



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2019 – 10:01 AM EDT

PDB ID : 4A0L  
Title : Structure of DDB1-DDB2-CUL4B-RBX1 bound to a 12 bp abasic site containing DNA-duplex  
Authors : Fischer, E.S.; Scrima, A.; Gut, H.; Thoma, N.H.  
Deposited on : 2011-09-09  
Resolution : 7.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

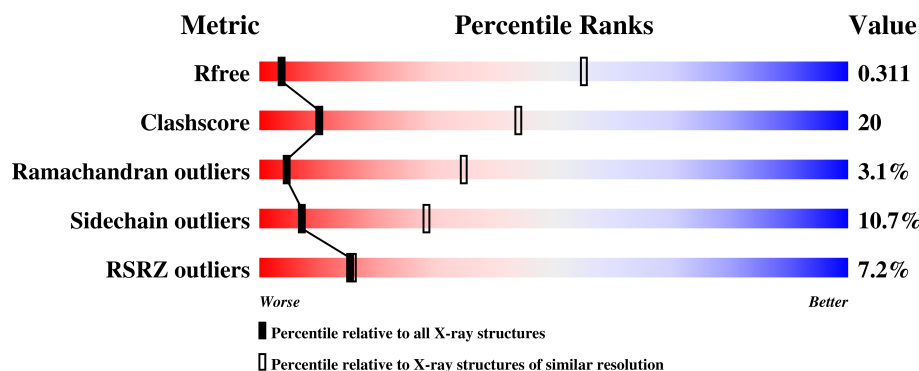
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 7.40 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))
$R_{free}$	111664	1067 (10.00-3.80)
Clashscore	122126	1146 (10.00-3.80)
Ramachandran outliers	120053	1071 (10.00-3.80)
Sidechain outliers	120020	1038 (10.00-3.80)
RSRZ outliers	108989	1012 (9.50-3.70)

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	1144	<div> <div>4%</div> <div>64%</div> <div>25%</div> <div>7%</div> <div>• •</div> </div>
1	C	1144	<div> <div>5%</div> <div>65%</div> <div>25%</div> <div>6%</div> <div>• •</div> </div>
2	B	382	<div> <div>19%</div> <div>74%</div> <div>16%</div> <div>•</div> <div>7%</div> </div>
2	D	382	<div> <div>6%</div> <div>74%</div> <div>17%</div> <div>•</div> <div>7%</div> </div>
3	E	726	<div> <div>6%</div> <div>59%</div> <div>32%</div> <div>6%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	726	
4	F	98	
4	I	98	
5	R	12	
5	T	12	
6	S	12	
6	U	12	

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
5	3DR	T	9	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35553 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 DNA DAMAGE-BINDING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1105	Total	C	N	O	S	0	0	0
			8517	5403	1417	1652	45			
1	C	1105	Total	C	N	O	S	0	0	0
			8537	5409	1428	1655	45			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
C	-3	GLY	-	expression tag	UNP Q16531
C	-2	GLY	-	expression tag	UNP Q16531
C	-1	GLY	-	expression tag	UNP Q16531
C	0	ARG	-	expression tag	UNP Q16531

- Molecule 2 is a protein called DNA DAMAGE-BINDING PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	355	Total	C	N	O	S	0	0	0
			2819	1792	492	524	11			
2	D	355	Total	C	N	O	S	0	0	0
			2843	1806	499	527	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	MET	-	expression tag	UNP Q2YDS1
B	77	HIS	-	expression tag	UNP Q2YDS1
B	78	HIS	-	expression tag	UNP Q2YDS1
B	79	HIS	-	expression tag	UNP Q2YDS1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	80	HIS	-	expression tag	UNP Q2YDS1
B	81	HIS	-	expression tag	UNP Q2YDS1
B	82	HIS	-	expression tag	UNP Q2YDS1
B	83	ARG	-	expression tag	UNP Q2YDS1
B	84	ARG	-	expression tag	UNP Q2YDS1
B	85	LEU	-	expression tag	UNP Q2YDS1
B	86	VAL	-	expression tag	UNP Q2YDS1
B	87	PRO	-	expression tag	UNP Q2YDS1
B	88	ARG	-	expression tag	UNP Q2YDS1
B	89	GLY	-	expression tag	UNP Q2YDS1
B	90	SER	-	expression tag	UNP Q2YDS1
B	91	GLY	-	expression tag	UNP Q2YDS1
B	92	GLY	-	expression tag	UNP Q2YDS1
B	93	ARG	-	expression tag	UNP Q2YDS1
B	180	GLN	LEU	variant	UNP Q2YDS1
B	214	ARG	TRP	variant	UNP Q2YDS1
D	76	MET	-	expression tag	UNP Q2YDS1
D	77	HIS	-	expression tag	UNP Q2YDS1
D	78	HIS	-	expression tag	UNP Q2YDS1
D	79	HIS	-	expression tag	UNP Q2YDS1
D	80	HIS	-	expression tag	UNP Q2YDS1
D	81	HIS	-	expression tag	UNP Q2YDS1
D	82	HIS	-	expression tag	UNP Q2YDS1
D	83	ARG	-	expression tag	UNP Q2YDS1
D	84	ARG	-	expression tag	UNP Q2YDS1
D	85	LEU	-	expression tag	UNP Q2YDS1
D	86	VAL	-	expression tag	UNP Q2YDS1
D	87	PRO	-	expression tag	UNP Q2YDS1
D	88	ARG	-	expression tag	UNP Q2YDS1
D	89	GLY	-	expression tag	UNP Q2YDS1
D	90	SER	-	expression tag	UNP Q2YDS1
D	91	GLY	-	expression tag	UNP Q2YDS1
D	92	GLY	-	expression tag	UNP Q2YDS1
D	93	ARG	-	expression tag	UNP Q2YDS1
D	180	GLN	LEU	variant	UNP Q2YDS1
D	214	ARG	TRP	variant	UNP Q2YDS1

- Molecule 3 is a protein called CULLIN-4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	709	Total	C	N	O	S	0	0	0
			5743	3659	979	1074	31			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	709	Total	C	N	O	S	0	0	0
			5773	3681	978	1082	32			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	189	GLY	-	expression tag	UNP Q13620
E	190	GLY	-	expression tag	UNP Q13620
E	191	GLY	-	expression tag	UNP Q13620
E	192	ARG	-	expression tag	UNP Q13620
H	189	GLY	-	expression tag	UNP Q13620
H	190	GLY	-	expression tag	UNP Q13620
H	191	GLY	-	expression tag	UNP Q13620
H	192	ARG	-	expression tag	UNP Q13620

- Molecule 4 is a protein called E3 UBIQUITIN-PROTEIN LIGASE RBX1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	21	Total	C	N	O	0	0	0
			175	118	31	26			
4	I	21	Total	C	N	O	0	0	0
			180	122	32	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	11	MET	-	expression tag	UNP P62878
I	11	MET	-	expression tag	UNP P62878

- Molecule 5 is a DNA chain called 12 BP THF CONTAINING DNA DUPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	R	12	Total	C	N	O	P	0	0	0
			234	111	41	70	12			
5	T	12	Total	C	N	O	P	0	0	0
			234	111	41	70	12			

- Molecule 6 is a DNA chain called 12 BP DNA DUPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	S	12	Total	C	N	O	P	0	0	0
			249	118	47	72	12			

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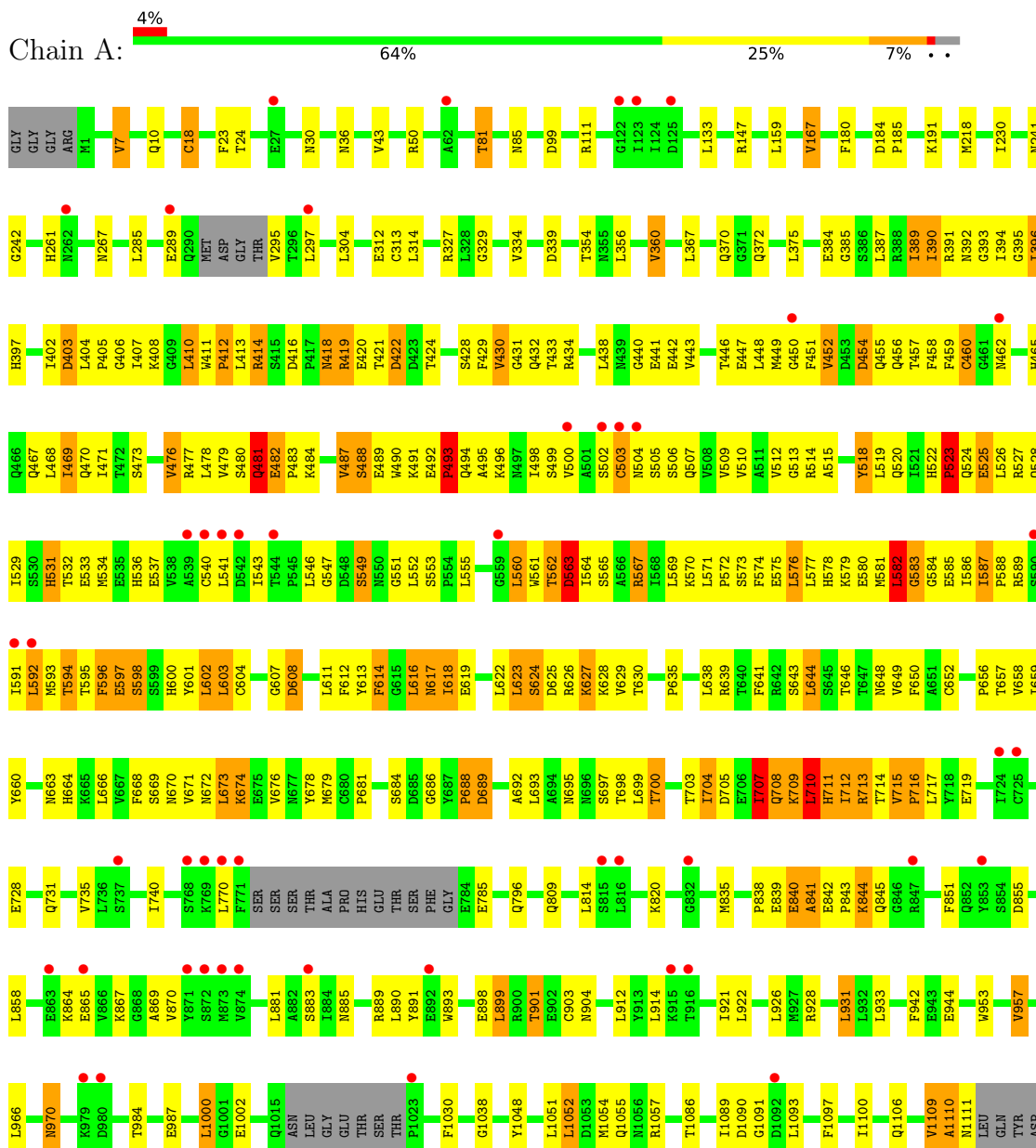
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	U	12	Total	C	N	O	P	0	0	0
			249	118	47	72	12			

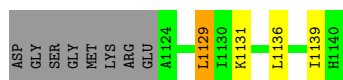
### 3 Residue-property plots

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.

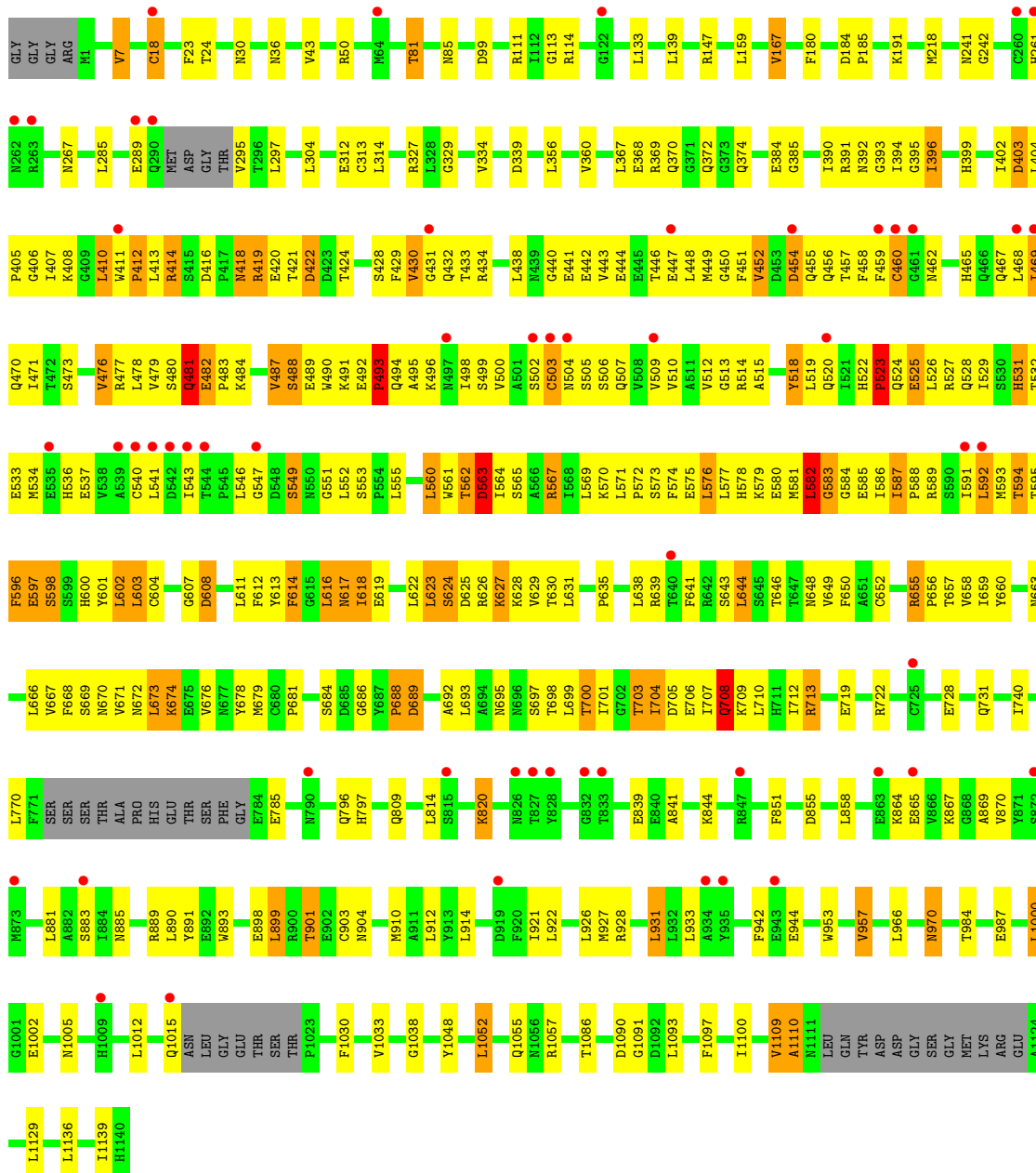
#### ● Molecule 1: DNA DAMAGE-BINDING PROTEIN 1



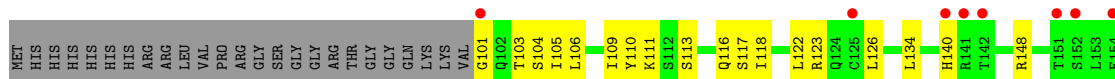
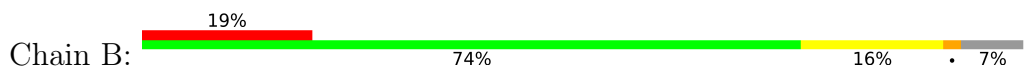


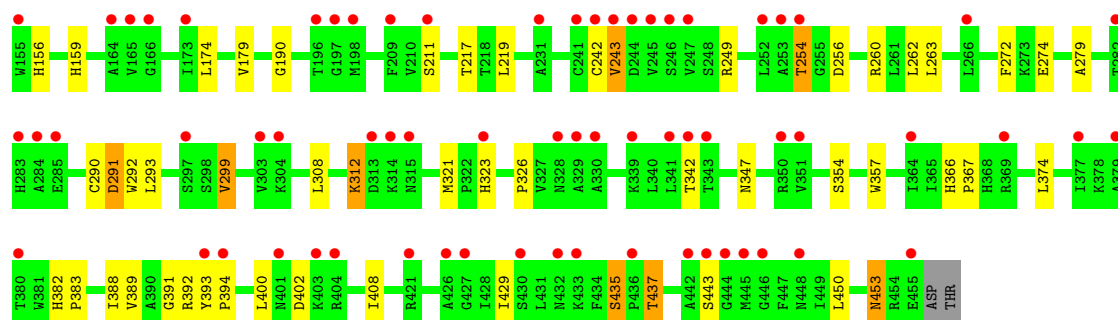


• Molecule 1: DNA DAMAGE-BINDING PROTEIN 1

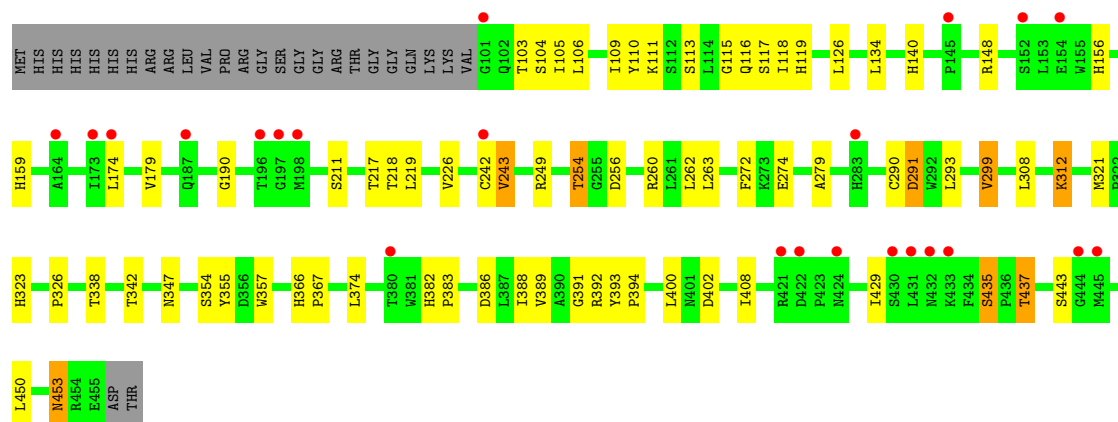
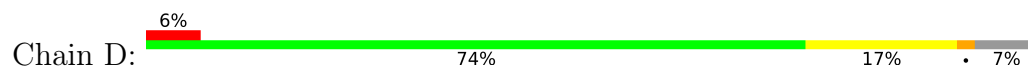


• Molecule 2: DNA DAMAGE-BINDING PROTEIN 2

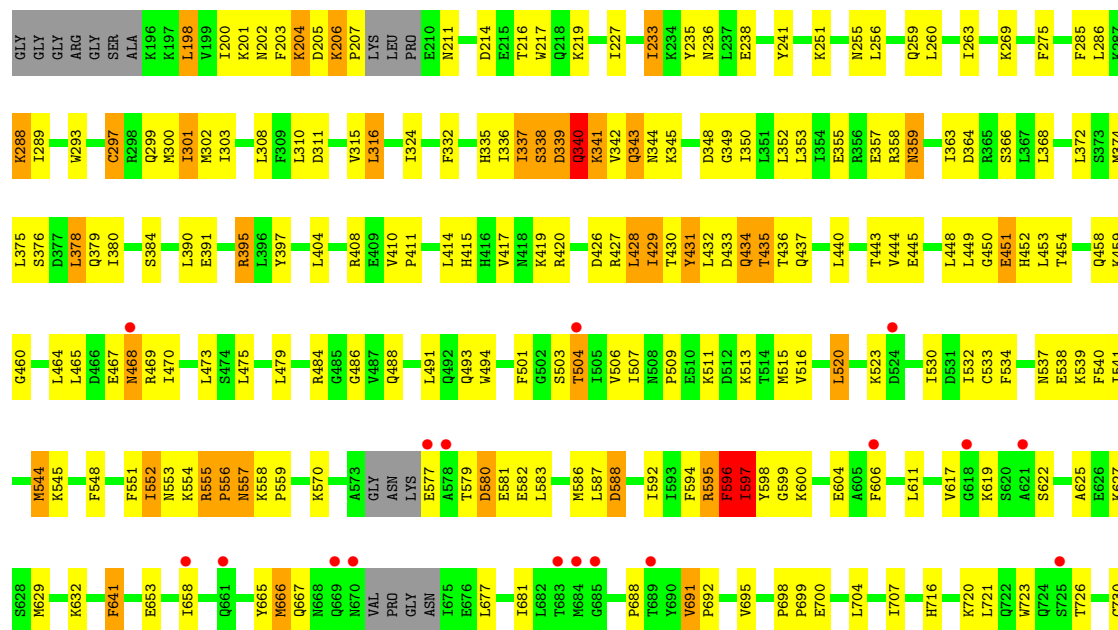


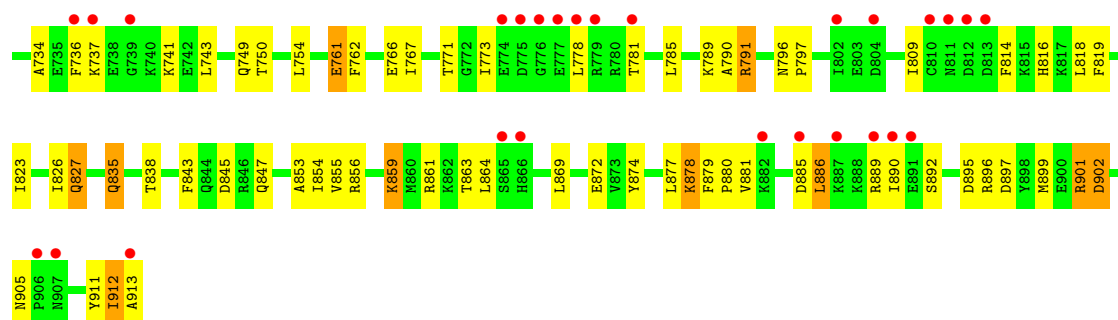


### • Molecule 2: DNA DAMAGE-BINDING PROTEIN 2

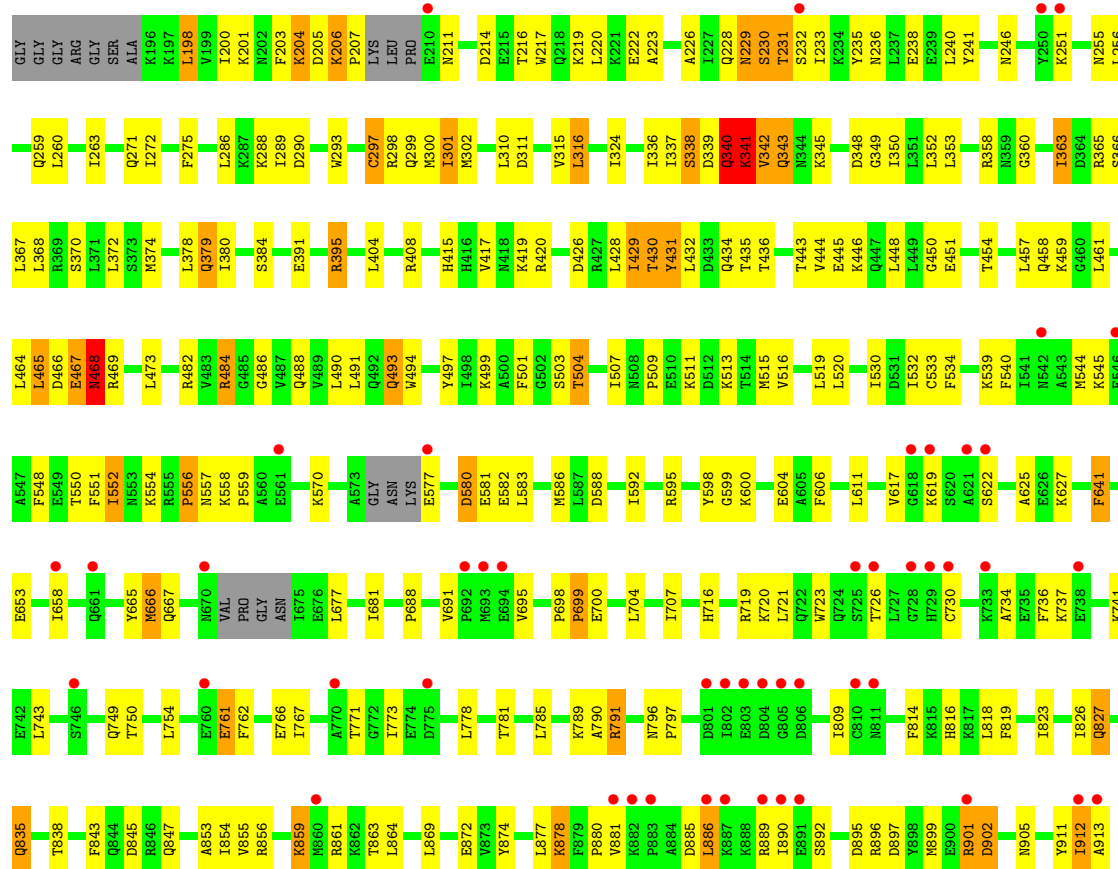


### • Molecule 3: CULLIN-4B

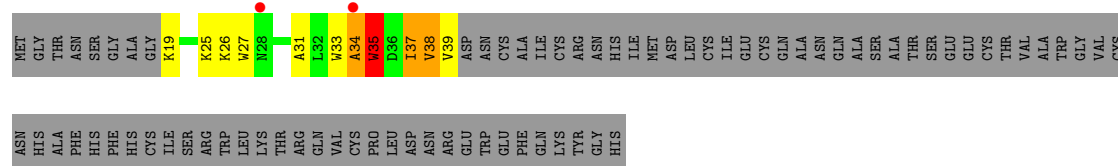




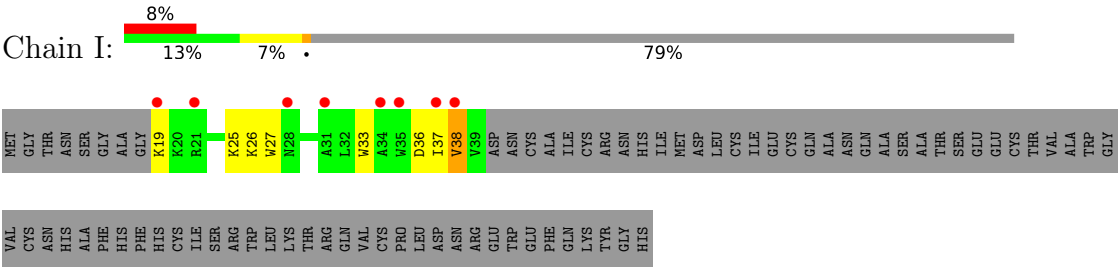
• Molecule 3: CULLIN-4B



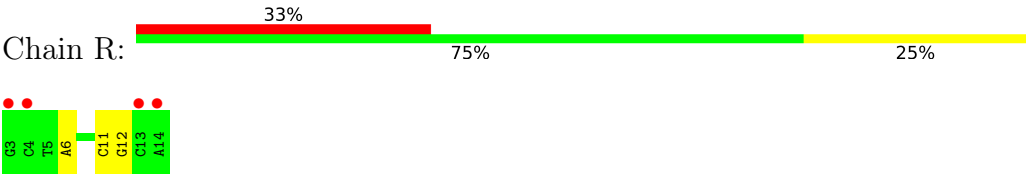
• Molecule 4: E3 UBIQUITIN-PROTEIN LIGASE RBX1



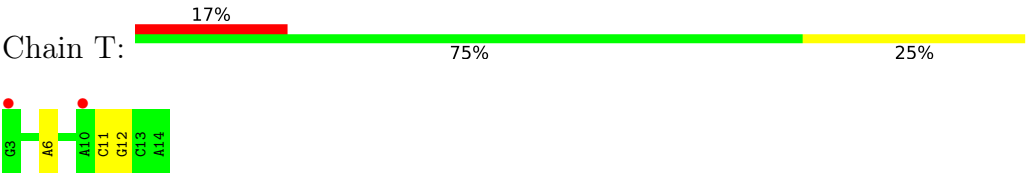
• Molecule 4: E3 UBIQUITIN-PROTEIN LIGASE RBX1



• Molecule 5: 12 BP THF CONTAINING DNA DUPLEX



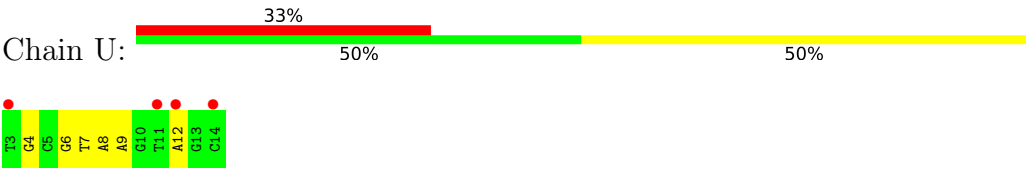
• Molecule 5: 12 BP THF CONTAINING DNA DUPLEX



• Molecule 6: 12 BP DNA DUPLEX



• Molecule 6: 12 BP DNA DUPLEX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.80Å 155.84Å 255.39Å 90.00° 94.17° 90.00°	Depositor
Resolution (Å)	29.86 – 7.40 29.86 – 7.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.86-7.40) 99.2 (29.86-7.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 7.23Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.318 , 0.320 0.313 , 0.311	Depositor DCC
$R_{free}$ test set	1355 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	444.7	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 213.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.76	EDS
Total number of atoms	35553	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	253.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.43	2/8668 (0.0%)	0.66	7/11756 (0.1%)
1	C	0.43	2/8688 (0.0%)	0.66	8/11783 (0.1%)
2	B	0.38	0/2891	0.60	0/3928
2	D	0.38	0/2917	0.60	0/3962
3	E	0.40	3/5831 (0.1%)	0.55	1/7832 (0.0%)
3	H	0.38	0/5865	0.54	0/7878
4	F	0.35	0/179	0.39	0/241
4	I	0.42	0/186	0.43	0/251
5	R	0.92	1/248 (0.4%)	1.13	0/377
5	T	0.92	1/248 (0.4%)	1.12	0/377
6	S	0.89	0/279	1.36	1/429 (0.2%)
6	U	0.88	0/279	1.36	1/429 (0.2%)
All	All	0.43	9/36279 (0.0%)	0.64	18/49243 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	582	LEU	C-N	6.82	1.45	1.33
1	A	582	LEU	C-N	6.78	1.45	1.33
3	E	579	THR	C-N	-5.89	1.20	1.34
3	E	376	SER	C-N	5.80	1.47	1.34
5	R	11	DC	C1'-N1	5.47	1.56	1.49
5	T	11	DC	C1'-N1	5.41	1.56	1.49
3	E	537	ASN	C-N	-5.21	1.22	1.34
1	C	18	CYS	CB-SG	-5.18	1.73	1.81
1	A	18	CYS	CB-SG	-5.16	1.73	1.81

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	624	SER	N-CA-C	7.04	130.01	111.00
1	C	624	SER	N-CA-C	7.02	129.95	111.00
1	A	688	PRO	N-CA-C	6.63	129.34	112.10
1	C	688	PRO	N-CA-C	6.56	129.16	112.10
1	A	689	ASP	N-CA-C	-6.55	93.32	111.00
1	C	689	ASP	N-CA-C	-6.45	93.59	111.00
6	U	4	DG	O4'-C1'-N9	6.19	112.33	108.00
6	S	4	DG	O4'-C1'-N9	6.07	112.25	108.00
1	C	688	PRO	CA-N-CD	-5.87	103.28	111.50
1	A	688	PRO	CA-N-CD	-5.85	103.31	111.50
1	C	624	SER	CB-CA-C	-5.84	99.00	110.10
1	A	624	SER	CB-CA-C	-5.81	99.07	110.10
1	C	710	LEU	N-CA-C	5.45	125.71	111.00
1	C	523	PRO	CA-N-CD	-5.28	104.11	111.50
1	A	422	ASP	CB-CG-OD2	5.24	123.02	118.30
3	E	376	SER	O-C-N	5.22	131.05	122.70
1	C	422	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	523	PRO	CA-N-CD	-5.19	104.23	111.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8517	0	8394	471	0
1	C	8537	0	8432	389	0
2	B	2819	0	2745	88	0
2	D	2843	0	2788	74	0
3	E	5743	0	5773	296	0
3	H	5773	0	5798	241	0
4	F	175	0	184	22	0
4	I	180	0	178	6	0
5	R	234	0	132	3	0
5	T	234	0	132	3	0
6	S	249	0	136	7	0
6	U	249	0	136	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	35553	0	34828	1424	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 20.

All (1424) 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)
3:E:555:ARG:CG	3:E:559:PRO:HD3	1.32	1.56
1:A:354:THR:CG2	1:A:712:ILE:HG21	1.37	1.53
3:E:552:ILE:CG2	3:E:597:ILE:HG12	1.42	1.48
3:H:365:ARG:CB	3:H:430:THR:HG22	1.44	1.45
3:E:555:ARG:HB3	3:E:559:PRO:CG	1.52	1.37
1:A:926:LEU:HD11	2:B:122:LEU:CD2	1.54	1.36
3:E:285:PHE:CE2	3:E:345:LYS:HD2	1.63	1.32
3:E:552:ILE:HG21	3:E:597:ILE:CG1	1.60	1.32
1:A:926:LEU:CD1	2:B:122:LEU:HD21	1.60	1.31
1:C:499:SER:HB3	3:H:238:GLU:CB	1.59	1.30
3:H:220:LEU:CD2	3:H:240:LEU:HD22	1.59	1.30
3:E:449:LEU:CD1	3:E:479:LEU:HD22	1.66	1.26
3:H:220:LEU:HD23	3:H:240:LEU:CD2	1.65	1.25
1:A:709:LYS:O	1:A:710:LEU:HD23	1.39	1.22
3:E:555:ARG:CB	3:E:559:PRO:HG3	1.69	1.21
1:C:841:ALA:O	2:D:104:SER:HA	1.36	1.20
1:A:354:THR:HG21	1:A:712:ILE:CG2	1.70	1.20
3:E:428:LEU:CD2	3:E:432:LEU:HD23	1.73	1.19
1:A:704:ILE:N	1:A:704:ILE:HD12	1.54	1.18
3:E:555:ARG:CG	3:E:559:PRO:CD	2.22	1.17
3:H:226:ALA:HB1	3:H:233:ILE:N	1.58	1.15
1:A:111:ARG:HG3	2:B:292:TRP:CZ2	1.80	1.15
1:A:394:ILE:HG23	1:A:705:ASP:HB3	1.25	1.14
1:A:354:THR:CG2	1:A:712:ILE:CG2	2.24	1.14
1:A:354:THR:HG21	1:A:712:ILE:HG21	1.16	1.13
3:E:449:LEU:HD11	3:E:479:LEU:HD22	1.22	1.13
3:E:285:PHE:CZ	3:E:345:LYS:HD2	1.83	1.13
3:E:555:ARG:HB3	3:E:559:PRO:CD	1.78	1.13
1:C:910:MET:HE1	2:D:105:ILE:HG21	1.25	1.13
1:A:111:ARG:NE	2:B:292:TRP:HE1	1.43	1.12
1:A:354:THR:HG23	1:A:712:ILE:HG21	1.32	1.10
3:E:494:TRP:CE3	3:E:540:PHE:HD2	1.70	1.10
1:A:562:THR:O	1:A:564:ILE:HG13	1.53	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:THR:O	1:C:564:ILE:HG13	1.52	1.09
3:E:340:GLN:HG2	3:E:341:LYS:N	1.65	1.09
3:H:365:ARG:CB	3:H:430:THR:CG2	2.30	1.08
1:A:714:THR:HG22	1:A:716:PRO:HD3	1.15	1.08
1:A:356:LEU:HD21	1:A:712:ILE:HG23	1.28	1.08
1:A:912:LEU:HD21	2:B:109:ILE:HG12	1.08	1.08
3:E:552:ILE:HD12	3:E:597:ILE:HD11	1.10	1.08
1:A:354:THR:HG21	1:A:712:ILE:CB	1.84	1.08
3:E:429:ILE:HG12	3:E:429:ILE:O	1.47	1.08
1:A:840:GLU:H	2:B:103:THR:CB	1.66	1.07
3:E:587:LEU:HD22	3:E:629:MET:SD	1.95	1.07
1:A:912:LEU:HD22	2:B:109:ILE:CG2	1.85	1.07
3:E:553:ASN:CB	3:E:598:TYR:HB2	1.84	1.07
1:A:664:HIS:HB2	1:A:1131:LYS:HE3	1.37	1.06
1:C:910:MET:CE	2:D:105:ILE:HG21	1.84	1.06
1:A:704:ILE:CD1	1:A:704:ILE:H	1.66	1.06
3:E:555:ARG:HB3	3:E:559:PRO:HG3	1.05	1.05
3:E:555:ARG:HG2	3:E:559:PRO:HD3	1.38	1.05
1:A:843:PRO:CB	2:B:104:SER:CB	2.36	1.04
3:E:374:MET:HG2	3:E:378:LEU:HD23	1.37	1.04
3:E:428:LEU:HD22	3:E:432:LEU:HD23	1.40	1.04
3:H:286:LEU:HD21	3:H:349:GLY:HA3	1.40	1.03
1:A:912:LEU:HD21	2:B:109:ILE:CG1	1.87	1.03
3:E:555:ARG:HG3	3:E:559:PRO:CD	1.85	1.03
1:A:704:ILE:HD12	1:A:704:ILE:H	0.87	1.02
1:A:111:ARG:CG	2:B:292:TRP:HZ2	1.71	1.02
3:E:555:ARG:CB	3:E:559:PRO:CD	2.36	1.02
3:H:272:ILE:HD11	3:H:340:GLN:HE22	1.17	1.02
3:H:363:ILE:HD13	3:H:363:ILE:C	1.79	1.02
1:A:356:LEU:CD2	1:A:712:ILE:HG23	1.90	1.02
3:E:552:ILE:HD12	3:E:597:ILE:CD1	1.90	1.01
1:C:111:ARG:HH22	2:D:290:CYS:HA	1.21	1.01
1:A:354:THR:CG2	1:A:712:ILE:HD12	1.90	1.01
1:A:354:THR:HG21	1:A:712:ILE:CD1	1.91	1.00
3:E:555:ARG:HG3	3:E:559:PRO:HD3	1.04	1.00
1:C:585:GLU:HG3	3:H:301:ILE:CG2	1.91	1.00
3:H:363:ILE:HD13	3:H:363:ILE:O	1.61	1.00
1:A:714:THR:CG2	1:A:716:PRO:HD3	1.90	0.99
3:E:397:TYR:CD2	3:E:444:VAL:HG13	1.96	0.99
1:C:708:GLN:NE2	1:C:708:GLN:HA	1.75	0.99
1:A:354:THR:CG2	1:A:712:ILE:CD1	2.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:912:LEU:CD2	2:B:109:ILE:HG12	1.92	0.98
3:H:220:LEU:HD23	3:H:240:LEU:HD22	0.99	0.98
3:E:555:ARG:CB	3:E:559:PRO:CG	2.33	0.97
3:E:720:LYS:HG3	4:F:34:ALA:HB2	1.47	0.97
3:H:465:LEU:HB3	3:H:497:TYR:CZ	2.01	0.96
1:A:111:ARG:HG3	2:B:292:TRP:HZ2	1.18	0.96
3:E:555:ARG:CB	3:E:559:PRO:HD3	1.95	0.96
1:A:708:GLN:O	1:A:709:LYS:HD3	1.67	0.95
3:H:353:LEU:HD22	3:H:363:ILE:CB	1.96	0.95
1:A:987:GLU:OE2	2:B:156:HIS:HE1	1.49	0.94
3:H:272:ILE:HD11	3:H:340:GLN:NE2	1.83	0.94
1:C:465:HIS:ND1	1:C:523:PRO:HD3	1.82	0.93
3:E:340:GLN:CG	3:E:341:LYS:H	1.80	0.93
3:H:428:LEU:HA	3:H:432:LEU:CB	1.98	0.93
1:A:465:HIS:ND1	1:A:523:PRO:HD3	1.82	0.93
3:H:457:LEU:HB2	3:H:493:GLN:HE21	1.32	0.93
4:F:37:ILE:HG13	4:F:38:VAL:N	1.83	0.93
3:E:340:GLN:CG	3:E:341:LYS:N	2.30	0.92
3:H:226:ALA:HB1	3:H:233:ILE:H	1.25	0.92
1:A:912:LEU:HD22	2:B:109:ILE:HG23	1.48	0.92
3:H:340:GLN:HG2	3:H:341:LYS:HG2	1.50	0.92
3:E:720:LYS:CG	4:F:34:ALA:HB2	2.00	0.92
3:H:353:LEU:HD22	3:H:363:ILE:CG1	2.00	0.92
3:H:417:VAL:HG22	3:H:448:LEU:HD13	1.49	0.92
1:A:715:VAL:O	1:A:715:VAL:HG12	1.71	0.91
1:C:507:GLN:NE2	1:C:552:LEU:HA	1.85	0.91
3:E:494:TRP:CE3	3:E:540:PHE:CD2	2.57	0.91
3:E:597:ILE:HG22	3:E:600:LYS:HG2	1.49	0.91
1:A:507:GLN:NE2	1:A:552:LEU:HA	1.85	0.91
3:E:588:ASP:HA	3:E:632:LYS:HZ1	1.32	0.91
3:E:286:LEU:HD21	3:E:349:GLY:HA3	1.52	0.91
3:H:223:ALA:CB	3:H:240:LEU:HD11	2.01	0.91
1:C:392:ASN:HB2	1:C:1012:LEU:O	1.70	0.90
1:C:111:ARG:NH2	2:D:290:CYS:HA	1.84	0.90
3:H:339:ASP:O	3:H:340:GLN:HB3	1.72	0.90
1:A:465:HIS:CE1	1:A:523:PRO:HD3	2.07	0.90
3:E:588:ASP:HA	3:E:632:LYS:NZ	1.86	0.90
1:C:18:CYS:HB2	1:C:313:CYS:SG	2.12	0.90
1:C:329:GLY:HA3	1:C:384:GLU:HG2	1.54	0.89
3:E:588:ASP:CA	3:E:632:LYS:HZ1	1.86	0.89
1:A:111:ARG:HE	2:B:292:TRP:HE1	1.20	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:338:SER:O	3:E:343:GLN:HB2	1.72	0.89
1:C:465:HIS:CE1	1:C:523:PRO:HD3	2.07	0.89
3:H:426:ASP:O	3:H:429:ILE:HG23	1.73	0.89
1:A:18:CYS:HB2	1:A:313:CYS:SG	2.12	0.88
1:A:329:GLY:HA3	1:A:384:GLU:HG2	1.54	0.88
1:A:714:THR:HG22	1:A:716:PRO:CD	2.03	0.88
2:D:323:HIS:NE2	2:D:342:THR:HG21	1.89	0.88
1:C:987:GLU:OE2	2:D:156:HIS:CE1	2.26	0.88
2:B:323:HIS:NE2	2:B:342:THR:HG21	1.88	0.88
1:C:578:HIS:CD2	1:C:623:LEU:HD12	2.09	0.87
1:A:23:PHE:H	1:A:30:ASN:HD22	1.21	0.87
1:A:578:HIS:CD2	1:A:623:LEU:HD12	2.09	0.87
3:E:552:ILE:CG2	3:E:597:ILE:CG1	2.35	0.87
3:E:552:ILE:CD1	3:E:597:ILE:HD11	2.00	0.87
3:H:226:ALA:CB	3:H:233:ILE:N	2.37	0.87
1:A:387:LEU:HG	1:A:717:LEU:HD11	1.56	0.87
1:C:910:MET:SD	2:D:105:ILE:HD13	2.15	0.87
3:H:340:GLN:HG2	3:H:341:LYS:N	1.87	0.86
1:C:649:VAL:HG12	1:C:650:PHE:H	1.39	0.86
3:H:226:ALA:CB	3:H:233:ILE:H	1.86	0.86
1:A:375:LEU:O	1:A:389:ILE:CA	2.23	0.85
3:E:340:GLN:CG	3:E:341:LYS:HG2	2.06	0.85
1:A:499:SER:HB3	3:E:238:GLU:CB	2.06	0.85
1:C:23:PHE:H	1:C:30:ASN:HD22	1.21	0.85
1:C:507:GLN:HE22	1:C:553:SER:H	1.24	0.85
1:C:111:ARG:CZ	2:D:290:CYS:SG	2.64	0.85
1:A:81:THR:HG21	1:A:85:ASN:HD22	1.41	0.85
1:A:520:GLN:HG3	1:A:529:ILE:HG13	1.59	0.85
4:F:38:VAL:O	4:F:39:VAL:HG23	1.77	0.84
1:A:649:VAL:HG12	1:A:650:PHE:H	1.38	0.84
3:H:353:LEU:HD22	3:H:363:ILE:HB	1.57	0.84
3:H:378:LEU:O	3:H:379:GLN:HB2	1.77	0.84
1:A:375:LEU:O	1:A:389:ILE:HA	1.78	0.84
3:E:428:LEU:HD23	3:E:432:LEU:HD23	1.58	0.84
3:E:595:ARG:O	3:E:596:PHE:CG	2.30	0.84
1:C:520:GLN:HG3	1:C:529:ILE:HG13	1.60	0.84
4:F:38:VAL:O	4:F:38:VAL:HG22	1.74	0.84
3:H:220:LEU:HD22	3:H:240:LEU:HD22	1.61	0.83
1:A:840:GLU:HG3	1:A:840:GLU:O	1.76	0.83
1:C:81:THR:HG21	1:C:85:ASN:HD22	1.41	0.83
1:C:841:ALA:O	2:D:104:SER:CA	2.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:926:LEU:HD11	2:B:122:LEU:HD21	0.85	0.83
1:C:430:VAL:HG13	3:H:246:ASN:HB3	1.58	0.83
1:A:714:THR:O	1:A:715:VAL:HB	1.77	0.83
1:A:111:ARG:CB	2:B:292:TRP:HZ2	1.91	0.83
1:A:446:THR:HG22	1:A:447:GLU:H	1.43	0.82
1:A:507:GLN:HE22	1:A:553:SER:H	1.25	0.82
4:F:38:VAL:C	4:F:39:VAL:HG23	1.99	0.82
1:A:394:ILE:HG23	1:A:705:ASP:CB	2.07	0.82
1:A:394:ILE:CG2	1:A:705:ASP:HB3	2.08	0.82
3:H:465:LEU:HB3	3:H:497:TYR:CE2	2.14	0.82
1:A:111:ARG:NE	2:B:292:TRP:NE1	2.26	0.82
1:A:404:LEU:HD21	3:E:200:ILE:HD11	1.61	0.82
1:A:585:GLU:OE2	3:E:301:ILE:HG23	1.79	0.82
3:E:332:PHE:CE1	3:E:336:ILE:HG21	2.14	0.82
3:H:461:LEU:HD22	3:H:493:GLN:HB3	1.61	0.82
1:A:509:VAL:HG23	1:A:543:ILE:HD13	1.62	0.81
1:A:987:GLU:OE2	2:B:156:HIS:CE1	2.33	0.81
1:C:585:GLU:OE2	3:H:301:ILE:HG23	1.79	0.81
1:C:482:GLU:CD	1:C:483:PRO:HD3	2.00	0.81
1:A:482:GLU:CD	1:A:483:PRO:HD3	2.00	0.81
1:C:446:THR:HG22	1:C:447:GLU:H	1.43	0.81
3:E:617:VAL:HG11	3:E:827:GLN:HB3	1.62	0.81
3:H:457:LEU:HB3	3:H:493:GLN:HG2	1.60	0.81
3:H:290:ASP:CG	3:H:367:LEU:HD13	2.02	0.81
1:C:926:LEU:CD2	2:D:105:ILE:HD11	2.10	0.81
3:H:340:GLN:HG2	3:H:341:LYS:H	1.46	0.81
1:A:534:MET:HE2	1:A:569:LEU:HD11	1.62	0.81
3:H:617:VAL:HG11	3:H:827:GLN:HB3	1.62	0.81
1:A:912:LEU:HD22	2:B:109:ILE:HG21	1.62	0.81
1:A:111:ARG:CB	2:B:292:TRP:CZ2	2.65	0.80
1:A:413:LEU:HB2	1:A:424:THR:HB	1.63	0.80
1:A:537:GLU:OE1	3:E:236:ASN:HB2	1.81	0.80
3:E:449:LEU:HD13	3:E:479:LEU:HD22	1.64	0.80
1:C:509:VAL:HG23	1:C:543:ILE:HD13	1.62	0.80
1:C:534:MET:HE2	1:C:569:LEU:HD11	1.63	0.80
1:C:987:GLU:OE2	2:D:156:HIS:HE1	1.62	0.80
1:A:356:LEU:HD21	1:A:712:ILE:CG2	2.10	0.80
3:E:595:ARG:C	3:E:596:PHE:CG	2.55	0.79
1:C:413:LEU:HB2	1:C:424:THR:HB	1.63	0.79
1:A:713:ARG:HG3	1:A:714:THR:H	1.47	0.79
1:C:430:VAL:HG22	3:H:246:ASN:HB3	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:PRO:HB2	1:C:422:ASP:OD2	1.83	0.79
1:C:705:ASP:OD1	1:C:707:ILE:HG13	1.83	0.79
1:A:111:ARG:HB3	2:B:290:CYS:SG	2.22	0.78
3:H:220:LEU:CD2	3:H:240:LEU:CD2	2.42	0.78
3:H:340:GLN:CG	3:H:341:LYS:HG2	2.12	0.78
1:A:708:GLN:O	1:A:709:LYS:CD	2.31	0.78
3:E:285:PHE:CE2	3:E:345:LYS:CD	2.58	0.78
1:A:578:HIS:NE2	1:A:623:LEU:HD12	1.99	0.78
1:C:814:LEU:HD11	2:D:106:LEU:HD13	1.66	0.78
1:A:111:ARG:CG	2:B:292:TRP:CZ2	2.53	0.78
3:E:491:LEU:HG	3:E:540:PHE:CZ	2.18	0.78
3:H:901:ARG:O	3:H:902:ASP:HB2	1.84	0.78
3:E:350:ILE:HA	3:E:368:LEU:HD21	1.65	0.78
3:E:339:ASP:CG	3:E:340:GLN:N	2.37	0.78
1:A:354:THR:HG21	1:A:712:ILE:HD12	1.59	0.77
1:A:708:GLN:O	1:A:709:LYS:CE	2.31	0.77
1:C:578:HIS:NE2	1:C:623:LEU:HD12	1.99	0.77
1:A:412:PRO:HB2	1:A:422:ASP:OD2	1.83	0.77
1:A:23:PHE:H	1:A:30:ASN:ND2	1.82	0.77
1:C:507:GLN:HE22	1:C:552:LEU:HA	1.48	0.77
1:A:507:GLN:HE22	1:A:552:LEU:HA	1.48	0.77
1:A:602:LEU:C	1:A:603:LEU:HD23	2.05	0.77
1:C:602:LEU:C	1:C:603:LEU:HD23	2.04	0.77
3:E:901:ARG:O	3:E:902:ASP:HB2	1.84	0.76
1:A:329:GLY:HA3	1:A:384:GLU:CG	2.15	0.76
1:C:649:VAL:HG12	1:C:650:PHE:N	2.00	0.76
1:C:708:GLN:HE21	1:C:708:GLN:HA	1.50	0.76
1:A:707:ILE:O	1:A:708:GLN:CB	2.33	0.76
1:A:709:LYS:O	1:A:710:LEU:CD2	2.30	0.76
1:C:23:PHE:H	1:C:30:ASN:ND2	1.82	0.76
1:A:649:VAL:HG12	1:A:650:PHE:N	2.00	0.76
3:E:417:VAL:HG21	3:E:449:LEU:HD21	1.66	0.76
1:A:450:GLY:HA3	1:A:479:VAL:CG2	2.17	0.75
1:A:664:HIS:C	1:A:1131:LYS:HE2	2.07	0.75
1:A:448:LEU:HB3	1:A:451:PHE:HD2	1.52	0.75
1:A:452:VAL:HG12	1:A:454:ASP:OD1	1.86	0.75
1:C:329:GLY:HA3	1:C:384:GLU:CG	2.16	0.75
3:E:587:LEU:HB3	3:E:632:LYS:HD3	1.67	0.75
3:H:340:GLN:NE2	3:H:342:VAL:HG22	2.01	0.75
1:A:838:PRO:HA	2:B:101:GLY:HA2	1.68	0.75
1:A:987:GLU:OE1	2:B:159:HIS:HB2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:VAL:HG12	1:C:454:ASP:OD1	1.86	0.74
3:E:595:ARG:O	3:E:596:PHE:CD2	2.40	0.74
4:F:35:TRP:HA	4:F:35:TRP:CE3	2.20	0.74
1:A:10:GLN:OE1	1:A:710:LEU:HD11	1.87	0.74
1:C:450:GLY:HA3	1:C:479:VAL:CG2	2.17	0.74
1:A:375:LEU:O	1:A:389:ILE:CB	2.36	0.74
1:C:585:GLU:CG	3:H:301:ILE:CG2	2.66	0.74
1:A:664:HIS:CB	1:A:1131:LYS:HE3	2.18	0.74
1:A:354:THR:HG22	1:A:712:ILE:CD1	2.17	0.74
1:A:589:ARG:NH1	3:E:241:TYR:HE2	1.85	0.74
1:C:928:ARG:HD2	2:D:437:THR:HG23	1.68	0.74
3:E:374:MET:HG2	3:E:378:LEU:CD2	2.15	0.74
3:H:457:LEU:HB2	3:H:493:GLN:NE2	2.03	0.74
1:A:451:PHE:CD1	1:A:470:GLN:HB2	2.23	0.73
1:C:469:ILE:HD11	1:C:476:VAL:HG23	1.69	0.73
1:C:585:GLU:HG3	3:H:301:ILE:HG21	1.68	0.73
3:H:293:TRP:CH2	3:H:370:SER:HB2	2.22	0.73
1:A:835:MET:HG2	1:A:845:GLN:O	1.88	0.73
1:A:469:ILE:HD11	1:A:476:VAL:HG23	1.69	0.73
1:A:657:THR:HG22	1:A:658:VAL:H	1.53	0.73
1:A:987:GLU:CD	2:B:156:HIS:CE1	2.61	0.73
1:C:910:MET:CE	2:D:105:ILE:HD13	2.19	0.73
1:A:844:LYS:O	1:A:845:GLN:HG3	1.88	0.73
1:A:111:ARG:HB2	2:B:292:TRP:CZ2	2.24	0.73
1:C:448:LEU:HB3	1:C:451:PHE:HD2	1.52	0.73
1:C:563:ASP:OD2	1:C:565:SER:HB3	1.87	0.73
1:A:926:LEU:HD21	2:B:122:LEU:CG	2.18	0.73
1:C:451:PHE:CD1	1:C:470:GLN:HB2	2.23	0.73
1:A:563:ASP:OD2	1:A:565:SER:HB3	1.87	0.72
1:A:354:THR:HG21	1:A:712:ILE:CG1	2.18	0.72
1:A:578:HIS:CD2	1:A:623:LEU:H	2.06	0.72
3:H:465:LEU:HD21	3:H:494:TRP:HD1	1.53	0.72
1:C:578:HIS:CD2	1:C:623:LEU:H	2.06	0.72
1:C:657:THR:HG22	1:C:658:VAL:H	1.52	0.72
1:C:841:ALA:HA	2:D:103:THR:O	1.90	0.72
3:E:353:LEU:CB	3:E:368:LEU:HD11	2.19	0.72
3:E:597:ILE:O	3:E:600:LYS:HE2	1.89	0.72
1:C:404:LEU:HD21	3:H:200:ILE:HD11	1.70	0.72
1:C:926:LEU:HD21	2:D:105:ILE:HD11	1.71	0.72
3:H:847:GLN:HB3	3:H:889:ARG:HD2	1.72	0.72
1:A:111:ARG:HG3	2:B:292:TRP:CE2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:585:GLU:OE2	3:H:301:ILE:CG2	2.38	0.72
3:H:461:LEU:CD2	3:H:493:GLN:HB3	2.18	0.72
1:A:912:LEU:CD2	2:B:109:ILE:CG1	2.62	0.72
3:E:597:ILE:O	3:E:600:LYS:HG2	1.88	0.72
1:C:1055:GLN:HE22	1:C:1090:ASP:H	1.36	0.72
1:A:387:LEU:HD11	1:A:735:VAL:HG21	1.72	0.72
1:A:664:HIS:HB2	1:A:1131:LYS:CE	2.18	0.72
1:A:842:GLU:O	1:A:844:LYS:HD3	1.90	0.72
1:A:840:GLU:N	2:B:103:THR:CB	2.48	0.72
1:C:537:GLU:OE1	3:H:236:ASN:HB2	1.89	0.72
1:A:465:HIS:HB2	1:A:467:GLN:HE21	1.54	0.71
1:C:589:ARG:NH1	3:H:241:TYR:CE2	2.58	0.71
1:A:1055:GLN:HE22	1:A:1090:ASP:H	1.37	0.71
1:C:469:ILE:HD13	1:C:470:GLN:N	2.06	0.71
1:C:465:HIS:O	1:C:467:GLN:HG3	1.89	0.71
1:A:394:ILE:HG22	1:A:395:GLY:N	2.05	0.71
3:E:847:GLN:HB3	3:E:889:ARG:HD2	1.72	0.71
1:C:465:HIS:HB2	1:C:467:GLN:HE21	1.54	0.71
3:E:555:ARG:HB2	3:E:559:PRO:HG3	1.68	0.71
1:A:465:HIS:O	1:A:467:GLN:HG3	1.89	0.71
1:A:450:GLY:HA3	1:A:479:VAL:HG21	1.73	0.71
1:A:889:ARG:HD3	1:A:901:THR:HB	1.73	0.71
3:H:229:ASN:C	3:H:231:THR:H	1.94	0.71
1:C:451:PHE:CE1	1:C:470:GLN:HB2	2.26	0.71
1:C:889:ARG:HD3	1:C:901:THR:HB	1.73	0.71
3:E:449:LEU:HD11	3:E:479:LEU:CD2	2.13	0.71
3:H:272:ILE:CD1	3:H:340:GLN:HE22	1.99	0.71
1:A:451:PHE:CE1	1:A:470:GLN:HB2	2.25	0.70
1:A:532:THR:HG22	1:A:533:GLU:N	2.06	0.70
1:A:652:CYS:HB3	1:A:676:VAL:O	1.91	0.70
1:C:399:HIS:NE2	1:C:703:THR:HG22	2.05	0.70
1:C:532:THR:HG22	1:C:533:GLU:N	2.06	0.70
1:C:585:GLU:CG	3:H:301:ILE:HG23	2.21	0.70
3:H:428:LEU:CA	3:H:432:LEU:CB	2.69	0.70
2:B:263:LEU:HB2	2:B:272:PHE:HB3	1.73	0.70
1:C:707:ILE:HG22	1:C:707:ILE:O	1.90	0.70
1:A:480:SER:O	1:A:484:LYS:HA	1.92	0.70
3:E:556:PRO:O	3:E:557:ASN:CG	2.30	0.70
3:H:457:LEU:CB	3:H:493:GLN:HE21	2.04	0.70
2:D:263:LEU:HB2	2:D:272:PHE:HB3	1.72	0.70
3:E:530:ILE:HA	3:E:534:PHE:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:VAL:O	1:A:715:VAL:CG1	2.40	0.70
1:C:561:TRP:O	1:C:587:ILE:CG2	2.40	0.70
3:E:429:ILE:O	3:E:429:ILE:CG1	2.35	0.69
3:H:223:ALA:HB2	3:H:240:LEU:HD11	1.72	0.69
1:C:450:GLY:HA3	1:C:479:VAL:HG21	1.73	0.69
1:A:469:ILE:HD13	1:A:470:GLN:N	2.06	0.69
3:E:597:ILE:O	3:E:600:LYS:CG	2.40	0.69
3:H:530:ILE:HA	3:H:534:PHE:HB2	1.73	0.69
1:C:652:CYS:HB3	1:C:676:VAL:O	1.91	0.69
4:F:37:ILE:HG13	4:F:38:VAL:H	1.57	0.69
1:C:430:VAL:HG13	3:H:246:ASN:CB	2.21	0.69
1:A:452:VAL:HG23	1:A:470:GLN:OE1	1.93	0.69
1:A:561:TRP:O	1:A:587:ILE:CG2	2.40	0.69
1:C:596:PHE:HE1	1:C:648:ASN:HA	1.58	0.69
3:E:428:LEU:HD22	3:E:432:LEU:CD2	2.20	0.69
3:H:336:ILE:O	3:H:342:VAL:HG11	1.91	0.69
1:C:592:LEU:HD23	1:C:593:MET:O	1.92	0.69
3:E:350:ILE:HG12	3:E:368:LEU:CD2	2.23	0.69
1:C:480:SER:O	1:C:484:LYS:HA	1.92	0.69
1:A:1051:LEU:HB2	1:A:1089:ILE:HD13	1.75	0.69
1:A:389:ILE:O	1:A:390:ILE:CB	2.40	0.69
3:E:339:ASP:O	3:E:340:GLN:HB3	1.93	0.69
1:A:596:PHE:HE1	1:A:648:ASN:HA	1.57	0.68
3:H:337:ILE:HG13	3:H:374:MET:CE	2.22	0.68
1:C:618:ILE:HG13	1:C:619:GLU:N	2.08	0.68
3:H:450:GLY:O	3:H:451:GLU:HB2	1.93	0.68
1:C:704:ILE:H	1:C:704:ILE:HD12	1.57	0.68
3:H:762:PHE:HB3	3:H:766:GLU:HG3	1.76	0.68
1:A:592:LEU:HD23	1:A:593:MET:O	1.92	0.68
3:E:598:TYR:CD2	3:E:878:LYS:O	2.46	0.68
3:E:340:GLN:HG2	3:E:341:LYS:HG2	1.76	0.68
1:A:926:LEU:HD11	2:B:122:LEU:HD23	1.70	0.68
1:A:618:ILE:HG13	1:A:619:GLU:N	2.07	0.68
1:C:402:ILE:CD1	3:H:198:LEU:HB3	2.23	0.68
3:E:417:VAL:HG21	3:E:449:LEU:CD2	2.24	0.68
3:E:762:PHE:HB3	3:E:766:GLU:HG3	1.76	0.68
1:A:111:ARG:NH1	2:B:290:CYS:SG	2.67	0.67
1:A:356:LEU:CD2	1:A:712:ILE:CG2	2.70	0.67
1:C:452:VAL:HG23	1:C:470:GLN:OE1	1.93	0.67
3:E:507:ILE:HD11	3:E:554:LYS:NZ	2.09	0.67
3:E:588:ASP:CA	3:E:632:LYS:NZ	2.53	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:VAL:CG1	3:H:246:ASN:HB3	2.24	0.67
3:E:450:GLY:C	3:E:452:HIS:H	1.97	0.67
3:E:594:PHE:C	3:E:596:PHE:H	1.96	0.67
1:C:499:SER:CB	3:H:238:GLU:CB	2.55	0.67
1:A:397:HIS:HB2	1:A:703:THR:CG2	2.25	0.67
1:A:354:THR:HG22	1:A:712:ILE:HD13	1.76	0.67
3:E:552:ILE:HG21	3:E:597:ILE:HG12	0.71	0.67
3:E:552:ILE:HG23	3:E:597:ILE:HG12	1.65	0.67
1:A:440:GLY:O	1:A:686:GLY:HA3	1.94	0.67
1:A:840:GLU:CG	1:A:840:GLU:O	2.43	0.67
1:A:912:LEU:CD2	2:B:109:ILE:CG2	2.69	0.67
1:C:440:GLY:O	1:C:686:GLY:HA3	1.94	0.67
1:C:926:LEU:HD21	2:D:126:LEU:HD11	1.76	0.66
3:E:374:MET:CG	3:E:378:LEU:HD23	2.20	0.66
1:A:714:THR:O	1:A:715:VAL:CB	2.44	0.66
1:A:111:ARG:HB2	2:B:292:TRP:HZ2	1.60	0.66
2:D:443:SER:HB2	2:D:450:LEU:HB2	1.76	0.66
4:F:35:TRP:HA	4:F:35:TRP:HE3	1.58	0.66
3:E:340:GLN:HG3	3:E:341:LYS:H	1.59	0.66
3:H:290:ASP:CG	3:H:367:LEU:CD1	2.64	0.66
1:A:710:LEU:O	1:A:711:HIS:C	2.34	0.66
1:A:460:CYS:HA	1:A:469:ILE:O	1.96	0.66
1:C:630:THR:CB	1:C:797:HIS:CE1	2.78	0.66
3:E:720:LYS:HG2	4:F:34:ALA:CB	2.26	0.66
1:A:354:THR:CG2	1:A:712:ILE:HD13	2.24	0.66
1:C:630:THR:HB	1:C:797:HIS:CE1	2.30	0.66
3:H:434:GLN:C	3:H:436:THR:H	1.99	0.66
1:A:536:HIS:CD2	1:A:563:ASP:HB3	2.31	0.66
1:C:926:LEU:HD22	2:D:105:ILE:CD1	2.26	0.66
3:E:332:PHE:CZ	3:E:336:ILE:HG21	2.31	0.66
3:E:599:GLY:HA2	3:E:879:PHE:HB3	1.78	0.66
2:B:443:SER:HB2	2:B:450:LEU:HB2	1.76	0.65
1:C:460:CYS:HA	1:C:469:ILE:O	1.95	0.65
1:C:564:ILE:HG22	1:C:564:ILE:O	1.96	0.65
3:H:363:ILE:C	3:H:363:ILE:CD1	2.53	0.65
1:A:926:LEU:HD21	2:B:122:LEU:HD11	1.78	0.65
3:H:911:TYR:O	3:H:912:ILE:HG13	1.96	0.65
1:C:582:LEU:O	1:C:583:GLY:O	2.14	0.65
3:E:555:ARG:CD	3:E:556:PRO:HD2	2.27	0.65
3:H:464:LEU:HB3	3:H:473:LEU:HD21	1.78	0.65
1:A:354:THR:HG23	1:A:712:ILE:CG2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:987:GLU:OE1	2:D:159:HIS:HB2	1.97	0.65
1:A:582:LEU:O	1:A:583:GLY:O	2.14	0.65
3:H:223:ALA:CB	3:H:240:LEU:CD1	2.75	0.65
3:H:340:GLN:HG2	3:H:341:LYS:CG	2.26	0.65
3:E:595:ARG:C	3:E:596:PHE:CD1	2.70	0.65
3:E:285:PHE:CZ	3:E:345:LYS:CD	2.71	0.65
3:E:494:TRP:HE3	3:E:540:PHE:HD2	1.41	0.65
1:C:536:HIS:CD2	1:C:563:ASP:HB3	2.31	0.65
1:C:394:ILE:HD12	1:C:706:GLU:HA	1.78	0.65
3:E:203:PHE:O	3:E:204:LYS:C	2.35	0.65
3:E:417:VAL:HG11	3:E:449:LEU:HD11	1.79	0.65
1:A:711:HIS:O	1:A:713:ARG:N	2.30	0.65
1:C:910:MET:HE1	2:D:105:ILE:CG2	2.16	0.65
1:A:562:THR:O	1:A:564:ILE:N	2.30	0.64
1:C:446:THR:CG2	1:C:447:GLU:H	2.05	0.64
3:E:720:LYS:CG	4:F:34:ALA:CB	2.74	0.64
1:A:564:ILE:HG22	1:A:564:ILE:O	1.96	0.64
1:C:507:GLN:HE22	1:C:553:SER:N	1.94	0.64
1:C:518:TYR:HD1	1:C:519:LEU:N	1.95	0.64
3:E:911:TYR:O	3:E:912:ILE:HG13	1.96	0.64
1:C:667:VAL:HG22	1:C:1015:GLN:O	1.98	0.64
3:E:339:ASP:CG	3:E:340:GLN:H	1.99	0.64
3:E:434:GLN:O	3:E:436:THR:N	2.30	0.64
3:E:594:PHE:O	3:E:596:PHE:N	2.30	0.64
3:H:434:GLN:O	3:H:436:THR:N	2.30	0.64
1:C:520:GLN:HG3	1:C:529:ILE:CG1	2.27	0.64
3:E:494:TRP:CZ3	3:E:540:PHE:HD2	2.14	0.64
3:H:203:PHE:O	3:H:204:LYS:C	2.35	0.64
3:H:230:SER:C	3:H:232:SER:H	2.00	0.64
1:A:589:ARG:NH1	3:E:241:TYR:CE2	2.65	0.64
3:E:415:HIS:O	3:E:419:LYS:HG2	1.97	0.64
1:A:507:GLN:NE2	1:A:553:SER:H	1.95	0.64
1:A:601:TYR:CE2	1:A:666:LEU:HD21	2.33	0.64
1:A:708:GLN:O	1:A:709:LYS:NZ	2.31	0.64
1:C:562:THR:O	1:C:564:ILE:N	2.30	0.64
3:E:450:GLY:O	3:E:452:HIS:N	2.30	0.64
3:E:555:ARG:O	3:E:557:ASN:N	2.30	0.64
1:A:715:VAL:N	1:A:716:PRO:CD	2.60	0.64
3:E:555:ARG:O	3:E:556:PRO:C	2.36	0.64
1:C:402:ILE:HD13	3:H:198:LEU:CB	2.28	0.64
3:H:467:GLU:HG2	3:H:469:ARG:HE	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:LEU:O	1:A:712:ILE:N	2.32	0.63
1:C:926:LEU:CD2	2:D:105:ILE:CD1	2.76	0.63
3:H:230:SER:O	3:H:232:SER:N	2.30	0.63
3:E:411:PRO:HG3	3:E:464:LEU:HD21	1.81	0.63
1:A:507:GLN:HE22	1:A:553:SER:N	1.95	0.63
1:C:430:VAL:CG2	3:H:246:ASN:HB3	2.27	0.63
1:C:601:TYR:CE2	1:C:666:LEU:HD21	2.33	0.63
3:H:229:ASN:O	3:H:231:THR:N	2.30	0.63
3:H:336:ILE:O	3:H:342:VAL:CB	2.45	0.63
3:H:599:GLY:H	3:H:878:LYS:HG2	1.63	0.63
1:A:476:VAL:HG13	1:A:490:TRP:HB3	1.81	0.63
3:E:431:TYR:O	3:E:432:LEU:HB2	1.98	0.63
3:E:595:ARG:HB2	3:E:596:PHE:CZ	2.33	0.63
1:A:518:TYR:HD1	1:A:519:LEU:N	1.96	0.63
3:E:359:ASN:OD1	3:E:359:ASN:N	2.32	0.63
1:A:414:ARG:CB	1:A:462:ASN:HD21	2.12	0.63
3:E:555:ARG:HD2	3:E:556:PRO:HD2	1.81	0.63
3:H:229:ASN:N	3:H:229:ASN:OD1	2.30	0.63
1:A:705:ASP:O	1:A:707:ILE:HG13	1.98	0.63
1:C:414:ARG:CB	1:C:462:ASN:HD21	2.12	0.62
2:D:249:ARG:HE	2:D:291:ASP:HB3	1.64	0.62
1:A:520:GLN:HG3	1:A:529:ILE:CG1	2.27	0.62
1:C:482:GLU:OE1	1:C:483:PRO:HD3	1.99	0.62
1:C:476:VAL:HG13	1:C:490:TRP:HB3	1.81	0.62
1:C:617:ASN:HD21	1:C:619:GLU:HB2	1.64	0.62
1:C:507:GLN:NE2	1:C:553:SER:H	1.94	0.62
3:H:340:GLN:CD	3:H:341:LYS:HG2	2.20	0.62
1:C:562:THR:HG22	1:C:563:ASP:N	2.14	0.62
1:A:7:VAL:HG13	1:A:1091:GLY:HA3	1.81	0.62
1:C:585:GLU:CD	3:H:301:ILE:HG23	2.19	0.62
1:C:839:GLU:H	2:D:103:THR:HG21	1.63	0.62
1:C:928:ARG:NH1	2:D:437:THR:CG2	2.62	0.62
1:C:7:VAL:HG13	1:C:1091:GLY:HA3	1.82	0.62
1:C:928:ARG:NH1	2:D:437:THR:HG23	2.14	0.62
3:E:340:GLN:HG3	3:E:341:LYS:HG2	1.82	0.62
3:E:397:TYR:CD2	3:E:444:VAL:CG1	2.78	0.62
2:B:249:ARG:HE	2:B:291:ASP:HB3	1.63	0.62
3:H:226:ALA:HB1	3:H:232:SER:C	2.18	0.62
1:A:591:ILE:O	1:A:592:LEU:HB2	2.00	0.62
1:A:926:LEU:HD21	2:B:122:LEU:CD1	2.30	0.62
1:C:926:LEU:HD22	2:D:105:ILE:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:720:LYS:HG2	4:F:34:ALA:HB2	1.82	0.62
1:A:354:THR:HG21	1:A:712:ILE:HB	1.78	0.61
1:A:582:LEU:HD13	1:A:583:GLY:H	1.64	0.61
3:E:598:TYR:HD2	3:E:878:LYS:O	1.83	0.61
1:A:562:THR:HG22	1:A:563:ASP:N	2.14	0.61
1:A:617:ASN:HD21	1:A:619:GLU:HB2	1.64	0.61
1:A:926:LEU:HD21	2:B:122:LEU:HG	1.80	0.61
1:C:928:ARG:CZ	2:D:437:THR:CG2	2.78	0.61
1:C:912:LEU:CD2	2:D:109:ILE:HD13	2.30	0.61
4:F:38:VAL:O	4:F:39:VAL:CG2	2.47	0.61
1:A:492:GLU:HG3	1:A:496:LYS:HB2	1.83	0.61
1:C:889:ARG:HG3	1:C:904:ASN:ND2	2.16	0.61
1:C:111:ARG:NH2	2:D:290:CYS:SG	2.73	0.61
1:A:657:THR:HG21	1:A:668:PHE:HB3	1.82	0.61
1:C:591:ILE:O	1:C:592:LEU:HB2	2.00	0.61
3:E:501:PHE:O	3:E:504:THR:HG22	2.01	0.61
5:R:12:DG:N2	6:S:6:DG:C2	2.69	0.61
1:A:889:ARG:HG3	1:A:904:ASN:ND2	2.16	0.61
5:T:12:DG:N2	6:U:6:DG:C2	2.69	0.61
1:A:482:GLU:OE1	1:A:483:PRO:HD3	1.99	0.61
1:C:396:ILE:H	1:C:396:ILE:HD13	1.66	0.60
3:H:415:HIS:O	3:H:419:LYS:HG2	2.00	0.60
1:A:394:ILE:CG2	1:A:395:GLY:N	2.64	0.60
3:H:465:LEU:HD21	3:H:494:TRP:CD1	2.35	0.60
3:H:501:PHE:O	3:H:504:THR:HG22	2.01	0.60
1:C:582:LEU:HD13	1:C:583:GLY:H	1.65	0.60
3:E:414:LEU:HB3	3:E:475:LEU:CD2	2.32	0.60
3:H:206:LYS:CB	3:H:207:PRO:CD	2.79	0.60
1:A:446:THR:CG2	1:A:447:GLU:H	2.05	0.60
1:C:492:GLU:HG3	1:C:496:LYS:HB2	1.83	0.60
1:A:387:LEU:CD1	1:A:735:VAL:HG21	2.31	0.60
3:H:290:ASP:OD1	3:H:367:LEU:CD1	2.50	0.60
3:E:286:LEU:HD21	3:E:349:GLY:CA	2.30	0.60
3:E:587:LEU:CB	3:E:632:LYS:HD3	2.31	0.60
1:A:912:LEU:HD21	2:B:109:ILE:CD1	2.31	0.60
1:A:589:ARG:HD3	3:E:241:TYR:OH	2.02	0.60
1:A:397:HIS:HB2	1:A:703:THR:HG23	1.84	0.59
1:C:392:ASN:HD22	1:C:1012:LEU:C	2.06	0.59
3:E:434:GLN:C	3:E:436:THR:H	2.03	0.59
1:A:889:ARG:HG3	1:A:904:ASN:HD21	1.67	0.59
3:E:596:PHE:N	3:E:596:PHE:CD1	2.69	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:SER:OG	1:A:575:GLU:HB2	2.02	0.59
1:A:673:LEU:HD23	1:A:674:LYS:H	1.67	0.59
1:C:851:PHE:HB3	1:C:858:LEU:HD22	1.85	0.59
3:H:446:LYS:HG3	3:H:484:ARG:HH22	1.67	0.59
3:E:337:ILE:O	3:E:342:VAL:CB	2.50	0.59
1:C:402:ILE:HD12	3:H:198:LEU:HB3	1.85	0.59
1:C:441:GLU:O	1:C:441:GLU:HG2	2.02	0.59
3:E:350:ILE:HA	3:E:368:LEU:CD2	2.32	0.59
3:E:375:LEU:HD22	3:E:380:ILE:HB	1.83	0.59
1:A:692:ALA:C	1:A:693:LEU:HD23	2.23	0.59
1:A:851:PHE:HB3	1:A:858:LEU:HD22	1.85	0.59
1:C:912:LEU:HD22	2:D:109:ILE:HD13	1.85	0.59
1:A:454:ASP:N	1:A:454:ASP:OD1	2.28	0.59
1:A:498:ILE:HD12	1:A:498:ILE:N	2.18	0.59
1:A:588:PRO:HB3	1:A:604:CYS:SG	2.43	0.59
1:C:890:LEU:HB3	1:C:903:CYS:HB2	1.84	0.59
3:E:374:MET:O	3:E:378:LEU:N	2.36	0.59
3:E:730:CYS:HB2	4:F:26:LYS:O	2.03	0.59
1:A:396:ILE:H	1:A:396:ILE:HD13	1.68	0.58
1:A:407:ILE:HG21	1:A:410:LEU:HD23	1.85	0.58
1:C:912:LEU:HD21	2:D:109:ILE:CD1	2.33	0.58
3:E:506:VAL:O	3:E:555:ARG:HD3	2.03	0.58
4:F:38:VAL:C	4:F:39:VAL:CG2	2.71	0.58
3:H:337:ILE:O	3:H:338:SER:C	2.41	0.58
3:H:444:VAL:HG12	3:H:448:LEU:HD12	1.84	0.58
1:A:167:VAL:HG13	1:A:180:PHE:HB3	1.84	0.58
1:A:922:LEU:HD23	1:A:957:VAL:HG13	1.84	0.58
1:C:498:ILE:N	1:C:498:ILE:HD12	2.18	0.58
1:C:889:ARG:HG3	1:C:904:ASN:HD21	1.67	0.58
1:A:432:GLN:NE2	3:E:207:PRO:HG3	2.18	0.58
3:E:375:LEU:HD23	3:E:380:ILE:HD12	1.85	0.58
1:A:841:ALA:N	2:B:103:THR:CB	2.65	0.58
3:H:519:LEU:HD21	3:H:552:ILE:HD11	1.85	0.58
1:A:441:GLU:HG2	1:A:441:GLU:O	2.02	0.58
1:C:446:THR:HG22	1:C:447:GLU:N	2.16	0.58
1:C:910:MET:HE1	2:D:105:ILE:HD13	1.86	0.58
3:H:340:GLN:O	3:H:341:LYS:C	2.41	0.58
3:H:604:GLU:HB2	3:H:641:PHE:CE2	2.39	0.58
1:A:926:LEU:CD2	2:B:122:LEU:HD11	2.33	0.58
1:C:414:ARG:HB3	1:C:462:ASN:HD21	1.68	0.58
1:C:573:SER:OG	1:C:575:GLU:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:ARG:HG2	1:C:489:GLU:HG3	1.86	0.58
1:C:692:ALA:C	1:C:693:LEU:HD23	2.23	0.58
1:A:433:THR:HG22	1:A:434:ARG:H	1.69	0.58
1:C:588:PRO:HB3	1:C:604:CYS:SG	2.43	0.58
1:C:600:HIS:HB2	1:C:616:LEU:O	2.04	0.58
1:A:432:GLN:HA	1:A:455:GLN:O	2.04	0.58
1:C:673:LEU:HD23	1:C:674:LYS:H	1.68	0.58
3:E:604:GLU:HB2	3:E:641:PHE:CE2	2.38	0.58
3:H:336:ILE:O	3:H:342:VAL:CG1	2.51	0.58
1:C:695:ASN:OD1	1:C:697:SER:N	2.30	0.58
3:E:491:LEU:HG	3:E:540:PHE:CE1	2.39	0.58
1:A:493:PRO:HB2	1:A:494:GLN:HE22	1.69	0.58
1:A:354:THR:CB	1:A:712:ILE:HD12	2.33	0.58
1:C:502:SER:O	1:C:503:CYS:HB2	2.04	0.58
1:C:814:LEU:HD11	2:D:106:LEU:CD1	2.32	0.58
1:C:903:CYS:HB3	1:C:942:PHE:CE2	2.38	0.58
1:C:953:TRP:CG	2:D:119:HIS:HE1	2.21	0.58
3:E:596:PHE:O	3:E:597:ILE:HG13	2.04	0.58
3:H:339:ASP:O	3:H:340:GLN:CB	2.48	0.58
3:H:464:LEU:HB3	3:H:473:LEU:CD2	2.32	0.58
1:A:502:SER:O	1:A:503:CYS:HB2	2.04	0.57
1:A:890:LEU:HB3	1:A:903:CYS:HB2	1.85	0.57
3:H:734:ALA:HB3	3:H:741:LYS:O	2.04	0.57
1:A:414:ARG:HG2	1:A:414:ARG:HH11	1.69	0.57
1:C:553:SER:O	1:C:571:LEU:HD12	2.03	0.57
3:H:730:CYS:HB2	4:I:26:LYS:O	2.03	0.57
6:U:7:DT:H73	6:U:8:DA:C6	2.39	0.57
1:A:481:GLN:HA	1:A:484:LYS:HZ3	1.68	0.57
1:C:402:ILE:HD13	3:H:198:LEU:HB3	1.86	0.57
1:C:414:ARG:HH11	1:C:414:ARG:HG2	1.69	0.57
1:A:709:LYS:C	1:A:710:LEU:HD23	2.21	0.57
1:A:903:CYS:HB3	1:A:942:PHE:CE2	2.39	0.57
1:C:167:VAL:HG13	1:C:180:PHE:HB3	1.84	0.57
1:C:407:ILE:HG21	1:C:410:LEU:HD23	1.85	0.57
1:C:430:VAL:HG12	1:C:431:GLY:N	2.19	0.57
1:C:481:GLN:HA	1:C:484:LYS:HZ3	1.68	0.57
3:E:734:ALA:HB3	3:E:741:LYS:O	2.04	0.57
3:H:228:GLN:HB3	3:H:229:ASN:OD1	2.04	0.57
6:S:7:DT:H73	6:S:8:DA:C6	2.39	0.57
1:A:553:SER:O	1:A:571:LEU:HD12	2.03	0.57
1:A:669:SER:O	1:A:670:ASN:C	2.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:CYS:O	2:B:254:THR:HG23	2.05	0.57
3:H:353:LEU:CD2	3:H:363:ILE:HB	2.33	0.57
1:C:922:LEU:HD23	1:C:957:VAL:HG13	1.85	0.57
1:A:503:CYS:SG	1:A:504:ASN:N	2.78	0.57
3:E:588:ASP:N	3:E:632:LYS:NZ	2.53	0.57
1:A:414:ARG:HB3	1:A:462:ASN:HD21	1.68	0.57
1:C:432:GLN:HA	1:C:455:GLN:O	2.04	0.57
1:C:910:MET:SD	2:D:105:ILE:HG21	2.44	0.57
3:E:417:VAL:HG11	3:E:449:LEU:CG	2.35	0.57
3:E:771:THR:HG23	3:E:773:ILE:HG12	1.86	0.57
4:F:38:VAL:O	4:F:38:VAL:CG2	2.48	0.57
3:H:337:ILE:HG21	3:H:374:MET:HE3	1.86	0.57
1:A:600:HIS:HB2	1:A:616:LEU:O	2.04	0.57
1:C:433:THR:HG22	1:C:434:ARG:H	1.69	0.57
1:C:493:PRO:HB2	1:C:494:GLN:HE22	1.70	0.57
1:C:578:HIS:CE1	1:C:623:LEU:HD12	2.39	0.57
1:C:589:ARG:NH1	3:H:241:TYR:HE2	2.02	0.57
1:A:111:ARG:CZ	2:B:292:TRP:HE1	2.14	0.56
3:H:771:THR:HG23	3:H:773:ILE:HG12	1.86	0.56
3:E:417:VAL:HG11	3:E:449:LEU:HD21	1.87	0.56
3:H:204:LYS:O	3:H:205:ASP:HB3	2.04	0.56
1:A:928:ARG:NH1	2:B:437:THR:HG23	2.21	0.56
1:C:503:CYS:SG	1:C:504:ASN:N	2.78	0.56
1:C:927:MET:SD	2:D:126:LEU:HD13	2.45	0.56
3:H:658:ILE:HG21	3:H:716:HIS:HE1	1.71	0.56
1:C:429:PHE:O	1:C:430:VAL:O	2.22	0.56
2:D:242:CYS:O	2:D:254:THR:HG23	2.04	0.56
3:H:353:LEU:HB3	3:H:363:ILE:HG13	1.87	0.56
1:A:430:VAL:HG12	1:A:431:GLY:N	2.19	0.56
1:A:578:HIS:CE1	1:A:623:LEU:HD12	2.40	0.56
1:C:1000:LEU:HD13	1:C:1002:GLU:HB2	1.88	0.56
3:E:410:VAL:HB	3:E:411:PRO:HD3	1.86	0.56
3:E:730:CYS:HB3	4:F:27:TRP:HA	1.88	0.56
1:A:477:ARG:HG2	1:A:489:GLU:HG3	1.86	0.56
1:C:669:SER:O	1:C:670:ASN:C	2.43	0.56
1:C:928:ARG:CZ	2:D:437:THR:HG21	2.35	0.56
3:E:467:GLU:HG2	3:E:469:ARG:HE	1.70	0.56
1:A:659:ILE:HG22	1:A:660:TYR:N	2.21	0.56
1:A:695:ASN:OD1	1:A:697:SER:N	2.30	0.56
1:A:354:THR:HG22	1:A:712:ILE:HG21	1.70	0.56
1:A:111:ARG:CZ	2:B:290:CYS:SG	2.94	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:518:TYR:CD1	1:C:519:LEU:N	2.74	0.56
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	1.88	0.56
1:A:664:HIS:CB	1:A:1131:LYS:CE	2.80	0.56
1:A:715:VAL:H	1:A:716:PRO:CD	2.18	0.56
3:E:339:ASP:HA	3:E:343:GLN:HB2	1.88	0.56
1:A:429:PHE:O	1:A:430:VAL:O	2.22	0.56
1:A:493:PRO:HB2	1:A:494:GLN:NE2	2.21	0.56
1:A:518:TYR:C	1:A:518:TYR:CD1	2.80	0.56
3:H:434:GLN:C	3:H:436:THR:N	2.59	0.56
1:A:587:ILE:HD11	3:E:308:LEU:CD2	2.36	0.55
1:A:703:THR:OG1	1:A:704:ILE:N	2.39	0.55
1:C:706:GLU:O	1:C:706:GLU:HG2	2.05	0.55
1:A:513:GLY:HA2	3:E:236:ASN:ND2	2.21	0.55
1:A:582:LEU:CD1	1:A:583:GLY:H	2.19	0.55
1:C:493:PRO:HB2	1:C:494:GLN:NE2	2.21	0.55
3:E:658:ILE:HG21	3:E:716:HIS:HE1	1.71	0.55
1:A:403:ASP:HA	1:A:698:THR:HG22	1.88	0.55
1:A:522:HIS:HB3	1:A:523:PRO:HD2	1.88	0.55
1:A:532:THR:CG2	1:A:533:GLU:N	2.69	0.55
1:C:582:LEU:CD1	1:C:583:GLY:H	2.20	0.55
1:A:663:ASN:O	1:A:1131:LYS:HE2	2.06	0.55
1:C:479:VAL:HG12	1:C:480:SER:N	2.22	0.55
1:A:446:THR:HG22	1:A:447:GLU:N	2.15	0.55
3:H:444:VAL:CG1	3:H:448:LEU:HD12	2.35	0.55
1:A:518:TYR:CD1	1:A:519:LEU:N	2.75	0.55
1:A:532:THR:OG1	1:A:574:PHE:HD2	1.90	0.55
1:C:522:HIS:HB3	1:C:523:PRO:HD2	1.89	0.55
1:A:448:LEU:HD23	1:A:451:PHE:CE2	2.42	0.55
1:A:479:VAL:HG12	1:A:480:SER:N	2.22	0.55
1:A:663:ASN:O	1:A:1131:LYS:CE	2.55	0.55
1:C:403:ASP:HA	1:C:698:THR:HG22	1.88	0.55
1:C:433:THR:HG22	1:C:434:ARG:N	2.22	0.55
1:C:525:GLU:OE2	1:C:527:ARG:NH2	2.39	0.55
1:C:502:SER:OG	1:C:543:ILE:HG12	2.07	0.55
1:A:432:GLN:HE22	3:E:207:PRO:CG	2.19	0.55
3:E:597:ILE:O	3:E:600:LYS:CE	2.53	0.55
3:E:734:ALA:HB1	3:E:736:PHE:CE2	2.42	0.55
3:H:730:CYS:HB3	4:I:27:TRP:HA	1.88	0.55
3:H:734:ALA:HB1	3:H:736:PHE:CE2	2.42	0.55
1:A:502:SER:OG	1:A:543:ILE:HG12	2.07	0.55
1:A:713:ARG:HG3	1:A:714:THR:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:226:ALA:O	3:H:232:SER:N	2.40	0.55
3:H:428:LEU:O	3:H:432:LEU:CB	2.55	0.55
3:H:457:LEU:CD1	3:H:490:LEU:HA	2.37	0.55
1:A:404:LEU:HD21	3:E:200:ILE:CD1	2.36	0.54
1:A:649:VAL:CG1	1:A:650:PHE:H	2.16	0.54
1:C:532:THR:OG1	1:C:574:PHE:HD2	1.90	0.54
3:E:357:GLU:O	3:E:427:ARG:NH2	2.41	0.54
1:A:926:LEU:CG	2:B:122:LEU:HD21	2.35	0.54
2:B:140:HIS:HB2	2:B:453:ASN:HB2	1.88	0.54
1:C:614:PHE:N	1:C:614:PHE:CD1	2.75	0.54
1:A:841:ALA:HA	2:B:103:THR:O	2.07	0.54
1:C:289:GLU:HA	1:C:295:VAL:HA	1.89	0.54
3:H:220:LEU:HD23	3:H:240:LEU:HD23	1.81	0.54
1:A:525:GLU:OE2	1:A:527:ARG:NE	2.41	0.54
1:C:1033:VAL:HG11	2:D:115:GLY:HA3	1.89	0.54
1:C:218:MET:CE	1:C:261:HIS:HD2	2.21	0.54
1:C:431:GLY:O	1:C:432:GLN:HB3	2.07	0.54
1:C:448:LEU:HD23	1:C:451:PHE:CE2	2.42	0.54
2:D:140:HIS:HB2	2:D:453:ASN:HB2	1.89	0.54
3:E:430:THR:O	3:E:431:TYR:CB	2.54	0.54
1:A:289:GLU:HA	1:A:295:VAL:HA	1.88	0.54
1:A:431:GLY:O	1:A:432:GLN:HB3	2.07	0.54
1:A:614:PHE:N	1:A:614:PHE:CD1	2.75	0.54
1:C:518:TYR:CD1	1:C:518:TYR:C	2.79	0.54
1:C:659:ILE:HG22	1:C:660:TYR:N	2.22	0.54
3:E:374:MET:CG	3:E:378:LEU:CD2	2.83	0.54
2:B:299:VAL:HA	2:B:326:PRO:HB3	1.89	0.54
3:E:553:ASN:CB	3:E:598:TYR:CB	2.73	0.54
1:C:285:LEU:HB3	1:C:297:LEU:HD11	1.89	0.54
2:D:299:VAL:HA	2:D:326:PRO:HB3	1.89	0.54
3:E:595:ARG:HB2	3:E:596:PHE:CE1	2.43	0.54
3:E:789:LYS:HB2	3:E:791:ARG:HH12	1.73	0.54
1:C:931:LEU:HD21	1:C:944:GLU:HG3	1.90	0.54
3:E:665:TYR:HD2	3:E:666:MET:SD	2.31	0.54
3:H:229:ASN:C	3:H:231:THR:N	2.61	0.54
1:A:111:ARG:CZ	2:B:292:TRP:NE1	2.71	0.53
1:A:525:GLU:OE2	1:A:527:ARG:NH2	2.39	0.53
1:C:641:PHE:CD2	1:C:679:MET:HE3	2.43	0.53
3:E:449:LEU:HD13	3:E:479:LEU:HB3	1.90	0.53
3:H:231:THR:O	3:H:232:SER:C	2.45	0.53
3:H:223:ALA:HB1	3:H:240:LEU:HD11	1.85	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:789:LYS:HB2	3:H:791:ARG:HH12	1.74	0.53
1:A:218:MET:CE	1:A:261:HIS:HD2	2.21	0.53
1:A:578:HIS:HD2	1:A:623:LEU:H	1.56	0.53
3:E:677:LEU:HD13	4:F:27:TRP:CE3	2.43	0.53
1:A:596:PHE:CZ	1:A:649:VAL:HG23	2.43	0.53
1:A:602:LEU:O	1:A:603:LEU:HD23	2.07	0.53
1:A:841:ALA:C	2:B:103:THR:O	2.46	0.53
3:E:767:ILE:O	3:E:771:THR:HG22	2.09	0.53
3:H:336:ILE:O	3:H:342:VAL:HG21	2.09	0.53
1:A:450:GLY:HA3	1:A:479:VAL:HG22	1.91	0.53
1:A:536:HIS:HB2	1:A:560:LEU:HD13	1.90	0.53
1:A:285:LEU:HB3	1:A:297:LEU:HD11	1.90	0.53
1:A:587:ILE:HD11	3:E:308:LEU:HD22	1.91	0.53
3:E:414:LEU:HB3	3:E:475:LEU:HD23	1.90	0.53
3:H:222:GLU:O	3:H:233:ILE:CB	2.57	0.53
3:H:338:SER:O	3:H:343:GLN:HB2	2.09	0.53
6:U:7:DT:H73	6:U:8:DA:N6	2.24	0.53
1:A:433:THR:HG22	1:A:434:ARG:N	2.23	0.53
1:C:596:PHE:CZ	1:C:649:VAL:HG23	2.43	0.53
1:C:602:LEU:O	1:C:603:LEU:HD23	2.08	0.53
1:C:622:LEU:C	1:C:622:LEU:HD12	2.29	0.53
3:E:507:ILE:HD11	3:E:554:LYS:HZ3	1.74	0.53
1:C:649:VAL:CG1	1:C:650:PHE:N	2.71	0.53
1:C:113:GLY:H	2:D:338:THR:HG22	1.74	0.53
3:H:226:ALA:HB2	3:H:233:ILE:CB	2.39	0.53
3:H:271:GLN:HB3	3:H:336:ILE:HD11	1.91	0.53
1:C:536:HIS:HB2	1:C:560:LEU:HD13	1.89	0.53
1:C:578:HIS:HD2	1:C:623:LEU:H	1.55	0.53
3:E:350:ILE:HG21	3:E:372:LEU:HD21	1.90	0.53
3:H:665:TYR:HD2	3:H:666:MET:SD	2.31	0.53
1:A:487:VAL:O	1:A:488:SER:HB2	2.09	0.52
1:A:622:LEU:HD12	1:A:622:LEU:C	2.29	0.52
1:C:532:THR:CG2	1:C:533:GLU:N	2.69	0.52
3:H:336:ILE:O	3:H:342:VAL:HB	2.07	0.52
3:H:365:ARG:O	3:H:431:TYR:CB	2.57	0.52
3:H:767:ILE:O	3:H:771:THR:HG22	2.09	0.52
1:A:869:ALA:HB2	2:B:106:LEU:CB	2.39	0.52
1:C:525:GLU:OE2	1:C:527:ARG:NE	2.41	0.52
3:E:704:LEU:HA	3:E:707:ILE:HG22	1.91	0.52
1:A:594:THR:CG2	1:A:595:THR:N	2.73	0.52
3:E:206:LYS:N	3:E:207:PRO:HD2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:677:LEU:HD13	4:I:27:TRP:CE3	2.44	0.52
6:S:7:DT:H73	6:S:8:DA:N6	2.24	0.52
1:C:659:ILE:HD12	1:C:659:ILE:H	1.75	0.52
2:B:217:THR:OG1	2:B:254:THR:HG21	2.09	0.52
1:C:912:LEU:HD21	2:D:109:ILE:HD11	1.92	0.52
1:A:658:VAL:HG12	1:A:658:VAL:O	2.09	0.52
1:A:664:HIS:O	1:A:1131:LYS:HE2	2.08	0.52
1:A:579:LYS:HG2	1:A:581:MET:HE3	1.92	0.52
1:A:931:LEU:HD21	1:A:944:GLU:HG3	1.91	0.52
1:C:487:VAL:O	1:C:488:SER:HB2	2.09	0.52
1:C:649:VAL:CG1	1:C:650:PHE:H	2.17	0.52
1:C:631:LEU:O	1:C:655:ARG:HB2	2.10	0.52
3:H:206:LYS:H	3:H:207:PRO:HD2	1.73	0.52
3:H:353:LEU:HD22	3:H:363:ILE:HG12	1.88	0.52
1:C:18:CYS:HB2	1:C:313:CYS:HG	1.72	0.52
1:C:594:THR:CG2	1:C:595:THR:N	2.73	0.52
2:D:217:THR:OG1	2:D:254:THR:HG21	2.10	0.52
3:E:417:VAL:HG11	3:E:449:LEU:CD1	2.40	0.52
1:A:448:LEU:HD23	1:A:451:PHE:HE2	1.75	0.52
1:C:402:ILE:O	1:C:698:THR:HB	2.10	0.52
1:A:408:LYS:HA	1:A:678:TYR:CE1	2.45	0.51
1:A:912:LEU:CD2	2:B:109:ILE:CD1	2.88	0.51
1:C:562:THR:C	1:C:564:ILE:N	2.64	0.51
1:C:561:TRP:HA	1:C:587:ILE:HG21	1.92	0.51
4:F:38:VAL:O	4:F:39:VAL:CB	2.57	0.51
1:C:402:ILE:CD1	3:H:198:LEU:CB	2.87	0.51
1:A:402:ILE:O	1:A:698:THR:HB	2.10	0.51
1:A:659:ILE:HD12	1:A:659:ILE:H	1.75	0.51
1:C:393:GLY:O	1:C:709:LYS:N	2.38	0.51
1:C:578:HIS:CE1	1:C:623:LEU:CD1	2.93	0.51
1:A:578:HIS:CE1	1:A:623:LEU:CD1	2.93	0.51
3:E:311:ASP:O	3:E:316:LEU:HB2	2.10	0.51
3:E:557:ASN:ND2	3:E:843:PHE:HZ	2.09	0.51
3:H:457:LEU:HD11	3:H:490:LEU:HA	1.93	0.51
1:A:838:PRO:CA	2:B:101:GLY:HA2	2.38	0.51
1:C:658:VAL:HG12	1:C:658:VAL:O	2.09	0.51
3:E:390:LEU:HD22	3:E:440:LEU:HD13	1.91	0.51
3:E:494:TRP:HE3	3:E:540:PHE:CD2	2.21	0.51
3:E:491:LEU:HA	3:E:540:PHE:CE2	2.46	0.51
1:A:573:SER:O	1:A:574:PHE:HB2	2.10	0.51
1:C:374:GLN:HG2	1:C:391:ARG:CB	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:600:LYS:HG3	3:E:878:LYS:HG3	1.91	0.51
3:H:704:LEU:HA	3:H:707:ILE:HG22	1.91	0.51
1:A:459:PHE:CD2	1:A:460:CYS:N	2.79	0.51
1:A:471:ILE:HA	1:A:476:VAL:HA	1.92	0.51
1:A:570:LYS:O	1:A:574:PHE:N	2.42	0.51
1:C:459:PHE:CD2	1:C:460:CYS:N	2.79	0.51
1:C:573:SER:O	1:C:574:PHE:HB2	2.10	0.51
3:E:340:GLN:O	3:E:344:ASN:OD1	2.28	0.51
1:C:451:PHE:HD1	1:C:470:GLN:HB2	1.74	0.51
3:H:206:LYS:N	3:H:207:PRO:HD2	2.26	0.51
3:H:600:LYS:HG3	3:H:878:LYS:HG3	1.91	0.51
3:H:598:TYR:HD1	3:H:878:LYS:O	1.94	0.51
3:H:338:SER:O	3:H:343:GLN:HG3	2.10	0.51
1:A:613:TYR:CE1	1:A:627:LYS:HB2	2.46	0.51
1:C:369:ARG:CB	1:C:668:PHE:CB	2.89	0.51
1:C:408:LYS:HA	1:C:678:TYR:CE1	2.46	0.51
1:C:454:ASP:N	1:C:454:ASP:OD1	2.28	0.51
1:A:711:HIS:O	1:A:711:HIS:CD2	2.64	0.51
1:C:970:ASN:OD1	2:D:119:HIS:ND1	2.42	0.51
3:E:340:GLN:HG2	3:E:341:LYS:H	1.42	0.51
3:E:428:LEU:HD22	3:E:432:LEU:HB3	1.91	0.51
3:H:864:LEU:HD23	3:H:869:LEU:HD12	1.92	0.51
1:A:987:GLU:CD	2:B:156:HIS:HE1	2.04	0.50
1:C:490:TRP:CG	1:C:491:LYS:N	2.79	0.50
1:C:671:VAL:O	1:C:673:LEU:N	2.38	0.50
1:A:416:ASP:OD1	1:A:418:ASN:HB2	2.11	0.50
1:A:814:LEU:HD21	2:B:110:TYR:HB2	1.93	0.50
1:C:613:TYR:CE1	1:C:627:LYS:HB2	2.46	0.50
1:C:430:VAL:HG22	3:H:246:ASN:HD22	1.76	0.50
3:H:311:ASP:O	3:H:316:LEU:HB2	2.10	0.50
1:A:394:ILE:CG2	1:A:395:GLY:H	2.24	0.50
1:A:612:PHE:CE2	1:A:628:LYS:HD2	2.47	0.50
1:A:671:VAL:O	1:A:673:LEU:N	2.38	0.50
1:C:471:ILE:HA	1:C:476:VAL:HA	1.92	0.50
1:C:430:VAL:HG22	3:H:246:ASN:CB	2.36	0.50
3:E:494:TRP:CH2	3:E:530:ILE:HG21	2.46	0.50
3:H:216:THR:HA	3:H:219:LYS:HB2	1.93	0.50
1:A:512:VAL:HB	1:A:515:ALA:HB3	1.93	0.50
3:E:761:GLU:HB3	3:E:809:ILE:HG22	1.94	0.50
3:H:457:LEU:HB3	3:H:493:GLN:CG	2.39	0.50
1:A:391:ARG:O	1:A:393:GLY:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:LEU:O	1:A:572:PRO:C	2.50	0.50
1:C:587:ILE:HD12	1:C:587:ILE:H	1.77	0.50
3:E:886:LEU:O	3:E:890:ILE:HG12	2.12	0.50
1:A:492:GLU:CG	1:A:496:LYS:HB2	2.42	0.50
1:C:512:VAL:HB	1:C:515:ALA:HB3	1.94	0.50
3:E:520:LEU:HD21	3:E:586:MET:HE3	1.93	0.50
1:A:1054:MET:SD	1:A:1129:LEU:HD11	2.52	0.50
3:E:523:LYS:CE	3:E:544:MET:HE2	2.42	0.50
3:H:345:LYS:HA	3:H:348:ASP:HB2	1.93	0.50
3:H:380:ILE:HG22	3:H:384:SER:HB2	1.94	0.50
3:H:494:TRP:CH2	3:H:530:ILE:HG21	2.46	0.50
1:A:561:TRP:HA	1:A:587:ILE:HG21	1.93	0.49
1:A:641:PHE:CD2	1:A:679:MET:HE3	2.47	0.49
1:A:893:TRP:HE3	1:A:899:LEU:HD13	1.77	0.49
1:A:912:LEU:CD2	2:B:109:ILE:HG23	2.33	0.49
1:C:399:HIS:CE1	1:C:703:THR:HG22	2.47	0.49
1:C:416:ASP:OD1	1:C:418:ASN:HB2	2.11	0.49
1:C:612:PHE:CE2	1:C:628:LYS:HD2	2.46	0.49
1:A:490:TRP:CG	1:A:491:LYS:N	2.79	0.49
1:A:668:PHE:CD1	1:A:668:PHE:N	2.80	0.49
2:B:256:ASP:OD2	2:B:260:ARG:HB2	2.12	0.49
1:C:448:LEU:HD23	1:C:451:PHE:HE2	1.75	0.49
3:E:587:LEU:CB	3:E:632:LYS:CD	2.90	0.49
1:C:490:TRP:CD2	1:C:491:LYS:N	2.81	0.49
1:C:695:ASN:OD1	1:C:698:THR:N	2.42	0.49
2:D:211:SER:HB3	2:D:243:VAL:HG13	1.95	0.49
3:E:216:THR:HA	3:E:219:LYS:HB2	1.93	0.49
3:E:350:ILE:HG12	3:E:368:LEU:HD22	1.91	0.49
1:C:707:ILE:O	1:C:708:GLN:O	2.30	0.49
1:C:928:ARG:NH1	2:D:437:THR:HG21	2.27	0.49
3:E:796:ASN:HB2	3:E:797:PRO:HD3	1.94	0.49
3:H:557:ASN:ND2	3:H:843:PHE:HZ	2.10	0.49
1:C:492:GLU:CG	1:C:496:LYS:HB2	2.42	0.49
1:C:570:LYS:O	1:C:574:PHE:N	2.41	0.49
3:E:864:LEU:HD23	3:E:869:LEU:HD12	1.92	0.49
1:A:1055:GLN:NE2	1:A:1090:ASP:H	2.09	0.49
1:A:354:THR:HB	1:A:712:ILE:HD12	1.93	0.49
1:A:602:LEU:HD13	1:A:602:LEU:C	2.33	0.49
1:C:602:LEU:HD13	1:C:602:LEU:C	2.33	0.49
1:C:893:TRP:HE3	1:C:899:LEU:HD13	1.77	0.49
1:A:664:HIS:O	1:A:1131:LYS:NZ	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:GLY:HA3	1:C:479:VAL:HG22	1.91	0.49
3:E:380:ILE:HG22	3:E:384:SER:HB2	1.95	0.49
3:E:555:ARG:NE	3:E:556:PRO:HD2	2.27	0.49
3:E:594:PHE:C	3:E:596:PHE:N	2.63	0.49
3:H:365:ARG:CB	3:H:430:THR:O	2.60	0.49
1:A:708:GLN:C	1:A:709:LYS:HD3	2.30	0.49
1:C:571:LEU:O	1:C:572:PRO:C	2.50	0.49
2:D:256:ASP:OD2	2:D:260:ARG:HB2	2.13	0.49
3:E:414:LEU:HG	3:E:479:LEU:HD12	1.94	0.49
1:A:562:THR:C	1:A:564:ILE:N	2.64	0.49
1:A:587:ILE:N	1:A:587:ILE:HD12	2.28	0.49
1:A:596:PHE:CE2	1:A:659:ILE:HG22	2.48	0.49
1:C:394:ILE:HG22	1:C:395:GLY:N	2.27	0.49
3:E:450:GLY:C	3:E:452:HIS:N	2.64	0.49
3:H:230:SER:C	3:H:232:SER:N	2.67	0.49
3:H:622:SER:HB3	3:H:625:ALA:HB2	1.95	0.49
1:A:641:PHE:CE2	1:A:650:PHE:HB2	2.48	0.49
1:A:912:LEU:CD2	2:B:109:ILE:HG21	2.38	0.49
1:C:1055:GLN:NE2	1:C:1090:ASP:H	2.09	0.49
1:C:707:ILE:CG2	1:C:707:ILE:O	2.60	0.49
3:E:397:TYR:CE2	3:E:444:VAL:CG1	2.96	0.49
3:H:886:LEU:O	3:H:890:ILE:HG12	2.12	0.49
1:A:459:PHE:O	1:A:460:CYS:HB3	2.13	0.48
1:A:840:GLU:O	1:A:841:ALA:O	2.30	0.48
3:E:345:LYS:HA	3:E:348:ASP:HB2	1.94	0.48
3:H:781:THR:HG22	3:H:826:ILE:HD13	1.95	0.48
1:A:490:TRP:CD2	1:A:491:LYS:N	2.81	0.48
1:A:514:ARG:HG3	1:A:514:ARG:HH11	1.77	0.48
2:B:211:SER:HB3	2:B:243:VAL:HG13	1.94	0.48
1:C:587:ILE:HD12	1:C:587:ILE:N	2.27	0.48
1:A:443:VAL:HG12	1:A:443:VAL:O	2.13	0.48
1:A:659:ILE:O	1:A:660:TYR:HB3	2.13	0.48
1:C:655:ARG:NH1	1:C:713:ARG:NE	2.60	0.48
3:E:339:ASP:HA	3:E:343:GLN:CB	2.43	0.48
3:E:426:ASP:O	3:E:429:ILE:HG23	2.12	0.48
3:E:622:SER:HB3	3:E:625:ALA:HB2	1.95	0.48
1:A:1136:LEU:O	1:A:1139:ILE:HG12	2.13	0.48
1:A:587:ILE:HD12	1:A:587:ILE:H	1.78	0.48
1:A:596:PHE:HZ	1:A:649:VAL:HG23	1.78	0.48
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.78	0.48
2:B:394:PRO:HB3	2:B:402:ASP:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:339:ASP:OD1	3:E:340:GLN:N	2.38	0.48
3:E:340:GLN:HG3	3:E:341:LYS:CD	2.43	0.48
3:H:761:GLU:HB3	3:H:809:ILE:HG22	1.94	0.48
1:A:385:GLY:HA3	1:A:719:GLU:O	2.14	0.48
1:A:450:GLY:O	1:A:477:ARG:NH2	2.45	0.48
1:A:695:ASN:OD1	1:A:698:THR:N	2.42	0.48
1:C:393:GLY:O	1:C:708:GLN:HA	2.14	0.48
1:C:459:PHE:O	1:C:460:CYS:HB3	2.13	0.48
1:C:596:PHE:HZ	1:C:649:VAL:HG23	1.78	0.48
1:C:722:ARG:NH2	2:D:110:TYR:CD2	2.82	0.48
1:A:432:GLN:HE22	3:E:207:PRO:HG3	1.79	0.48
3:E:781:THR:HG22	3:E:826:ILE:HD13	1.94	0.48
3:H:337:ILE:HG13	3:H:374:MET:HE1	1.96	0.48
3:H:796:ASN:HB2	3:H:797:PRO:HD3	1.94	0.48
1:A:433:THR:O	1:A:434:ARG:HG3	2.14	0.48
1:C:641:PHE:HB2	1:C:681:PRO:HG3	1.95	0.48
2:D:394:PRO:HB3	2:D:402:ASP:HB3	1.96	0.48
3:E:233:ILE:H	3:E:233:ILE:HD13	1.78	0.48
3:E:587:LEU:HB2	3:E:632:LYS:HE3	1.95	0.48
1:A:638:LEU:O	1:A:639:ARG:HG2	2.14	0.48
1:C:392:ASN:CB	1:C:1012:LEU:O	2.54	0.48
1:C:596:PHE:CE2	1:C:659:ILE:HG22	2.47	0.48
1:C:641:PHE:CE2	1:C:650:PHE:HB2	2.48	0.48
1:A:594:THR:HG23	1:A:595:THR:N	2.28	0.48
1:A:679:MET:C	1:A:679:MET:SD	2.92	0.48
1:C:657:THR:HG22	1:C:658:VAL:N	2.24	0.48
1:C:659:ILE:O	1:C:660:TYR:HB3	2.13	0.48
3:H:681:ILE:HD11	3:H:721:LEU:HD22	1.95	0.48
1:A:396:ILE:HD13	1:A:396:ILE:N	2.29	0.48
1:A:459:PHE:CG	1:A:460:CYS:N	2.82	0.48
1:A:711:HIS:CG	1:A:711:HIS:O	2.66	0.48
3:E:588:ASP:N	3:E:632:LYS:HZ1	2.09	0.48
3:H:582:GLU:O	3:H:586:MET:HG2	2.14	0.48
1:A:479:VAL:CG1	1:A:480:SER:N	2.77	0.48
1:C:514:ARG:HG3	1:C:514:ARG:HH11	1.78	0.48
1:C:731:GLN:HA	1:C:796:GLN:HE21	1.78	0.48
1:C:770:LEU:HD13	1:C:865:GLU:HB2	1.95	0.48
3:E:203:PHE:O	3:E:205:ASP:N	2.47	0.48
3:E:892:SER:O	3:E:896:ARG:HD3	2.14	0.48
2:B:272:PHE:HE2	2:B:312:LYS:HA	1.79	0.47
1:C:385:GLY:HA3	1:C:719:GLU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:582:GLU:O	3:E:586:MET:HG2	2.14	0.47
3:H:358:ARG:O	3:H:420:ARG:NH1	2.47	0.47
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.44	0.47
1:A:457:THR:HG22	1:A:458:PHE:N	2.29	0.47
1:C:679:MET:SD	1:C:679:MET:C	2.92	0.47
3:H:892:SER:O	3:H:896:ARG:HD3	2.14	0.47
1:A:414:ARG:HB3	1:A:462:ASN:ND2	2.29	0.47
1:A:707:ILE:H	1:A:707:ILE:HG13	1.35	0.47
1:C:1136:LEU:O	1:C:1139:ILE:HG12	2.13	0.47
1:C:414:ARG:HB3	1:C:462:ASN:ND2	2.29	0.47
1:C:450:GLY:O	1:C:477:ARG:NH2	2.46	0.47
3:E:555:ARG:HA	3:E:555:ARG:HD2	1.61	0.47
3:E:681:ILE:HD11	3:E:721:LEU:HD22	1.95	0.47
1:A:641:PHE:HB2	1:A:681:PRO:HG3	1.95	0.47
1:C:402:ILE:HG22	1:C:403:ASP:H	1.80	0.47
1:C:403:ASP:O	1:C:405:PRO:HD3	2.15	0.47
1:C:459:PHE:CG	1:C:460:CYS:N	2.82	0.47
1:C:579:LYS:HG2	1:C:581:MET:HE3	1.95	0.47
1:C:638:LEU:O	1:C:639:ARG:HG2	2.15	0.47
2:D:272:PHE:HE2	2:D:312:LYS:HA	1.79	0.47
1:A:402:ILE:HD13	3:E:198:LEU:HB3	1.97	0.47
3:E:355:GLU:O	3:E:359:ASN:OD1	2.32	0.47
1:A:403:ASP:O	1:A:405:PRO:HD3	2.15	0.47
1:A:715:VAL:H	1:A:716:PRO:HD3	1.80	0.47
1:C:479:VAL:CG1	1:C:480:SER:N	2.77	0.47
3:E:206:LYS:CB	3:E:207:PRO:CD	2.92	0.47
1:A:490:TRP:O	1:A:491:LYS:HB2	2.14	0.47
1:A:531:HIS:ND1	1:A:532:THR:N	2.63	0.47
1:A:843:PRO:N	2:B:104:SER:CB	2.78	0.47
1:A:926:LEU:CD2	2:B:122:LEU:HD21	2.44	0.47
1:C:23:PHE:N	1:C:30:ASN:ND2	2.59	0.47
1:C:443:VAL:HG12	1:C:443:VAL:O	2.13	0.47
3:E:847:GLN:HE22	3:E:885:ASP:HB3	1.80	0.47
1:A:1048:TYR:O	1:A:1052:LEU:HB2	2.15	0.47
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.96	0.47
1:A:656:PRO:HG2	1:A:676:VAL:HG23	1.97	0.47
1:C:184:ASP:HB2	1:C:185:PRO:CD	2.44	0.47
1:C:407:ILE:CD1	1:C:699:LEU:HB2	2.45	0.47
1:C:532:THR:HG22	1:C:533:GLU:H	1.80	0.47
1:C:594:THR:HG23	1:C:595:THR:N	2.28	0.47
1:C:708:GLN:HE21	1:C:708:GLN:CA	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ILE:CD1	1:A:699:LEU:HB2	2.45	0.47
1:C:585:GLU:OE2	3:H:301:ILE:HG12	2.15	0.47
1:A:218:MET:HE2	1:A:261:HIS:HD2	1.79	0.47
1:A:396:ILE:O	1:A:396:ILE:HD13	2.15	0.47
1:C:396:ILE:HD13	1:C:396:ILE:O	2.15	0.47
1:C:433:THR:O	1:C:434:ARG:HG3	2.14	0.47
3:E:341:LYS:HD2	3:E:341:LYS:H	1.79	0.47
1:A:714:THR:HG22	1:A:715:VAL:N	2.30	0.47
1:A:770:LEU:HD13	1:A:865:GLU:HB2	1.95	0.47
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.50	0.47
1:C:457:THR:HG22	1:C:458:PHE:N	2.29	0.47
1:C:113:GLY:N	2:D:338:THR:HG22	2.29	0.47
3:E:417:VAL:CG2	3:E:449:LEU:HD21	2.43	0.47
3:E:597:ILE:N	3:E:600:LYS:HE2	2.29	0.47
3:E:587:LEU:HB2	3:E:632:LYS:CD	2.44	0.47
1:A:451:PHE:HD1	1:A:470:GLN:HB2	1.73	0.46
1:A:512:VAL:O	1:A:515:ALA:HB3	2.15	0.46
1:A:579:LYS:HE3	1:A:581:MET:CE	2.45	0.46
1:A:840:GLU:O	1:A:841:ALA:C	2.54	0.46
1:C:531:HIS:ND1	1:C:532:THR:N	2.63	0.46
1:C:643:SER:OG	1:C:644:LEU:N	2.46	0.46
1:C:889:ARG:HD2	1:C:891:TYR:CZ	2.50	0.46
3:E:859:LYS:HB3	3:E:859:LYS:HE3	1.80	0.46
1:A:402:ILE:HG22	1:A:403:ASP:H	1.80	0.46
1:A:432:GLN:HE22	3:E:207:PRO:HG2	1.80	0.46
1:C:218:MET:HE2	1:C:261:HIS:HD2	1.80	0.46
1:C:356:LEU:HD21	1:C:712:ILE:HD13	1.96	0.46
1:C:438:LEU:CD1	1:C:684:SER:HB2	2.46	0.46
1:C:704:ILE:H	1:C:704:ILE:CD1	2.21	0.46
1:C:114:ARG:NH2	2:D:386:ASP:OD2	2.47	0.46
3:E:350:ILE:HG12	3:E:368:LEU:HD23	1.94	0.46
3:E:414:LEU:HG	3:E:479:LEU:CD1	2.45	0.46
3:H:205:ASP:O	3:H:205:ASP:CG	2.53	0.46
3:H:430:THR:O	3:H:431:TYR:CB	2.61	0.46
3:H:911:TYR:CE2	3:H:913:ALA:HB2	2.50	0.46
1:A:451:PHE:HE1	1:A:470:GLN:HB2	1.79	0.46
1:A:360:VAL:HG22	2:B:113:SER:O	2.15	0.46
1:C:1048:TYR:O	1:C:1052:LEU:HB2	2.15	0.46
1:C:579:LYS:HE3	1:C:581:MET:CE	2.45	0.46
1:C:596:PHE:CZ	1:C:659:ILE:HG22	2.50	0.46
1:A:560:LEU:HG	1:A:565:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:ILE:CD1	1:C:396:ILE:N	2.78	0.46
3:E:299:GLN:HA	3:E:302:MET:HE3	1.97	0.46
3:E:555:ARG:HE	3:E:556:PRO:HD2	1.80	0.46
3:E:599:GLY:H	3:E:878:LYS:HG2	1.80	0.46
1:A:664:HIS:O	1:A:1131:LYS:CE	2.64	0.46
1:A:442:GLU:HG3	1:A:443:VAL:H	1.81	0.46
1:A:869:ALA:CB	2:B:106:LEU:CB	2.93	0.46
1:C:512:VAL:O	1:C:515:ALA:HB3	2.15	0.46
1:C:560:LEU:HG	1:C:565:SER:OG	2.16	0.46
1:A:596:PHE:CZ	1:A:659:ILE:HG22	2.50	0.46
1:A:709:LYS:C	1:A:710:LEU:CG	2.84	0.46
3:E:341:LYS:O	3:E:345:LYS:HG2	2.15	0.46
3:H:223:ALA:HB1	3:H:240:LEU:CD1	2.43	0.46
1:A:657:THR:HG22	1:A:658:VAL:N	2.24	0.46
1:C:43:VAL:HG21	1:C:50:ARG:CZ	2.46	0.46
3:E:597:ILE:HG22	3:E:597:ILE:O	2.15	0.46
4:F:33:TRP:O	4:F:34:ALA:O	2.34	0.46
1:A:396:ILE:N	1:A:396:ILE:CD1	2.78	0.46
1:A:438:LEU:CD1	1:A:684:SER:HB2	2.45	0.46
1:C:841:ALA:C	2:D:104:SER:HA	2.25	0.46
3:H:226:ALA:CB	3:H:233:ILE:CB	2.94	0.46
3:H:698:PRO:O	3:H:700:GLU:N	2.48	0.46
3:H:847:GLN:HE22	3:H:885:ASP:HB3	1.80	0.46
1:C:490:TRP:O	1:C:491:LYS:HB2	2.15	0.46
3:E:350:ILE:HD13	3:E:372:LEU:CD2	2.45	0.46
3:E:698:PRO:O	3:E:700:GLU:N	2.48	0.46
3:E:720:LYS:HG3	4:F:34:ALA:CB	2.34	0.46
1:A:587:ILE:CD1	1:A:587:ILE:H	2.29	0.46
1:A:407:ILE:HD11	1:A:699:LEU:HB2	1.98	0.46
1:C:184:ASP:HB2	1:C:185:PRO:HD2	1.97	0.46
1:C:656:PRO:HG2	1:C:676:VAL:HG23	1.97	0.46
1:C:1005:ASN:ND2	2:D:113:SER:O	2.46	0.46
1:C:442:GLU:HG3	1:C:443:VAL:H	1.81	0.45
1:C:869:ALA:H	1:C:885:ASN:ND2	2.14	0.45
1:C:953:TRP:HB2	1:C:970:ASN:HB2	1.98	0.45
1:A:715:VAL:O	1:A:716:PRO:C	2.55	0.45
1:A:953:TRP:HZ2	2:B:123:ARG:NH1	2.15	0.45
1:C:546:LEU:O	1:C:549:SER:HB3	2.16	0.45
1:C:597:GLU:O	1:C:598:SER:HB3	2.16	0.45
3:E:911:TYR:CE2	3:E:913:ALA:HB2	2.50	0.45
1:C:513:GLY:HA2	3:H:236:ASN:ND2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:VAL:HG22	1:A:526:LEU:CD1	2.47	0.45
3:E:332:PHE:CZ	3:E:336:ILE:HD12	2.51	0.45
3:E:417:VAL:HG11	3:E:449:LEU:CD2	2.47	0.45
3:E:558:LYS:N	3:E:559:PRO:HD2	2.32	0.45
1:C:926:LEU:CD2	2:D:126:LEU:HD11	2.45	0.45
3:H:340:GLN:NE2	3:H:342:VAL:CG2	2.76	0.45
1:A:411:TRP:HB2	1:A:460:CYS:SG	2.56	0.45
1:C:564:ILE:HG22	1:C:582:LEU:CD1	2.47	0.45
1:C:407:ILE:HD11	1:C:699:LEU:HB2	1.99	0.45
2:D:388:ILE:O	2:D:408:ILE:HA	2.17	0.45
3:E:341:LYS:CD	3:E:341:LYS:H	2.29	0.45
3:E:691:VAL:HA	3:E:692:PRO:HD3	1.85	0.45
3:H:491:LEU:HG	3:H:540:PHE:CZ	2.51	0.45
1:A:643:SER:OG	1:A:644:LEU:N	2.47	0.45
1:A:835:MET:CG	1:A:845:GLN:O	2.61	0.45
3:E:269:LYS:HD2	3:E:335:HIS:CE1	2.52	0.45
3:E:434:GLN:C	3:E:436:THR:N	2.68	0.45
1:A:1109:VAL:O	1:A:1111:ASN:N	2.42	0.45
1:A:589:ARG:CZ	3:E:241:TYR:CE2	3.00	0.45
1:A:657:THR:CG2	1:A:668:PHE:HB3	2.47	0.45
1:A:707:ILE:HB	1:A:708:GLN:H	1.45	0.45
1:A:354:THR:HG22	1:A:712:ILE:HD12	1.84	0.45
1:A:889:ARG:CD	1:A:901:THR:HB	2.45	0.45
1:C:390:ILE:HG22	1:C:391:ARG:N	2.32	0.45
1:C:655:ARG:NH1	1:C:713:ARG:HE	2.15	0.45
3:H:350:ILE:HG21	3:H:372:LEU:HD21	1.98	0.45
6:S:7:DT:C7	6:S:8:DA:C6	2.99	0.45
1:A:629:VAL:HG23	1:A:630:THR:N	2.31	0.45
1:A:953:TRP:HB2	1:A:970:ASN:HB2	1.97	0.45
1:C:411:TRP:HB2	1:C:460:CYS:SG	2.57	0.45
3:E:580:ASP:HA	3:E:583:LEU:HB3	1.99	0.45
3:H:436:THR:O	3:H:436:THR:HG22	2.16	0.45
3:H:580:ASP:HA	3:H:583:LEU:HB3	1.98	0.45
3:H:720:LYS:HB3	4:I:36:ASP:HB2	1.98	0.45
1:A:564:ILE:HG22	1:A:582:LEU:CD1	2.47	0.45
1:C:528:GLN:HG2	1:C:528:GLN:O	2.17	0.45
3:E:507:ILE:HD11	3:E:554:LYS:HZ2	1.80	0.45
1:A:312:GLU:HG3	1:A:327:ARG:HD2	1.98	0.45
1:A:43:VAL:HG21	1:A:50:ARG:CZ	2.46	0.45
1:A:597:GLU:O	1:A:598:SER:HB3	2.17	0.45
1:A:841:ALA:CA	2:B:103:THR:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:GLU:HB3	3:H:201:LYS:HB2	1.98	0.45
3:H:861:ARG:NH1	3:H:872:GLU:OE2	2.50	0.45
6:U:7:DT:C7	6:U:8:DA:C6	3.00	0.45
1:A:312:GLU:HG3	1:A:327:ARG:CD	2.47	0.44
1:A:397:HIS:HB2	1:A:703:THR:HG22	1.99	0.44
1:A:528:GLN:HG2	1:A:528:GLN:O	2.17	0.44
1:A:532:THR:CG2	1:A:533:GLU:H	2.30	0.44
1:A:546:LEU:O	1:A:549:SER:HB3	2.17	0.44
1:A:740:ILE:HG23	1:A:785:GLU:HG3	1.99	0.44
1:C:580:GLU:OE2	1:C:626:ARG:HD2	2.17	0.44
1:C:629:VAL:HG23	1:C:630:THR:N	2.31	0.44
1:C:692:ALA:O	1:C:693:LEU:HD23	2.17	0.44
3:E:545:LYS:HB3	3:E:545:LYS:HE2	1.82	0.44
1:A:564:ILE:O	1:A:582:LEU:HD12	2.17	0.44
1:C:312:GLU:HG3	1:C:327:ARG:HD2	1.98	0.44
1:C:396:ILE:HD13	1:C:396:ILE:N	2.29	0.44
1:C:476:VAL:HG22	1:C:526:LEU:CD1	2.47	0.44
1:C:607:GLY:HA2	1:C:635:PRO:HB3	1.99	0.44
1:A:580:GLU:OE2	1:A:626:ARG:HD2	2.17	0.44
1:A:659:ILE:CG2	1:A:660:TYR:N	2.79	0.44
3:E:494:TRP:CZ3	3:E:540:PHE:HB3	2.52	0.44
3:H:340:GLN:HE21	3:H:340:GLN:HB3	1.52	0.44
3:H:391:GLU:HG2	3:H:395:ARG:HH22	1.81	0.44
3:H:853:ALA:HA	3:H:856:ARG:HG2	2.00	0.44
3:H:719:ARG:HD3	4:I:33:TRP:CE3	2.53	0.44
4:I:37:ILE:O	4:I:38:VAL:C	2.56	0.44
1:A:478:LEU:HB3	1:A:488:SER:HB3	1.99	0.44
1:A:692:ALA:O	1:A:693:LEU:HD23	2.17	0.44
1:A:869:ALA:H	1:A:885:ASN:ND2	2.15	0.44
1:C:1057:ARG:HH12	1:C:1110:ALA:HB3	1.83	0.44
1:C:889:ARG:CD	1:C:901:THR:HB	2.45	0.44
3:E:275:PHE:CE2	3:E:289:ILE:HD13	2.53	0.44
3:E:391:GLU:HG2	3:E:395:ARG:HH22	1.81	0.44
3:H:336:ILE:O	3:H:342:VAL:CG2	2.65	0.44
1:A:953:TRP:CZ2	2:B:123:ARG:NH1	2.86	0.44
1:C:659:ILE:CG2	1:C:660:TYR:N	2.80	0.44
3:H:558:LYS:N	3:H:559:PRO:HD2	2.32	0.44
3:H:749:GLN:HG2	3:H:785:LEU:HD11	2.00	0.44
3:E:293:TRP:O	3:E:297:CYS:HB2	2.18	0.44
3:E:743:LEU:HD22	3:E:823:ILE:HD11	2.00	0.44
3:E:853:ALA:HA	3:E:856:ARG:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:275:PHE:CE2	3:H:289:ILE:HD13	2.53	0.44
3:H:736:PHE:HB2	3:H:737:LYS:H	1.62	0.44
1:A:419:ARG:HD3	1:A:421:THR:O	2.18	0.44
1:A:429:PHE:O	1:A:456:GLN:HG3	2.18	0.44
1:C:740:ILE:HG23	1:C:785:GLU:HG3	2.00	0.44
1:C:921:ILE:HB	1:C:933:LEU:HB2	1.99	0.44
3:E:375:LEU:CD2	3:E:380:ILE:HD12	2.48	0.44
3:E:556:PRO:C	3:E:557:ASN:CG	2.77	0.44
3:H:743:LEU:HD22	3:H:823:ILE:HD11	2.00	0.44
1:A:1057:ARG:HH12	1:A:1110:ALA:HB3	1.82	0.44
1:A:562:THR:O	1:A:563:ASP:C	2.56	0.44
1:A:926:LEU:HD21	2:B:122:LEU:CD2	2.48	0.44
1:A:921:ILE:HB	1:A:933:LEU:HB2	1.99	0.44
3:E:336:ILE:HG22	3:E:337:ILE:HD13	2.00	0.44
3:H:293:TRP:O	3:H:297:CYS:HB2	2.18	0.44
3:E:622:SER:HB3	3:E:625:ALA:CB	2.48	0.43
5:T:12:DG:C2	6:U:6:DG:C2	3.06	0.43
1:A:582:LEU:CD1	1:A:583:GLY:N	2.81	0.43
1:A:607:GLY:HA2	1:A:635:PRO:HB3	1.99	0.43
1:C:312:GLU:HG3	1:C:327:ARG:CD	2.47	0.43
1:C:430:VAL:O	1:C:456:GLN:HB2	2.19	0.43
1:C:447:GLU:O	1:C:448:LEU:HD12	2.18	0.43
1:C:139:LEU:HG	2:D:355:TYR:HB2	1.99	0.43
3:E:749:GLN:HG2	3:E:785:LEU:HD11	2.00	0.43
3:H:353:LEU:HD12	3:H:368:LEU:HD21	1.99	0.43
3:H:854:ILE:HD13	3:H:890:ILE:HD13	2.00	0.43
2:B:323:HIS:CD2	2:B:342:THR:HG21	2.53	0.43
2:B:388:ILE:O	2:B:408:ILE:HA	2.17	0.43
1:C:428:SER:OG	1:C:456:GLN:HG2	2.19	0.43
1:C:602:LEU:HD22	1:C:603:LEU:N	2.33	0.43
3:E:861:ARG:NH1	3:E:872:GLU:OE2	2.51	0.43
3:H:741:LYS:HG2	3:H:818:LEU:O	2.19	0.43
1:A:926:LEU:HD21	2:B:122:LEU:HD21	2.01	0.43
2:B:382:HIS:CG	2:B:383:PRO:HD2	2.54	0.43
2:D:383:PRO:HG3	2:D:435:SER:O	2.18	0.43
3:E:555:ARG:HD2	3:E:556:PRO:CD	2.47	0.43
3:E:741:LYS:HG2	3:E:818:LEU:O	2.19	0.43
5:R:12:DG:C2	6:S:6:DG:C2	3.06	0.43
1:A:611:LEU:HD23	1:A:611:LEU:C	2.39	0.43
1:C:429:PHE:O	1:C:456:GLN:HG3	2.18	0.43
1:C:564:ILE:O	1:C:582:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:229:ASN:O	3:H:231:THR:HG23	2.18	0.43
3:H:750:THR:O	3:H:754:LEU:HB2	2.19	0.43
1:A:602:LEU:HD22	1:A:603:LEU:N	2.34	0.43
1:A:912:LEU:CD2	2:B:109:ILE:HD13	2.48	0.43
2:B:105:ILE:HD12	2:B:126:LEU:HD21	2.01	0.43
2:B:367:PRO:HG2	2:B:392:ARG:HG3	2.01	0.43
1:C:534:MET:HE1	1:C:569:LEU:HD21	2.00	0.43
3:E:340:GLN:HG3	3:E:341:LYS:CG	2.46	0.43
1:A:448:LEU:HA	1:A:448:LEU:HD12	1.80	0.43
1:A:707:ILE:HG22	1:A:709:LYS:HZ1	1.83	0.43
1:A:708:GLN:C	1:A:709:LYS:HE2	2.39	0.43
1:C:673:LEU:HD23	1:C:674:LYS:N	2.33	0.43
3:H:466:ASP:O	3:H:468:ASN:N	2.51	0.43
1:A:1097:PHE:O	1:A:1100:ILE:HG12	2.18	0.43
1:A:428:SER:OG	1:A:456:GLN:HG2	2.19	0.43
1:C:655:ARG:HH11	1:C:655:ARG:CG	2.31	0.43
1:C:655:ARG:NH2	1:C:713:ARG:HD3	2.34	0.43
3:H:300:MET:C	3:H:302:MET:H	2.22	0.43
3:H:341:LYS:HE3	3:H:341:LYS:HB3	1.79	0.43
3:H:337:ILE:HG21	3:H:374:MET:CE	2.48	0.43
1:A:603:LEU:N	1:A:603:LEU:HD23	2.33	0.43
1:A:586:ILE:HG21	1:A:608:ASP:N	2.34	0.43
1:C:419:ARG:HD3	1:C:421:THR:O	2.18	0.43
1:C:478:LEU:HB3	1:C:488:SER:HB3	1.99	0.43
3:E:300:MET:C	3:E:302:MET:H	2.22	0.43
3:E:227:ILE:HD11	3:E:303:ILE:HG13	2.01	0.43
3:H:457:LEU:CD1	3:H:493:GLN:HB2	2.49	0.43
3:H:507:ILE:HD11	3:H:554:LYS:HB3	2.00	0.43
5:R:6:DA:C2	6:S:12:DA:C2	3.07	0.43
1:C:1097:PHE:O	1:C:1100:ILE:HG12	2.19	0.43
1:C:567:ARG:HB3	1:C:579:LYS:HA	2.01	0.43
3:E:450:GLY:HA2	3:E:453:LEU:HD21	2.01	0.43
1:A:494:GLN:O	1:A:495:ALA:HB3	2.19	0.42
1:A:562:THR:C	1:A:564:ILE:H	2.23	0.42
2:B:391:GLY:HA3	2:B:429:ILE:O	2.19	0.42
1:C:603:LEU:HD23	1:C:603:LEU:N	2.34	0.42
1:C:611:LEU:HD23	1:C:611:LEU:C	2.40	0.42
1:C:893:TRP:CE3	1:C:899:LEU:HD13	2.54	0.42
3:E:468:ASN:HD22	3:E:468:ASN:C	2.22	0.42
3:E:509:PRO:C	3:E:511:LYS:H	2.23	0.42
3:E:854:ILE:HD13	3:E:890:ILE:HD13	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:467:GLU:O	3:H:468:ASN:CB	2.66	0.42
3:H:622:SER:HB3	3:H:625:ALA:CB	2.48	0.42
1:C:562:THR:C	1:C:564:ILE:H	2.23	0.42
2:D:382:HIS:CG	2:D:383:PRO:HD2	2.54	0.42
3:E:201:LYS:O	3:E:202:ASN:HB2	2.18	0.42
3:E:311:ASP:HA	3:E:315:VAL:HG23	2.00	0.42
5:T:6:DA:C2	6:U:12:DA:C2	3.07	0.42
1:A:230:ILE:HD11	1:A:285:LEU:HD21	2.02	0.42
1:A:505:SER:OG	1:A:506:SER:N	2.52	0.42
1:C:582:LEU:CD1	1:C:583:GLY:N	2.81	0.42
2:D:367:PRO:HG2	2:D:392:ARG:HG3	2.01	0.42
3:H:311:ASP:HA	3:H:315:VAL:HG23	2.01	0.42
1:A:23:PHE:N	1:A:30:ASN:ND2	2.59	0.42
1:A:414:ARG:CG	1:A:414:ARG:HH11	2.32	0.42
1:A:430:VAL:O	1:A:456:GLN:HB2	2.18	0.42
1:A:586:ILE:HG22	1:A:607:GLY:H	1.83	0.42
1:A:842:GLU:O	1:A:844:LYS:CD	2.65	0.42
1:C:586:ILE:HG22	1:C:607:GLY:H	1.82	0.42
1:C:641:PHE:CD1	1:C:641:PHE:C	2.93	0.42
3:E:599:GLY:N	3:E:878:LYS:HG2	2.34	0.42
3:H:415:HIS:HB3	3:H:419:LYS:HZ1	1.84	0.42
1:A:567:ARG:HB3	1:A:579:LYS:HA	2.01	0.42
2:B:383:PRO:HG3	2:B:435:SER:O	2.18	0.42
1:C:494:GLN:O	1:C:495:ALA:HB3	2.19	0.42
2:D:391:GLY:HA3	2:D:429:ILE:O	2.20	0.42
3:E:397:TYR:CD1	3:E:448:LEU:HD11	2.55	0.42
3:E:750:THR:O	3:E:754:LEU:HB2	2.19	0.42
3:H:467:GLU:O	3:H:468:ASN:HB3	2.20	0.42
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.55	0.42
1:C:413:LEU:HB3	1:C:414:ARG:H	1.69	0.42
1:A:447:GLU:O	1:A:448:LEU:HD12	2.18	0.42
1:C:448:LEU:HA	1:C:448:LEU:HD12	1.80	0.42
1:C:500:VAL:HG12	1:C:541:LEU:HD12	2.01	0.42
1:C:699:LEU:HD13	1:C:700:THR:N	2.35	0.42
3:E:363:ILE:O	3:E:364:ASP:C	2.58	0.42
3:E:523:LYS:CE	3:E:544:MET:CE	2.98	0.42
1:C:1030:PHE:CZ	1:C:1038:GLY:HA3	2.54	0.42
3:E:338:SER:O	3:E:343:GLN:CB	2.57	0.42
3:E:390:LEU:CD2	3:E:440:LEU:HD13	2.50	0.42
3:E:533:CYS:HB2	3:E:534:PHE:HD1	1.85	0.42
1:A:23:PHE:N	1:A:30:ASN:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:VAL:HG12	1:A:541:LEU:HD12	2.01	0.42
1:A:578:HIS:CG	1:A:623:LEU:HD12	2.54	0.42
1:C:451:PHE:HE1	1:C:470:GLN:HB2	1.79	0.42
1:C:505:SER:OG	1:C:506:SER:N	2.52	0.42
1:C:562:THR:O	1:C:563:ASP:C	2.56	0.42
2:D:279:ALA:HB1	2:D:299:VAL:HG22	2.02	0.42
3:E:552:ILE:CG2	3:E:597:ILE:CD1	2.97	0.42
3:E:736:PHE:HB2	3:E:737:LYS:H	1.62	0.42
3:H:445:GLU:OE2	3:H:482:ARG:NE	2.53	0.42
3:H:468:ASN:C	3:H:468:ASN:HD22	2.23	0.42
3:H:509:PRO:C	3:H:511:LYS:H	2.22	0.42
2:B:347:ASN:HA	2:B:366:HIS:O	2.20	0.42
2:D:105:ILE:HD12	2:D:126:LEU:HD21	2.01	0.42
3:H:340:GLN:O	3:H:343:GLN:N	2.52	0.42
3:H:466:ASP:O	3:H:467:GLU:C	2.55	0.42
3:H:855:VAL:O	3:H:859:LYS:HB2	2.20	0.42
1:A:1055:GLN:HE22	1:A:1090:ASP:N	2.11	0.41
1:A:502:SER:O	1:A:503:CYS:CB	2.68	0.41
1:A:407:ILE:HD13	1:A:699:LEU:HD23	2.01	0.41
1:C:368:GLU:O	1:C:629:VAL:HB	2.20	0.41
1:C:576:LEU:C	1:C:577:LEU:HD23	2.41	0.41
3:E:855:VAL:O	3:E:859:LYS:HB2	2.20	0.41
1:C:523:PRO:HB3	1:C:524:GLN:NE2	2.35	0.41
1:C:532:THR:CG2	1:C:533:GLU:H	2.30	0.41
1:C:586:ILE:HG21	1:C:608:ASP:N	2.34	0.41
3:E:606:PHE:CZ	3:E:838:THR:HG23	2.55	0.41
1:A:24:THR:H	1:A:30:ASN:ND2	2.18	0.41
1:A:641:PHE:CD1	1:A:641:PHE:C	2.93	0.41
1:A:708:GLN:C	1:A:709:LYS:CD	2.88	0.41
2:B:354:SER:HA	2:B:357:TRP:CE2	2.56	0.41
1:C:24:THR:H	1:C:30:ASN:ND2	2.18	0.41
1:C:111:ARG:NE	2:D:290:CYS:SG	2.93	0.41
3:E:340:GLN:HE21	3:E:340:GLN:HB3	1.66	0.41
2:B:279:ALA:HB1	2:B:299:VAL:HG22	2.02	0.41
1:C:565:SER:CB	1:C:567:ARG:HH11	2.34	0.41
1:C:407:ILE:HD13	1:C:699:LEU:HD23	2.01	0.41
3:E:397:TYR:CG	3:E:444:VAL:HG13	2.50	0.41
3:E:494:TRP:CZ3	3:E:540:PHE:CD2	3.00	0.41
3:H:606:PHE:CZ	3:H:838:THR:HG23	2.55	0.41
3:H:698:PRO:HA	3:H:699:PRO:HD3	1.98	0.41
1:A:111:ARG:NH2	2:B:292:TRP:CD1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ILE:O	1:A:713:ARG:O	2.38	0.41
2:D:354:SER:HA	2:D:357:TRP:CE2	2.56	0.41
3:H:465:LEU:HG	3:H:497:TYR:CD2	2.55	0.41
1:A:708:GLN:C	1:A:709:LYS:CE	2.88	0.41
2:D:347:ASN:HA	2:D:366:HIS:O	2.20	0.41
3:E:410:VAL:HG21	3:E:460:GLY:HA3	2.02	0.41
3:H:341:LYS:HD2	3:H:341:LYS:H	1.85	0.41
3:H:533:CYS:HB2	3:H:534:PHE:HD1	1.85	0.41
1:A:576:LEU:C	1:A:577:LEU:HD23	2.41	0.41
1:C:565:SER:OG	1:C:567:ARG:NH1	2.54	0.41
3:E:288:LYS:HD3	3:E:288:LYS:HA	1.88	0.41
3:E:299:GLN:HA	3:E:302:MET:CE	2.51	0.41
3:E:358:ARG:HG3	3:E:427:ARG:HH12	1.86	0.41
3:E:464:LEU:HB3	3:E:473:LEU:CD2	2.51	0.41
3:E:899:MET:HA	3:E:911:TYR:O	2.21	0.41
1:A:394:ILE:HG22	1:A:395:GLY:H	1.82	0.41
1:A:643:SER:O	1:A:644:LEU:C	2.59	0.41
1:A:705:ASP:OD1	1:A:705:ASP:C	2.59	0.41
3:H:206:LYS:CB	3:H:207:PRO:HD3	2.50	0.41
3:H:298:ARG:CZ	3:H:298:ARG:HB3	2.50	0.41
3:H:545:LYS:HE2	3:H:545:LYS:HB3	1.82	0.41
1:A:565:SER:CB	1:A:567:ARG:HH11	2.34	0.41
1:A:703:THR:OG1	1:A:704:ILE:HD12	2.20	0.41
1:C:404:LEU:HD12	1:C:429:PHE:CZ	2.55	0.41
1:C:643:SER:O	1:C:644:LEU:C	2.59	0.41
1:C:926:LEU:HD21	2:D:105:ILE:CD1	2.43	0.41
2:D:323:HIS:CD2	2:D:342:THR:HG21	2.53	0.41
3:E:404:LEU:HD22	3:E:408:ARG:HH21	1.86	0.41
3:E:538:GLU:HA	3:E:541:ILE:HG22	2.03	0.41
3:H:741:LYS:HA	3:H:819:PHE:CE1	2.56	0.41
1:A:448:LEU:HB3	1:A:451:PHE:CD2	2.43	0.41
1:A:523:PRO:HB3	1:A:524:GLN:NE2	2.36	0.41
1:A:699:LEU:HD13	1:A:700:THR:N	2.35	0.41
3:H:299:GLN:HA	3:H:302:MET:CE	2.51	0.41
1:A:561:TRP:O	1:A:587:ILE:HG21	2.19	0.41
1:C:457:THR:CG2	1:C:459:PHE:O	2.69	0.41
3:E:436:THR:O	3:E:436:THR:HG22	2.20	0.41
3:E:468:ASN:HD21	3:E:470:ILE:HG23	1.86	0.41
3:H:272:ILE:HD11	3:H:340:GLN:CD	2.41	0.41
3:H:494:TRP:CE3	3:H:540:PHE:HD2	2.38	0.41
3:H:499:LYS:HE2	3:H:550:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:8:DA:C2	6:S:9:DA:N6	2.88	0.41
1:A:664:HIS:C	1:A:1131:LYS:CE	2.84	0.40
1:C:1055:GLN:HE22	1:C:1090:ASP:N	2.11	0.40
1:C:414:ARG:HH11	1:C:414:ARG:CG	2.32	0.40
1:C:701:ILE:HD12	1:C:701:ILE:H	1.86	0.40
1:C:820:LYS:H	1:C:820:LYS:HG2	1.79	0.40
2:D:218:THR:CG2	2:D:226:VAL:HG13	2.51	0.40
3:E:741:LYS:HA	3:E:819:PHE:CE1	2.56	0.40
3:E:835:GLN:HA	3:E:838:THR:HG22	2.03	0.40
3:H:404:LEU:HD22	3:H:408:ARG:HH21	1.86	0.40
3:H:457:LEU:CB	3:H:493:GLN:HG2	2.43	0.40
6:U:8:DA:C2	6:U:9:DA:N6	2.88	0.40
1:A:404:LEU:HD12	1:A:429:PHE:CZ	2.56	0.40
1:A:870:VAL:HA	1:A:883:SER:O	2.21	0.40
1:C:487:VAL:O	1:C:487:VAL:HG23	2.21	0.40
3:H:226:ALA:HB1	3:H:232:SER:CA	2.51	0.40
3:H:293:TRP:CZ3	3:H:370:SER:HB2	2.53	0.40
1:A:329:GLY:HA3	1:A:384:GLU:HG3	2.00	0.40
1:A:413:LEU:HD13	1:A:468:LEU:HD23	2.03	0.40
1:A:565:SER:OG	1:A:567:ARG:NH1	2.54	0.40
1:A:709:LYS:C	1:A:710:LEU:HG	2.40	0.40
1:C:870:VAL:HA	1:C:883:SER:O	2.21	0.40
3:E:449:LEU:O	3:E:453:LEU:HD13	2.21	0.40
3:E:596:PHE:O	3:E:597:ILE:CG1	2.68	0.40
1:A:457:THR:CG2	1:A:459:PHE:O	2.69	0.40
1:C:1057:ARG:NH1	1:C:1109:VAL:O	2.55	0.40
3:E:681:ILE:HD12	4:F:31:ALA:HB3	2.03	0.40
3:H:198:LEU:HA	3:H:198:LEU:HD22	1.92	0.40
3:H:290:ASP:OD1	3:H:367:LEU:HD13	2.16	0.40
3:H:859:LYS:HB3	3:H:859:LYS:HE3	1.80	0.40
3:H:899:MET:HA	3:H:911:TYR:O	2.21	0.40
1:A:893:TRP:CE3	1:A:899:LEU:HD13	2.54	0.40
1:C:413:LEU:HD13	1:C:468:LEU:HD23	2.03	0.40
1:C:452:VAL:HG22	1:C:477:ARG:NH1	2.37	0.40
1:C:928:ARG:HH11	2:D:437:THR:HG23	1.82	0.40
3:E:358:ARG:O	3:E:420:ARG:NH2	2.55	0.40
3:E:445:GLU:O	3:E:449:LEU:HB2	2.21	0.40
3:H:835:GLN:HA	3:H:838:THR:HG22	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	1095/1144 (96%)	948 (87%)	105 (10%)	42 (4%)	3	30
1	C	1095/1144 (96%)	967 (88%)	97 (9%)	31 (3%)	5	37
2	B	353/382 (92%)	333 (94%)	16 (4%)	4 (1%)	16	58
2	D	353/382 (92%)	333 (94%)	16 (4%)	4 (1%)	16	58
3	E	701/726 (97%)	603 (86%)	73 (10%)	25 (4%)	4	32
3	H	701/726 (97%)	604 (86%)	72 (10%)	25 (4%)	4	32
4	F	19/98 (19%)	14 (74%)	2 (10%)	3 (16%)	0	4
4	I	19/98 (19%)	16 (84%)	2 (10%)	1 (5%)	2	25
All	All	4336/4700 (92%)	3818 (88%)	383 (9%)	135 (3%)	4	35

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	LEU
1	A	390	ILE
1	A	430	VAL
1	A	583	GLY
1	A	598	SER
1	A	672	ASN
1	A	707	ILE
1	A	708	GLN
1	A	711	HIS
1	A	712	ILE
1	A	713	ARG
1	A	715	VAL
1	A	841	ALA
1	C	367	LEU
1	C	430	VAL
1	C	583	GLY
1	C	598	SER

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Mol	Chain	Res	Type
1	C	672	ASN
1	C	674	LYS
1	C	708	GLN
3	E	204	LYS
3	E	431	TYR
3	E	515	MET
3	E	556	PRO
3	E	595	ARG
3	E	597	ILE
3	E	902	ASP
4	F	34	ALA
4	F	38	VAL
3	H	204	LYS
3	H	431	TYR
3	H	515	MET
3	H	902	ASP
4	I	38	VAL
1	A	389	ILE
1	A	392	ASN
1	A	549	SER
1	A	562	THR
1	A	563	ASP
1	A	584	GLY
1	A	674	LYS
1	A	855	ASP
1	A	1110	ALA
2	B	117	SER
1	C	547	GLY
1	C	549	SER
1	C	562	THR
1	C	563	ASP
1	C	584	GLY
1	C	855	ASP
1	C	1110	ALA
2	D	117	SER
3	E	337	ILE
3	E	435	THR
3	E	596	PHE
3	E	761	GLU
3	E	880	PRO
3	E	912	ILE
3	H	206	LYS

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Mol	Chain	Res	Type
3	H	230	SER
3	H	231	THR
3	H	338	SER
3	H	435	THR
3	H	761	GLU
3	H	880	PRO
3	H	912	ILE
1	A	372	GLN
1	A	418	ASN
1	A	449	MET
1	A	481	GLN
1	A	547	GLY
1	A	624	SER
1	A	644	LEU
1	A	710	LEU
1	A	1109	VAL
1	C	418	ASN
1	C	449	MET
1	C	481	GLN
1	C	624	SER
1	C	644	LEU
1	C	1109	VAL
3	E	557	ASN
3	H	340	GLN
3	H	341	LYS
3	H	468	ASN
1	A	36	ASN
1	A	488	SER
2	B	190	GLY
1	C	36	ASN
1	C	372	GLN
1	C	488	SER
1	C	503	CYS
2	D	190	GLY
3	E	338	SER
3	E	340	GLN
3	E	451	GLU
3	E	699	PRO
3	H	699	PRO
1	A	503	CYS
1	A	592	LEU
1	C	242	GLY

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Mol	Chain	Res	Type
1	C	592	LEU
2	D	291	ASP
3	E	790	ALA
3	H	360	GLY
3	H	467	GLU
3	H	556	PRO
3	H	790	ALA
1	A	242	GLY
1	A	460	CYS
2	B	291	ASP
1	C	460	CYS
4	F	35	TRP
1	A	493	PRO
1	A	551	GLY
2	B	118	ILE
1	C	493	PRO
1	C	551	GLY
2	D	118	ILE
3	E	301	ILE
3	E	688	PRO
3	E	881	VAL
3	H	301	ILE
3	H	688	PRO
3	H	881	VAL
1	A	406	GLY
1	C	406	GLY
3	E	516	VAL
3	H	516	VAL
1	A	523	PRO
1	A	716	PRO
1	C	523	PRO
3	E	206	LYS
3	E	486	GLY
3	H	486	GLY

### 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	938/1000 (94%)	847 (90%)	91 (10%)	9	32
1	C	944/1000 (94%)	854 (90%)	90 (10%)	9	33
2	B	306/335 (91%)	283 (92%)	23 (8%)	15	45
2	D	313/335 (93%)	290 (93%)	23 (7%)	15	46
3	E	625/660 (95%)	535 (86%)	90 (14%)	3	19
3	H	631/660 (96%)	548 (87%)	83 (13%)	4	22
4	F	17/83 (20%)	13 (76%)	4 (24%)	1	5
4	I	16/83 (19%)	14 (88%)	2 (12%)	5	23
All	All	3790/4156 (91%)	3384 (89%)	406 (11%)	7	28

All (406) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	81	THR
1	A	99	ASP
1	A	133	LEU
1	A	147	ARG
1	A	159	LEU
1	A	167	VAL
1	A	191	LYS
1	A	241	ASN
1	A	267	ASN
1	A	304	LEU
1	A	314	LEU
1	A	334	VAL
1	A	339	ASP
1	A	360	VAL
1	A	370	GLN
1	A	396	ILE
1	A	403	ASP
1	A	410	LEU
1	A	412	PRO
1	A	414	ARG
1	A	419	ARG
1	A	420	GLU
1	A	452	VAL
1	A	454	ASP
1	A	469	ILE
1	A	473	SER

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Mol	Chain	Res	Type
1	A	476	VAL
1	A	481	GLN
1	A	482	GLU
1	A	487	VAL
1	A	493	PRO
1	A	510	VAL
1	A	518	TYR
1	A	523	PRO
1	A	525	GLU
1	A	531	HIS
1	A	540	CYS
1	A	555	LEU
1	A	560	LEU
1	A	563	ASP
1	A	567	ARG
1	A	576	LEU
1	A	582	LEU
1	A	587	ILE
1	A	594	THR
1	A	596	PHE
1	A	597	GLU
1	A	602	LEU
1	A	603	LEU
1	A	608	ASP
1	A	614	PHE
1	A	616	LEU
1	A	617	ASN
1	A	618	ILE
1	A	623	LEU
1	A	625	ASP
1	A	627	LYS
1	A	646	THR
1	A	673	LEU
1	A	688	PRO
1	A	689	ASP
1	A	700	THR
1	A	704	ILE
1	A	707	ILE
1	A	709	LYS
1	A	710	LEU
1	A	728	GLU
1	A	809	GLN

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Mol	Chain	Res	Type
1	A	820	LYS
1	A	839	GLU
1	A	840	GLU
1	A	844	LYS
1	A	864	LYS
1	A	867	LYS
1	A	881	LEU
1	A	898	GLU
1	A	899	LEU
1	A	901	THR
1	A	914	LEU
1	A	931	LEU
1	A	957	VAL
1	A	966	LEU
1	A	970	ASN
1	A	984	THR
1	A	1000	LEU
1	A	1052	LEU
1	A	1086	THR
1	A	1093	LEU
1	A	1106	GLN
1	A	1129	LEU
2	B	111	LYS
2	B	116	GLN
2	B	134	LEU
2	B	148	ARG
2	B	174	LEU
2	B	179	VAL
2	B	219	LEU
2	B	243	VAL
2	B	254	THR
2	B	262	LEU
2	B	274	GLU
2	B	293	LEU
2	B	299	VAL
2	B	308	LEU
2	B	312	LYS
2	B	321	MET
2	B	374	LEU
2	B	389	VAL
2	B	393	TYR
2	B	400	LEU

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Mol	Chain	Res	Type
2	B	435	SER
2	B	437	THR
2	B	453	ASN
1	C	7	VAL
1	C	81	THR
1	C	99	ASP
1	C	133	LEU
1	C	147	ARG
1	C	159	LEU
1	C	167	VAL
1	C	191	LYS
1	C	241	ASN
1	C	267	ASN
1	C	304	LEU
1	C	314	LEU
1	C	334	VAL
1	C	339	ASP
1	C	360	VAL
1	C	370	GLN
1	C	396	ILE
1	C	403	ASP
1	C	410	LEU
1	C	412	PRO
1	C	414	ARG
1	C	419	ARG
1	C	420	GLU
1	C	452	VAL
1	C	454	ASP
1	C	469	ILE
1	C	473	SER
1	C	476	VAL
1	C	481	GLN
1	C	482	GLU
1	C	487	VAL
1	C	493	PRO
1	C	510	VAL
1	C	518	TYR
1	C	523	PRO
1	C	525	GLU
1	C	531	HIS
1	C	540	CYS
1	C	555	LEU

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Mol	Chain	Res	Type
1	C	560	LEU
1	C	563	ASP
1	C	567	ARG
1	C	576	LEU
1	C	582	LEU
1	C	587	ILE
1	C	594	THR
1	C	596	PHE
1	C	597	GLU
1	C	602	LEU
1	C	603	LEU
1	C	608	ASP
1	C	614	PHE
1	C	616	LEU
1	C	617	ASN
1	C	618	ILE
1	C	623	LEU
1	C	625	ASP
1	C	627	LYS
1	C	646	THR
1	C	655	ARG
1	C	663	ASN
1	C	673	LEU
1	C	688	PRO
1	C	689	ASP
1	C	700	THR
1	C	703	THR
1	C	704	ILE
1	C	708	GLN
1	C	713	ARG
1	C	728	GLU
1	C	809	GLN
1	C	820	LYS
1	C	844	LYS
1	C	864	LYS
1	C	867	LYS
1	C	881	LEU
1	C	898	GLU
1	C	899	LEU
1	C	901	THR
1	C	914	LEU
1	C	931	LEU

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Mol	Chain	Res	Type
1	C	957	VAL
1	C	966	LEU
1	C	970	ASN
1	C	984	THR
1	C	1000	LEU
1	C	1052	LEU
1	C	1086	THR
1	C	1093	LEU
1	C	1129	LEU
2	D	111	LYS
2	D	116	GLN
2	D	134	LEU
2	D	148	ARG
2	D	174	LEU
2	D	179	VAL
2	D	219	LEU
2	D	243	VAL
2	D	254	THR
2	D	262	LEU
2	D	274	GLU
2	D	293	LEU
2	D	299	VAL
2	D	308	LEU
2	D	312	LYS
2	D	321	MET
2	D	374	LEU
2	D	389	VAL
2	D	393	TYR
2	D	400	LEU
2	D	435	SER
2	D	437	THR
2	D	453	ASN
3	E	198	LEU
3	E	211	ASN
3	E	214	ASP
3	E	217	TRP
3	E	233	ILE
3	E	235	TYR
3	E	251	LYS
3	E	255	ASN
3	E	256	LEU
3	E	259	GLN

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Mol	Chain	Res	Type
3	E	260	LEU
3	E	263	ILE
3	E	288	LYS
3	E	297	CYS
3	E	310	LEU
3	E	316	LEU
3	E	324	ILE
3	E	339	ASP
3	E	340	GLN
3	E	341	LYS
3	E	343	GLN
3	E	352	LEU
3	E	359	ASN
3	E	366	SER
3	E	378	LEU
3	E	379	GLN
3	E	395	ARG
3	E	428	LEU
3	E	429	ILE
3	E	433	ASP
3	E	434	GLN
3	E	435	THR
3	E	437	GLN
3	E	443	THR
3	E	451	GLU
3	E	454	THR
3	E	458	GLN
3	E	459	LYS
3	E	465	LEU
3	E	468	ASN
3	E	484	ARG
3	E	488	GLN
3	E	493	GLN
3	E	503	SER
3	E	504	THR
3	E	513	LYS
3	E	520	LEU
3	E	532	ILE
3	E	539	LYS
3	E	544	MET
3	E	548	PHE
3	E	551	PHE

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Mol	Chain	Res	Type
3	E	552	ILE
3	E	555	ARG
3	E	570	LYS
3	E	577	GLU
3	E	580	ASP
3	E	581	GLU
3	E	588	ASP
3	E	592	ILE
3	E	596	PHE
3	E	597	ILE
3	E	611	LEU
3	E	619	LYS
3	E	627	LYS
3	E	641	PHE
3	E	653	GLU
3	E	666	MET
3	E	667	GLN
3	E	691	VAL
3	E	695	VAL
3	E	723	TRP
3	E	726	THR
3	E	778	LEU
3	E	791	ARG
3	E	814	PHE
3	E	816	HIS
3	E	827	GLN
3	E	835	GLN
3	E	845	ASP
3	E	859	LYS
3	E	863	THR
3	E	874	TYR
3	E	877	LEU
3	E	878	LYS
3	E	886	LEU
3	E	895	ASP
3	E	897	ASP
3	E	901	ARG
3	E	905	ASN
4	F	19	LYS
4	F	25	LYS
4	F	35	TRP
4	F	37	ILE

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Mol	Chain	Res	Type
3	H	198	LEU
3	H	211	ASN
3	H	214	ASP
3	H	217	TRP
3	H	229	ASN
3	H	235	TYR
3	H	251	LYS
3	H	255	ASN
3	H	256	LEU
3	H	259	GLN
3	H	260	LEU
3	H	263	ILE
3	H	288	LYS
3	H	297	CYS
3	H	310	LEU
3	H	316	LEU
3	H	324	ILE
3	H	340	GLN
3	H	341	LYS
3	H	342	VAL
3	H	343	GLN
3	H	352	LEU
3	H	363	ILE
3	H	366	SER
3	H	379	GLN
3	H	395	ARG
3	H	429	ILE
3	H	430	THR
3	H	443	THR
3	H	454	THR
3	H	458	GLN
3	H	459	LYS
3	H	465	LEU
3	H	468	ASN
3	H	484	ARG
3	H	488	GLN
3	H	493	GLN
3	H	503	SER
3	H	504	THR
3	H	513	LYS
3	H	520	LEU
3	H	532	ILE

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Mol	Chain	Res	Type
3	H	539	LYS
3	H	544	MET
3	H	548	PHE
3	H	551	PHE
3	H	552	ILE
3	H	556	PRO
3	H	570	LYS
3	H	577	GLU
3	H	580	ASP
3	H	581	GLU
3	H	588	ASP
3	H	592	ILE
3	H	595	ARG
3	H	611	LEU
3	H	619	LYS
3	H	627	LYS
3	H	641	PHE
3	H	653	GLU
3	H	666	MET
3	H	667	GLN
3	H	691	VAL
3	H	695	VAL
3	H	723	TRP
3	H	726	THR
3	H	778	LEU
3	H	791	ARG
3	H	814	PHE
3	H	816	HIS
3	H	827	GLN
3	H	835	GLN
3	H	845	ASP
3	H	859	LYS
3	H	863	THR
3	H	874	TYR
3	H	877	LEU
3	H	878	LYS
3	H	886	LEU
3	H	895	ASP
3	H	897	ASP
3	H	901	ARG
3	H	905	ASN
4	I	19	LYS

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Mol	Chain	Res	Type
4	I	25	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	30	ASN
1	A	85	ASN
1	A	156	ASN
1	A	241	ASN
1	A	261	HIS
1	A	374	GLN
1	A	397	HIS
1	A	455	GLN
1	A	462	ASN
1	A	467	GLN
1	A	481	GLN
1	A	494	GLN
1	A	507	GLN
1	A	524	GLN
1	A	536	HIS
1	A	578	HIS
1	A	634	GLN
1	A	648	ASN
1	A	727	GLN
1	A	796	GLN
1	A	885	ASN
1	A	904	ASN
1	A	907	ASN
1	A	908	ASN
1	A	1034	ASN
1	A	1055	GLN
2	B	156	HIS
2	B	269	HIS
2	B	370	GLN
2	B	453	ASN
1	C	4	ASN
1	C	30	ASN
1	C	85	ASN
1	C	156	ASN
1	C	241	ASN
1	C	261	HIS

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Mol	Chain	Res	Type
1	C	374	GLN
1	C	392	ASN
1	C	455	GLN
1	C	456	GLN
1	C	462	ASN
1	C	467	GLN
1	C	481	GLN
1	C	494	GLN
1	C	507	GLN
1	C	524	GLN
1	C	536	HIS
1	C	578	HIS
1	C	634	GLN
1	C	648	ASN
1	C	708	GLN
1	C	727	GLN
1	C	796	GLN
1	C	797	HIS
1	C	885	ASN
1	C	904	ASN
1	C	907	ASN
1	C	908	ASN
1	C	1034	ASN
1	C	1055	GLN
2	D	107	HIS
2	D	269	HIS
2	D	370	GLN
2	D	412	ASN
2	D	453	ASN
3	E	255	ASN
3	E	259	GLN
3	E	340	GLN
3	E	343	GLN
3	E	379	GLN
3	E	402	GLN
3	E	434	GLN
3	E	468	ASN
3	E	557	ASN
3	E	716	HIS
3	E	744	GLN
3	E	827	GLN
3	E	847	GLN

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Mol	Chain	Res	Type
3	E	849	GLN
3	E	905	ASN
3	E	910	ASN
3	H	246	ASN
3	H	255	ASN
3	H	340	GLN
3	H	343	GLN
3	H	379	GLN
3	H	402	GLN
3	H	434	GLN
3	H	468	ASN
3	H	493	GLN
3	H	557	ASN
3	H	716	HIS
3	H	744	GLN
3	H	827	GLN
3	H	847	GLN
3	H	849	GLN
3	H	905	ASN
3	H	910	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
5	3DR	R	9	5	8,11,12	0.48	0	9,14,17	1.08	0
5	3DR	T	9	5	8,11,12	0.50	0	9,14,17	1.08	0

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
5	3DR	R	9	5	-	0/3/15/16	0/1/1/1
5	3DR	T	9	5	-	0/3/15/16	0/1/1/1

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.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	1105/1144 (96%)	0.42	49 (4%) 34 31	98, 183, 251, 326	0
1	C	1105/1144 (96%)	0.49	55 (4%) 29 28	130, 197, 349, 378	0
2	B	355/382 (92%)	1.05	74 (20%) 1 3	275, 328, 394, 423	0
2	D	355/382 (92%)	0.66	23 (6%) 19 19	193, 275, 343, 370	0
3	E	709/726 (97%)	0.44	44 (6%) 20 20	131, 321, 394, 414	0
3	H	709/726 (97%)	0.49	49 (6%) 17 17	226, 289, 381, 399	0
4	F	21/98 (21%)	0.78	2 (9%) 8 10	368, 383, 396, 398	0
4	I	21/98 (21%)	1.53	8 (38%) 0 1	340, 358, 380, 389	0
5	R	11/12 (91%)	1.86	4 (36%) 0 1	301, 317, 376, 403	0
5	T	11/12 (91%)	1.32	2 (18%) 1 3	257, 344, 355, 356	0
6	S	12/12 (100%)	1.74	4 (33%) 0 2	317, 326, 386, 386	0
6	U	12/12 (100%)	1.69	4 (33%) 0 2	286, 320, 350, 363	0
All	All	4426/4748 (93%)	0.54	318 (7%) 15 16	98, 240, 379, 423	0

All (318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	775	ASP	10.5
1	C	542	ASP	7.1
3	E	810	CYS	6.3
1	C	503	CYS	5.8
2	D	430	SER	5.8
1	A	770	LEU	5.6
2	B	342	THR	5.3
3	E	779	ARG	5.3
3	H	618	GLY	5.2
1	C	502	SER	5.1
1	A	872	SER	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	542	ASP	4.6
2	D	242	CYS	4.6
2	B	380	THR	4.6
1	A	540	CYS	4.6
1	A	832	GLY	4.5
2	D	197	GLY	4.5
2	B	350	ARG	4.4
6	U	14	DC	4.4
1	C	540	CYS	4.4
2	B	242	CYS	4.4
2	B	283	HIS	4.3
1	A	771	PHE	4.2
1	C	544	THR	4.2
6	S	14	DC	4.2
3	E	774	GLU	4.1
1	C	872	SER	4.1
3	H	803	GLU	4.1
2	B	379	ALA	4.1
1	C	262	ASN	4.1
2	B	284	ALA	4.0
3	H	621	ALA	3.9
2	B	152	SER	3.8
6	U	11	DT	3.8
1	A	590	SER	3.7
1	A	865	GLU	3.7
3	E	684	MET	3.7
1	C	1015	GLN	3.7
3	H	805	GLY	3.7
2	D	432	ASN	3.6
2	B	394	PRO	3.6
3	E	577	GLU	3.6
3	E	811	ASN	3.6
5	R	3	DG	3.6
1	A	815	SER	3.6
2	B	154	GLU	3.5
2	B	244	ASP	3.5
2	B	197	GLY	3.5
3	E	669	GLN	3.5
1	C	934	ALA	3.5
3	H	728	GLY	3.5
3	H	890	ILE	3.5
1	C	541	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
3	H	804	ASP	3.4
2	D	101	GLY	3.4
3	H	577	GLU	3.4
3	E	685	GLY	3.3
3	H	250	TYR	3.3
6	S	13	DG	3.3
2	B	164	ALA	3.3
1	A	768	SER	3.3
3	E	882	LYS	3.3
2	B	426	ALA	3.3
1	A	502	SER	3.3
1	A	544	THR	3.3
2	D	152	SER	3.3
3	H	725	SER	3.3
1	A	591	ILE	3.3
3	E	578	ALA	3.3
3	H	251	LYS	3.3
1	A	769	LYS	3.2
1	C	469	ILE	3.2
1	C	260	CYS	3.2
1	A	539	ALA	3.2
4	I	28	ASN	3.2
3	H	729	HIS	3.2
1	C	461	GLY	3.2
1	A	883	SER	3.2
1	A	503	CYS	3.1
1	C	815	SER	3.1
1	C	261	HIS	3.1
5	T	3	DG	3.1
2	B	142	THR	3.1
5	R	14	DA	3.1
2	B	432	ASN	3.1
2	B	430	SER	3.1
3	H	860	MET	3.1
2	D	431	LEU	3.0
2	B	433	LYS	3.0
3	H	810	CYS	3.0
3	H	694	GLU	3.0
1	C	832	GLY	3.0
1	C	520	GLN	3.0
3	E	776	GLY	3.0
3	E	889	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	916	THR	2.9
1	C	504	ASN	2.9
1	C	591	ILE	2.9
2	D	173	ILE	2.9
3	E	683	THR	2.9
2	B	243	VAL	2.9
3	E	813	ASP	2.9
1	A	873	MET	2.9
1	A	915	LYS	2.9
1	A	289	GLU	2.9
3	E	621	ALA	2.8
3	H	881	VAL	2.8
2	B	343	THR	2.8
1	C	547	GLY	2.8
3	E	778	LEU	2.8
1	C	847	ARG	2.8
2	B	254	THR	2.8
3	E	661	GLN	2.8
2	B	241	CYS	2.8
2	D	174	LEU	2.8
2	D	283	HIS	2.8
1	C	865	GLU	2.7
1	A	592	LEU	2.7
1	C	431	GLY	2.7
3	E	907	ASN	2.7
2	B	445	MET	2.7
2	B	231	ALA	2.7
3	H	693	MET	2.7
2	D	422	ASP	2.7
3	H	658	ILE	2.7
2	D	444	GLY	2.7
1	C	790	ASN	2.7
3	E	777	GLU	2.7
3	H	733	LYS	2.7
3	H	882	LYS	2.7
2	B	364	ILE	2.7
2	B	196	THR	2.7
3	E	618	GLY	2.7
2	D	380	THR	2.7
2	D	424	ASN	2.7
2	B	393	TYR	2.7
2	B	285	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	460	CYS	2.7
2	D	154	GLU	2.7
2	B	455	GLU	2.7
1	A	262	ASN	2.6
2	B	442	ALA	2.6
3	H	210	GLU	2.6
3	H	619	LYS	2.6
1	A	863	GLU	2.6
2	D	145	PRO	2.6
3	H	661	GLN	2.6
1	C	18	CYS	2.6
2	B	448	ASN	2.6
3	H	738	GLU	2.6
1	C	289	GLU	2.6
2	B	282	THR	2.6
1	C	290	GLN	2.6
3	H	802	ILE	2.6
1	C	943	GLU	2.6
1	C	468	LEU	2.6
3	H	806	ASP	2.6
2	D	196	THR	2.6
2	B	245	VAL	2.6
1	A	541	LEU	2.6
1	A	874	VAL	2.5
1	A	725	CYS	2.5
2	B	421	ARG	2.5
3	E	890	ILE	2.5
3	E	885	ASP	2.5
2	B	351	VAL	2.5
1	A	27	GLU	2.5
1	C	447	GLU	2.5
1	C	725	CYS	2.5
3	E	524	ASP	2.5
1	A	980	ASP	2.5
1	A	737	SER	2.5
2	B	304	LYS	2.5
2	B	443	SER	2.5
1	A	979	LYS	2.4
1	A	871	TYR	2.4
3	E	804	ASP	2.4
2	B	403	LYS	2.4
2	B	297	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	827	THR	2.4
2	B	151	THR	2.4
2	B	198	MET	2.4
3	E	725	SER	2.4
3	H	886	LEU	2.4
2	B	404	ARG	2.4
3	H	891	GLU	2.4
2	B	427	GLY	2.4
2	B	246	SER	2.4
1	C	411	TRP	2.4
2	B	166	GLY	2.4
4	I	34	ALA	2.4
2	B	444	GLY	2.4
3	E	891	GLU	2.4
1	A	1023	PRO	2.4
2	B	140	HIS	2.4
1	A	122	GLY	2.4
3	H	542	ASN	2.4
1	C	454	ASP	2.4
3	E	504	THR	2.4
2	B	341	LEU	2.4
5	T	10	DA	2.4
3	E	737	LYS	2.4
1	A	1092	ASP	2.3
4	I	19	LYS	2.3
2	B	252	LEU	2.3
2	B	330	ALA	2.3
1	C	543	ILE	2.3
2	D	198	MET	2.3
3	H	901	ARG	2.3
3	H	726	THR	2.3
3	E	913	ALA	2.3
2	D	164	ALA	2.3
3	H	730	CYS	2.3
2	B	211	SER	2.3
1	C	935	TYR	2.3
4	I	21	ARG	2.3
1	C	826	ASN	2.3
2	B	323	HIS	2.3
3	H	546	GLU	2.3
1	C	64	MET	2.3
3	H	775	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	640	THR	2.3
3	E	468	ASN	2.3
4	I	38	VAL	2.2
3	H	770	ALA	2.2
1	A	816	LEU	2.2
2	D	187	GLN	2.2
3	E	736	PHE	2.2
3	H	232	SER	2.2
2	B	314	LYS	2.2
5	R	4	DC	2.2
2	B	446	GLY	2.2
1	C	459	PHE	2.2
3	H	692	PRO	2.2
1	C	535	GLU	2.2
2	B	369	ARG	2.2
2	B	315	ASN	2.2
1	C	883	SER	2.2
3	H	801	ASP	2.2
1	C	592	LEU	2.2
3	H	760	GLU	2.2
2	B	377	ILE	2.2
6	S	8	DA	2.2
1	C	863	GLU	2.2
2	B	266	LEU	2.2
4	I	31	ALA	2.2
2	B	313	ASP	2.2
3	E	812	ASP	2.2
6	U	3	DT	2.2
1	C	828	TYR	2.2
2	B	101	GLY	2.1
4	F	34	ALA	2.1
1	A	847	ARG	2.1
4	F	28	ASN	2.1
2	B	329	ALA	2.1
1	C	509	VAL	2.1
2	B	328	ASN	2.1
3	E	670	ASN	2.1
6	S	9	DA	2.1
3	H	883	PRO	2.1
2	B	436	PRO	2.1
1	A	504	ASN	2.1
1	A	450	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	724	ILE	2.1
3	E	802	ILE	2.1
2	B	165	VAL	2.1
3	H	670	ASN	2.1
2	B	303	VAL	2.1
3	E	658	ILE	2.1
1	A	62	ALA	2.1
1	C	263	ARG	2.1
1	C	1009	HIS	2.1
2	B	209	PHE	2.1
2	B	155	TRP	2.1
3	E	906	PRO	2.1
1	C	873	MET	2.1
2	D	433	LYS	2.1
1	A	123	ILE	2.1
3	E	887	LYS	2.1
2	B	141	ARG	2.1
5	R	13	DC	2.1
2	B	125	CYS	2.1
2	D	445	MET	2.1
3	H	913	ALA	2.1
3	H	889	ARG	2.1
1	C	833	THR	2.1
3	E	606	PHE	2.1
1	A	500	VAL	2.1
1	A	853	TYR	2.1
2	D	421	ARG	2.1
6	U	12	DA	2.1
1	A	559	GLY	2.1
3	H	746	SER	2.1
3	E	781	THR	2.1
1	A	462	ASN	2.1
1	A	892	GLU	2.1
2	B	173	ILE	2.1
3	E	689	THR	2.1
4	I	37	ILE	2.1
1	A	125	ASP	2.0
1	C	122	GLY	2.0
1	C	539	ALA	2.0
3	E	739	GLY	2.0
3	H	887	LYS	2.0
2	B	339	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	E	865	SER	2.0
4	I	35	TRP	2.0
1	A	297	LEU	2.0
2	B	247	VAL	2.0
2	B	401	ASN	2.0
2	B	253	ALA	2.0
3	H	912	ILE	2.0
1	C	497	ASN	2.0
1	C	919	ASP	2.0
3	H	622	SER	2.0
3	H	811	ASN	2.0
3	E	866	HIS	2.0
3	H	561	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	3DR	T	9	11/12	0.69	0.68	347,358,362,362	0
5	3DR	R	9	11/12	0.78	0.38	318,324,336,339	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.