



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:57 AM GMT

PDB ID : 2QRV
Title : Structure of Dnmt3a-Dnmt3L C-terminal domain complex
Authors : Jia, D.; Cheng, X.
Deposited on : 2007-07-29
Resolution : 2.89 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

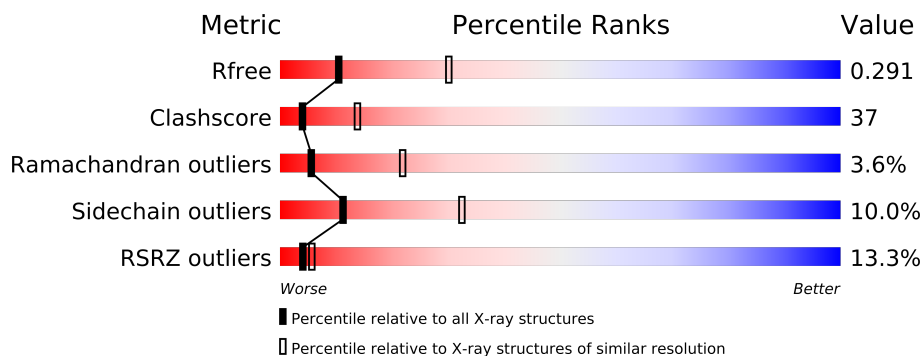
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.89 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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	295	
1	D	295	
1	E	295	
1	H	295	
2	B	230	
2	C	230	
2	F	230	
2	G	230	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14657 atoms, of which 0 are hydrogen and 0 are deuterium.

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 (cytosine-5)-methyltransferase3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2143	1370	379	381	13			
1	D	267	Total	C	N	O	S	0	0	0
			2111	1350	372	376	13			
1	E	270	Total	C	N	O	S	0	0	0
			2128	1361	375	379	13			
1	H	267	Total	C	N	O	S	0	0	0
			2111	1350	372	376	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	MET	-	EXPRESSION TAG	UNP Q9Y6K1
A	615	GLY	-	EXPRESSION TAG	UNP Q9Y6K1
A	616	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
A	617	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
A	618	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
A	619	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
A	620	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
A	621	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
A	622	MET	-	EXPRESSION TAG	UNP Q9Y6K1
D	614	MET	-	EXPRESSION TAG	UNP Q9Y6K1
D	615	GLY	-	EXPRESSION TAG	UNP Q9Y6K1
D	616	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
D	617	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
D	618	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
D	619	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
D	620	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
D	621	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
D	622	MET	-	EXPRESSION TAG	UNP Q9Y6K1
E	614	MET	-	EXPRESSION TAG	UNP Q9Y6K1
E	615	GLY	-	EXPRESSION TAG	UNP Q9Y6K1
E	616	HIS	-	EXPRESSION TAG	UNP Q9Y6K1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	617	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
E	618	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
E	619	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
E	620	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
E	621	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
E	622	MET	-	EXPRESSION TAG	UNP Q9Y6K1
H	614	MET	-	EXPRESSION TAG	UNP Q9Y6K1
H	615	GLY	-	EXPRESSION TAG	UNP Q9Y6K1
H	616	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
H	617	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
H	618	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
H	619	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
H	620	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
H	621	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
H	622	MET	-	EXPRESSION TAG	UNP Q9Y6K1

- Molecule 2 is a protein called DNA (cytosine-5)-methyltransferase3-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	186	Total	C	N	O	S	0	0	0
			1515	991	254	266	4			
2	C	186	Total	C	N	O	S	0	0	0
			1515	991	254	266	4			
2	F	186	Total	C	N	O	S	0	0	0
			1515	991	254	266	4			
2	G	186	Total	C	N	O	S	0	0	0
			1515	991	254	266	4			

There are 12 discrepancies between the modelled and reference sequences:

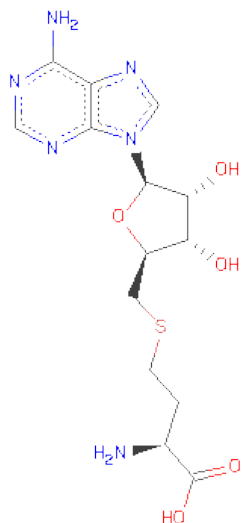
Chain	Residue	Modelled	Actual	Comment	Reference
B	157	GLY	-	EXPRESSION TAG	UNP Q9UJW3
B	158	SER	-	EXPRESSION TAG	UNP Q9UJW3
B	159	MET	-	EXPRESSION TAG	UNP Q9UJW3
C	157	GLY	-	EXPRESSION TAG	UNP Q9UJW3
C	158	SER	-	EXPRESSION TAG	UNP Q9UJW3
C	159	MET	-	EXPRESSION TAG	UNP Q9UJW3
F	157	GLY	-	EXPRESSION TAG	UNP Q9UJW3
F	158	SER	-	EXPRESSION TAG	UNP Q9UJW3
F	159	MET	-	EXPRESSION TAG	UNP Q9UJW3
G	157	GLY	-	EXPRESSION TAG	UNP Q9UJW3
G	158	SER	-	EXPRESSION TAG	UNP Q9UJW3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	159	MET	-	EXPRESSION TAG	UNP Q9UJW3

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



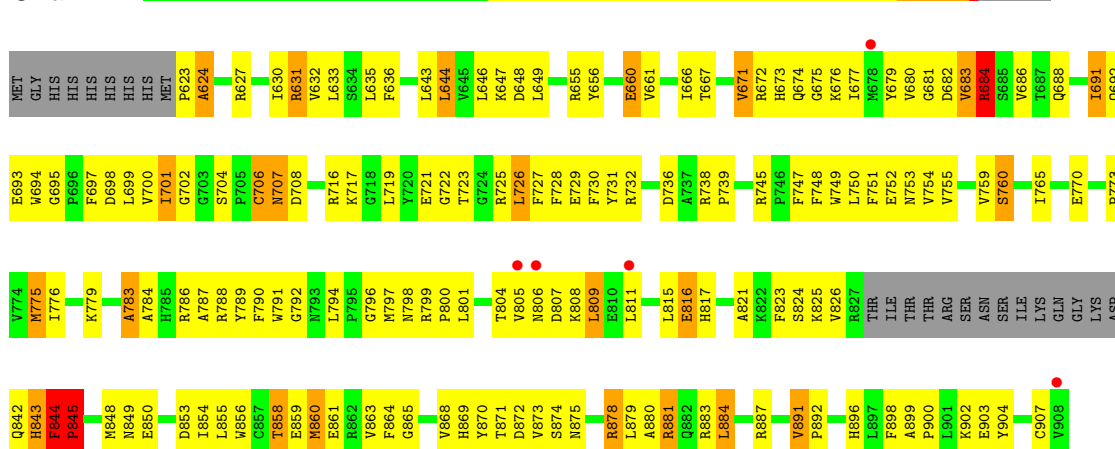
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	H	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

3 Residue-property plots

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

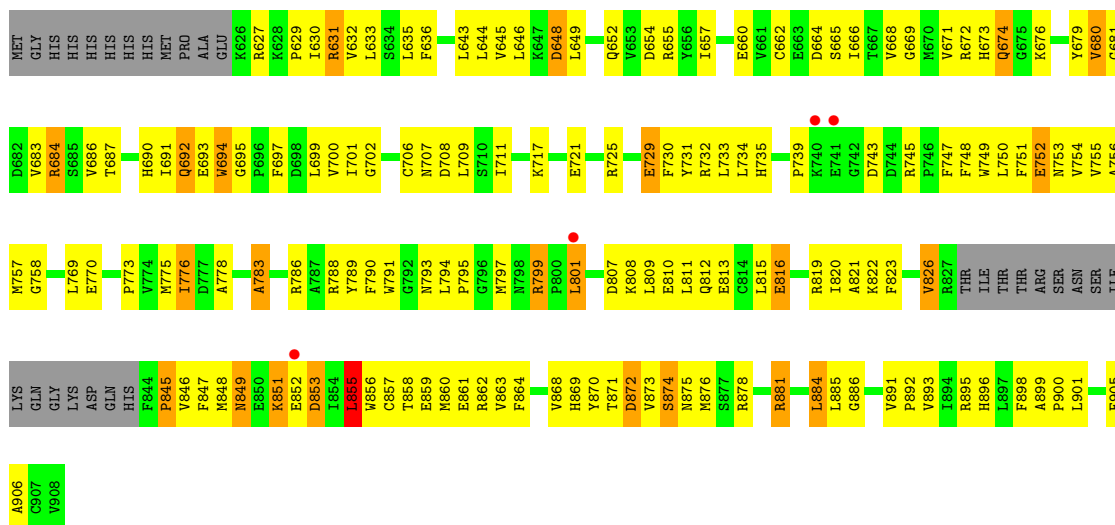
• Molecule 1: DNA (cytosine-5)-methyltransferase3A

Chain A:



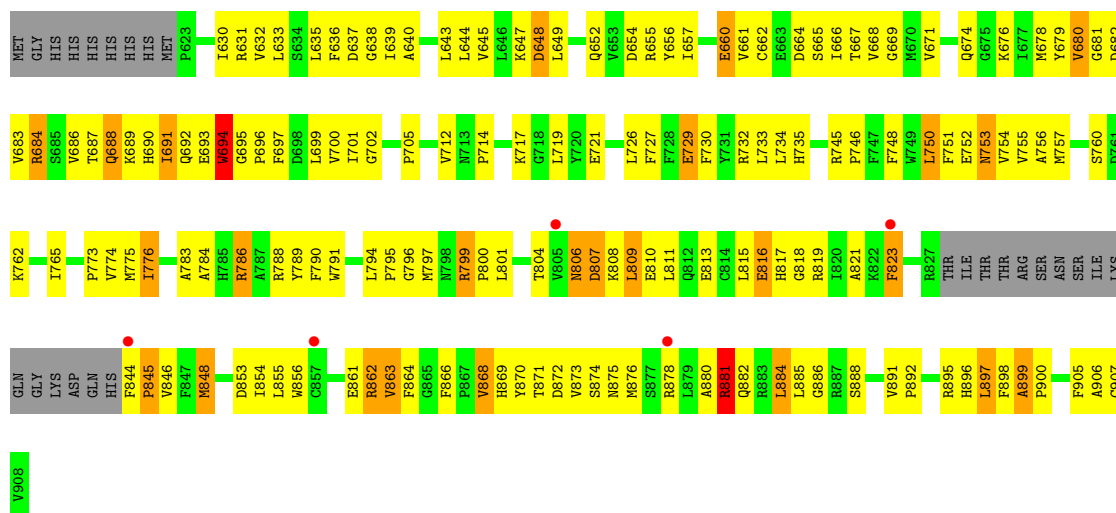
• Molecule 1: DNA (cytosine-5)-methyltransferase3A

Chain D:



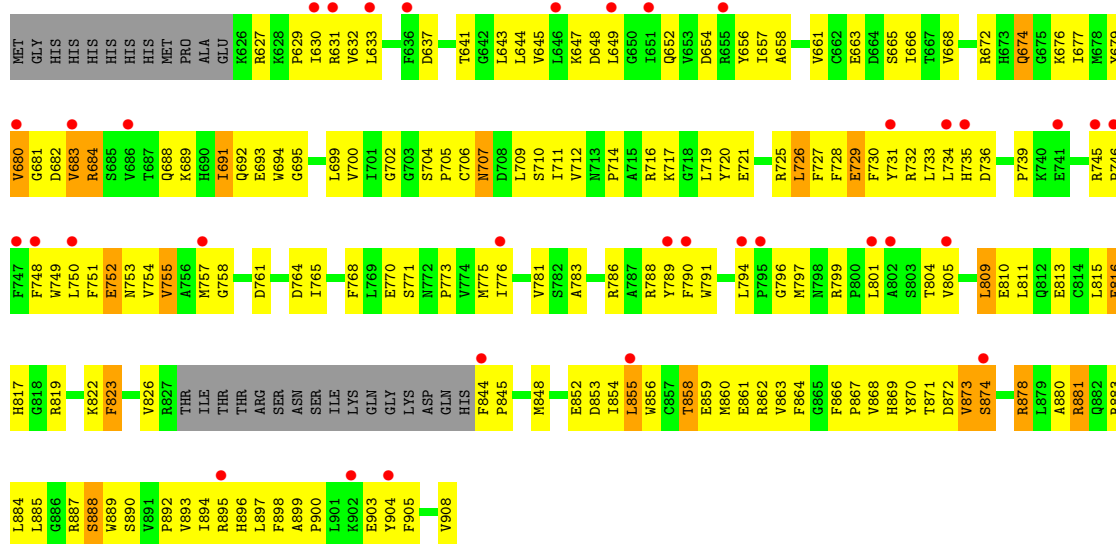
• Molecule 1: DNA (cytosine-5)-methyltransferase3A

Chain E:



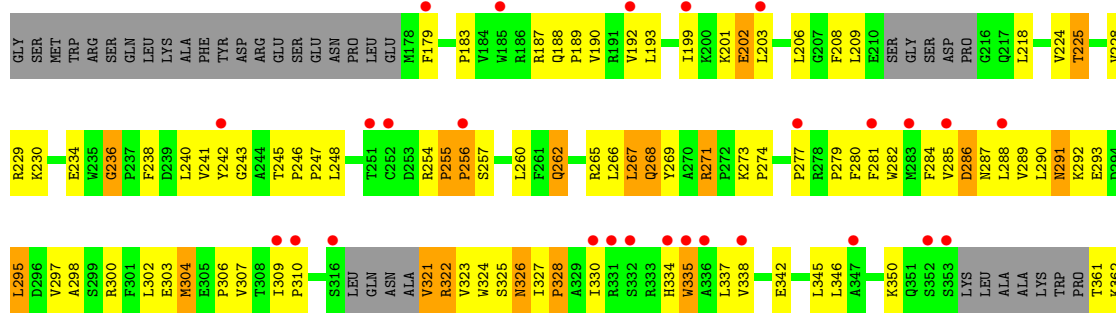
• Molecule 1: DNA (cytosine-5)-methyltransferase3A

Chain H:



• Molecule 2: DNA (cytosine-5)-methyltransferase3-like

Chain B:



A347	•
Q348	•
N349	•
K350	•
Q351	
S352	
S353	•
LYS	
LEU	
ALA	
ALA	
LYS	
THR	
PRO	
T361	
K362	•
L363	•
V364	•
K365	•
N366	•
C367	•
F368	•
L369	
P370	
L371	
R372	
E373	•
Y374	
F375	
K376	
Y377	•
F378	•
S379	
THR	
GLU	
LEU	
THR	
SER	
SER	
LEU	

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	401.88Å 401.88Å 49.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.90 – 2.89 43.85 – 2.90	Depositor EDS
% Data completeness (in resolution range)	81.9 (38.90-2.89) 92.7 (43.85-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.281 0.278 , 0.291	Depositor DCC
R_{free} test set	3124 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	77.8	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 57.5	EDS
Estimated twinning fraction	0.014 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 65264 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14657	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.55	0/2196	0.83	2/2973 (0.1%)
1	D	0.52	0/2162	0.76	2/2926 (0.1%)
1	E	0.58	0/2180	0.78	1/2951 (0.0%)
1	H	0.44	0/2162	0.65	0/2926
2	B	0.41	0/1560	0.61	0/2120
2	C	0.37	0/1560	0.59	0/2120
2	F	0.35	0/1560	0.58	0/2120
2	G	0.36	0/1560	0.54	0/2120
All	All	0.47	0/14940	0.69	5/20256 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	844	PHE	C-N-CD	-13.46	91.00	120.60
1	D	875	ASN	N-CA-C	-6.49	93.47	111.00
1	A	644	LEU	CA-CB-CG	6.20	129.55	115.30
1	D	872	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	E	881	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2143	0	2076	174	0
1	D	2111	0	2052	172	0
1	E	2128	0	2067	170	0
1	H	2111	0	2052	195	0
2	B	1515	0	1484	122	0
2	C	1515	0	1484	93	0
2	F	1515	0	1484	109	0
2	G	1515	0	1484	105	0
3	A	26	0	19	1	0
3	D	26	0	19	0	0
3	E	26	0	19	1	0
3	H	26	0	19	2	0
All	All	14657	0	14259	1076	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 37.

All (1076) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:786:ARG:HG3	1:E:786:ARG:HH11	1.19	1.06
1:E:655:ARG:HH12	1:E:695:GLY:HA3	1.20	1.05
2:B:271:ARG:HH11	2:B:271:ARG:HG3	1.13	1.05
1:E:854:ILE:HG22	1:E:855:LEU:H	1.18	1.05
1:A:843:HIS:O	1:A:845:PRO:HD3	1.59	1.02
1:D:655:ARG:HH12	1:D:695:GLY:HA3	1.25	1.01
1:E:873:VAL:HG23	1:E:874:SER:H	1.22	1.01
1:A:811:LEU:HD13	1:A:826:VAL:HG13	1.43	1.00
1:D:874:SER:HB2	1:D:876:MET:HB2	1.40	0.99
2:F:262:GLN:HA	2:F:262:GLN:HE21	1.26	0.97
2:F:363:LEU:H	2:F:363:LEU:HD22	1.29	0.97
1:E:662:CYS:O	1:E:666:ILE:HG13	1.65	0.96
1:H:871:THR:OG1	1:H:881:ARG:HD3	1.65	0.95
2:B:260:LEU:HD21	2:B:298:ALA:HA	1.49	0.94
1:D:680:VAL:HG12	1:D:681:GLY:H	1.33	0.93
1:A:655:ARG:HH12	1:A:695:GLY:HA3	1.33	0.92
1:A:725:ARG:HH12	2:B:297:VAL:HG21	1.32	0.92
2:B:363:LEU:H	2:B:363:LEU:HD22	1.34	0.92
2:B:248:LEU:H	2:B:287:ASN:HD21	1.17	0.91
1:A:632:VAL:HG22	1:A:699:LEU:HB3	1.51	0.91
1:E:680:VAL:HG12	1:E:681:GLY:H	1.36	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:858:THR:HG22	1:A:868:VAL:HG12	1.51	0.89
2:C:326:ASN:HD22	2:C:326:ASN:H	1.19	0.89
1:A:878:ARG:HH11	1:A:878:ARG:HG2	1.36	0.88
2:G:300:ARG:HH11	1:H:732:ARG:NH1	1.71	0.88
2:G:262:GLN:HE21	2:G:262:GLN:HA	1.40	0.87
1:A:686:VAL:O	1:A:732:ARG:NH2	2.07	0.87
2:G:300:ARG:HH11	1:H:732:ARG:HH12	1.18	0.86
1:H:815:LEU:HA	1:H:859:GLU:HG2	1.55	0.86
1:E:776:ILE:HD11	1:E:801:LEU:HD21	1.57	0.86
2:B:201:LYS:HB3	2:B:202:GLU:OE1	1.76	0.86
2:G:300:ARG:CZ	1:H:684:ARG:HB2	2.06	0.86
2:G:273:LYS:HB3	2:G:274:PRO:HD2	1.56	0.85
2:F:326:ASN:H	2:F:326:ASN:HD22	1.18	0.85
1:D:648:ASP:HB3	1:D:895:ARG:HH12	1.40	0.85
1:H:732:ARG:HH21	1:H:733:LEU:HD21	1.41	0.84
1:E:752:GLU:HG2	1:E:753:ASN:H	1.43	0.84
1:H:773:PRO:HD3	1:H:791:TRP:NE1	1.93	0.84
2:G:311:ASP:HB2	2:G:363:LEU:HD11	1.59	0.84
2:C:310:PRO:HG2	2:C:338:VAL:HG21	1.60	0.83
1:A:667:THR:O	1:A:671:VAL:HG23	1.78	0.83
2:F:273:LYS:HB3	2:F:274:PRO:HD2	1.60	0.83
1:A:843:HIS:C	1:A:845:PRO:HD3	1.99	0.82
1:D:680:VAL:HG12	1:D:681:GLY:N	1.89	0.82
1:D:786:ARG:HG3	1:D:786:ARG:HH11	1.42	0.82
2:F:202:GLU:HG2	2:F:361:THR:HG23	1.62	0.81
1:E:655:ARG:NH1	1:E:695:GLY:HA3	1.95	0.81
2:G:256:PRO:HB3	2:G:290:LEU:HD23	1.61	0.81
1:D:631:ARG:HH11	1:D:631:ARG:HB2	1.45	0.81
1:H:860:MET:HG2	1:H:864:PHE:HE1	1.42	0.81
1:H:873:VAL:HG23	1:H:874:SER:H	1.45	0.81
1:A:739:PRO:HG3	1:A:745:ARG:NH2	1.94	0.81
1:A:643:LEU:HG	1:A:647:LYS:HE3	1.61	0.81
2:B:271:ARG:NH1	2:B:271:ARG:HG3	1.84	0.81
1:A:725:ARG:NH1	2:B:297:VAL:HG21	1.95	0.80
2:C:202:GLU:HG2	2:C:361:THR:HG23	1.64	0.80
1:E:691:ILE:HD11	1:E:733:LEU:HD12	1.62	0.80
2:C:285:VAL:HG22	2:C:323:VAL:HG22	1.63	0.80
1:A:809:LEU:HD12	1:A:809:LEU:H	1.47	0.80
1:A:750:LEU:HD12	1:A:791:TRP:O	1.82	0.79
1:A:874:SER:HA	1:D:856:TRP:CE2	2.18	0.79
2:B:273:LYS:HB3	2:B:274:PRO:HD2	1.65	0.79
2:C:294:ASP:CG	1:D:725:ARG:HH22	1.86	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:648:ASP:HB3	1:D:895:ARG:NH1	1.97	0.79
1:H:682:ASP:OD2	1:H:684:ARG:HD3	1.83	0.79
2:B:188:GLN:HB3	2:B:189:PRO:HD2	1.64	0.79
1:D:684:ARG:H	1:D:684:ARG:HD3	1.47	0.79
1:E:786:ARG:NH1	1:E:786:ARG:HG3	1.96	0.78
1:E:854:ILE:HG22	1:E:855:LEU:N	1.98	0.78
2:C:247:PRO:HA	2:C:287:ASN:HD22	1.46	0.78
1:A:858:THR:HG22	1:A:868:VAL:CG1	2.12	0.78
1:H:732:ARG:HE	1:H:733:LEU:CD2	1.96	0.78
2:C:188:GLN:HB3	2:C:189:PRO:HD2	1.65	0.78
1:D:655:ARG:NH1	1:D:695:GLY:HA3	1.97	0.78
1:A:655:ARG:NH1	1:A:695:GLY:HA3	1.99	0.78
1:H:773:PRO:HD3	1:H:791:TRP:HE1	1.45	0.78
1:H:858:THR:HG22	1:H:868:VAL:CG1	2.13	0.78
1:D:755:VAL:HA	1:D:789:TYR:CD2	2.19	0.78
1:H:897:LEU:O	1:H:900:PRO:HD2	1.82	0.77
2:B:326:ASN:HD22	2:B:326:ASN:H	1.31	0.77
1:D:801:LEU:HD12	1:D:801:LEU:H	1.48	0.77
1:A:672:ARG:HG3	1:A:870:TYR:CE1	2.19	0.77
1:H:873:VAL:HG23	1:H:874:SER:N	2.00	0.77
1:E:861:GLU:OE1	1:E:869:HIS:N	2.18	0.77
2:G:187:ARG:O	2:G:376:LYS:HB2	1.85	0.77
1:E:873:VAL:HG23	1:E:874:SER:N	2.00	0.77
1:D:871:THR:OG1	1:D:881:ARG:HD3	1.85	0.76
2:C:260:LEU:HD21	2:C:298:ALA:HA	1.64	0.76
1:E:732:ARG:NH2	1:E:733:LEU:HD21	2.00	0.76
1:E:776:ILE:CD1	1:E:801:LEU:HD21	2.15	0.76
1:D:664:ASP:O	1:D:668:VAL:HG23	1.85	0.76
2:G:232:VAL:HG21	2:G:266:LEU:HD22	1.68	0.76
1:E:680:VAL:HG12	1:E:681:GLY:N	2.02	0.75
1:H:880:ALA:O	1:H:884:LEU:HD13	1.86	0.75
1:A:649:LEU:O	1:A:902:LYS:HE2	1.87	0.75
2:B:202:GLU:HG2	2:B:361:THR:HG23	1.67	0.75
1:H:683:VAL:HG22	3:H:8:SAH:N1	2.00	0.75
1:A:843:HIS:O	1:A:845:PRO:CD	2.35	0.75
2:F:202:GLU:HG2	2:F:361:THR:CG2	2.17	0.74
1:E:683:VAL:HG23	1:E:684:ARG:HD3	1.68	0.74
1:D:857:CYS:O	1:D:861:GLU:HG3	1.88	0.74
2:F:193:LEU:HB2	2:F:238:PHE:CE2	2.23	0.74
1:A:723:THR:HB	1:A:726:LEU:HD12	1.69	0.74
2:C:273:LYS:HB3	2:C:274:PRO:HD2	1.67	0.74
2:F:193:LEU:HB2	2:F:238:PHE:CD2	2.23	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:794:LEU:O	1:A:797:MET:HG3	1.88	0.73
1:H:691:ILE:HG22	1:H:692:GLN:N	2.01	0.73
2:C:310:PRO:CG	2:C:338:VAL:HG21	2.19	0.73
1:D:652:GLN:HB2	1:D:906:ALA:HB3	1.69	0.73
2:G:192:VAL:HG22	2:G:240:LEU:HB3	1.70	0.73
1:A:804:THR:HG22	1:A:806:ASN:H	1.52	0.73
2:F:248:LEU:H	2:F:287:ASN:ND2	1.86	0.73
1:A:878:ARG:NH1	1:A:878:ARG:HG2	1.99	0.73
1:E:788:ARG:HH11	1:E:788:ARG:HG2	1.54	0.72
2:C:228:VAL:HG12	2:C:229:ARG:N	2.02	0.72
1:E:752:GLU:HG2	1:E:753:ASN:N	2.02	0.72
2:B:262:GLN:NE2	2:B:265:ARG:HE	1.88	0.72
1:A:684:ARG:H	1:A:684:ARG:HD3	1.54	0.72
1:E:801:LEU:HD12	1:E:801:LEU:H	1.55	0.72
2:C:192:VAL:HG21	2:C:203:LEU:HD21	1.71	0.71
2:B:248:LEU:H	2:B:287:ASN:ND2	1.87	0.71
2:F:240:LEU:HA	2:F:281:PHE:O	1.91	0.71
1:A:823:PHE:CZ	1:A:842:GLN:HA	2.26	0.71
1:H:732:ARG:HE	1:H:733:LEU:HD22	1.54	0.71
1:A:680:VAL:HG12	1:A:681:GLY:N	2.04	0.71
2:B:248:LEU:N	2:B:287:ASN:HD21	1.87	0.71
1:D:648:ASP:CB	1:D:895:ARG:HH12	2.04	0.71
2:G:281:PHE:HE2	2:G:328:PRO:HD3	1.55	0.71
2:B:267:LEU:HD13	2:B:268:GLN:NE2	2.06	0.71
2:G:248:LEU:H	2:G:287:ASN:ND2	1.89	0.71
2:B:268:GLN:HE21	2:B:268:GLN:N	1.89	0.71
2:G:247:PRO:HA	2:G:287:ASN:ND2	2.06	0.70
2:F:192:VAL:HG21	2:F:203:LEU:HD21	1.72	0.70
1:H:755:VAL:HG21	1:H:775:MET:SD	2.31	0.70
2:B:248:LEU:N	2:B:287:ASN:ND2	2.38	0.70
2:F:191:ARG:HH21	2:F:237:PRO:HB2	1.56	0.70
1:H:704:SER:HG	1:H:751:PHE:HZ	1.39	0.70
1:H:786:ARG:HG3	1:H:786:ARG:HH11	1.56	0.70
1:H:871:THR:CB	1:H:881:ARG:HD3	2.22	0.70
1:D:801:LEU:HD12	1:D:801:LEU:N	2.07	0.70
1:E:866:PHE:HE2	1:E:888:SER:HG	1.40	0.70
2:F:363:LEU:CD2	2:F:363:LEU:H	2.03	0.70
1:H:844:PHE:HB3	1:H:852:GLU:HG2	1.72	0.70
1:E:891:VAL:HB	1:E:892:PRO:HD3	1.74	0.70
2:C:260:LEU:CD2	2:C:298:ALA:HA	2.21	0.69
2:C:376:LYS:HD3	2:C:378:PHE:CE2	2.26	0.69
1:A:680:VAL:HG12	1:A:681:GLY:H	1.57	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:823:PHE:CD1	1:H:823:PHE:N	2.57	0.69
2:B:292:LYS:HA	2:B:295:LEU:HD22	1.73	0.69
1:H:666:ILE:HA	1:H:679:TYR:HE2	1.56	0.69
1:E:810:GLU:N	1:E:810:GLU:OE2	2.24	0.69
1:A:881:ARG:O	1:A:884:LEU:HB2	1.93	0.69
2:B:260:LEU:HD21	2:B:298:ALA:CA	2.21	0.69
2:B:240:LEU:HA	2:B:281:PHE:O	1.93	0.69
1:E:753:ASN:ND2	1:E:754:VAL:HG22	2.08	0.69
1:D:686:VAL:O	1:D:732:ARG:NH2	2.26	0.68
1:A:856:TRP:HB2	1:A:859:GLU:HG3	1.75	0.68
2:F:262:GLN:HA	2:F:262:GLN:NE2	2.05	0.68
2:G:199:ILE:HG22	2:G:203:LEU:HB2	1.75	0.68
1:D:680:VAL:CG1	1:D:681:GLY:H	2.07	0.68
1:H:732:ARG:NH2	1:H:733:LEU:HD21	2.08	0.68
2:B:267:LEU:HD13	2:B:268:GLN:HE22	1.57	0.68
2:G:262:GLN:NE2	2:G:262:GLN:HA	2.09	0.68
2:G:369:LEU:HB2	2:G:370:PRO:HD3	1.75	0.68
1:H:861:GLU:OE1	1:H:869:HIS:N	2.27	0.67
1:D:683:VAL:HG23	1:D:684:ARG:N	2.09	0.67
1:D:752:GLU:HG2	1:D:753:ASN:N	2.08	0.67
1:E:854:ILE:CG2	1:E:855:LEU:H	2.00	0.67
1:E:705:PRO:HG2	1:E:726:LEU:HD12	1.77	0.67
1:A:853:ASP:OD2	1:A:854:ILE:N	2.27	0.67
1:A:729:GLU:OE2	1:A:732:ARG:NH1	2.26	0.67
2:G:306:PRO:HB3	2:G:324:TRP:CZ2	2.30	0.67
1:A:683:VAL:HG22	3:A:1:SAH:N1	2.10	0.67
2:B:229:ARG:HA	2:B:269:TYR:CD1	2.30	0.67
1:A:859:GLU:O	1:A:863:VAL:HG23	1.95	0.67
1:H:712:VAL:O	1:H:714:PRO:HD3	1.93	0.67
2:G:363:LEU:HD22	2:G:363:LEU:H	1.60	0.66
2:F:187:ARG:HH12	2:F:373:GLU:HA	1.59	0.66
1:E:630:ILE:HG22	1:E:652:GLN:O	1.95	0.66
1:D:855:LEU:HD23	1:D:856:TRP:H	1.60	0.66
1:H:730:PHE:CE2	1:H:734:LEU:HD12	2.30	0.66
1:E:667:THR:O	1:E:671:VAL:HG23	1.96	0.66
1:E:750:LEU:HD11	1:E:897:LEU:HD13	1.78	0.66
1:H:729:GLU:O	1:H:733:LEU:HD23	1.95	0.66
2:F:228:VAL:HG12	2:F:229:ARG:H	1.60	0.66
1:A:786:ARG:HH21	1:A:788:ARG:NH2	1.93	0.66
1:E:717:LYS:HB3	1:E:721:GLU:HB2	1.78	0.66
2:F:282:TRP:H	2:F:326:ASN:HD21	1.44	0.66
2:B:262:GLN:HE22	2:B:265:ARG:HE	1.40	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:256:PRO:HB3	2:B:290:LEU:HD23	1.76	0.66
2:G:262:GLN:HE22	2:G:265:ARG:HE	1.44	0.66
2:B:291:ASN:O	2:B:295:LEU:HD13	1.96	0.66
1:D:691:ILE:HD11	1:D:733:LEU:HD12	1.78	0.65
2:F:363:LEU:N	2:F:363:LEU:HD22	2.08	0.65
2:G:260:LEU:HD21	2:G:298:ALA:HA	1.77	0.65
1:E:815:LEU:HD11	1:E:846:VAL:CG1	2.26	0.65
2:G:202:GLU:HG2	2:G:361:THR:CG2	2.26	0.65
1:H:860:MET:HG2	1:H:864:PHE:CE1	2.28	0.65
2:C:202:GLU:O	2:C:206:LEU:HD23	1.96	0.65
2:C:376:LYS:HD3	2:C:378:PHE:HE2	1.62	0.65
2:B:285:VAL:HG13	2:B:323:VAL:HG22	1.77	0.65
1:H:719:LEU:HB2	1:H:761:ASP:OD2	1.96	0.65
2:C:268:GLN:HG2	1:D:735:HIS:CE1	2.32	0.65
1:A:631:ARG:HD2	1:A:698:ASP:OD1	1.96	0.65
1:A:869:HIS:CE1	1:D:872:ASP:HB3	2.32	0.64
1:D:786:ARG:HG3	1:D:786:ARG:NH1	2.12	0.64
2:C:247:PRO:HA	2:C:287:ASN:ND2	2.11	0.64
1:H:890:SER:OG	1:H:892:PRO:HD2	1.97	0.64
1:H:895:ARG:O	1:H:899:ALA:HB2	1.97	0.64
2:F:248:LEU:H	2:F:287:ASN:HD21	1.44	0.64
1:H:755:VAL:HG21	1:H:775:MET:CE	2.28	0.64
2:F:193:LEU:HD13	2:F:238:PHE:CZ	2.31	0.64
2:G:228:VAL:HG12	2:G:229:ARG:H	1.60	0.64
2:F:228:VAL:HG12	2:F:229:ARG:N	2.12	0.64
2:G:310:PRO:HG2	2:G:338:VAL:HG21	1.80	0.64
1:D:672:ARG:HD2	1:D:870:TYR:CD1	2.33	0.64
1:E:872:ASP:HB3	1:H:869:HIS:CE1	2.33	0.63
2:G:228:VAL:HG12	2:G:229:ARG:N	2.13	0.63
2:F:230:LYS:N	2:F:230:LYS:HD2	2.12	0.63
2:G:262:GLN:CA	2:G:262:GLN:HE21	2.10	0.63
2:B:199:ILE:HD11	2:B:242:TYR:CE2	2.33	0.63
1:D:709:LEU:HD13	1:D:757:MET:HE1	1.80	0.63
1:E:815:LEU:HD11	1:E:846:VAL:HG11	1.80	0.63
1:E:801:LEU:HD12	1:E:801:LEU:N	2.12	0.63
1:D:794:LEU:O	1:D:797:MET:HG3	1.98	0.63
1:A:684:ARG:HB2	2:B:300:ARG:CZ	2.29	0.63
2:G:202:GLU:O	2:G:206:LEU:HD23	1.99	0.63
2:G:202:GLU:HG2	2:G:361:THR:HG23	1.79	0.63
1:D:748:PHE:HB3	1:D:794:LEU:CD2	2.28	0.63
1:E:649:LEU:HD22	1:E:899:ALA:HA	1.79	0.63
2:B:245:THR:HB	2:B:289:VAL:HG11	1.81	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:867:PRO:O	1:H:870:TYR:HB2	1.99	0.62
2:F:230:LYS:H	2:F:230:LYS:HD2	1.64	0.62
2:C:311:ASP:HB2	2:C:363:LEU:HD11	1.82	0.62
1:A:682:ASP:OD2	1:A:684:ARG:HD3	1.99	0.62
2:B:293:GLU:N	2:B:293:GLU:OE2	2.33	0.62
2:B:363:LEU:CD2	2:B:363:LEU:H	2.11	0.62
2:B:267:LEU:CD1	2:B:268:GLN:HE22	2.12	0.62
1:H:819:ARG:HD2	1:H:848:MET:SD	2.40	0.62
1:H:716:ARG:HG2	1:H:716:ARG:HH11	1.64	0.62
2:B:247:PRO:HA	2:B:287:ASN:ND2	2.15	0.61
1:H:860:MET:O	1:H:863:VAL:HB	2.00	0.61
1:H:810:GLU:H	1:H:810:GLU:CD	2.04	0.61
2:B:199:ILE:HG22	2:B:203:LEU:HB2	1.81	0.61
2:B:376:LYS:HD3	2:B:378:PHE:CE2	2.35	0.61
1:H:691:ILE:HG21	1:H:736:ASP:O	2.00	0.61
2:C:198:ASP:HB3	2:C:220:HIS:ND1	2.15	0.61
1:E:875:ASN:HB3	1:H:878:ARG:HD2	1.82	0.61
1:D:717:LYS:HB3	1:D:721:GLU:HB2	1.83	0.61
1:H:711:ILE:HD11	1:H:758:GLY:N	2.16	0.61
2:B:287:ASN:HA	2:B:321:VAL:HG23	1.83	0.61
1:H:796:GLY:O	1:H:799:ARG:HG3	1.99	0.61
2:B:282:TRP:CZ3	2:B:302:LEU:HD22	2.35	0.61
1:H:801:LEU:N	1:H:801:LEU:HD12	2.16	0.61
1:A:824:SER:O	1:A:825:LYS:HG2	2.00	0.61
2:G:193:LEU:HB2	2:G:238:PHE:CD2	2.35	0.61
1:H:649:LEU:HD21	1:H:895:ARG:HG2	1.81	0.61
1:H:717:LYS:O	1:H:721:GLU:HB2	2.00	0.61
1:D:683:VAL:HG23	1:D:729:GLU:HG2	1.83	0.61
2:B:268:GLN:HE21	2:B:268:GLN:CA	2.11	0.61
1:D:730:PHE:CE2	1:D:751:PHE:HB2	2.35	0.61
2:G:248:LEU:H	2:G:287:ASN:HD21	1.49	0.61
1:D:749:TRP:CZ3	1:D:769:LEU:HD13	2.36	0.60
1:E:816:GLU:O	1:E:819:ARG:HG3	2.01	0.60
1:H:815:LEU:HA	1:H:859:GLU:CG	2.29	0.60
1:D:786:ARG:NH1	1:D:864:PHE:HE2	1.98	0.60
1:E:729:GLU:OE2	2:F:301:PHE:HE1	1.84	0.60
2:C:228:VAL:HG12	2:C:229:ARG:H	1.64	0.60
1:H:844:PHE:N	1:H:845:PRO:HD3	2.17	0.60
1:E:655:ARG:HH12	1:E:695:GLY:CA	2.06	0.60
2:F:191:ARG:HB2	2:F:239:ASP:OD1	2.01	0.60
2:B:271:ARG:NH1	2:B:271:ARG:CG	2.60	0.60
1:D:820:ILE:O	1:D:847:PHE:N	2.30	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:688:GLN:HE21	1:E:692:GLN:NE2	2.00	0.60
1:A:811:LEU:CD1	1:A:826:VAL:HG13	2.27	0.60
2:B:202:GLU:OE1	2:B:202:GLU:N	2.35	0.60
2:B:248:LEU:HD21	2:B:288:LEU:O	2.01	0.60
1:H:641:THR:O	1:H:645:VAL:HG23	2.02	0.60
2:G:327:ILE:O	2:G:330:ILE:HB	2.01	0.60
1:A:633:LEU:HD13	1:A:697:PHE:CZ	2.37	0.59
2:F:190:VAL:HB	2:F:375:PHE:CD1	2.37	0.59
2:C:240:LEU:HA	2:C:281:PHE:O	2.01	0.59
1:E:786:ARG:NH1	1:E:864:PHE:CE2	2.70	0.59
1:D:635:LEU:HD12	1:D:730:PHE:HD1	1.67	0.59
1:H:668:VAL:HG22	1:H:873:VAL:HG21	1.83	0.59
2:G:260:LEU:CD2	2:G:298:ALA:HA	2.33	0.59
2:B:346:LEU:O	2:B:350:LYS:HG2	2.02	0.59
1:H:883:ARG:HD3	1:H:887:ARG:NH2	2.18	0.59
1:D:855:LEU:HD23	1:D:856:TRP:N	2.18	0.59
1:H:799:ARG:HH22	1:H:899:ALA:HB3	1.68	0.59
2:B:285:VAL:HG22	2:B:323:VAL:HG22	1.85	0.59
1:E:635:LEU:HD12	1:E:730:PHE:CD1	2.38	0.59
1:E:874:SER:HA	1:H:856:TRP:CE2	2.38	0.59
1:H:732:ARG:HE	1:H:733:LEU:HD21	1.68	0.59
2:F:198:ASP:HB3	2:F:220:HIS:ND1	2.18	0.59
1:E:872:ASP:OD1	1:H:869:HIS:ND1	2.32	0.59
1:H:811:LEU:HD13	1:H:811:LEU:O	2.03	0.59
1:E:643:LEU:O	1:E:647:LYS:HG3	2.02	0.59
1:A:809:LEU:HD12	1:A:809:LEU:N	2.15	0.58
2:C:228:VAL:CG1	2:C:229:ARG:N	2.65	0.58
1:H:680:VAL:HG12	1:H:681:GLY:H	1.68	0.58
1:A:635:LEU:HD12	1:A:730:PHE:CD1	2.38	0.58
1:E:729:GLU:O	1:E:733:LEU:HD23	2.03	0.58
2:C:187:ARG:O	2:C:376:LYS:HB2	2.02	0.58
2:F:248:LEU:N	2:F:287:ASN:ND2	2.50	0.58
2:B:192:VAL:HG22	2:B:240:LEU:HB3	1.84	0.58
2:C:245:THR:HB	2:C:289:VAL:HG11	1.85	0.58
1:H:754:VAL:HA	1:H:788:ARG:HD3	1.85	0.58
1:H:786:ARG:HG3	1:H:786:ARG:NH1	2.19	0.58
1:A:843:HIS:N	1:A:843:HIS:ND1	2.51	0.58
2:G:300:ARG:NH1	1:H:732:ARG:NH1	2.49	0.58
2:G:310:PRO:CG	2:G:338:VAL:HG21	2.33	0.58
1:A:874:SER:HA	1:D:856:TRP:NE1	2.18	0.58
2:B:203:LEU:HD13	2:B:368:PHE:CD1	2.39	0.58
2:C:202:GLU:HG2	2:C:361:THR:CG2	2.32	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:671:VAL:HG11	1:H:816:GLU:HG2	1.86	0.58
2:B:179:PHE:HE2	2:B:280:PHE:H	1.52	0.58
1:D:649:LEU:HD22	1:D:899:ALA:HA	1.86	0.58
1:A:811:LEU:O	1:A:811:LEU:HG	2.02	0.58
2:B:203:LEU:HG	2:B:209:LEU:HD11	1.86	0.58
2:G:306:PRO:HB3	2:G:324:TRP:CE2	2.39	0.58
2:F:372:ARG:HH11	2:F:372:ARG:HG2	1.69	0.58
2:C:346:LEU:O	2:C:350:LYS:HG2	2.04	0.58
2:F:291:ASN:O	2:F:295:LEU:HD13	2.04	0.57
2:G:300:ARG:NH1	1:H:732:ARG:HH12	1.96	0.57
1:D:855:LEU:CD2	1:D:859:GLU:HB2	2.35	0.57
2:C:228:VAL:CG1	2:C:229:ARG:H	2.17	0.57
2:F:310:PRO:HG2	2:F:338:VAL:HG21	1.85	0.57
1:H:858:THR:HG22	1:H:868:VAL:HG12	1.87	0.57
1:E:752:GLU:HB2	1:E:790:PHE:CE2	2.39	0.57
1:E:688:GLN:NE2	1:E:692:GLN:NE2	2.52	0.57
1:E:669:GLY:HA3	1:E:679:TYR:OH	2.05	0.57
2:G:248:LEU:N	2:G:287:ASN:ND2	2.52	0.57
1:D:673:HIS:C	1:D:674:GLN:HG2	2.24	0.57
1:E:752:GLU:O	1:E:753:ASN:HB2	2.05	0.57
1:A:786:ARG:NH1	1:A:864:PHE:CE2	2.73	0.57
2:F:290:LEU:HB2	2:F:295:LEU:CD1	2.35	0.57
1:E:688:GLN:HE21	1:E:692:GLN:HE22	1.53	0.57
1:E:755:VAL:HA	1:E:789:TYR:CD2	2.40	0.57
1:A:776:ILE:HD11	1:A:801:LEU:HD21	1.86	0.57
1:A:656:TYR:HD2	1:A:677:ILE:HG12	1.69	0.57
1:H:755:VAL:HA	1:H:789:TYR:CD2	2.39	0.56
1:D:702:GLY:O	1:D:751:PHE:HA	2.05	0.56
1:H:868:VAL:O	1:H:869:HIS:HB2	2.06	0.56
1:D:633:LEU:HB2	1:D:697:PHE:CD2	2.40	0.56
1:H:734:LEU:HD11	1:H:749:TRP:CE3	2.39	0.56
2:C:271:ARG:HG3	2:C:271:ARG:HH11	1.69	0.56
1:A:872:ASP:HB3	1:D:869:HIS:CE1	2.41	0.56
2:C:248:LEU:H	2:C:287:ASN:ND2	2.03	0.56
1:H:810:GLU:OE2	1:H:810:GLU:N	2.38	0.56
2:F:286:ASP:OD2	2:F:290:LEU:HG	2.05	0.56
2:C:246:PRO:HG2	2:C:259:TYR:OH	2.05	0.56
1:E:823:PHE:CD1	1:E:823:PHE:N	2.72	0.56
2:C:230:LYS:HD2	2:C:230:LYS:H	1.70	0.56
2:C:309:ILE:HG13	2:C:321:VAL:HG12	1.88	0.56
1:E:801:LEU:HA	1:E:896:HIS:CE1	2.41	0.56
1:A:786:ARG:NH1	1:A:864:PHE:HE2	2.03	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:635:LEU:HD12	1:D:730:PHE:CD1	2.40	0.56
2:C:230:LYS:N	2:C:230:LYS:HD2	2.20	0.56
2:B:361:THR:N	2:B:363:LEU:CD2	2.69	0.56
1:A:680:VAL:CG1	1:A:681:GLY:H	2.19	0.56
1:D:752:GLU:O	1:D:753:ASN:HB2	2.05	0.56
2:B:260:LEU:CD2	2:B:298:ALA:HA	2.29	0.56
1:H:691:ILE:CG2	1:H:692:GLN:N	2.69	0.56
2:C:201:LYS:HB3	2:C:202:GLU:OE1	2.05	0.56
1:H:726:LEU:O	1:H:729:GLU:HB2	2.05	0.56
1:A:770:GLU:OE2	2:B:229:ARG:NH1	2.39	0.56
1:H:632:VAL:HG12	1:H:633:LEU:N	2.21	0.56
2:C:310:PRO:HG2	2:C:338:VAL:CG2	2.35	0.56
1:E:632:VAL:HG13	1:E:699:LEU:HG	1.88	0.56
1:E:652:GLN:HB2	1:E:906:ALA:HB3	1.86	0.56
1:D:861:GLU:OE1	1:D:869:HIS:N	2.39	0.56
1:A:691:ILE:HG22	1:A:692:GLN:N	2.21	0.56
1:D:732:ARG:NH2	1:D:733:LEU:HD21	2.21	0.55
2:B:262:GLN:HA	2:B:262:GLN:HE21	1.70	0.55
1:A:680:VAL:CG1	1:A:681:GLY:N	2.70	0.55
2:B:326:ASN:ND2	2:B:326:ASN:H	2.03	0.55
1:H:666:ILE:HA	1:H:679:TYR:CE2	2.40	0.55
1:A:878:ARG:HH12	1:A:879:LEU:HD23	1.71	0.55
1:H:684:ARG:HA	1:H:732:ARG:HH22	1.70	0.55
2:B:291:ASN:HB3	2:B:293:GLU:OE2	2.06	0.55
1:D:752:GLU:HG2	1:D:753:ASN:H	1.69	0.55
1:A:853:ASP:CG	1:A:854:ILE:N	2.59	0.55
1:A:671:VAL:HG11	1:D:816:GLU:HG2	1.89	0.55
1:H:799:ARG:NH2	1:H:900:PRO:HD3	2.21	0.55
2:C:199:ILE:HD11	2:C:242:TYR:CE2	2.42	0.55
2:B:285:VAL:HG13	2:B:323:VAL:CG2	2.36	0.55
1:H:699:LEU:HA	1:H:748:PHE:O	2.07	0.55
1:D:748:PHE:HA	1:D:793:ASN:HD21	1.70	0.55
2:B:203:LEU:HG	2:B:209:LEU:CD1	2.37	0.55
1:D:700:VAL:O	1:D:749:TRP:HA	2.07	0.55
1:D:739:PRO:HB3	1:D:743:ASP:OD2	2.06	0.55
1:E:660:GLU:HB3	1:E:666:ILE:HG12	1.89	0.55
1:E:752:GLU:CG	1:E:753:ASN:N	2.69	0.55
1:E:732:ARG:NH2	1:E:733:LEU:CD2	2.68	0.55
2:G:230:LYS:H	2:G:230:LYS:HD2	1.72	0.55
2:B:306:PRO:HB3	2:B:324:TRP:CE2	2.42	0.55
1:A:748:PHE:HB3	1:A:794:LEU:HD23	1.88	0.55
1:A:704:SER:HG	1:A:751:PHE:HZ	1.54	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:750:LEU:HD12	1:H:791:TRP:O	2.07	0.55
1:H:710:SER:O	1:H:716:ARG:HD3	2.06	0.55
2:G:372:ARG:HH11	2:G:372:ARG:HG2	1.71	0.55
2:B:228:VAL:HG12	2:B:229:ARG:N	2.20	0.55
1:A:816:GLU:HG2	1:D:671:VAL:HG11	1.88	0.55
1:H:656:TYR:HD2	1:H:677:ILE:HG23	1.71	0.55
2:C:282:TRP:H	2:C:326:ASN:HD21	1.55	0.55
2:C:326:ASN:HD22	2:C:326:ASN:N	1.91	0.55
1:E:874:SER:C	1:E:876:MET:H	2.10	0.54
1:A:643:LEU:HD23	1:A:673:HIS:ND1	2.22	0.54
1:E:748:PHE:HB3	1:E:794:LEU:HD23	1.89	0.54
1:A:635:LEU:HD12	1:A:730:PHE:HD1	1.70	0.54
1:D:819:ARG:NH1	1:D:853:ASP:OD1	2.40	0.54
1:A:716:ARG:HG2	1:A:716:ARG:HH11	1.70	0.54
2:F:208:PHE:C	2:F:209:LEU:HD12	2.27	0.54
2:B:266:LEU:N	2:B:266:LEU:HD23	2.22	0.54
1:E:683:VAL:HG23	1:E:684:ARG:H	1.72	0.54
2:G:240:LEU:HA	2:G:281:PHE:O	2.07	0.54
2:F:324:TRP:O	2:F:325:SER:HB2	2.08	0.54
2:C:324:TRP:O	2:C:325:SER:HB2	2.07	0.54
2:B:199:ILE:HG21	2:B:368:PHE:HE1	1.71	0.54
2:G:326:ASN:HD22	2:G:326:ASN:H	1.56	0.54
2:C:303:GLU:O	2:C:304:MET:HB3	2.08	0.54
1:E:726:LEU:O	1:E:729:GLU:HB2	2.08	0.54
2:G:183:PRO:O	2:G:187:ARG:HG3	2.08	0.54
1:A:844:PHE:O	1:A:853:ASP:O	2.25	0.54
1:H:688:GLN:NE2	1:H:692:GLN:NE2	2.56	0.54
2:G:199:ILE:HG22	2:G:199:ILE:O	2.08	0.54
1:A:660:GLU:OE2	1:A:661:VAL:N	2.41	0.54
2:B:203:LEU:HD11	2:B:208:PHE:HD1	1.72	0.53
1:D:752:GLU:HB2	1:D:790:PHE:CE2	2.43	0.53
2:F:187:ARG:NH1	2:F:373:GLU:HA	2.21	0.53
1:H:739:PRO:HG3	1:H:745:ARG:NH2	2.23	0.53
1:A:849:ASN:O	1:A:850:GLU:HB2	2.08	0.53
2:B:303:GLU:O	2:B:304:MET:HB3	2.07	0.53
1:H:733:LEU:N	1:H:733:LEU:HD22	2.24	0.53
1:H:889:TRP:NE1	3:H:8:SAH:N	2.56	0.53
1:D:711:ILE:HD11	1:D:758:GLY:N	2.24	0.53
2:G:192:VAL:HG21	2:G:203:LEU:HD21	1.89	0.53
1:D:739:PRO:HG3	1:D:745:ARG:NH2	2.23	0.53
2:B:286:ASP:O	2:B:321:VAL:HG22	2.08	0.53
1:D:858:THR:HG23	1:D:868:VAL:CG1	2.39	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:869:HIS:HE1	1:D:872:ASP:HB3	1.73	0.53
1:H:873:VAL:O	1:H:874:SER:O	2.26	0.53
1:H:716:ARG:HG2	1:H:716:ARG:NH1	2.23	0.53
1:H:810:GLU:HG2	1:H:813:GLU:CB	2.38	0.53
1:E:694:TRP:HA	1:E:694:TRP:HE3	1.73	0.53
1:H:704:SER:OG	1:H:751:PHE:HZ	1.90	0.53
1:E:866:PHE:HE2	1:E:888:SER:OG	1.91	0.53
2:C:293:GLU:OE2	2:C:293:GLU:N	2.38	0.53
1:H:817:HIS:C	1:H:817:HIS:CD2	2.82	0.53
2:G:190:VAL:HB	2:G:375:PHE:CD1	2.43	0.53
2:C:264:HIS:CD2	1:D:731:TYR:HE2	2.25	0.53
1:E:815:LEU:CD1	1:E:846:VAL:HG11	2.39	0.53
2:B:193:LEU:HD22	2:B:238:PHE:CE1	2.44	0.53
1:A:875:ASN:CG	1:D:878:ARG:HD2	2.29	0.53
1:E:699:LEU:HD11	1:E:701:ILE:CG2	2.39	0.53
2:G:232:VAL:CG2	2:G:266:LEU:HD22	2.37	0.52
1:E:694:TRP:HA	1:E:694:TRP:CE3	2.44	0.52
1:E:666:ILE:HG23	1:E:679:TYR:CD2	2.43	0.52
1:A:861:GLU:OE1	1:A:869:HIS:N	2.42	0.52
1:H:682:ASP:OD2	1:H:682:ASP:C	2.48	0.52
1:D:848:MET:O	1:D:851:LYS:N	2.35	0.52
2:C:363:LEU:HD22	2:C:363:LEU:H	1.75	0.52
1:H:652:GLN:HG2	1:H:908:VAL:CB	2.39	0.52
1:E:898:PHE:C	1:E:900:PRO:HD2	2.30	0.52
2:G:363:LEU:N	2:G:363:LEU:HD22	2.22	0.52
1:A:643:LEU:HD23	1:A:673:HIS:CG	2.45	0.52
1:E:712:VAL:O	1:E:714:PRO:HD3	2.09	0.52
1:E:873:VAL:CG2	1:E:874:SER:H	2.04	0.52
2:G:281:PHE:CE2	2:G:328:PRO:HD3	2.40	0.52
2:F:191:ARG:NH2	2:F:237:PRO:HB2	2.23	0.52
2:G:268:GLN:HG2	1:H:735:HIS:NE2	2.25	0.52
2:C:290:LEU:HB2	2:C:295:LEU:CD1	2.39	0.52
2:G:311:ASP:CB	2:G:363:LEU:HD11	2.36	0.52
1:A:649:LEU:HD22	1:A:902:LYS:HE3	1.91	0.52
1:E:794:LEU:O	1:E:797:MET:HG3	2.10	0.52
2:F:303:GLU:O	2:F:304:MET:HB3	2.08	0.52
1:A:799:ARG:NH2	1:A:900:PRO:HD3	2.24	0.52
1:D:874:SER:HB2	1:D:876:MET:CB	2.27	0.52
1:H:799:ARG:NH2	1:H:896:HIS:O	2.43	0.52
1:H:700:VAL:O	1:H:749:TRP:HA	2.10	0.52
2:B:346:LEU:HD23	2:B:346:LEU:O	2.09	0.52
1:E:636:PHE:HE2	1:E:726:LEU:HD13	1.75	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:686:VAL:O	1:E:732:ARG:NH2	2.43	0.52
2:B:192:VAL:HG21	2:B:203:LEU:HD21	1.91	0.52
1:D:643:LEU:HD23	1:D:673:HIS:CD2	2.45	0.52
2:C:262:GLN:HA	2:C:262:GLN:NE2	2.24	0.52
1:H:693:GLU:C	1:H:695:GLY:H	2.12	0.52
1:D:753:ASN:ND2	1:D:754:VAL:HG22	2.25	0.52
2:C:209:LEU:HD12	2:C:209:LEU:N	2.25	0.52
1:E:753:ASN:HD22	1:E:754:VAL:N	2.08	0.52
1:E:633:LEU:HB3	1:E:700:VAL:HG22	1.92	0.52
2:C:304:MET:HB2	2:C:331:ARG:NH2	2.25	0.52
2:G:198:ASP:HB3	2:G:220:HIS:CG	2.45	0.52
1:H:706:CYS:HB2	1:H:754:VAL:HG13	1.92	0.52
2:C:346:LEU:O	2:C:346:LEU:HD23	2.10	0.52
1:E:817:HIS:CE1	1:H:674:GLN:HB3	2.45	0.52
1:H:750:LEU:HD11	1:H:790:PHE:HD2	1.75	0.51
1:H:788:ARG:HH11	1:H:788:ARG:HG2	1.75	0.51
1:A:868:VAL:O	1:A:869:HIS:HB2	2.10	0.51
1:H:776:ILE:HD11	1:H:801:LEU:HD21	1.93	0.51
1:D:810:GLU:HG2	1:D:813:GLU:CB	2.40	0.51
2:F:260:LEU:CD2	2:F:298:ALA:HA	2.40	0.51
1:A:872:ASP:HB3	1:D:869:HIS:HE1	1.74	0.51
2:F:327:ILE:O	2:F:330:ILE:HB	2.10	0.51
1:D:645:VAL:HG11	1:D:895:ARG:HA	1.92	0.51
1:A:643:LEU:CG	1:A:647:LYS:HE3	2.38	0.51
2:B:203:LEU:HD13	2:B:368:PHE:HD1	1.75	0.51
1:E:786:ARG:NH1	1:E:864:PHE:HE2	2.07	0.51
2:G:324:TRP:O	2:G:325:SER:HB2	2.10	0.51
2:F:306:PRO:HB3	2:F:324:TRP:CE2	2.45	0.51
1:A:799:ARG:NH2	1:A:896:HIS:O	2.43	0.51
2:G:184:VAL:C	2:G:186:ARG:H	2.14	0.51
1:E:871:THR:HB	1:E:881:ARG:HG2	1.92	0.51
1:E:748:PHE:HB3	1:E:794:LEU:CD2	2.41	0.51
1:A:671:VAL:CG1	1:D:816:GLU:HG2	2.41	0.51
1:D:747:PHE:O	1:D:793:ASN:ND2	2.39	0.51
2:B:286:ASP:OD1	2:B:322:ARG:HG3	2.11	0.51
1:A:633:LEU:HD13	1:A:697:PHE:CE1	2.46	0.51
1:A:854:ILE:HG22	1:A:855:LEU:N	2.25	0.51
1:H:801:LEU:HD12	1:H:801:LEU:H	1.76	0.51
1:D:749:TRP:HZ3	1:D:769:LEU:HD13	1.75	0.51
1:E:687:THR:O	1:E:690:HIS:HB2	2.11	0.51
1:D:783:ALA:O	1:D:826:VAL:HG22	2.10	0.51
2:G:322:ARG:HH22	2:G:340:GLU:CD	2.12	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:633:LEU:HB2	1:D:697:PHE:CE2	2.46	0.51
2:B:201:LYS:HE3	2:B:202:GLU:OE1	2.11	0.51
1:D:711:ILE:HD11	1:D:757:MET:C	2.31	0.51
1:H:629:PRO:HB2	1:H:654:ASP:HB2	1.92	0.51
1:E:693:GLU:C	1:E:695:GLY:H	2.14	0.50
1:E:730:PHE:CE2	1:E:751:PHE:HB2	2.46	0.50
2:F:234:GLU:C	2:F:236:GLY:H	2.14	0.50
1:E:788:ARG:NH1	1:E:788:ARG:HG2	2.21	0.50
2:B:271:ARG:CG	2:B:271:ARG:HH11	2.00	0.50
1:H:856:TRP:HB2	1:H:859:GLU:OE1	2.11	0.50
1:E:684:ARG:HD3	1:E:684:ARG:H	1.76	0.50
2:B:282:TRP:HZ3	2:B:302:LEU:HD22	1.76	0.50
1:A:858:THR:CG2	1:A:868:VAL:HG12	2.33	0.50
1:D:683:VAL:CG2	1:D:684:ARG:N	2.74	0.50
1:E:635:LEU:HD12	1:E:730:PHE:HD1	1.76	0.50
2:F:256:PRO:HB3	2:F:290:LEU:HD23	1.93	0.50
1:E:689:LYS:O	1:E:693:GLU:HB2	2.12	0.50
2:F:229:ARG:O	2:F:233:GLU:HG3	2.11	0.50
1:H:809:LEU:HD12	1:H:809:LEU:H	1.75	0.50
2:C:300:ARG:NH1	1:D:684:ARG:HB2	2.27	0.50
2:G:209:LEU:N	2:G:209:LEU:HD12	2.26	0.50
1:A:796:GLY:O	1:A:799:ARG:CG	2.59	0.50
1:D:680:VAL:HG11	1:D:686:VAL:HG22	1.92	0.50
2:F:310:PRO:CG	2:F:338:VAL:HG21	2.41	0.50
2:C:246:PRO:HG2	2:C:259:TYR:CZ	2.47	0.50
2:G:291:ASN:HB3	2:G:293:GLU:OE2	2.11	0.50
2:B:202:GLU:O	2:B:206:LEU:HD23	2.11	0.50
1:D:630:ILE:HG22	1:D:652:GLN:O	2.11	0.50
1:H:645:VAL:HG21	1:H:894:ILE:HB	1.93	0.50
2:F:224:VAL:HG11	2:F:266:LEU:HD11	1.92	0.50
2:F:201:LYS:HB3	2:F:202:GLU:OE1	2.12	0.50
1:A:656:TYR:CD2	1:A:677:ILE:HG12	2.46	0.50
1:D:874:SER:C	1:D:876:MET:H	2.06	0.50
1:A:729:GLU:OE2	2:B:300:ARG:NH1	2.45	0.50
1:D:708:ASP:OD2	1:D:717:LYS:HB2	2.12	0.50
1:E:817:HIS:CD2	1:E:817:HIS:C	2.85	0.50
1:E:807:ASP:O	1:E:809:LEU:HG	2.12	0.50
1:H:684:ARG:HD3	1:H:684:ARG:H	1.77	0.49
2:F:199:ILE:HG22	2:F:203:LEU:HB2	1.93	0.49
1:E:745:ARG:HG3	1:E:746:PRO:HD2	1.93	0.49
1:A:865:GLY:O	1:A:891:VAL:HB	2.12	0.49
1:A:773:PRO:HB3	1:A:791:TRP:CE2	2.48	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:643:LEU:HG	1:E:647:LYS:HE3	1.93	0.49
1:E:643:LEU:HB2	1:E:656:TYR:CE1	2.47	0.49
1:H:627:ARG:NH1	1:H:903:GLU:HA	2.26	0.49
2:B:290:LEU:HB2	2:B:295:LEU:CD1	2.42	0.49
1:E:753:ASN:ND2	1:E:754:VAL:H	2.10	0.49
1:E:686:VAL:HG12	1:E:733:LEU:HD11	1.93	0.49
2:B:310:PRO:HG3	2:B:338:VAL:HG21	1.95	0.49
2:B:183:PRO:O	2:B:187:ARG:HG3	2.12	0.49
1:D:632:VAL:HG21	1:D:646:LEU:HD11	1.94	0.49
1:E:680:VAL:CG1	1:E:681:GLY:H	2.17	0.49
2:C:191:ARG:HH21	2:C:237:PRO:HB2	1.78	0.49
2:G:368:PHE:O	2:G:371:LEU:HB2	2.12	0.49
1:E:668:VAL:HG22	1:E:873:VAL:HG21	1.93	0.49
1:D:874:SER:HB2	1:D:876:MET:H	1.78	0.49
1:E:810:GLU:HG2	1:E:813:GLU:CB	2.42	0.49
1:A:700:VAL:O	1:A:749:TRP:HA	2.12	0.49
2:G:346:LEU:HD23	2:G:346:LEU:O	2.13	0.49
1:D:631:ARG:HH11	1:D:631:ARG:CB	2.21	0.49
1:E:699:LEU:HD11	1:E:701:ILE:HG23	1.95	0.49
2:F:326:ASN:N	2:F:326:ASN:HD22	1.92	0.49
1:D:776:ILE:CG2	1:D:790:PHE:HD1	2.25	0.49
1:H:754:VAL:HA	1:H:788:ARG:CD	2.42	0.49
1:D:885:LEU:O	1:D:886:GLY:C	2.52	0.49
2:B:287:ASN:HA	2:B:321:VAL:CG2	2.43	0.48
1:A:716:ARG:NH1	1:A:716:ARG:HG2	2.28	0.48
1:A:759:VAL:HG23	1:A:760:SER:N	2.28	0.48
1:A:630:ILE:HG12	1:A:632:VAL:HG23	1.95	0.48
2:F:367:CYS:O	2:F:370:PRO:HD2	2.13	0.48
1:D:691:ILE:HG22	1:D:692:GLN:N	2.27	0.48
1:A:775:MET:SD	1:A:776:ILE:N	2.86	0.48
2:G:263:PHE:CE2	2:G:284:PHE:HB2	2.48	0.48
2:G:309:ILE:HG13	2:G:309:ILE:O	2.13	0.48
1:E:786:ARG:CG	1:E:786:ARG:NH1	2.70	0.48
1:D:858:THR:HG23	1:D:868:VAL:HG13	1.95	0.48
1:A:684:ARG:HB2	2:B:300:ARG:NH1	2.28	0.48
1:D:709:LEU:HD13	1:D:757:MET:CE	2.42	0.48
2:F:198:ASP:HB3	2:F:220:HIS:CG	2.49	0.48
1:E:817:HIS:CD2	1:E:818:GLY:N	2.82	0.48
1:D:876:MET:SD	1:D:884:LEU:CD2	3.01	0.48
1:A:869:HIS:HB3	1:D:869:HIS:CE1	2.48	0.48
2:F:256:PRO:O	2:F:259:TYR:HD1	1.96	0.48
2:C:243:GLY:O	2:C:284:PHE:HA	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:290:LEU:HD22	2:G:294:ASP:HB3	1.95	0.48
1:H:668:VAL:HG22	1:H:873:VAL:CG2	2.43	0.48
1:A:874:SER:HA	1:D:856:TRP:CZ2	2.49	0.48
1:A:823:PHE:HZ	1:A:842:GLN:HA	1.79	0.48
2:F:243:GLY:O	2:F:284:PHE:HA	2.14	0.48
1:H:861:GLU:OE2	1:H:881:ARG:NH1	2.46	0.48
2:C:279:PRO:HB2	2:C:281:PHE:HE1	1.77	0.48
2:B:209:LEU:N	2:B:209:LEU:HD12	2.28	0.48
2:G:267:LEU:HD22	2:G:267:LEU:O	2.14	0.48
1:A:869:HIS:ND1	1:D:869:HIS:HB3	2.29	0.48
2:F:199:ILE:O	2:F:199:ILE:HG22	2.14	0.48
1:E:794:LEU:HD13	1:E:897:LEU:O	2.14	0.48
2:B:234:GLU:C	2:B:236:GLY:H	2.16	0.48
1:H:691:ILE:CD1	1:H:733:LEU:HD12	2.44	0.48
1:E:773:PRO:HD3	1:E:791:TRP:NE1	2.29	0.48
1:H:682:ASP:OD2	1:H:683:VAL:N	2.47	0.47
2:F:326:ASN:ND2	2:F:326:ASN:H	1.99	0.47
1:H:717:LYS:HB3	1:H:721:GLU:CB	2.44	0.47
2:F:372:ARG:HD2	2:F:377:TYR:HB2	1.96	0.47
2:C:327:ILE:O	2:C:330:ILE:HB	2.14	0.47
1:D:657:ILE:HD12	1:D:697:PHE:CZ	2.49	0.47
1:H:773:PRO:CD	1:H:791:TRP:NE1	2.70	0.47
1:A:647:LYS:HZ1	1:A:673:HIS:HB3	1.78	0.47
1:E:632:VAL:HG12	1:E:633:LEU:N	2.29	0.47
2:C:264:HIS:O	2:C:268:GLN:NE2	2.47	0.47
1:H:885:LEU:O	1:H:888:SER:OG	2.32	0.47
1:A:666:ILE:HG12	1:A:679:TYR:CE2	2.48	0.47
2:C:326:ASN:ND2	2:C:326:ASN:H	1.98	0.47
1:A:804:THR:HG22	1:A:805:VAL:N	2.30	0.47
2:G:201:LYS:HB3	2:G:202:GLU:OE1	2.13	0.47
1:D:810:GLU:CD	1:D:810:GLU:H	2.17	0.47
1:H:861:GLU:OE1	1:H:868:VAL:HA	2.14	0.47
2:B:361:THR:N	2:B:363:LEU:HD23	2.28	0.47
2:F:224:VAL:HG11	2:F:266:LEU:CD1	2.45	0.47
1:E:727:PHE:CE1	1:E:765:ILE:HG23	2.49	0.47
1:D:748:PHE:CE1	1:D:795:PRO:HD3	2.50	0.47
1:E:686:VAL:CG1	1:E:733:LEU:HD11	2.44	0.47
2:F:202:GLU:O	2:F:206:LEU:HD23	2.13	0.47
1:H:732:ARG:NE	1:H:733:LEU:HD21	2.30	0.47
2:G:290:LEU:HB3	2:G:294:ASP:HB2	1.96	0.47
1:H:819:ARG:CD	1:H:848:MET:SD	3.02	0.47
1:D:748:PHE:HB3	1:D:794:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:786:ARG:NH1	1:H:864:PHE:HE2	2.12	0.47
2:G:204:THR:OG1	2:G:209:LEU:HD22	2.15	0.47
2:F:247:PRO:HA	2:F:287:ASN:ND2	2.29	0.47
1:H:663:GLU:O	1:H:666:ILE:HB	2.14	0.47
2:G:346:LEU:O	2:G:350:LYS:HG2	2.14	0.47
1:A:623:PRO:O	1:A:624:ALA:HB2	2.14	0.47
1:E:885:LEU:O	1:E:886:GLY:C	2.51	0.47
1:H:720:TYR:HH	1:H:764:ASP:CG	2.17	0.47
1:D:662:CYS:O	1:D:666:ILE:HG13	2.14	0.47
2:G:300:ARG:NH1	1:H:684:ARG:HB2	2.29	0.47
1:A:680:VAL:HG21	1:A:694:TRP:CH2	2.50	0.47
1:E:702:GLY:O	1:E:751:PHE:HA	2.15	0.47
2:C:290:LEU:HB2	2:C:295:LEU:HD13	1.96	0.47
2:G:257:SER:OG	1:H:725:ARG:NH2	2.47	0.47
2:C:300:ARG:NH1	1:D:729:GLU:OE2	2.48	0.47
2:B:282:TRP:H	2:B:326:ASN:HD21	1.62	0.47
1:D:752:GLU:CG	1:D:753:ASN:N	2.75	0.47
2:B:376:LYS:HD3	2:B:378:PHE:HE2	1.77	0.47
1:H:706:CYS:CB	1:H:754:VAL:HG13	2.45	0.47
2:G:198:ASP:HB3	2:G:220:HIS:ND1	2.30	0.47
2:G:293:GLU:OE2	2:G:293:GLU:N	2.46	0.47
1:D:873:VAL:HG23	1:D:874:SER:N	2.29	0.47
1:H:871:THR:HB	1:H:881:ARG:HD3	1.96	0.47
1:E:683:VAL:HG23	1:E:684:ARG:N	2.29	0.46
1:D:855:LEU:HD21	1:D:859:GLU:HB2	1.97	0.46
1:E:633:LEU:HB2	1:E:697:PHE:CD2	2.50	0.46
1:E:755:VAL:HG13	1:E:756:ALA:N	2.30	0.46
1:D:699:LEU:HA	1:D:748:PHE:O	2.15	0.46
1:D:871:THR:CB	1:D:881:ARG:HD3	2.46	0.46
1:H:691:ILE:HD11	1:H:733:LEU:HD12	1.96	0.46
1:H:691:ILE:HG22	1:H:692:GLN:H	1.80	0.46
1:D:648:ASP:CG	1:D:895:ARG:HH12	2.19	0.46
1:A:816:GLU:HG2	1:D:671:VAL:CG1	2.45	0.46
1:D:629:PRO:HB2	1:D:654:ASP:HB2	1.97	0.46
1:H:823:PHE:HD1	1:H:823:PHE:N	2.12	0.46
2:F:188:GLN:N	2:F:188:GLN:OE1	2.49	0.46
1:A:686:VAL:HG13	1:A:694:TRP:CZ3	2.50	0.46
1:D:645:VAL:CG1	1:D:895:ARG:HA	2.45	0.46
1:D:635:LEU:O	1:D:636:PHE:HB2	2.16	0.46
1:D:693:GLU:C	1:D:695:GLY:H	2.18	0.46
1:H:873:VAL:CG2	1:H:874:SER:N	2.71	0.46
1:E:671:VAL:CG1	1:H:816:GLU:HG2	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:346:LEU:HD23	2:C:346:LEU:C	2.36	0.46
2:C:262:GLN:HE21	2:C:262:GLN:CA	2.29	0.46
1:H:854:ILE:HG22	1:H:855:LEU:N	2.30	0.46
1:D:819:ARG:CZ	1:D:846:VAL:HG21	2.46	0.46
1:D:801:LEU:CD1	1:D:801:LEU:H	2.21	0.46
2:G:208:PHE:C	2:G:209:LEU:HD12	2.36	0.46
1:H:709:LEU:HD13	1:H:753:ASN:ND2	2.30	0.46
1:H:661:VAL:O	1:H:661:VAL:HG22	2.16	0.46
2:B:188:GLN:HB3	2:B:189:PRO:CD	2.42	0.46
2:G:202:GLU:HG2	2:G:361:THR:HG21	1.97	0.46
2:G:267:LEU:HD12	2:G:268:GLN:HE22	1.79	0.46
1:E:631:ARG:NH1	1:E:696:PRO:O	2.48	0.46
2:F:268:GLN:OE1	2:F:271:ARG:NH1	2.49	0.46
1:A:869:HIS:CE1	1:D:869:HIS:HB3	2.51	0.46
1:E:699:LEU:HD12	1:E:700:VAL:N	2.30	0.46
1:A:755:VAL:HG23	1:A:789:TYR:CE1	2.51	0.46
2:F:218:LEU:C	2:F:218:LEU:HD23	2.37	0.46
1:E:810:GLU:H	1:E:810:GLU:CD	2.17	0.46
2:F:369:LEU:HB2	2:F:370:PRO:HD3	1.98	0.46
2:F:245:THR:HB	2:F:289:VAL:HG11	1.97	0.46
2:B:309:ILE:HG13	2:B:309:ILE:O	2.15	0.46
1:H:705:PRO:HG2	1:H:726:LEU:HD12	1.97	0.45
2:B:203:LEU:CD1	2:B:208:PHE:HD1	2.29	0.45
2:B:229:ARG:HA	2:B:269:TYR:HD1	1.79	0.45
1:A:860:MET:O	1:A:864:PHE:HD1	1.98	0.45
2:F:372:ARG:NH1	2:F:372:ARG:HG2	2.31	0.45
2:B:218:LEU:C	2:B:218:LEU:HD23	2.37	0.45
2:G:300:ARG:HG2	1:H:732:ARG:NH1	2.31	0.45
1:H:732:ARG:NE	1:H:733:LEU:CD2	2.72	0.45
2:B:268:GLN:NE2	2:B:268:GLN:CA	2.79	0.45
1:H:866:PHE:O	1:H:867:PRO:C	2.55	0.45
1:A:801:LEU:HD12	1:A:801:LEU:N	2.31	0.45
1:H:752:GLU:CG	1:H:753:ASN:N	2.79	0.45
2:F:279:PRO:CB	2:F:281:PHE:HE1	2.29	0.45
2:F:184:VAL:HA	2:F:187:ARG:NE	2.31	0.45
1:E:643:LEU:HD22	1:E:656:TYR:CG	2.50	0.45
1:H:794:LEU:O	1:H:797:MET:HG3	2.16	0.45
2:G:268:GLN:HG2	1:H:735:HIS:CE1	2.51	0.45
2:G:322:ARG:NH2	2:G:340:GLU:OE1	2.33	0.45
2:B:202:GLU:H	2:B:202:GLU:CD	2.20	0.45
2:G:232:VAL:O	2:G:232:VAL:HG12	2.17	0.45
1:H:657:ILE:CG2	1:H:680:VAL:CG2	2.95	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:248:LEU:HG	2:B:287:ASN:ND2	2.32	0.45
2:G:310:PRO:HG2	2:G:338:VAL:CG2	2.46	0.45
2:G:203:LEU:HG	2:G:209:LEU:HD11	1.99	0.45
2:B:228:VAL:CG1	2:B:229:ARG:N	2.79	0.45
1:A:693:GLU:C	1:A:695:GLY:H	2.19	0.45
1:E:753:ASN:HD22	1:E:754:VAL:HG22	1.79	0.45
1:E:682:ASP:OD2	1:E:684:ARG:HG2	2.16	0.45
2:F:224:VAL:CB	2:F:266:LEU:HD11	2.46	0.45
2:F:188:GLN:HB3	2:F:189:PRO:CD	2.47	0.45
2:C:221:VAL:HG21	2:C:235:TRP:CH2	2.52	0.45
2:C:234:GLU:C	2:C:236:GLY:H	2.20	0.45
1:D:691:ILE:HD11	1:D:733:LEU:CD1	2.44	0.45
1:A:773:PRO:HD3	1:A:791:TRP:NE1	2.32	0.45
2:F:192:VAL:HG21	2:F:203:LEU:CD2	2.42	0.45
1:D:776:ILE:CG2	1:D:790:PHE:CD1	3.00	0.45
1:E:817:HIS:ND1	1:H:674:GLN:HB3	2.32	0.45
2:G:230:LYS:N	2:G:230:LYS:HD2	2.32	0.45
1:D:812:GLN:OE1	1:D:821:ALA:N	2.34	0.45
2:C:300:ARG:CZ	1:D:684:ARG:HB2	2.47	0.45
2:G:372:ARG:HG2	2:G:372:ARG:NH1	2.31	0.45
1:D:810:GLU:HG2	1:D:813:GLU:H	1.82	0.45
1:E:796:GLY:O	1:E:799:ARG:HG3	2.17	0.45
1:D:680:VAL:CG1	1:D:681:GLY:N	2.61	0.45
2:B:202:GLU:HG2	2:B:361:THR:CG2	2.43	0.45
1:D:819:ARG:HD2	1:D:848:MET:SD	2.56	0.45
2:B:199:ILE:O	2:B:199:ILE:HG22	2.17	0.45
1:A:891:VAL:N	1:A:892:PRO:CD	2.79	0.45
1:E:735:HIS:NE2	2:F:268:GLN:CG	2.80	0.45
2:G:188:GLN:OE1	2:G:188:GLN:N	2.50	0.45
1:D:786:ARG:NH1	1:D:864:PHE:CE2	2.83	0.44
2:G:255:PRO:HA	2:G:256:PRO:HD3	1.90	0.44
1:E:732:ARG:HD3	2:F:301:PHE:CE1	2.52	0.44
1:A:717:LYS:HD2	1:A:722:GLY:HA3	1.99	0.44
2:C:369:LEU:HB2	2:C:370:PRO:HD3	1.99	0.44
1:E:664:ASP:O	1:E:668:VAL:HG23	2.17	0.44
1:E:875:ASN:ND2	1:H:856:TRP:HD1	2.15	0.44
2:G:376:LYS:HD3	2:G:378:PHE:CE2	2.53	0.44
1:H:702:GLY:O	1:H:751:PHE:HA	2.16	0.44
1:E:810:GLU:HG2	1:E:813:GLU:H	1.82	0.44
1:E:816:GLU:CD	1:E:862:ARG:HH22	2.21	0.44
1:E:719:LEU:HG	1:E:719:LEU:O	2.16	0.44
1:E:638:GLY:HA2	1:E:660:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:725:ARG:HH12	2:B:297:VAL:CG2	2.17	0.44
1:H:781:VAL:CG1	1:H:892:PRO:HB2	2.48	0.44
1:H:893:VAL:O	1:H:896:HIS:HB3	2.17	0.44
2:B:326:ASN:HD22	2:B:326:ASN:N	1.98	0.44
1:E:844:PHE:O	1:E:846:VAL:N	2.51	0.44
1:A:875:ASN:HB3	1:D:878:ARG:CD	2.47	0.44
2:C:221:VAL:HG21	2:C:235:TRP:CZ3	2.52	0.44
2:B:325:SER:OG	2:B:327:ILE:HG13	2.18	0.44
2:G:347:ALA:O	2:G:351:GLN:HG3	2.17	0.44
1:A:808:LYS:HG2	1:A:808:LYS:H	1.56	0.44
1:A:775:MET:CE	1:A:787:ALA:HB1	2.48	0.44
2:C:271:ARG:HG3	2:C:271:ARG:NH1	2.33	0.44
1:A:865:GLY:O	1:A:891:VAL:CB	2.66	0.44
1:E:657:ILE:HG12	1:E:678:MET:HB3	2.00	0.44
2:B:330:ILE:O	2:B:330:ILE:HG13	2.17	0.44
2:C:231:ASP:N	2:C:231:ASP:OD1	2.49	0.44
2:C:326:ASN:ND2	2:C:326:ASN:N	2.62	0.44
1:D:786:ARG:HH21	1:D:788:ARG:NH2	2.16	0.44
1:D:652:GLN:HG3	1:D:906:ALA:O	2.17	0.44
1:E:819:ARG:HD2	1:E:848:MET:SD	2.58	0.44
1:A:899:ALA:HB3	1:A:900:PRO:CD	2.48	0.44
1:A:871:THR:HG1	1:A:881:ARG:HH11	1.64	0.44
1:H:717:LYS:HB3	1:H:721:GLU:HB2	1.98	0.44
1:A:728:PHE:HA	1:A:731:TYR:HB3	2.00	0.44
2:F:262:GLN:HE22	2:F:265:ARG:HE	1.65	0.44
1:E:753:ASN:ND2	1:E:754:VAL:N	2.66	0.44
1:E:691:ILE:HG22	1:E:692:GLN:N	2.32	0.44
2:G:248:LEU:N	2:G:287:ASN:HD22	2.15	0.44
2:C:208:PHE:C	2:C:209:LEU:HD12	2.38	0.44
1:A:719:LEU:HG	1:A:719:LEU:O	2.18	0.44
2:F:346:LEU:C	2:F:346:LEU:HD23	2.37	0.44
1:E:872:ASP:HB3	1:H:869:HIS:HE1	1.81	0.44
2:G:310:PRO:O	2:G:363:LEU:HD12	2.17	0.44
1:E:699:LEU:CD1	1:E:701:ILE:HG23	2.48	0.44
2:F:361:THR:N	2:F:363:LEU:HD23	2.33	0.44
1:E:868:VAL:O	1:E:869:HIS:HB2	2.18	0.44
2:B:309:ILE:HA	2:B:310:PRO:HD3	1.78	0.44
2:G:303:GLU:O	2:G:304:MET:HB3	2.18	0.44
1:H:689:LYS:O	1:H:692:GLN:OE1	2.36	0.43
2:G:256:PRO:CB	2:G:290:LEU:HD23	2.39	0.43
1:H:873:VAL:O	1:H:874:SER:C	2.57	0.43
2:F:267:LEU:HD12	2:F:268:GLN:HE22	1.83	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:706:CYS:SG	1:A:707:ASN:N	2.90	0.43
1:D:811:LEU:HD13	1:D:811:LEU:O	2.17	0.43
1:E:648:ASP:OD2	1:E:895:ARG:NH1	2.46	0.43
2:F:326:ASN:N	2:F:326:ASN:ND2	2.63	0.43
1:H:890:SER:O	1:H:893:VAL:HB	2.17	0.43
1:H:788:ARG:NH1	1:H:788:ARG:HG2	2.33	0.43
2:B:289:VAL:O	2:B:289:VAL:HG22	2.19	0.43
1:A:739:PRO:HG3	1:A:745:ARG:CZ	2.48	0.43
1:A:738:ARG:HA	1:A:747:PHE:CE2	2.52	0.43
1:A:750:LEU:HD11	1:A:790:PHE:HD2	1.83	0.43
2:C:199:ILE:HG21	2:C:368:PHE:HE1	1.82	0.43
2:F:228:VAL:CG1	2:F:229:ARG:H	2.29	0.43
1:D:810:GLU:OE1	1:D:813:GLU:CB	2.67	0.43
1:H:752:GLU:O	1:H:753:ASN:HB2	2.17	0.43
2:B:335:TRP:O	2:B:337:LEU:N	2.46	0.43
2:F:309:ILE:HG13	2:F:321:VAL:HG12	2.00	0.43
1:H:757:MET:HE3	1:H:757:MET:HB2	1.83	0.43
1:A:883:ARG:O	1:A:887:ARG:HG2	2.18	0.43
1:A:699:LEU:HG	1:A:701:ILE:HG23	2.00	0.43
1:A:869:HIS:HB3	1:D:869:HIS:ND1	2.33	0.43
2:G:203:LEU:CG	2:G:209:LEU:HD11	2.47	0.43
2:F:229:ARG:HG2	2:F:233:GLU:OE1	2.18	0.43
2:C:262:GLN:HA	2:C:262:GLN:HE21	1.82	0.43
2:F:346:LEU:HD23	2:F:346:LEU:O	2.19	0.43
1:D:822:LYS:NZ	1:D:852:GLU:OE2	2.49	0.43
1:A:672:ARG:CG	1:A:870:TYR:CE1	2.97	0.43
1:H:822:LYS:HB2	1:H:823:PHE:CE1	2.53	0.43
1:A:855:LEU:HD23	1:A:855:LEU:HA	1.84	0.43
1:E:630:ILE:HD11	1:E:699:LEU:HD23	2.01	0.43
2:C:363:LEU:CD2	2:C:363:LEU:H	2.31	0.43
2:G:193:LEU:HB2	2:G:238:PHE:CE2	2.52	0.43
1:E:881:ARG:HH22	1:H:872:ASP:CG	2.22	0.43
2:F:346:LEU:O	2:F:350:LYS:HG2	2.18	0.43
1:E:757:MET:HE2	1:E:762:LYS:N	2.34	0.43
1:H:728:PHE:HE2	1:H:768:PHE:CZ	2.35	0.43
2:C:198:ASP:HB3	2:C:220:HIS:CG	2.53	0.43
1:D:687:THR:O	1:D:690:HIS:HB2	2.18	0.43
1:A:646:LEU:HA	1:A:646:LEU:HD23	1.84	0.43
2:G:234:GLU:C	2:G:236:GLY:H	2.20	0.43
1:H:815:LEU:HA	1:H:859:GLU:OE2	2.19	0.43
1:A:635:LEU:O	1:A:636:PHE:HB2	2.19	0.43
2:B:255:PRO:HA	2:B:256:PRO:HD3	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:786:ARG:HG3	1:A:786:ARG:HH11	1.83	0.43
2:G:228:VAL:CG1	2:G:229:ARG:N	2.82	0.43
1:E:786:ARG:HB3	1:E:788:ARG:HH12	1.84	0.43
1:D:859:GLU:O	1:D:863:VAL:HG23	2.18	0.43
1:D:711:ILE:HG12	1:D:756:ALA:O	2.19	0.43
1:H:899:ALA:N	1:H:900:PRO:HD2	2.34	0.43
1:A:649:LEU:CD2	1:A:902:LYS:HE3	2.49	0.43
2:F:246:PRO:HA	2:F:247:PRO:HD3	1.92	0.43
2:C:192:VAL:HG21	2:C:203:LEU:CD2	2.45	0.43
2:B:190:VAL:HG22	2:B:192:VAL:HG23	2.00	0.43
1:A:749:TRP:CZ3	1:A:792:GLY:HA2	2.53	0.43
1:E:735:HIS:NE2	2:F:268:GLN:HG2	2.33	0.43
2:F:260:LEU:CD2	2:F:297:VAL:HG12	2.49	0.43
2:F:258:TRP:CE2	2:F:262:GLN:HG3	2.53	0.43
1:D:750:LEU:HD13	1:D:794:LEU:HD12	2.00	0.43
1:A:682:ASP:OD2	1:A:684:ARG:CD	2.66	0.43
1:A:739:PRO:HD3	1:A:747:PHE:CG	2.53	0.43
2:F:199:ILE:HG22	2:F:203:LEU:N	2.34	0.43
1:A:666:ILE:HA	1:A:679:TYR:CE2	2.53	0.43
2:C:218:LEU:HD23	2:C:218:LEU:C	2.40	0.43
1:D:694:TRP:HA	1:D:694:TRP:HE3	1.84	0.43
2:B:257:SER:O	2:B:260:LEU:N	2.52	0.43
2:B:286:ASP:OD2	2:B:289:VAL:HG12	2.18	0.43
1:A:878:ARG:CG	1:A:878:ARG:HH11	2.15	0.43
2:F:282:TRP:CZ3	2:F:302:LEU:HD22	2.54	0.43
2:C:289:VAL:HG22	2:C:289:VAL:O	2.19	0.43
2:C:306:PRO:HB3	2:C:324:TRP:CE2	2.54	0.43
2:F:219:LYS:HE2	2:F:235:TRP:CD2	2.54	0.43
2:G:269:TYR:CD2	2:G:269:TYR:N	2.87	0.43
1:E:774:VAL:O	1:E:776:ILE:HG22	2.19	0.42
1:D:773:PRO:HD3	1:D:791:TRP:NE1	2.34	0.42
2:C:345:LEU:HD12	2:C:349:ASN:OD1	2.18	0.42
1:D:876:MET:SD	1:D:884:LEU:HD23	2.59	0.42
2:B:260:LEU:CD2	2:B:298:ALA:CA	2.94	0.42
1:D:868:VAL:O	1:D:869:HIS:HB2	2.18	0.42
1:H:730:PHE:CE2	1:H:751:PHE:HB2	2.54	0.42
1:A:675:GLY:O	1:A:677:ILE:N	2.52	0.42
2:B:307:VAL:HG13	2:B:334:HIS:ND1	2.35	0.42
2:C:199:ILE:O	2:C:203:LEU:HB2	2.19	0.42
2:F:228:VAL:CG1	2:F:229:ARG:N	2.80	0.42
1:H:720:TYR:CD1	1:H:720:TYR:N	2.87	0.42
2:F:267:LEU:C	2:F:267:LEU:HD13	2.39	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:727:PHE:CE1	1:A:765:ILE:HG23	2.54	0.42
1:A:783:ALA:O	1:A:826:VAL:HG22	2.20	0.42
1:D:862:ARG:NH1	1:D:868:VAL:HG21	2.33	0.42
1:H:730:PHE:CZ	1:H:734:LEU:HD12	2.54	0.42
2:C:279:PRO:CB	2:C:281:PHE:HE1	2.32	0.42
1:H:632:VAL:CG1	1:H:633:LEU:N	2.82	0.42
2:G:326:ASN:ND2	2:G:326:ASN:H	2.18	0.42
1:H:692:GLN:OE1	1:H:692:GLN:N	2.52	0.42
1:H:786:ARG:NH1	1:H:864:PHE:CE2	2.88	0.42
1:A:775:MET:HE1	1:A:787:ALA:HB1	2.01	0.42
1:H:904:TYR:C	1:H:905:PHE:CD1	2.92	0.42
1:E:687:THR:O	1:E:690:HIS:N	2.53	0.42
2:F:257:SER:O	2:F:260:LEU:N	2.53	0.42
1:A:632:VAL:CG1	1:A:633:LEU:N	2.82	0.42
2:G:363:LEU:CD2	2:G:363:LEU:H	2.28	0.42
1:D:819:ARG:HH21	1:D:859:GLU:CD	2.21	0.42
1:A:880:ALA:O	1:A:881:ARG:C	2.58	0.42
1:H:883:ARG:HD3	1:H:887:ARG:HH22	1.85	0.42
2:F:372:ARG:CD	2:F:377:TYR:HB2	2.50	0.42
2:B:230:LYS:N	2:B:230:LYS:HD2	2.35	0.42
1:E:876:MET:CG	1:E:880:ALA:HB3	2.50	0.42
1:D:699:LEU:HG	1:D:701:ILE:HG23	2.02	0.42
1:A:691:ILE:HG21	1:A:736:ASP:O	2.18	0.42
2:B:342:GLU:O	2:B:345:LEU:HB3	2.19	0.42
2:G:245:THR:HB	2:G:289:VAL:HG11	2.02	0.42
2:G:300:ARG:NH1	1:H:729:GLU:OE2	2.48	0.42
1:A:683:VAL:HG23	1:A:684:ARG:H	1.85	0.42
1:D:815:LEU:CD1	1:D:846:VAL:HG12	2.50	0.42
2:B:267:LEU:HD22	2:B:267:LEU:O	2.20	0.42
1:H:630:ILE:HG13	1:H:905:PHE:CE2	2.55	0.42
1:A:849:ASN:O	1:A:850:GLU:CB	2.68	0.42
1:E:690:HIS:O	1:E:694:TRP:N	2.49	0.42
1:H:728:PHE:HA	1:H:731:TYR:HB3	2.02	0.42
1:D:778:ALA:HB2	1:D:893:VAL:HG21	2.02	0.42
1:E:878:ARG:O	1:E:882:GLN:HB2	2.20	0.42
1:E:639:ILE:O	1:E:870:TYR:OH	2.28	0.42
1:H:871:THR:HB	1:H:881:ARG:CG	2.50	0.42
1:D:657:ILE:CG2	1:D:680:VAL:HG23	2.50	0.42
1:A:632:VAL:HG12	1:A:633:LEU:N	2.33	0.42
1:A:856:TRP:HB2	1:A:859:GLU:CG	2.47	0.42
1:E:699:LEU:HA	1:E:748:PHE:O	2.20	0.42
1:E:881:ARG:NH2	1:H:872:ASP:OD2	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:687:THR:O	1:D:690:HIS:N	2.53	0.42
1:E:639:ILE:O	1:E:640:ALA:HB3	2.19	0.42
1:A:779:LYS:HA	1:A:784:ALA:O	2.20	0.42
1:E:786:ARG:HB3	1:E:788:ARG:NH1	2.35	0.42
1:A:730:PHE:CE2	1:A:751:PHE:HB2	2.54	0.42
2:F:273:LYS:CB	2:F:274:PRO:HD2	2.42	0.42
1:D:848:MET:O	1:D:849:ASN:C	2.59	0.42
1:D:773:PRO:HB2	1:D:789:TYR:HD1	1.84	0.42
2:F:247:PRO:HA	2:F:287:ASN:HD22	1.85	0.42
2:C:368:PHE:CD2	2:C:368:PHE:N	2.86	0.42
1:E:888:SER:HA	3:E:5:SAH:C	2.49	0.42
2:F:187:ARG:HB3	2:F:375:PHE:HA	2.01	0.42
1:A:706:CYS:HB2	1:A:754:VAL:HG13	2.00	0.42
2:B:243:GLY:O	2:B:284:PHE:HA	2.20	0.42
1:A:627:ARG:HH12	1:A:903:GLU:HA	1.85	0.42
1:H:898:PHE:N	1:H:898:PHE:CD2	2.86	0.42
2:F:260:LEU:HD21	2:F:298:ALA:HA	2.02	0.41
1:H:811:LEU:CD2	1:H:826:VAL:HG13	2.50	0.41
1:D:898:PHE:O	1:D:901:LEU:HB2	2.20	0.41
2:G:346:LEU:HD23	2:G:346:LEU:C	2.40	0.41
1:D:694:TRP:CE3	1:D:694:TRP:HA	2.55	0.41
2:F:282:TRP:H	2:F:326:ASN:ND2	2.15	0.41
1:D:755:VAL:HG13	1:D:756:ALA:N	2.35	0.41
2:C:229:ARG:HA	2:C:269:TYR:CD1	2.55	0.41
2:G:184:VAL:HG13	2:G:185:TRP:N	2.34	0.41
2:F:271:ARG:HG3	2:F:271:ARG:HH11	1.85	0.41
2:G:196:PHE:O	2:G:197:GLU:HG2	2.20	0.41
1:E:876:MET:SD	1:E:884:LEU:HD22	2.60	0.41
1:D:683:VAL:HG23	1:D:684:ARG:H	1.83	0.41
2:C:229:ARG:HB2	1:D:770:GLU:OE1	2.21	0.41
2:B:208:PHE:C	2:B:209:LEU:HD12	2.41	0.41
2:F:224:VAL:HB	2:F:266:LEU:HD11	2.01	0.41
2:C:179:PHE:HE2	2:C:280:PHE:H	1.60	0.41
2:C:343:LEU:HA	2:C:343:LEU:HD12	1.94	0.41
2:B:224:VAL:O	2:B:225:THR:C	2.59	0.41
2:B:248:LEU:HD11	2:B:288:LEU:HB2	2.02	0.41
1:A:633:LEU:CD2	1:A:635:LEU:HD21	2.50	0.41
2:C:363:LEU:N	2:C:363:LEU:HD22	2.33	0.41
2:G:285:VAL:HG13	2:G:323:VAL:HG22	2.02	0.41
1:A:815:LEU:HD11	1:A:821:ALA:HB2	2.02	0.41
1:A:683:VAL:HG23	1:A:684:ARG:HD3	2.02	0.41
1:E:898:PHE:O	1:E:900:PRO:N	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:199:ILE:CG2	2:G:203:LEU:HB2	2.47	0.41
1:A:796:GLY:O	1:A:799:ARG:HG2	2.20	0.41
2:F:224:VAL:CG1	2:F:266:LEU:HD11	2.50	0.41
2:B:327:ILE:HA	2:B:328:PRO:HD3	1.93	0.41
1:E:874:SER:C	1:E:876:MET:N	2.74	0.41
1:A:811:LEU:HD23	1:A:821:ALA:HB1	2.01	0.41
2:F:311:ASP:HB2	2:F:363:LEU:HD11	2.01	0.41
1:A:702:GLY:O	1:A:751:PHE:HA	2.21	0.41
1:A:872:ASP:CG	1:D:881:ARG:HH22	2.24	0.41
2:G:262:GLN:NE2	2:G:265:ARG:HE	2.12	0.41
1:E:896:HIS:O	1:E:898:PHE:N	2.53	0.41
1:A:804:THR:CG2	1:A:805:VAL:N	2.83	0.41
1:H:801:LEU:N	1:H:801:LEU:CD1	2.83	0.41
1:A:691:ILE:HD12	1:A:691:ILE:HA	1.81	0.41
1:A:799:ARG:NH2	1:A:900:PRO:CD	2.84	0.41
1:E:645:VAL:HG11	1:E:895:ARG:HA	2.03	0.41
1:E:784:ALA:HB2	1:E:863:VAL:HG13	2.02	0.41
1:D:627:ARG:HG3	1:D:627:ARG:H	1.71	0.41
2:C:294:ASP:OD2	1:D:725:ARG:NH2	2.54	0.41
2:B:203:LEU:HD11	2:B:208:PHE:CD1	2.53	0.41
1:A:799:ARG:HA	1:A:800:PRO:HD3	1.83	0.41
1:H:672:ARG:HA	1:H:672:ARG:HD3	1.84	0.41
1:E:811:LEU:HD12	1:E:821:ALA:HB1	2.02	0.41
1:D:669:GLY:HA3	1:D:679:TYR:OH	2.21	0.41
1:E:876:MET:HG3	1:E:880:ALA:CB	2.51	0.41
2:C:241:VAL:O	2:C:282:TRP:HA	2.20	0.41
2:G:203:LEU:HD23	2:G:209:LEU:HD11	2.02	0.41
1:A:898:PHE:O	1:A:899:ALA:C	2.58	0.41
1:H:804:THR:HG22	1:H:805:VAL:N	2.36	0.41
1:D:891:VAL:N	1:D:892:PRO:CD	2.84	0.41
1:E:788:ARG:NH1	1:E:788:ARG:CG	2.84	0.41
1:A:699:LEU:HA	1:A:748:PHE:O	2.20	0.41
1:A:682:ASP:C	1:A:682:ASP:OD2	2.58	0.41
2:B:368:PHE:CD2	2:B:368:PHE:N	2.89	0.41
2:B:346:LEU:C	2:B:346:LEU:HD23	2.41	0.41
1:D:899:ALA:HB3	1:D:900:PRO:CD	2.51	0.41
1:D:810:GLU:OE2	1:D:810:GLU:N	2.53	0.41
1:A:752:GLU:O	1:A:753:ASN:HB2	2.21	0.41
2:F:339:SER:O	2:F:343:LEU:HB2	2.21	0.41
1:H:727:PHE:CZ	1:H:765:ILE:HG23	2.55	0.41
1:H:643:LEU:HG	1:H:647:LYS:HE3	2.02	0.41
2:C:297:VAL:O	2:C:301:PHE:HB2	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:863:VAL:HG12	1:H:864:PHE:N	2.36	0.41
1:E:856:TRP:CE2	1:H:874:SER:HA	2.55	0.41
1:A:873:VAL:O	1:A:874:SER:OG	2.26	0.41
1:D:860:MET:O	1:D:863:VAL:HB	2.21	0.41
2:B:241:VAL:O	2:B:282:TRP:HA	2.21	0.41
1:D:630:ILE:HA	1:D:905:PHE:CD2	2.56	0.41
1:E:905:PHE:O	1:E:906:ALA:C	2.60	0.41
1:H:783:ALA:O	1:H:826:VAL:HG22	2.21	0.41
1:D:898:PHE:O	1:D:899:ALA:C	2.59	0.41
1:A:801:LEU:HD12	1:A:801:LEU:H	1.85	0.41
1:H:752:GLU:HG2	1:H:753:ASN:N	2.36	0.41
1:D:632:VAL:HG13	1:D:699:LEU:HB3	2.03	0.40
2:C:189:PRO:HB3	2:C:378:PHE:HZ	1.86	0.40
1:A:817:HIS:CD2	1:D:674:GLN:HA	2.56	0.40
2:F:325:SER:OG	2:F:327:ILE:HG13	2.21	0.40
1:H:853:ASP:CG	1:H:854:ILE:N	2.74	0.40
1:A:717:LYS:HB3	1:A:721:GLU:HB2	2.02	0.40
1:D:808:LYS:HG2	1:D:808:LYS:H	1.71	0.40
2:F:202:GLU:OE1	2:F:202:GLU:N	2.45	0.40
1:H:732:ARG:CZ	1:H:733:LEU:HD21	2.51	0.40
1:E:684:ARG:HB2	2:F:300:ARG:CZ	2.52	0.40
1:E:729:GLU:OE2	2:F:300:ARG:NH1	2.55	0.40
1:D:815:LEU:HD11	1:D:846:VAL:HG12	2.03	0.40
1:D:652:GLN:CD	1:D:906:ALA:HB1	2.41	0.40
2:B:203:LEU:CG	2:B:209:LEU:HD11	2.50	0.40
1:H:816:GLU:CD	1:H:862:ARG:NH2	2.75	0.40
1:H:632:VAL:HG22	1:H:699:LEU:HB3	2.03	0.40
1:E:794:LEU:HA	1:E:795:PRO:HD2	1.95	0.40
1:H:801:LEU:CD1	1:H:801:LEU:H	2.35	0.40
2:B:179:PHE:CE2	2:B:279:PRO:HA	2.56	0.40
1:H:745:ARG:HA	1:H:746:PRO:HD3	1.93	0.40
1:E:804:THR:HB	1:E:806:ASN:O	2.21	0.40
1:H:770:GLU:O	1:H:771:SER:HB3	2.22	0.40
1:D:632:VAL:HG12	1:D:633:LEU:N	2.37	0.40
2:B:246:PRO:HA	2:B:247:PRO:HD3	1.91	0.40
1:H:873:VAL:C	1:H:874:SER:O	2.60	0.40
2:F:248:LEU:N	2:F:287:ASN:HD22	2.16	0.40
1:D:706:CYS:CB	1:D:754:VAL:HG13	2.52	0.40
1:H:657:ILE:HG22	1:H:680:VAL:HG23	2.03	0.40
1:H:748:PHE:HB3	1:H:794:LEU:HD23	2.02	0.40
1:H:637:ASP:CB	1:H:658:ALA:HB1	2.51	0.40
2:F:257:SER:O	2:F:258:TRP:C	2.60	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:203:LEU:HG	2:G:209:LEU:CD1	2.51	0.40
1:H:748:PHE:HZ	1:H:904:TYR:CD2	2.38	0.40
2:C:258:TRP:CE2	2:C:262:GLN:HG3	2.57	0.40
1:D:799:ARG:CZ	1:D:896:HIS:CE1	3.05	0.40
2:C:265:ARG:HG2	2:C:265:ARG:HH11	1.87	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	268/295 (91%)	228 (85%)	30 (11%)	10 (4%)	5	20
1	D	263/295 (89%)	221 (84%)	35 (13%)	7 (3%)	8	30
1	E	266/295 (90%)	223 (84%)	34 (13%)	9 (3%)	6	23
1	H	263/295 (89%)	226 (86%)	29 (11%)	8 (3%)	7	27
2	B	178/230 (77%)	135 (76%)	34 (19%)	9 (5%)	3	10
2	C	178/230 (77%)	138 (78%)	32 (18%)	8 (4%)	4	14
2	F	178/230 (77%)	136 (76%)	36 (20%)	6 (3%)	6	23
2	G	178/230 (77%)	138 (78%)	33 (18%)	7 (4%)	5	18
All	All	1772/2100 (84%)	1445 (82%)	263 (15%)	64 (4%)	5	22

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	845	PRO
1	D	849	ASN
1	E	845	PRO
1	H	874	SER
1	H	888	SER
1	A	676	LYS
1	A	707	ASN

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Mol	Chain	Res	Type
1	A	884	LEU
1	E	897	LEU
2	G	328	PRO
1	A	624	ALA
2	B	277	PRO
2	B	291	ASN
2	B	328	PRO
2	C	277	PRO
2	C	328	PRO
1	D	845	PRO
2	F	277	PRO
2	F	328	PRO
2	G	277	PRO
1	H	707	ASN
1	H	726	LEU
1	A	684	ARG
1	A	708	ASP
1	A	726	LEU
1	A	783	ALA
1	A	844	PHE
2	B	225	THR
2	B	304	MET
2	B	362	LYS
2	C	236	GLY
2	C	304	MET
1	D	676	LYS
1	D	783	ALA
1	D	855	LEU
1	D	874	SER
1	E	808	LYS
1	E	899	ALA
2	F	304	MET
2	G	225	THR
2	G	236	GLY
1	H	676	LYS
1	H	873	VAL
2	B	256	PRO
1	E	637	ASP
1	E	676	LYS
1	E	694	TRP
1	E	783	ALA
2	F	236	GLY

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Mol	Chain	Res	Type
2	C	336	ALA
2	G	304	MET
1	E	680	VAL
2	B	236	GLY
2	C	278	ARG
2	G	256	PRO
2	B	254	ARG
2	F	256	PRO
1	H	680	VAL
1	H	691	ILE
2	C	272	PRO
2	C	276	SER
1	D	680	VAL
2	F	272	PRO
2	G	278	ARG

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	224/259 (86%)	196 (88%)	28 (12%)	7	19
1	D	222/259 (86%)	194 (87%)	28 (13%)	7	18
1	E	223/259 (86%)	188 (84%)	35 (16%)	4	11
1	H	222/259 (86%)	203 (91%)	19 (9%)	15	41
2	B	166/210 (79%)	153 (92%)	13 (8%)	18	46
2	C	166/210 (79%)	154 (93%)	12 (7%)	21	51
2	F	166/210 (79%)	155 (93%)	11 (7%)	24	57
2	G	166/210 (79%)	157 (95%)	9 (5%)	31	69
All	All	1555/1876 (83%)	1400 (90%)	155 (10%)	11	32

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	631	ARG
1	A	644	LEU

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Mol	Chain	Res	Type
1	A	648	ASP
1	A	660	GLU
1	A	671	VAL
1	A	674	GLN
1	A	683	VAL
1	A	684	ARG
1	A	688	GLN
1	A	691	ILE
1	A	701	ILE
1	A	706	CYS
1	A	760	SER
1	A	775	MET
1	A	798	ASN
1	A	807	ASP
1	A	809	LEU
1	A	816	GLU
1	A	843	HIS
1	A	845	PRO
1	A	848	MET
1	A	858	THR
1	A	860	MET
1	A	878	ARG
1	A	881	ARG
1	A	891	VAL
1	A	904	TYR
1	A	907	CYS
2	B	202	GLU
2	B	255	PRO
2	B	262	GLN
2	B	267	LEU
2	B	268	GLN
2	B	271	ARG
2	B	286	ASP
2	B	295	LEU
2	B	321	VAL
2	B	322	ARG
2	B	326	ASN
2	B	335	TRP
2	B	363	LEU
2	C	191	ARG
2	C	231	ASP
2	C	239	ASP

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Mol	Chain	Res	Type
2	C	257	SER
2	C	268	GLN
2	C	294	ASP
2	C	301	PHE
2	C	308	THR
2	C	321	VAL
2	C	326	ASN
2	C	328	PRO
2	C	335	TRP
1	D	631	ARG
1	D	644	LEU
1	D	648	ASP
1	D	660	GLU
1	D	665	SER
1	D	674	GLN
1	D	684	ARG
1	D	692	GLN
1	D	694	TRP
1	D	707	ASN
1	D	729	GLU
1	D	734	LEU
1	D	752	GLU
1	D	775	MET
1	D	776	ILE
1	D	799	ARG
1	D	801	LEU
1	D	807	ASP
1	D	809	LEU
1	D	816	GLU
1	D	823	PHE
1	D	826	VAL
1	D	845	PRO
1	D	851	LYS
1	D	853	ASP
1	D	855	LEU
1	D	881	ARG
1	D	884	LEU
1	E	644	LEU
1	E	648	ASP
1	E	654	ASP
1	E	660	GLU
1	E	661	VAL

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Mol	Chain	Res	Type
1	E	665	SER
1	E	674	GLN
1	E	684	ARG
1	E	688	GLN
1	E	691	ILE
1	E	694	TRP
1	E	729	GLU
1	E	734	LEU
1	E	750	LEU
1	E	753	ASN
1	E	760	SER
1	E	775	MET
1	E	776	ILE
1	E	786	ARG
1	E	799	ARG
1	E	800	PRO
1	E	806	ASN
1	E	807	ASP
1	E	809	LEU
1	E	816	GLU
1	E	823	PHE
1	E	845	PRO
1	E	848	MET
1	E	853	ASP
1	E	862	ARG
1	E	863	VAL
1	E	868	VAL
1	E	881	ARG
1	E	884	LEU
1	E	907	CYS
2	F	230	LYS
2	F	231	ASP
2	F	237	PRO
2	F	239	ASP
2	F	262	GLN
2	F	268	GLN
2	F	291	ASN
2	F	294	ASP
2	F	326	ASN
2	F	335	TRP
2	F	363	LEU
2	G	191	ARG

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Mol	Chain	Res	Type
2	G	196	PHE
2	G	262	GLN
2	G	268	GLN
2	G	286	ASP
2	G	301	PHE
2	G	326	ASN
2	G	335	TRP
2	G	337	LEU
1	H	631	ARG
1	H	644	LEU
1	H	648	ASP
1	H	665	SER
1	H	674	GLN
1	H	683	VAL
1	H	684	ARG
1	H	694	TRP
1	H	707	ASN
1	H	729	GLU
1	H	752	GLU
1	H	755	VAL
1	H	809	LEU
1	H	816	GLU
1	H	823	PHE
1	H	855	LEU
1	H	858	THR
1	H	878	ARG
1	H	881	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	688	GLN
1	A	753	ASN
2	B	262	GLN
2	B	264	HIS
2	B	268	GLN
2	B	287	ASN
2	B	313	HIS
2	B	326	ASN
2	C	262	GLN
2	C	264	HIS
2	C	268	GLN

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Mol	Chain	Res	Type
2	C	287	ASN
2	C	326	ASN
1	D	707	ASN
1	D	753	ASN
1	D	896	HIS
1	E	688	GLN
1	E	753	ASN
1	E	817	HIS
1	E	896	HIS
2	F	262	GLN
2	F	264	HIS
2	F	287	ASN
2	F	313	HIS
2	F	326	ASN
2	G	262	GLN
2	G	268	GLN
2	G	287	ASN
2	G	326	ASN
1	H	688	GLN
1	H	753	ASN
1	H	817	HIS
1	H	882	GLN
1	H	896	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands 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$
3	SAH	A	1	-	28,28,28	1.93	8 (28%)	40,40,40	2.60	11 (27%)
3	SAH	D	4	-	28,28,28	1.88	5 (17%)	40,40,40	2.52	11 (27%)
3	SAH	E	5	-	28,28,28	1.93	9 (32%)	40,40,40	2.23	11 (27%)
3	SAH	H	8	-	28,28,28	1.96	7 (25%)	40,40,40	2.78	12 (30%)

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
3	SAH	A	1	-	-	0/15/31/31	0/1/3/3
3	SAH	D	4	-	-	0/15/31/31	0/1/3/3
3	SAH	E	5	-	-	0/15/31/31	0/1/3/3
3	SAH	H	8	-	-	1/15/31/31	0/1/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	SAH	C1'-N9	-5.11	1.32	1.48
3	E	5	SAH	C1'-N9	-5.07	1.32	1.48
3	A	1	SAH	C1'-N9	-4.54	1.34	1.48
3	H	8	SAH	C1'-N9	-4.50	1.34	1.48
3	A	1	SAH	O4'-C1'	4.07	1.47	1.41
3	H	8	SAH	O4'-C1'	4.04	1.47	1.41
3	H	8	SAH	C4-N9	3.94	1.43	1.37
3	H	8	SAH	C5'-SD	-3.87	1.73	1.81
3	D	4	SAH	C5'-SD	-3.85	1.73	1.81
3	E	5	SAH	C2-N3	3.80	1.39	1.32
3	E	5	SAH	O4'-C1'	3.77	1.47	1.41
3	D	4	SAH	C4-N9	3.71	1.43	1.37
3	A	1	SAH	C4-N9	3.63	1.43	1.37
3	D	4	SAH	C2-N3	3.26	1.38	1.32
3	A	1	SAH	C2-N3	3.25	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	8	SAH	C2-N3	3.01	1.38	1.32
3	E	5	SAH	C5'-SD	-2.65	1.75	1.81
3	E	5	SAH	C5'-C4'	2.57	1.59	1.52
3	A	1	SAH	C5'-C4'	2.52	1.59	1.52
3	E	5	SAH	C4-N9	2.49	1.41	1.37
3	E	5	SAH	C8-N7	-2.47	1.29	1.34
3	A	1	SAH	C2'-C3'	2.43	1.60	1.53
3	D	4	SAH	C5'-C4'	2.42	1.59	1.52
3	A	1	SAH	C8-N7	-2.27	1.30	1.34
3	E	5	SAH	C2-N1	2.26	1.38	1.33
3	A	1	SAH	C5'-SD	-2.22	1.76	1.81
3	E	5	SAH	CA-C	2.04	1.60	1.53
3	H	8	SAH	C8-N9	2.03	1.39	1.36
3	H	8	SAH	C8-N7	-2.01	1.30	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	SAH	O4'-C1'-C2'	-9.22	92.63	106.77
3	H	8	SAH	O4'-C1'-N9	8.43	116.28	108.44
3	E	5	SAH	N3-C2-N1	-8.37	121.71	128.71
3	A	1	SAH	N3-C2-N1	-7.65	122.31	128.71
3	H	8	SAH	N3-C2-N1	-7.55	122.39	128.71
3	D	4	SAH	N3-C2-N1	-7.04	122.82	128.71
3	H	8	SAH	CB-CG-SD	-6.52	100.99	113.57
3	D	4	SAH	O4'-C4'-C5'	-6.31	92.07	108.91
3	D	4	SAH	O4'-C1'-C2'	-6.08	97.45	106.77
3	D	4	SAH	C8-N9-C1'	4.85	135.94	126.38
3	A	1	SAH	C8-N9-C1'	4.83	135.89	126.38
3	H	8	SAH	C8-N9-C1'	4.76	135.77	126.38
3	E	5	SAH	C8-N9-C1'	4.71	135.66	126.38
3	H	8	SAH	C4'-O4'-C1'	-4.67	104.68	109.75
3	D	4	SAH	C4'-O4'-C1'	-4.65	104.69	109.75
3	A	1	SAH	CB-CG-SD	-4.35	105.18	113.57
3	A	1	SAH	C8-N9-C4	-4.32	103.60	106.90
3	H	8	SAH	C8-N9-C4	-4.22	103.68	106.90
3	D	4	SAH	CB-CG-SD	-3.97	105.91	113.57
3	H	8	SAH	O4'-C1'-C2'	-3.96	100.69	106.77
3	E	5	SAH	C1'-N9-C4	-3.95	119.81	126.64
3	E	5	SAH	CB-CG-SD	-3.91	106.03	113.57
3	D	4	SAH	C1'-N9-C4	-3.82	120.03	126.64
3	D	4	SAH	C8-N9-C4	-3.76	104.03	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	8	SAH	CG-CB-CA	3.59	119.24	113.22
3	A	1	SAH	C1'-N9-C4	-3.56	120.48	126.64
3	H	8	SAH	C1'-N9-C4	-3.53	120.54	126.64
3	E	5	SAH	CG-CB-CA	3.40	118.92	113.22
3	A	1	SAH	CB-CA-N	3.31	118.24	110.14
3	E	5	SAH	C8-N9-C4	-3.12	104.52	106.90
3	E	5	SAH	O4'-C1'-C2'	-2.91	102.31	106.77
3	E	5	SAH	C2-N1-C6	2.90	124.01	118.77
3	H	8	SAH	C2-N1-C6	2.80	123.83	118.77
3	D	4	SAH	CG-CB-CA	2.60	117.58	113.22
3	E	5	SAH	C3'-C2'-C1'	2.51	104.84	100.91
3	A	1	SAH	C2-N1-C6	2.48	123.24	118.77
3	D	4	SAH	C2-N1-C6	2.45	123.20	118.77
3	H	8	SAH	O4'-C4'-C3'	2.43	110.10	105.17
3	A	1	SAH	C3'-C2'-C1'	2.43	104.70	100.91
3	E	5	SAH	C4'-C5'-SD	-2.42	106.08	113.53
3	A	1	SAH	C2'-C1'-N9	2.41	119.45	113.27
3	D	4	SAH	CB-CA-N	2.25	115.65	110.14
3	A	1	SAH	C5-C6-N6	2.10	125.48	120.72
3	E	5	SAH	O4'-C4'-C5'	-2.04	103.47	108.91
3	H	8	SAH	C4'-C5'-SD	-2.03	107.27	113.53

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	8	SAH	C2'-C1'-N9-C8

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	272/295 (92%)	0.16	5 (1%) 65 74	30, 64, 106, 146	0
1	D	267/295 (90%)	0.05	4 (1%) 70 79	37, 75, 122, 157	0
1	E	270/295 (91%)	0.17	5 (1%) 64 72	27, 67, 111, 132	0
1	H	267/295 (90%)	0.52	35 (13%) 4 6	51, 101, 138, 170	0
2	B	186/230 (80%)	0.90	33 (17%) 2 3	55, 121, 187, 207	0
2	C	186/230 (80%)	1.05	40 (21%) 1 2	61, 118, 189, 206	0
2	F	186/230 (80%)	1.07	37 (19%) 2 2	66, 121, 189, 210	0
2	G	186/230 (80%)	2.53	84 (45%) 1 0	109, 163, 201, 210	0
All	All	1820/2100 (86%)	0.70	243 (13%) 4 5	27, 93, 181, 210	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	321	VAL	19.9
2	G	309	ILE	13.6
2	G	334	HIS	12.8
2	F	331	ARG	12.5
2	G	331	ARG	12.3
2	F	315	GLY	12.0
2	F	334	HIS	10.8
2	G	308	THR	10.4
2	G	222	VAL	10.1
2	C	316	SER	9.4
2	C	361	THR	9.1
2	F	336	ALA	9.0
2	B	352	SER	8.6
2	F	314	GLY	8.2
2	G	353	SER	8.0
2	F	310	PRO	7.7

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Mol	Chain	Res	Type	RSRZ
2	C	315	GLY	7.4
2	G	344	SER	7.4
2	F	316	SER	7.1
2	G	310	PRO	6.9
2	C	314	GLY	6.9
2	F	251	THR	6.8
2	G	252	CYS	6.7
2	G	350	LYS	6.7
2	G	216	GLY	6.5
2	G	221	VAL	6.5
2	G	280	PHE	6.4
2	B	203	LEU	6.4
2	G	196	PHE	6.3
2	G	279	PRO	6.2
2	C	313	HIS	6.1
2	G	364	VAL	6.1
2	G	328	PRO	6.0
2	G	253	ASP	6.0
2	B	336	ALA	5.8
2	G	185	TRP	5.7
2	C	349	ASN	5.7
2	G	180	GLU	5.7
2	B	334	HIS	5.6
2	G	316	SER	5.5
2	G	335	TRP	5.4
2	G	182	VAL	5.4
2	G	217	GLN	5.2
2	G	348	GLN	5.2
2	G	241	VAL	5.1
2	G	311	ASP	5.1
2	F	276	SER	5.1
2	G	186	ARG	5.0
2	G	368	PHE	4.9
1	H	790	PHE	4.9
2	C	348	GLN	4.9
2	G	192	VAL	4.8
2	F	363	LEU	4.8
2	G	315	GLY	4.8
2	C	352	SER	4.8
2	G	302	LEU	4.7
2	B	364	VAL	4.7
2	G	288	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
2	C	192	VAL	4.7
2	C	336	ALA	4.7
2	G	259	TYR	4.7
2	G	307	VAL	4.7
2	G	362	LYS	4.6
2	F	353	SER	4.6
2	G	282	TRP	4.6
2	G	199	ILE	4.6
2	C	341	GLU	4.5
2	F	330	ILE	4.5
2	B	353	SER	4.5
2	C	310	PRO	4.5
2	C	179	PHE	4.4
1	H	686	VAL	4.3
2	B	242	TYR	4.3
2	G	367	CYS	4.3
2	G	327	ILE	4.3
2	G	324	TRP	4.3
2	G	284	PHE	4.2
2	B	192	VAL	4.2
2	C	274	PRO	4.2
2	G	235	TRP	4.1
2	F	279	PRO	4.1
2	G	343	LEU	4.1
2	G	349	ASN	4.1
2	C	208	PHE	4.1
2	C	248	LEU	4.1
1	H	805	VAL	4.0
2	B	252	CYS	4.0
2	F	252	CYS	4.0
2	G	203	LEU	3.9
1	H	748	PHE	3.9
2	F	364	VAL	3.9
2	F	313	HIS	3.9
1	E	805	VAL	3.9
2	G	312	VAL	3.9
2	C	368	PHE	3.8
1	H	630	ILE	3.8
2	C	240	LEU	3.8
2	C	288	LEU	3.8
2	G	289	VAL	3.8
2	G	377	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
2	G	314	GLY	3.8
2	G	179	PHE	3.7
2	G	251	THR	3.7
2	B	285	VAL	3.7
2	G	195	LEU	3.7
2	G	206	LEU	3.7
2	G	178	MET	3.7
2	F	182	VAL	3.6
2	G	181	THR	3.6
2	F	352	SER	3.6
2	F	274	PRO	3.6
2	C	252	CYS	3.6
1	H	646	LEU	3.6
2	F	335	TRP	3.6
2	F	343	LEU	3.5
2	C	251	THR	3.5
1	H	731	TYR	3.5
2	B	310	PRO	3.5
1	H	844	PHE	3.5
2	G	183	PRO	3.4
2	G	270	ALA	3.4
2	G	232	VAL	3.4
1	A	806	ASN	3.3
2	C	376	LYS	3.3
1	E	844	PHE	3.3
2	G	285	VAL	3.3
2	F	203	LEU	3.2
2	C	365	LYS	3.2
2	C	367	CYS	3.2
1	H	683	VAL	3.2
2	C	345	LEU	3.2
2	C	369	LEU	3.2
2	G	223	ASP	3.2
2	F	347	ALA	3.2
2	B	371	LEU	3.2
2	G	283	MET	3.1
1	D	740	LYS	3.1
2	G	378	PHE	3.1
2	B	185	TRP	3.1
2	F	277	PRO	3.0
2	G	273	LYS	3.0
2	F	333	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	235	TRP	3.0
2	G	374	TYR	2.9
1	E	878	ARG	2.9
1	H	750	LEU	2.9
2	F	209	LEU	2.9
2	C	206	LEU	2.9
2	G	271	ARG	2.9
2	G	229	ARG	2.9
2	G	190	VAL	2.8
1	H	631	ARG	2.8
1	A	805	VAL	2.8
1	H	794	LEU	2.8
2	C	370	PRO	2.8
1	H	633	LEU	2.8
2	G	346	LEU	2.8
2	B	179	PHE	2.8
2	B	338	VAL	2.8
2	G	340	GLU	2.8
2	B	316	SER	2.8
1	H	802	ALA	2.8
2	B	256	PRO	2.7
2	F	332	SER	2.7
2	G	323	VAL	2.7
2	B	309	ILE	2.7
2	G	363	LEU	2.7
1	H	649	LEU	2.7
1	D	801	LEU	2.7
2	B	332	SER	2.7
2	G	304	MET	2.7
1	H	895	ARG	2.6
2	F	181	THR	2.6
2	B	331	ARG	2.6
2	G	336	ALA	2.6
1	H	734	LEU	2.6
2	B	368	PHE	2.6
1	H	745	ARG	2.6
1	H	801	LEU	2.6
2	G	337	LEU	2.6
2	B	277	PRO	2.6
1	H	776	ILE	2.6
1	H	746	PRO	2.5
2	F	338	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	251	THR	2.5
2	F	309	ILE	2.5
2	G	272	PRO	2.5
2	B	335	TRP	2.5
2	C	334	HIS	2.5
2	B	347	ALA	2.5
2	B	281	PHE	2.5
2	C	378	PHE	2.5
2	F	311	ASP	2.5
2	F	216	GLY	2.4
2	C	328	PRO	2.4
2	G	366	ASN	2.4
1	H	655	ARG	2.4
1	H	741	GLU	2.4
2	C	209	LEU	2.3
2	F	195	LEU	2.3
1	E	823	PHE	2.3
1	H	651	ILE	2.3
2	C	351	GLN	2.3
2	B	288	LEU	2.3
2	B	379	SER	2.3
1	E	857	CYS	2.3
1	H	636	PHE	2.3
1	H	680	VAL	2.2
2	B	365	LYS	2.2
2	C	203	LEU	2.2
1	H	735	HIS	2.2
2	F	288	LEU	2.2
2	B	363	LEU	2.2
2	C	333	ARG	2.2
2	F	193	LEU	2.2
1	H	874	SER	2.2
2	G	365	LYS	2.2
2	C	217	GLN	2.2
2	G	184	VAL	2.2
1	H	789	TYR	2.2
1	H	855	LEU	2.1
1	D	852	GLU	2.1
2	G	338	VAL	2.1
2	B	199	ILE	2.1
2	C	347	ALA	2.1
1	D	741	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	904	TYR	2.1
2	B	330	ILE	2.1
1	H	757	MET	2.1
2	F	275	GLY	2.1
1	A	811	LEU	2.0
2	C	363	LEU	2.0
2	C	371	LEU	2.0
1	H	795	PRO	2.0
2	G	255	PRO	2.0
1	H	747	PHE	2.0
2	G	301	PHE	2.0
1	A	678	MET	2.0
1	A	908	VAL	2.0
2	B	283	MET	2.0
2	G	277	PRO	2.0
1	H	902	LYS	2.0
2	F	374	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SAH	A	1	26/26	0.22	0.02	38,67,84,95	0
3	SAH	D	4	26/26	0.19	-0.28	40,59,71,73	0
3	SAH	H	8	26/26	0.17	-0.80	49,104,112,114	0
3	SAH	E	5	26/26	0.16	-0.82	31,56,66,69	0

6.5 Other polymers ⓘ

There are no such residues in this entry.