	134	GLN
1	E	135	GLU
1	E	152	LEU
1	E	176	THR
1	E	205	ASP
1	E	221	LEU
1	E	240	GLU
1	E	246	ILE
1	E	272	TYR
1	E	273	LEU

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Mol	Chain	Res	Type
1	E	276	SER
1	E	294	ASN
1	E	295	THR
1	E	297	ARG
1	E	298	LYS
1	E	308	SER
1	E	321	MET
1	E	331	ASP
1	E	353	GLN
1	E	359	ILE
1	E	370	ILE
1	E	376	LEU
1	E	384	GLN
1	E	396	ASP
1	E	402	LEU
1	E	408	ASP
1	E	443	LYS
1	E	444	LYS
1	E	445	THR
1	E	449	LYS
1	E	451	LEU
1	E	452	SER
1	E	462	GLU
1	E	466	HIS
1	E	468	ASP
1	E	469	ILE
1	E	474	ARG
1	E	494	GLN
1	E	508	ASN
1	E	514	LEU
1	E	515	LEU
1	E	522	ASP
1	E	529	LEU
1	E	555	LEU
1	E	575	ILE
1	E	594	GLU
1	E	599	ASN
1	E	612	ASN
1	E	613	LYS
1	E	618	THR
1	E	620	ILE
1	E	626	ASP

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Mol	Chain	Res	Type
1	E	627	LYS
1	E	637	ASN
1	E	644	LYS
1	E	648	GLU
1	E	666	ASN
1	E	678	SER
1	E	685	SER
1	E	708	GLU
1	E	744	THR
1	E	746	ARG
1	E	747	TYR
1	E	755	ARG
1	E	777	VAL
1	E	783	LEU
1	E	817	LEU
1	E	824	LEU
1	E	846	LYS
1	E	858	LYS
1	E	902	LEU
1	E	915	SER
1	E	918	ARG
1	E	925	TYR
1	E	928	LEU
1	E	948	ARG
1	E	1019	VAL
1	E	1020	GLU
1	E	1026	LYS
1	E	1042	ASP
1	E	1053	ARG
1	E	1071	THR
1	E	1095	LEU
1	E	1098	LYS
1	E	1105	SER
1	E	1114	LYS
1	E	1120	ASP
1	E	1141	LYS
1	E	1152	ILE
1	E	1163	TRP
1	E	1168	VAL
1	E	1184	GLU
1	E	1215	LEU
1	E	1218	ARG

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Mol	Chain	Res	Type
1	E	1221	LYS
1	E	1226	LEU
1	E	1229	LEU
1	E	1244	ARG
1	E	1250	MET
1	E	1267	LEU
1	E	1270	LEU
1	E	1277	GLN
1	E	1289	GLU
1	G	0	ASN
1	G	10	LYS
1	G	17	LEU
1	G	28	LEU
1	G	43	ARG
1	G	68	SER
1	G	70	CYS
1	G	72	SER
1	G	74	ASP
1	G	91	ASP
1	G	94	LEU
1	G	102	LYS
1	G	110	SER
1	G	117	GLU
1	G	121	ASN
1	G	125	GLN
1	G	129	ASP
1	G	134	GLN
1	G	157	SER
1	G	176	THR
1	G	178	TYR
1	G	187	LYS
1	G	202	ARG
1	G	205	ASP
1	G	227	GLU
1	G	241	GLU
1	G	246	ILE
1	G	272	TYR
1	G	273	LEU
1	G	289	PHE
1	G	295	THR
1	G	297	ARG
1	G	298	LYS

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Mol	Chain	Res	Type
1	G	310	GLN
1	G	323	VAL
1	G	325	PHE
1	G	343	GLU
1	G	350	THR
1	G	367	GLU
1	G	369	SER
1	G	377	LEU
1	G	397	LYS
1	G	402	LEU
1	G	403	SER
1	G	408	ASP
1	G	422	THR
1	G	453	LEU
1	G	462	GLU
1	G	466	HIS
1	G	505	LYS
1	G	509	GLN
1	G	512	LYS
1	G	513	ASP
1	G	515	LEU
1	G	521	ASP
1	G	529	LEU
1	G	532	GLN
1	G	533	THR
1	G	538	HIS
1	G	555	LEU
1	G	557	LYS
1	G	594	GLU
1	G	598	LEU
1	G	599	ASN
1	G	612	ASN
1	G	618	THR
1	G	637	ASN
1	G	639	LYS
1	G	652	GLU
1	G	668	MET
1	G	681	PHE
1	G	744	THR
1	G	747	TYR
1	G	749	SER
1	G	765	THR

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Mol	Chain	Res	Type
1	G	772	SER
1	G	777	VAL
1	G	783	LEU
1	G	804	HIS
1	G	814	GLU
1	G	817	LEU
1	G	824	LEU
1	G	846	LYS
1	G	858	LYS
1	G	863	PHE
1	G	890	SER
1	G	918	ARG
1	G	925	TYR
1	G	928	LEU
1	G	930	ASP
1	G	949	MET
1	G	957	LEU
1	G	1016	ARG
1	G	1019	VAL
1	G	1020	GLU
1	G	1048	THR
1	G	1052	LEU
1	G	1053	ARG
1	G	1095	LEU
1	G	1105	SER
1	G	1166	ARG
1	G	1173	GLU
1	G	1184	GLU
1	G	1206	LYS
1	G	1209	SER
1	G	1215	LEU
1	G	1217	MET
1	G	1218	ARG
1	G	1220	SER
1	G	1226	LEU
1	G	1228	TYR
1	G	1229	LEU
1	G	1244	ARG
1	G	1250	MET
1	G	1267	LEU
1	G	1269	LEU
1	G	1270	LEU

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Mol	Chain	Res	Type
1	G	1277	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	ASN
1	A	185	ASN
1	A	271	ASN
1	A	507	GLN
1	A	547	GLN
1	A	634	ASN
1	A	843	HIS
1	A	1245	GLN
1	C	271	ASN
1	C	405	GLN
1	C	634	ASN
1	C	1277	GLN
1	E	843	HIS
1	G	108	GLN
1	G	532	GLN
1	G	634	ASN
1	G	901	ASN
1	G	1299	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	23/43 (53%)	8 (34%)	0
2	D	23/43 (53%)	8 (34%)	1 (4%)
2	F	23/43 (53%)	7 (30%)	0
2	H	23/43 (53%)	7 (30%)	0
All	All	92/172 (53%)	30 (32%)	1 (1%)

All (30) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-10	C
2	B	-8	G
2	B	-6	U
2	B	-5	G

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Mol	Chain	Res	Type
2	B	-4	U
2	B	-3	A
2	B	1	A
2	B	4	U
2	D	-10	C
2	D	-8	G
2	D	-6	U
2	D	-5	G
2	D	-4	U
2	D	-3	A
2	D	1	A
2	D	5	U
2	F	-15	U
2	F	-10	C
2	F	-8	G
2	F	-6	U
2	F	-5	G
2	F	-3	A
2	F	1	A
2	H	-15	U
2	H	-10	C
2	H	-8	G
2	H	-6	U
2	H	-5	G
2	H	-3	A
2	H	1	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	-5	G

## 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

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, 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	1268/1302 (97%)	-0.02	4 (0%) 93 94	43, 67, 93, 144	0
1	C	1268/1302 (97%)	0.05	12 (0%) 84 85	51, 75, 105, 152	0
1	E	1262/1302 (96%)	0.18	27 (2%) 64 64	50, 78, 125, 166	0
1	G	1253/1302 (96%)	0.07	12 (0%) 82 83	48, 81, 126, 166	0
2	B	25/43 (58%)	-0.07	0 100 100	42, 53, 69, 99	0
2	D	25/43 (58%)	0.04	0 100 100	57, 70, 87, 93	0
2	F	25/43 (58%)	0.01	0 100 100	47, 54, 84, 112	0
2	H	25/43 (58%)	0.03	0 100 100	48, 60, 76, 97	0
All	All	5151/5380 (95%)	0.07	55 (1%) 80 81	42, 74, 117, 166	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	550	ASP	5.3
1	E	78	ASN	4.7
1	C	1162	ASN	4.5
1	E	266	ILE	4.0
1	E	568	CYS	3.8
1	C	699	LYS	3.7
1	E	76	LEU	3.6
1	A	0	ASN	3.4
1	E	555	LEU	3.3
1	G	478	ILE	3.2
1	C	1195	ILE	3.2
1	E	391	ILE	3.2
1	E	71	ILE	3.1
1	E	92	ASP	3.0
1	E	82	VAL	3.0
1	A	1162	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	96	LYS	3.0
1	E	549	GLU	3.0
1	E	79	TYR	2.8
1	E	119	PHE	2.8
1	G	1177	LEU	2.8
1	E	450	TYR	2.7
1	G	331	ASP	2.7
1	A	968	ARG	2.7
1	E	95	GLN	2.7
1	E	100	SER	2.6
1	C	550	ASP	2.6
1	E	444	LYS	2.6
1	E	1195	ILE	2.5
1	C	700	ASN	2.5
1	G	1015	GLY	2.4
1	E	128	ILE	2.4
1	E	98	PHE	2.4
1	C	1183	ILE	2.4
1	E	548	SER	2.4
1	G	1222	THR	2.3
1	A	1016	ARG	2.3
1	G	1016	ARG	2.3
1	G	393	PHE	2.3
1	E	553	ASN	2.3
1	C	686	GLU	2.3
1	C	1022	GLN	2.2
1	E	439	GLU	2.2
1	G	1187	HIS	2.2
1	G	1151	LEU	2.2
1	G	1124	PHE	2.2
1	E	273	LEU	2.2
1	C	78	ASN	2.2
1	E	88	LYS	2.1
1	G	132	LYS	2.1
1	C	1199	SER	2.1
1	C	376	LEU	2.1
1	C	1204	PHE	2.0
1	E	565	PHE	2.0
1	G	1218	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å <sup>2</sup> )	Q<0.9
3	MG	C	1401	1/1	0.92	0.47	9.10	56,56,56,56	0
3	MG	G	1401	1/1	0.94	0.26	1.82	56,56,56,56	0
3	MG	E	1401	1/1	0.94	0.15	-2.32	78,78,78,78	0
3	MG	A	1401	1/1	0.95	0.16	-2.45	56,56,56,56	0
3	MG	B	200	1/1	0.93	0.07	-	61,61,61,61	0
3	MG	D	200	1/1	0.97	0.08	-	61,61,61,61	0
3	MG	H	200	1/1	0.95	0.12	-	61,61,61,61	0
3	MG	F	200	1/1	0.99	0.06	-	62,62,62,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.