



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 05:07 pm BST

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

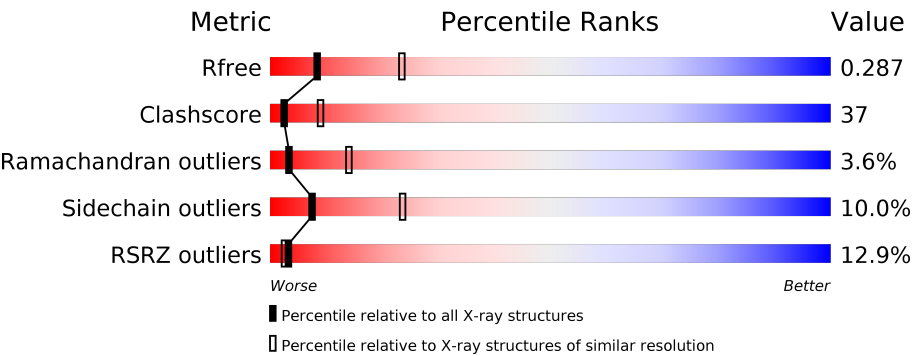
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	295	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>38%45%8%8%</div></div>
1	D	295	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>38%44%8%9%</div></div>
1	E	295	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>38%44%8%8%</div></div>
1	H	295	<div><div>8%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>35%49%7%9%</div></div>
2	B	230	<div><div>16%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>40%33%8%19%</div></div>
2	C	230	<div><div>16%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>39%38%19%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	230	<div><div></div><div>16%</div><div>39%</div><div>37%</div><div>5%</div><div>19%</div></div>
2	G	230	<div><div></div><div>38%</div><div>40%</div><div>37%</div><div>•</div><div>19%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14657 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 (cytosine-5)-methyltransferase 3A.

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)-methyltransferase 3-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:

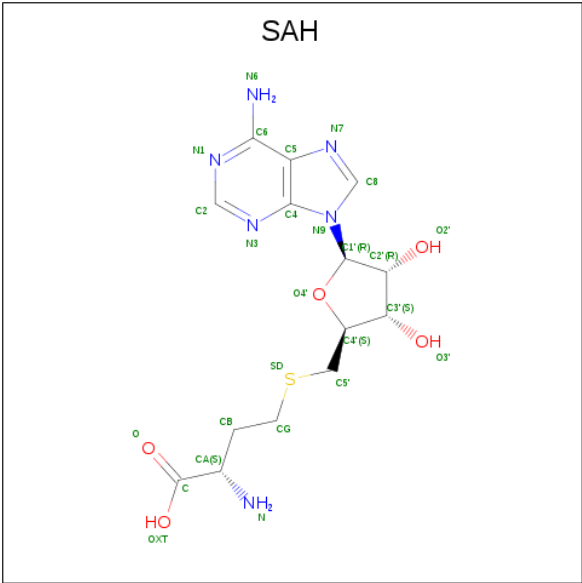
Chain	Residue	Modelled	Actual	Comment	Reference
B	157	GLY	-	EXPRESSION TAG	UNP Q9UJW3
B	158	SER	-	EXPRESSION TAG	UNP Q9UJW3
B	159	MET	-	EXPRESSION TAG	UNP Q9UJW3
C	157	GLY	-	EXPRESSION TAG	UNP Q9UJW3
C	158	SER	-	EXPRESSION TAG	UNP Q9UJW3
C	159	MET	-	EXPRESSION TAG	UNP Q9UJW3
F	157	GLY	-	EXPRESSION TAG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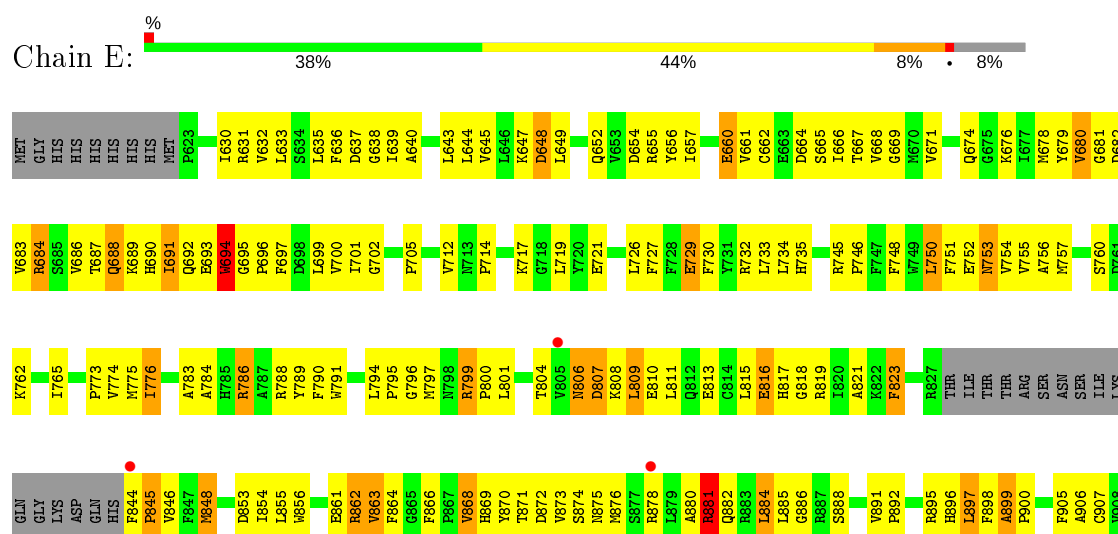
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Chain	Residue	Modelled	Actual	Comment	Reference
G	159	MET	-	EXPRESSION TAG	UNP Q9UJW3

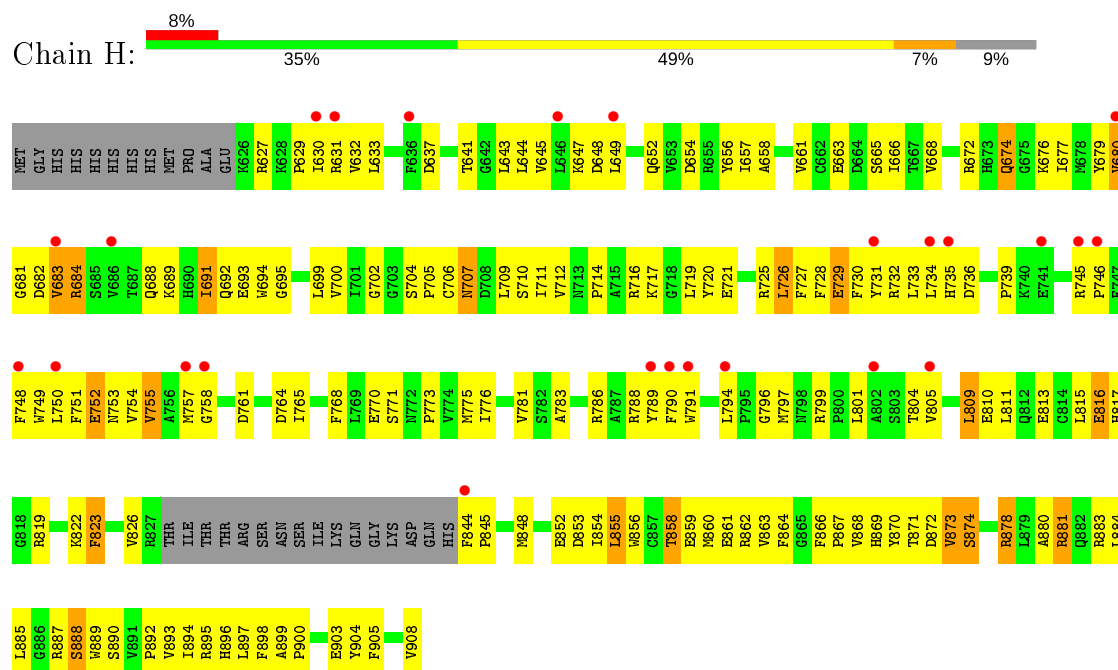
- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



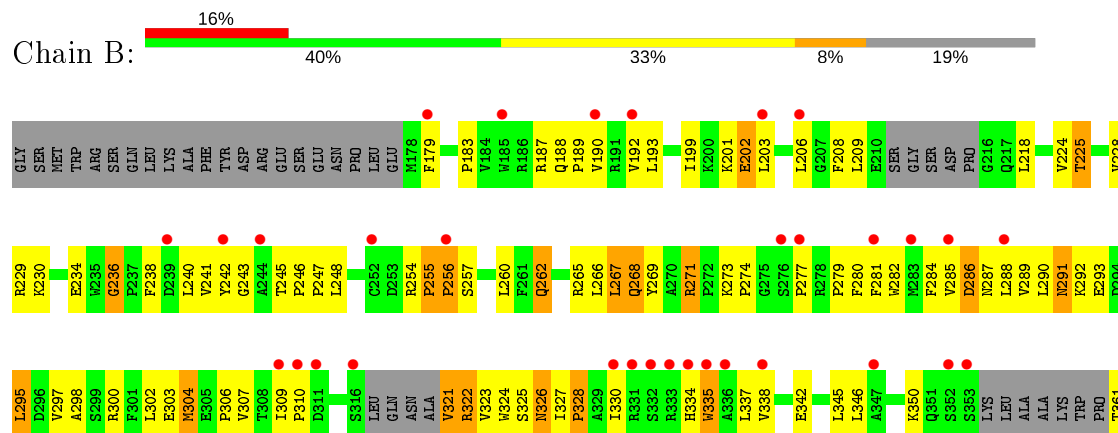
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	H	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

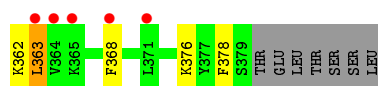


- Molecule 1: DNA (cytosine-5)-methyltransferase 3A

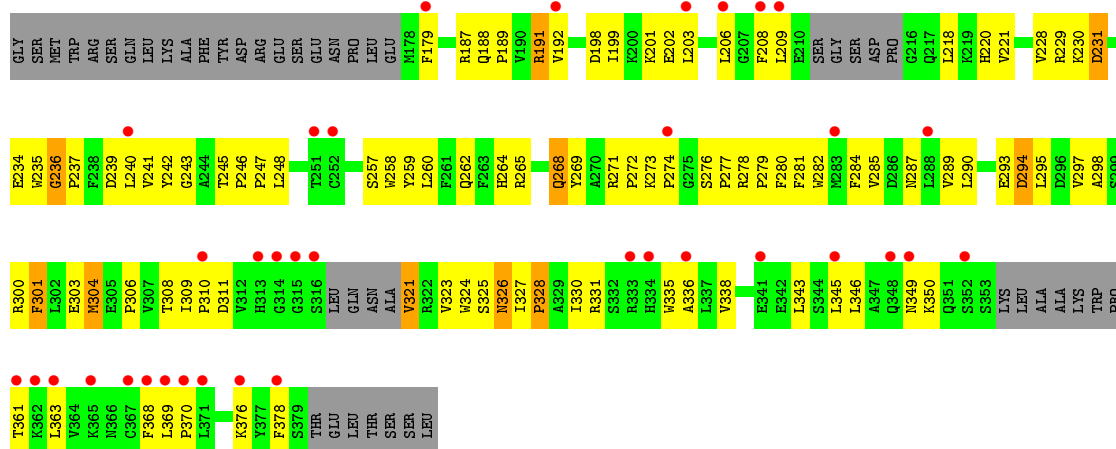


- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

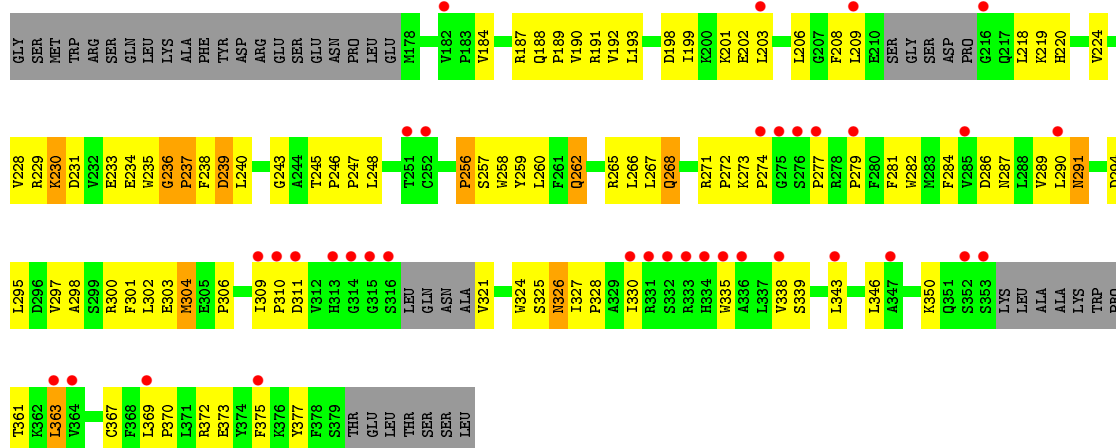




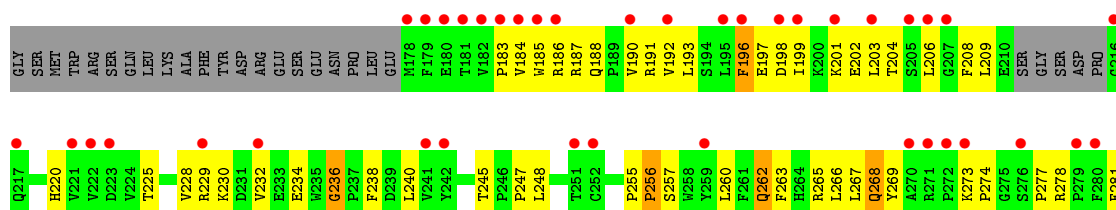
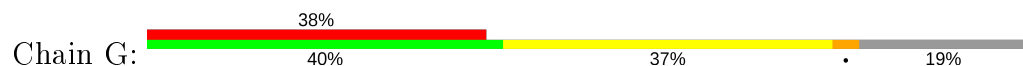
• Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

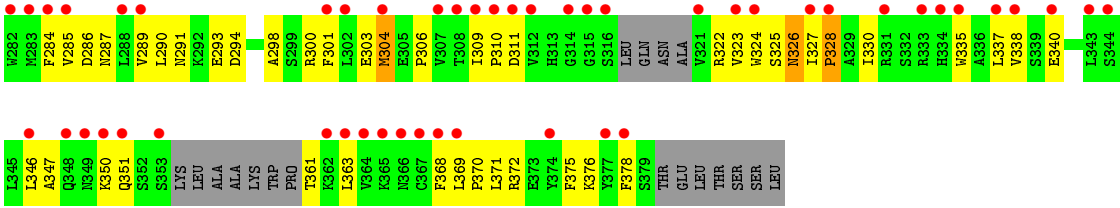


• Molecule 2: DNA (cytosine-5)-methyltransferase 3-like



• Molecule 2: DNA (cytosine-5)-methyltransferase 3-like





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	401.88 Å 401.88 Å 49.69 Å 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 2.90 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.281 0.271 , 0.287	Depositor DCC
R_{free} test set	3313 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	77.8	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 79.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for h,-h-k,-l	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.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 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	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

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 37.

All (1076) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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
1:A:858:THR:HG22	1:A:868:VAL:HG12	1.51	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:655:ARG:NH1	1:E:695:GLY:HA3	1.95	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:643:LEU:HG	1:A:647:LYS:HE3	1.61	0.81
1:A:739:PRO:HG3	1:A:745:ARG:NH2	1.94	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
1:A:809:LEU:HD12	1:A:809:LEU:H	1.47	0.80
2:C:285:VAL:HG22	2:C:323:VAL:HG22	1.63	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	Interatomic distance (Å)	Clash overlap (Å)
1:D:648:ASP:HB3	1:D:895:ARG:NH1	1.97	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:H:682:ASP:OD2	1:H:684:ARG:HD3	1.83	0.79
2:C:247:PRO:HA	2:C:287:ASN:HD22	1.46	0.78
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
1:A:858:THR:HG22	1:A:868:VAL:CG1	2.12	0.78
2:C:188:GLN:HB3	2:C:189:PRO:HD2	1.65	0.78
1:H:732:ARG:HE	1:H:733:LEU:CD2	1.96	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:D:755:VAL:HA	1:D:789:TYR:CD2	2.19	0.78
1:H:858:THR:HG22	1:H:868:VAL:CG1	2.13	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:E:861:GLU:OE1	1:E:869:HIS:N	2.18	0.77
1:H:873:VAL:HG23	1:H:874:SER:N	2.00	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:D:664:ASP:O	1:D:668:VAL:HG23	1.85	0.76
1:E:776:ILE:CD1	1:E:801:LEU:HD21	2.15	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
1:A:723:THR:HB	1:A:726:LEU:HD12	1.69	0.74
2:F:193:LEU:HB2	2:F:238:PHE:CE2	2.23	0.74
2:C:273:LYS:HB3	2:C:274:PRO:HD2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:193:LEU:HB2	2:F:238:PHE:CD2	2.23	0.73
1:A:794:LEU:O	1:A:797:MET:HG3	1.88	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:H:691:ILE:HG22	1:H:692:GLN:N	2.01	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
2:C:228:VAL:HG12	2:C:229:ARG:N	2.02	0.72
1:E:788:ARG:HH11	1:E:788:ARG:HG2	1.54	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
1:A:823:PHE:CZ	1:A:842:GLN:HA	2.26	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:680:VAL:HG12	1:A:681:GLY:N	2.04	0.71
1:H:732:ARG:HE	1:H:733:LEU:HD22	1.54	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:F:192:VAL:HG21	2:F:203:LEU:HD21	1.72	0.70
2:G:247:PRO:HA	2:G:287:ASN:ND2	2.06	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:E:891:VAL:HB	1:E:892:PRO:HD3	1.74	0.70
1:H:844:PHE:HB3	1:H:852:GLU:HG2	1.72	0.70
2:C:260:LEU:CD2	2:C:298:ALA:HA	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:292:LYS:HA	2:B:295:LEU:HD22	1.73	0.69
1:H:823:PHE:CD1	1:H:823:PHE:N	2.57	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:240:LEU:HA	2:B:281:PHE:O	1.93	0.69
2:B:260:LEU:HD21	2:B:298:ALA:CA	2.21	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
2:B:267:LEU:HD13	2:B:268:GLN:HE22	1.57	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: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: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:H:861:GLU:OE1	1:H:869:HIS:N	2.27	0.67
1:E:854:ILE:CG2	1:E:855:LEU:H	2.00	0.67
1:A:853:ASP:OD2	1:A:854:ILE:N	2.27	0.67
1:E:705:PRO:HG2	1:E:726:LEU:HD12	1.77	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
1:E:630:ILE:HG22	1:E:652:GLN:O	1.95	0.66
2:F:187:ARG:HH12	2:F:373:GLU:HA	1.59	0.66
2:G:363:LEU:HD22	2:G:363:LEU:H	1.60	0.66
1:D:855:LEU:HD23	1:D:856:TRP:H	1.60	0.66
1:E:667:THR:O	1:E:671:VAL:HG23	1.96	0.66
1:H:730:PHE:CE2	1:H:734:LEU:HD12	2.30	0.66
1:E:750:LEU:HD11	1:E:897:LEU:HD13	1.78	0.66
2:F:228:VAL:HG12	2:F:229:ARG:H	1.60	0.66
1:H:729:GLU:O	1:H:733:LEU:HD23	1.95	0.66
1:A:786:ARG:HH21	1:A:788:ARG:NH2	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:717:LYS:HB3	1:E:721:GLU:HB2	1.78	0.66
2:B:256:PRO:HB3	2:B:290:LEU:HD23	1.76	0.66
2:B:262:GLN:HE22	2:B:265:ARG:HE	1.40	0.66
2:F:282:TRP:H	2:F:326:ASN:HD21	1.44	0.66
2:B:291:ASN:O	2:B:295:LEU:HD13	1.96	0.66
2:G:262:GLN:HE22	2:G:265:ARG:HE	1.44	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:B:285:VAL:HG13	2:B:323:VAL:HG22	1.77	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
1:H:719:LEU:HB2	1:H:761:ASP:OD2	1.96	0.65
1:A:631:ARG:HD2	1:A:698:ASP:OD1	1.96	0.65
2:C:268:GLN:HG2	1:D:735:HIS:CE1	2.32	0.65
1:A:869:HIS:CE1	1:D:872:ASP:HB3	2.32	0.64
2:C:247:PRO:HA	2:C:287:ASN:ND2	2.11	0.64
1:D:786:ARG:HG3	1:D:786:ARG:NH1	2.12	0.64
1:H:890:SER:OG	1:H:892:PRO:HD2	1.97	0.64
2:F:248:LEU:H	2:F:287:ASN:HD21	1.44	0.64
1:H:895:ARG:O	1:H:899:ALA:HB2	1.97	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
1:D:672:ARG:HD2	1:D:870:TYR:CD1	2.33	0.64
2:G:310:PRO:HG2	2:G:338:VAL:HG21	1.80	0.64
2:F:230:LYS:N	2:F:230:LYS:HD2	2.12	0.63
2:G:228:VAL:HG12	2:G:229:ARG:N	2.13	0.63
1:E:872:ASP:HB3	1:H:869:HIS:CE1	2.33	0.63
2:B:199:ILE:HD11	2:B:242:TYR:CE2	2.33	0.63
2:G:262:GLN:CA	2:G:262:GLN:HE21	2.10	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:A:684:ARG:HB2	2:B:300:ARG:CZ	2.29	0.63
1:D:794:LEU:O	1:D:797:MET:HG3	1.98	0.63
2:G:202:GLU:O	2:G:206:LEU:HD23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:867:PRO:O	1:H:870:TYR:HB2	1.99	0.62
2:C:311:ASP:HB2	2:C:363:LEU:HD11	1.82	0.62
2:F:230:LYS:H	2:F:230:LYS:HD2	1.64	0.62
1:A:682:ASP:OD2	1:A:684:ARG:HD3	1.99	0.62
2:B:293:GLU:OE2	2:B:293:GLU:N	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:810:GLU:H	1:H:810:GLU:CD	2.04	0.61
1:H:860:MET:O	1:H:863:VAL:HB	2.00	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
2:C:198:ASP:HB3	2:C:220:HIS:ND1	2.15	0.61
1:H:691:ILE:HG21	1:H:736:ASP:O	2.00	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
2:B:282:TRP:CZ3	2:B:302:LEU:HD22	2.35	0.61
1:H:796:GLY:O	1:H:799:ARG:HG3	1.99	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:801:LEU:N	1:H:801:LEU:HD12	2.16	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
2:B:268:GLN:HE21	2:B:268:GLN:CA	2.11	0.61
1:D:683:VAL:HG23	1:D:729:GLU:HG2	1.83	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
2:C:228:VAL:HG12	2:C:229:ARG:H	1.64	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
1:H:844:PHE:N	1:H:845:PRO:HD3	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:815:LEU:HA	1:H:859:GLU:CG	2.29	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
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
2:G:327:ILE:O	2:G:330:ILE:HB	2.01	0.60
1:H:641:THR:O	1:H:645:VAL:HG23	2.02	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:D:635:LEU:HD12	1:D:730:PHE:HD1	1.67	0.59
1:E:786:ARG:NH1	1:E:864:PHE:CE2	2.70	0.59
2:B:346:LEU:O	2:B:350:LYS:HG2	2.02	0.59
2:G:260:LEU:CD2	2:G:298:ALA:HA	2.33	0.59
1:H:668:VAL:HG22	1:H:873:VAL:HG21	1.83	0.59
1:H:883:ARG:HD3	1:H:887:ARG:NH2	2.18	0.59
2:B:285:VAL:HG22	2:B:323:VAL:HG22	1.85	0.59
1:D:855:LEU:HD23	1:D:856:TRP:N	2.18	0.59
1:E:635:LEU:HD12	1:E:730:PHE:CD1	2.38	0.59
1:H:799:ARG:HH22	1:H:899:ALA:HB3	1.68	0.59
1:E:874:SER:HA	1:H:856:TRP:CE2	2.38	0.59
2:F:198:ASP:HB3	2:F:220:HIS:ND1	2.18	0.59
1:H:732:ARG:HE	1:H:733:LEU:HD21	1.68	0.59
1:E:643:LEU:O	1:E:647:LYS:HG3	2.02	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: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
2:B:192:VAL:HG22	2:B:240:LEU:HB3	1.84	0.58
2:C:187:ARG:O	2:C:376:LYS:HB2	2.02	0.58
1:E:729:GLU:O	1:E:733:LEU:HD23	2.03	0.58
2:F:248:LEU:N	2:F:287:ASN:ND2	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:HIS:N	1:A:843:HIS:ND1	2.51	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:G:310:PRO:CG	2:G:338:VAL:HG21	2.33	0.58
2:G:300:ARG:NH1	1:H:732:ARG:NH1	2.49	0.58
2:B:179:PHE:HE2	2:B:280:PHE:H	1.52	0.58
2:C:202:GLU:HG2	2:C:361:THR:CG2	2.32	0.58
1:E:671:VAL:HG11	1:H:816:GLU:HG2	1.86	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:C:346:LEU:O	2:C:350:LYS:HG2	2.04	0.58
2:F:372:ARG:HH11	2:F:372:ARG:HG2	1.69	0.58
2:G:306:PRO:HB3	2:G:324:TRP:CE2	2.39	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
2:C:228:VAL:CG1	2:C:229:ARG:H	2.17	0.57
1:D:855:LEU:CD2	1:D:859:GLU:HB2	2.35	0.57
2:F:310:PRO:HG2	2:F:338:VAL:HG21	1.85	0.57
1:E:752:GLU:HB2	1:E:790:PHE:CE2	2.39	0.57
1:H:858:THR:HG22	1:H:868:VAL:HG12	1.87	0.57
1:E:688:GLN:NE2	1:E:692:GLN:NE2	2.52	0.57
1:D:673:HIS:C	1:D:674:GLN:HG2	2.24	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: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:A:656:TYR:HD2	1:A:677:ILE:HG12	1.69	0.57
1:A:776:ILE:HD11	1:A:801:LEU:HD21	1.86	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:D:702:GLY:O	1:D:751:PHE:HA	2.05	0.56
1:H:755:VAL:HA	1:H:789:TYR:CD2	2.39	0.56
2:C:271:ARG:HG3	2:C:271:ARG:HH11	1.69	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
1:H:868:VAL:O	1:H:869:HIS:HB2	2.06	0.56
2:C:246:PRO:HG2	2:C:259:TYR:OH	2.05	0.56
2:C:248:LEU:H	2:C:287:ASN:ND2	2.03	0.56
1:E:823:PHE:CD1	1:E:823:PHE:N	2.72	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:810:GLU:OE2	1:H:810:GLU:N	2.38	0.56
1:A:872:ASP:HB3	1:D:869:HIS:CE1	2.41	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
2:F:286:ASP:OD2	2:F:290:LEU:HG	2.05	0.56
1:A:786:ARG:NH1	1:A:864:PHE:HE2	2.03	0.56
2:C:230:LYS:N	2:C:230:LYS:HD2	2.20	0.56
1:D:635:LEU:HD12	1:D:730:PHE:CD1	2.40	0.56
1:E:801:LEU:HA	1:E:896:HIS:CE1	2.41	0.56
1:A:680:VAL:CG1	1:A:681:GLY:H	2.19	0.56
2:B:361:THR:N	2:B:363:LEU:CD2	2.69	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
2:C:201:LYS:HB3	2:C:202:GLU:OE1	2.05	0.56
1:H:691:ILE:CG2	1:H:692:GLN:N	2.69	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:652:GLN:HB2	1:E:906:ALA:HB3	1.86	0.56
1:E:632:VAL:HG13	1:E:699:LEU:HG	1.88	0.56
1:A:691:ILE:HG22	1:A:692:GLN:N	2.21	0.56
1:D:861:GLU:OE1	1:D:869:HIS:N	2.39	0.56
2:B:262:GLN:HA	2:B:262:GLN:HE21	1.70	0.55
1:D:732:ARG:NH2	1:D:733:LEU:HD21	2.21	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
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:H:684:ARG:HA	1:H:732:ARG:HH22	1.70	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
2:B:285:VAL:HG13	2:B:323:VAL:CG2	2.36	0.55
2:C:199:ILE:HD11	2:C:242:TYR:CE2	2.42	0.55
1:H:699:LEU:HA	1:H:748:PHE:O	2.07	0.55
1:H:799:ARG:NH2	1:H:900:PRO:HD3	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:748:PHE:HA	1:D:793:ASN:HD21	1.70	0.55
2:B:306:PRO:HB3	2:B:324:TRP:CE2	2.42	0.55
1:E:660:GLU:HB3	1:E:666:ILE:HG12	1.89	0.55
1:E:732:ARG:NH2	1:E:733:LEU:CD2	2.68	0.55
1:E:752:GLU:CG	1:E:753:ASN:N	2.69	0.55
2:G:230:LYS:H	2:G:230:LYS:HD2	1.72	0.55
1:A:704:SER:HG	1:A:751:PHE:HZ	1.54	0.55
1:A:748:PHE:HB3	1:A:794:LEU:HD23	1.88	0.55
2:G:372:ARG:HH11	2:G:372:ARG:HG2	1.71	0.55
1:H:710:SER:O	1:H:716:ARG:HD3	2.06	0.55
1:H:750:LEU:HD12	1:H:791:TRP:O	2.07	0.55
1:A:816:GLU:HG2	1:D:671:VAL:HG11	1.88	0.55
2:B:228:VAL:HG12	2:B:229:ARG:N	2.20	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: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:E:874:SER:C	1:E:876:MET:H	2.10	0.54
1:A:716:ARG:HG2	1:A:716:ARG:HH11	1.70	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
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
2:C:324:TRP:O	2:C:325:SER:HB2	2.07	0.54
1:E:683:VAL:HG23	1:E:684:ARG:H	1.72	0.54
2:F:324:TRP:O	2:F:325:SER:HB2	2.08	0.54
2:G:240:LEU:HA	2:G:281:PHE:O	2.07	0.54
2:B:199:ILE:HG21	2:B:368:PHE:HE1	1.71	0.54
2:C:303:GLU:O	2:C:304:MET:HB3	2.08	0.54
2:G:326:ASN:HD22	2:G:326:ASN:H	1.56	0.54
1:A:844:PHE:O	1:A:853:ASP:O	2.25	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:660:GLU:OE2	1:A:661:VAL:N	2.41	0.54
2:G:199:ILE:HG22	2:G:199:ILE:O	2.08	0.54
1:H:688:GLN:NE2	1:H:692:GLN:NE2	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:739:PRO:HG3	1:D:745:ARG:NH2	2.23	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: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:A:869:HIS:HE1	1:D:872:ASP:HB3	1.73	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
1:E:694:TRP:HA	1:E:694:TRP:HE3	1.73	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:H:873:VAL:O	1:H:874:SER:O	2.26	0.53
2:C:293:GLU:OE2	2:C:293:GLU:N	2.38	0.53
1:E:866:PHE:HE2	1:E:888:SER:OG	1.91	0.53
1:H:704:SER:OG	1:H:751:PHE:HZ	1.90	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:A:875:ASN:CG	1:D:878:ARG:HD2	2.29	0.53
2:B:193:LEU:HD22	2:B:238:PHE:CE1	2.44	0.53
1:E:815:LEU:CD1	1:E:846:VAL:HG11	2.39	0.53
1:E:699:LEU:HD11	1:E:701:ILE:CG2	2.39	0.53
1:E:694:TRP:HA	1:E:694:TRP:CE3	2.44	0.52
2:G:232:VAL:CG2	2:G:266:LEU:HD22	2.37	0.52
1:A:861:GLU:OE1	1:A:869:HIS:N	2.42	0.52
2:C:363:LEU:HD22	2:C:363:LEU:H	1.75	0.52
1:D:848:MET:O	1:D:851:LYS:N	2.35	0.52
1:E:666:ILE:HG23	1:E:679:TYR:CD2	2.43	0.52
1:H:682:ASP:OD2	1:H:682:ASP:C	2.48	0.52
1:H:652:GLN:HG2	1:H:908:VAL:CB	2.39	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: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
2:C:290:LEU:HB2	2:C:295:LEU:CD1	2.39	0.52
1:E:873:VAL:CG2	1:E:874:SER:H	2.04	0.52
2:F:191:ARG:NH2	2:F:237:PRO:HB2	2.23	0.52
2:G:281:PHE:CE2	2:G:328:PRO:HD3	2.40	0.52
2:G:268:GLN:HG2	1:H:735:HIS:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:LEU:HD22	1:A:902:LYS:HE3	1.91	0.52
1:A:799:ARG:NH2	1:A:900:PRO:HD3	2.24	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
2:G:311:ASP:CB	2:G:363:LEU:HD11	2.36	0.52
2:B:346:LEU:HD23	2:B:346:LEU:O	2.09	0.52
1:D:874:SER:HB2	1:D:876:MET:CB	2.27	0.52
1:H:700:VAL:O	1:H:749:TRP:HA	2.10	0.52
1:H:799:ARG:NH2	1:H:896:HIS:O	2.43	0.52
2:B:192:VAL:HG21	2:B:203:LEU:HD21	1.91	0.52
2:C:262:GLN:HA	2:C:262:GLN:NE2	2.24	0.52
1:D:643:LEU:HD23	1:D:673:HIS:CD2	2.45	0.52
1:E:636:PHE:HE2	1:E:726:LEU:HD13	1.75	0.52
1:E:686:VAL:O	1:E:732:ARG:NH2	2.43	0.52
1:H:693:GLU:C	1:H:695:GLY:H	2.12	0.52
2:C:209:LEU:HD12	2:C:209:LEU:N	2.25	0.52
1:D:753:ASN:ND2	1:D:754:VAL:HG22	2.25	0.52
2:C:304:MET:HB2	2:C:331:ARG:NH2	2.25	0.52
1:E:633:LEU:HB3	1:E:700:VAL:HG22	1.92	0.52
1:E:753:ASN:HD22	1:E:754:VAL:N	2.08	0.52
2:G:198:ASP:HB3	2:G:220:HIS:CG	2.45	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:706:CYS:HB2	1:H:754:VAL:HG13	1.92	0.52
1:H:788:ARG:HH11	1:H:788:ARG:HG2	1.75	0.51
1:H:750:LEU:HD11	1:H:790:PHE:HD2	1.75	0.51
1:A:868:VAL:O	1:A:869:HIS:HB2	2.10	0.51
1:D:810:GLU:HG2	1:D:813:GLU:CB	2.40	0.51
1:H:776:ILE:HD11	1:H:801:LEU:HD21	1.93	0.51
1:A:872:ASP:HB3	1:D:869:HIS:HE1	1.74	0.51
2:F:260:LEU:CD2	2:F:298:ALA:HA	2.40	0.51
2:F:327:ILE:O	2:F:330:ILE:HB	2.10	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:D:645:VAL:HG11	1:D:895:ARG:HA	1.92	0.51
1:A:799:ARG:NH2	1:A:896:HIS:O	2.43	0.51
1:E:786:ARG:NH1	1:E:864:PHE:HE2	2.07	0.51
1:E:871:THR:HB	1:E:881:ARG:HG2	1.92	0.51
2:F:306:PRO:HB3	2:F:324:TRP:CE2	2.45	0.51
2:G:184:VAL:C	2:G:186:ARG:H	2.14	0.51
2:G:324:TRP:O	2:G:325:SER:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:286:ASP:OD1	2:B:322:ARG:HG3	2.11	0.51
1:D:749:TRP:HZ3	1:D:769:LEU:HD13	1.75	0.51
1:D:783:ALA:O	1:D:826:VAL:HG22	2.10	0.51
1:E:687:THR:O	1:E:690:HIS:HB2	2.11	0.51
2:G:322:ARG:HH22	2:G:340:GLU:CD	2.12	0.51
1:H:801:LEU:HD12	1:H:801:LEU:H	1.76	0.51
2:B:201:LYS:HE3	2:B:202:GLU:OE1	2.11	0.51
1:D:633:LEU:HB2	1:D:697:PHE:CE2	2.46	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
2:B:271:ARG:CG	2:B:271:ARG:HH11	2.00	0.50
2:B:282:TRP:HZ3	2:B:302:LEU:HD22	1.76	0.50
1:E:684:ARG:HD3	1:E:684:ARG:H	1.76	0.50
1:E:788:ARG:NH1	1:E:788:ARG:HG2	2.21	0.50
1:H:856:TRP:HB2	1:H:859:GLU:OE1	2.11	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
1:A:796:GLY:O	1:A:799:ARG:CG	2.59	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
2:C:246:PRO:HG2	2:C:259:TYR:CZ	2.47	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: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
2:F:224:VAL:HG11	2:F:266:LEU:HD11	1.92	0.50
1:H:645:VAL:HG21	1:H:894:ILE:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:TYR:CD2	1:A:677:ILE:HG12	2.46	0.50
2:F:201:LYS:HB3	2:F:202:GLU:OE1	2.12	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:D:874:SER:C	1:D:876:MET:H	2.06	0.50
1:E:807:ASP:O	1:E:809:LEU:HG	2.12	0.50
1:E:817:HIS:CD2	1:E:817:HIS:C	2.85	0.50
2:F:199:ILE:HG22	2:F:203:LEU:HB2	1.93	0.49
1:H:684:ARG:HD3	1:H:684:ARG:H	1.77	0.49
1:A:865:GLY:O	1:A:891:VAL:HB	2.12	0.49
1:E:745:ARG:HG3	1:E:746:PRO:HD2	1.93	0.49
1:A:773:PRO:HB3	1:A:791:TRP:CE2	2.48	0.49
1:E:643:LEU:HB2	1:E:656:TYR:CE1	2.47	0.49
1:E:643:LEU:HG	1:E:647:LYS:HE3	1.93	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
2:B:183:PRO:O	2:B:187:ARG:HG3	2.12	0.49
2:B:310:PRO:HG3	2:B:338:VAL:HG21	1.95	0.49
1:E:686:VAL:HG12	1:E:733:LEU:HD11	1.93	0.49
1:E:753:ASN:ND2	1:E:754:VAL:H	2.10	0.49
2:C:191:ARG:HH21	2:C:237:PRO:HB2	1.78	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:G:368:PHE:O	2:G:371:LEU:HB2	2.12	0.49
1:D:874:SER:HB2	1:D:876:MET:H	1.78	0.49
1:E:668:VAL:HG22	1:E:873:VAL:HG21	1.93	0.49
1:A:700:VAL:O	1:A:749:TRP:HA	2.12	0.49
1:E:810:GLU:HG2	1:E:813:GLU:CB	2.42	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
1:D:776:ILE:CG2	1:D:790:PHE:HD1	2.25	0.49
1:D:885:LEU:O	1:D:886:GLY:C	2.52	0.49
2:F:326:ASN:N	2:F:326:ASN:HD22	1.92	0.49
1:H:754:VAL:HA	1:H:788:ARG:CD	2.42	0.49
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
2:B:287:ASN:HA	2:B:321:VAL:CG2	2.43	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:A:775:MET:SD	1:A:776:ILE:N	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:691:ILE:HG22	1:D:692:GLN:N	2.27	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: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
1:D:858:THR:HG23	1:D:868:VAL:HG13	1.95	0.48
1:E:786:ARG:CG	1:E:786:ARG:NH1	2.70	0.48
1:E:817:HIS:CD2	1:E:818:GLY:N	2.82	0.48
2:F:198:ASP:HB3	2:F:220:HIS:CG	2.49	0.48
1:A:869:HIS:HB3	1:D:869:HIS:CE1	2.48	0.48
2:C:243:GLY:O	2:C:284:PHE:HA	2.14	0.48
1:D:876:MET:SD	1:D:884:LEU:CD2	3.01	0.48
2:F:256:PRO:O	2:F:259:TYR:HD1	1.96	0.48
1:A:823:PHE:HZ	1:A:842:GLN:HA	1.79	0.48
1:A:874:SER:HA	1:D:856:TRP:CZ2	2.49	0.48
2:F:243:GLY:O	2:F:284:PHE:HA	2.14	0.48
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
2:C:279:PRO:HB2	2:C:281:PHE:HE1	1.77	0.48
1:H:861:GLU:OE2	1:H:881:ARG:NH1	2.46	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
2:B:234:GLU:C	2:B:236:GLY:H	2.16	0.48
1:A:869:HIS:ND1	1:D:869:HIS:HB3	2.29	0.48
1:E:794:LEU:HD13	1:E:897:LEU:O	2.14	0.48
2:F:199:ILE:O	2:F:199:ILE:HG22	2.14	0.48
1:E:773:PRO:HD3	1:E:791:TRP:NE1	2.29	0.48
1:H:691:ILE:CD1	1:H:733:LEU:HD12	2.44	0.48
2:C:327:ILE:O	2:C:330:ILE:HB	2.14	0.47
2:F:326:ASN:ND2	2:F:326:ASN:H	1.99	0.47
2:F:372:ARG:HD2	2:F:377:TYR:HB2	1.96	0.47
1:H:682:ASP:OD2	1:H:683:VAL:N	2.47	0.47
1:H:717:LYS:HB3	1:H:721:GLU:CB	2.44	0.47
1:A:647:LYS:HZ1	1:A:673:HIS:HB3	1.78	0.47
1:A:666:ILE:HG12	1:A:679:TYR:CE2	2.48	0.47
2:C:264:HIS:O	2:C:268:GLN:NE2	2.47	0.47
1:D:657:ILE:HD12	1:D:697:PHE:CZ	2.49	0.47
1:E:632:VAL:HG12	1:E:633:LEU:N	2.29	0.47
1:H:773:PRO:CD	1:H:791:TRP:NE1	2.70	0.47
1:H:885:LEU:O	1:H:888:SER:OG	2.32	0.47
1:A:804:THR:HG22	1:A:805:VAL:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:326:ASN:ND2	2:C:326:ASN:H	1.98	0.47
1:D:810:GLU:CD	1:D:810:GLU:H	2.17	0.47
2:G:201:LYS:HB3	2:G:202:GLU:OE1	2.13	0.47
2:B:361:THR:N	2:B:363:LEU:HD23	2.28	0.47
1:E:727:PHE:CE1	1:E:765:ILE:HG23	2.49	0.47
2:F:224:VAL:HG11	2:F:266:LEU:CD1	2.45	0.47
1:H:861:GLU:OE1	1:H:868:VAL:HA	2.14	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
2:G:290:LEU:HB3	2:G:294:ASP:HB2	1.96	0.47
1:H:732:ARG:NE	1:H:733:LEU:HD21	2.30	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
2:G:204:THR:OG1	2:G:209:LEU:HD22	2.15	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:D:662:CYS:O	1:D:666:ILE:HG13	2.14	0.47
1:E:885:LEU:O	1:E:886:GLY:C	2.51	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
1:H:720:TYR:HH	1:H:764:ASP:CG	2.17	0.47
1:H:786:ARG:NH1	1:H:864:PHE:HE2	2.12	0.47
1:A:680:VAL:HG21	1:A:694:TRP:CH2	2.50	0.47
2:C:290:LEU:HB2	2:C:295:LEU:HD13	1.96	0.47
1:E:702:GLY:O	1:E:751:PHE:HA	2.15	0.47
2:G:300:ARG:NH1	1:H:684:ARG:HB2	2.29	0.47
2:G:257:SER:OG	1:H:725:ARG:NH2	2.47	0.47
2:B:282:TRP:H	2:B:326:ASN:HD21	1.62	0.47
2:B:376:LYS:HD3	2:B:378:PHE:HE2	1.77	0.47
2:C:300:ARG:NH1	1:D:729:GLU:OE2	2.48	0.47
1:D:752:GLU:CG	1:D:753:ASN:N	2.75	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:H:706:CYS:CB	1:H:754:VAL:HG13	2.45	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: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:683:VAL:HG23	1:E:684:ARG:N	2.29	0.46
1:E:755:VAL:HG13	1:E:756:ALA:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:648:ASP:CG	1:D:895:ARG:HH12	2.19	0.46
1:H:691:ILE:HG22	1:H:692:GLN:H	1.80	0.46
1:H:691:ILE:HD11	1:H:733:LEU:HD12	1.96	0.46
2:F:188:GLN:N	2:F:188:GLN:OE1	2.49	0.46
1:H:823:PHE:HD1	1:H:823:PHE:N	2.12	0.46
1:A:686:VAL:HG13	1:A:694:TRP:CZ3	2.50	0.46
1:D:635:LEU:O	1:D:636:PHE:HB2	2.16	0.46
1:D:645:VAL:CG1	1:D:895:ARG:HA	2.45	0.46
2:C:262:GLN:HE21	2:C:262:GLN:CA	2.29	0.46
2:C:346:LEU:HD23	2:C:346:LEU:C	2.36	0.46
1:D:693:GLU:C	1:D:695:GLY:H	2.18	0.46
1:E:671:VAL:CG1	1:H:816:GLU:HG2	2.46	0.46
1:H:854:ILE:HG22	1:H:855:LEU:N	2.30	0.46
1:H:873:VAL:CG2	1:H:874:SER:N	2.71	0.46
1:D:801:LEU:CD1	1:D:801:LEU:H	2.21	0.46
1:D:819:ARG:CZ	1:D:846:VAL:HG21	2.46	0.46
2:G:208:PHE:C	2:G:209:LEU:HD12	2.36	0.46
1:H:661:VAL:O	1:H:661:VAL:HG22	2.16	0.46
1:H:709:LEU:HD13	1:H:753:ASN:ND2	2.30	0.46
2:B:188:GLN:HB3	2:B:189:PRO:CD	2.42	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
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:A:755:VAL:HG23	1:A:789:TYR:CE1	2.51	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
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:245:THR:HB	2:F:289:VAL:HG11	1.97	0.46
2:F:369:LEU:HB2	2:F:370:PRO:HD3	1.98	0.46
2:B:309:ILE:HG13	2:B:309:ILE:O	2.15	0.46
1:A:860:MET:O	1:A:864:PHE:HD1	1.98	0.45
2:B:203:LEU:CD1	2:B:208:PHE:HD1	2.29	0.45
2:B:218:LEU:HD23	2:B:218:LEU:C	2.37	0.45
2:B:229:ARG:HA	2:B:269:TYR:HD1	1.79	0.45
2:F:372:ARG:NH1	2:F:372:ARG:HG2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:705:PRO:HG2	1:H:726:LEU:HD12	1.97	0.45
1:A:801:LEU:HD12	1:A:801:LEU:N	2.31	0.45
2:B:268:GLN:NE2	2:B:268:GLN:CA	2.79	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
1:H:752:GLU:CG	1:H:753:ASN:N	2.79	0.45
1:H:866:PHE:O	1:H:867:PRO:C	2.55	0.45
1:E:643:LEU:HD22	1:E:656:TYR:CG	2.50	0.45
2:F:184:VAL:HA	2:F:187:ARG:NE	2.31	0.45
2:F:279:PRO:CB	2:F:281:PHE:HE1	2.29	0.45
2:G:322:ARG:NH2	2:G:340:GLU:OE1	2.33	0.45
2:G:268:GLN:HG2	1:H:735:HIS:CE1	2.51	0.45
1:H:794:LEU:O	1:H:797:MET:HG3	2.16	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
2:B:228:VAL:CG1	2:B:229:ARG:N	2.79	0.45
2:B:248:LEU:HG	2:B:287:ASN:ND2	2.32	0.45
2:G:203:LEU:HG	2:G:209:LEU:HD11	1.99	0.45
2:G:310:PRO:HG2	2:G:338:VAL:CG2	2.46	0.45
1:A:693:GLU:C	1:A:695:GLY:H	2.19	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:E:682:ASP:OD2	1:E:684:ARG:HG2	2.16	0.45
1:E:753:ASN:HD22	1:E:754:VAL:HG22	1.79	0.45
2:F:188:GLN:HB3	2:F:189:PRO:CD	2.47	0.45
2:F:224:VAL:CB	2:F:266:LEU:HD11	2.46	0.45
1:A:773:PRO:HD3	1:A:791:TRP:NE1	2.32	0.45
1:D:691:ILE:HD11	1:D:733:LEU:CD1	2.44	0.45
1:D:776:ILE:CG2	1:D:790:PHE:CD1	3.00	0.45
2:F:192:VAL:HG21	2:F:203:LEU:CD2	2.42	0.45
1:E:817:HIS:ND1	1:H:674:GLN:HB3	2.32	0.45
1:D:812:GLN:OE1	1:D:821:ALA:N	2.34	0.45
2:G:230:LYS:N	2:G:230:LYS:HD2	2.32	0.45
2:C:300:ARG:CZ	1:D:684:ARG:HB2	2.47	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
2:G:372:ARG:NH1	2:G:372:ARG:HG2	2.31	0.45
1:A:891:VAL:N	1:A:892:PRO:CD	2.79	0.45
2:B:199:ILE:O	2:B:199:ILE:HG22	2.17	0.45
2:B:202:GLU:HG2	2:B:361:THR:CG2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:680:VAL:CG1	1:D:681:GLY:N	2.61	0.45
1:D:819:ARG:HD2	1:D:848:MET:SD	2.56	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: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:D:786:ARG:NH1	1:D:864:PHE:CE2	2.83	0.44
1:E:732:ARG:HD3	2:F:301:PHE:CE1	2.52	0.44
2:G:255:PRO:HA	2:G:256:PRO:HD3	1.90	0.44
1:E:664:ASP:O	1:E:668:VAL:HG23	2.17	0.44
1:E:719:LEU:HG	1:E:719:LEU:O	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: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:A:725:ARG:HH12	2:B:297:VAL:CG2	2.17	0.44
1:A:808:LYS:HG2	1:A:808:LYS:H	1.56	0.44
1:A:875:ASN:HB3	1:D:878:ARG:CD	2.47	0.44
2:B:326:ASN:HD22	2:B:326:ASN:N	1.98	0.44
2:B:325:SER:OG	2:B:327:ILE:HG13	2.18	0.44
2:C:221:VAL:HG21	2:C:235:TRP:CZ3	2.52	0.44
1:E:638:GLY:HA2	1:E:660:GLU:OE1	2.18	0.44
1:E:844:PHE:O	1:E:846:VAL:N	2.51	0.44
2:G:347:ALA:O	2:G:351:GLN:HG3	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
1:A:775:MET:CE	1:A:787:ALA:HB1	2.48	0.44
1:A:865:GLY:O	1:A:891:VAL:CB	2.66	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:271:ARG:HG3	2:C:271:ARG:NH1	2.33	0.44
1:E:657:ILE:HG12	1:E:678:MET:HB3	2.00	0.44
1:A:899:ALA:HB3	1:A:900:PRO:CD	2.48	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:728:PHE:HA	1:A:731:TYR:HB3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:LEU:O	1:A:719:LEU:HG	2.18	0.44
2:C:208:PHE:C	2:C:209:LEU:HD12	2.38	0.44
1:E:691:ILE:HG22	1:E:692:GLN:N	2.32	0.44
1:E:753:ASN:ND2	1:E:754:VAL:N	2.66	0.44
2:F:262:GLN:HE22	2:F:265:ARG:HE	1.65	0.44
2:F:346:LEU:C	2:F:346:LEU:HD23	2.37	0.44
2:G:248:LEU:N	2:G:287:ASN:HD22	2.15	0.44
1:E:699:LEU:CD1	1:E:701:ILE:HG23	2.48	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
2:B:309:ILE:HA	2:B:310:PRO:HD3	1.78	0.44
1:E:868:VAL:O	1:E:869:HIS:HB2	2.18	0.44
2:F:361:THR:N	2:F:363:LEU:HD23	2.33	0.44
2:G:303:GLU:O	2:G:304:MET:HB3	2.18	0.44
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:267:LEU:HD12	2:F:268:GLN:HE22	1.83	0.43
2:G:256:PRO:CB	2:G:290:LEU:HD23	2.39	0.43
1:H:689:LYS:O	1:H:692:GLN:OE1	2.36	0.43
1:H:873:VAL:O	1:H:874:SER:C	2.57	0.43
2:F:326:ASN:N	2:F:326:ASN:ND2	2.63	0.43
1:H:788:ARG:NH1	1:H:788:ARG:HG2	2.33	0.43
1:H:890:SER:O	1:H:893:VAL:HB	2.17	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
1:A:883:ARG:O	1:A:887:ARG:HG2	2.18	0.43
2:B:289:VAL:O	2:B:289:VAL:HG22	2.19	0.43
2:B:335:TRP:O	2:B:337:LEU:N	2.46	0.43
2:C:199:ILE:HG21	2:C:368:PHE:HE1	1.82	0.43
1:D:810:GLU:OE1	1:D:813:GLU:CB	2.67	0.43
2:F:228:VAL:CG1	2:F:229:ARG:H	2.29	0.43
2:F:309:ILE:HG13	2:F:321:VAL:HG12	2.00	0.43
1:H:752:GLU:O	1:H:753:ASN:HB2	2.17	0.43
1:H:757:MET:HE3	1:H:757:MET:HB2	1.83	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:C:262:GLN:HA	2:C:262:GLN:HE21	1.82	0.43
1:D:822:LYS:NZ	1:D:852:GLU:OE2	2.49	0.43
2:F:229:ARG:HG2	2:F:233:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:346:LEU:HD23	2:F:346:LEU:O	2.19	0.43
2:G:203:LEU:CG	2:G:209:LEU:HD11	2.47	0.43
1:A:855:LEU:HD23	1:A:855:LEU:HA	1.84	0.43
1:A:672:ARG:CG	1:A:870:TYR:CE1	2.97	0.43
2:C:363:LEU:CD2	2:C:363:LEU:H	2.31	0.43
1:E:630:ILE:HD11	1:E:699:LEU:HD23	2.01	0.43
1:E:757:MET:HE2	1:E:762:LYS:N	2.34	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
2:G:193:LEU:HB2	2:G:238:PHE:CE2	2.52	0.43
1:H:728:PHE:HE2	1:H:768:PHE:CZ	2.35	0.43
1:H:822:LYS:HB2	1:H:823:PHE:CE1	2.53	0.43
1:A:646:LEU:HA	1:A:646:LEU:HD23	1.84	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
2:G:234:GLU:C	2:G:236:GLY:H	2.20	0.43
1:A:635:LEU:O	1:A:636:PHE:HB2	2.19	0.43
1:A:786:ARG:HG3	1:A:786:ARG:HH11	1.83	0.43
2:B:255:PRO:HA	2:B:256:PRO:HD3	1.84	0.43
2:G:228:VAL:CG1	2:G:229:ARG:N	2.82	0.43
1:H:815:LEU:HA	1:H:859:GLU:OE2	2.19	0.43
1:A:649:LEU:CD2	1:A:902:LYS:HE3	2.49	0.43
1:A:749:TRP:CZ3	1:A:792:GLY:HA2	2.53	0.43
2:B:190:VAL:HG22	2:B:192:VAL:HG23	2.00	0.43
2:C:192:VAL:HG21	2:C:203:LEU:CD2	2.45	0.43
1:D:711:ILE:HG12	1:D:756:ALA:O	2.19	0.43
1:D:859:GLU:O	1:D:863:VAL:HG23	2.18	0.43
1:E:735:HIS:NE2	2:F:268:GLN:HG2	2.33	0.43
1:E:786:ARG:HB3	1:E:788:ARG:HH12	1.84	0.43
2:F:246:PRO:HA	2:F:247:PRO:HD3	1.92	0.43
1:H:899:ALA:N	1:H:900:PRO:HD2	2.34	0.43
1:A:666:ILE:HA	1:A:679:TYR:CE2	2.53	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: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
1:D:750:LEU:HD13	1:D:794:LEU:HD12	2.00	0.43
2:F:199:ILE:HG22	2:F:203:LEU:N	2.34	0.43
2:F:258:TRP:CE2	2:F:262:GLN:HG3	2.53	0.43
2:F:260:LEU:CD2	2:F:297:VAL:HG12	2.49	0.43
1:A:878:ARG:CG	1:A:878:ARG:HH11	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:282:TRP:CZ3	2:F:302:LEU:HD22	2.54	0.43
2:G:269:TYR:CD2	2:G:269:TYR:N	2.87	0.43
2:C:345:LEU:HD12	2:C:349:ASN:OD1	2.18	0.42
1:D:773:PRO:HD3	1:D:791:TRP:NE1	2.34	0.42
1:E:774:VAL:O	1:E:776:ILE:HG22	2.19	0.42
1:A:675:GLY:O	1:A:677:ILE:N	2.52	0.42
2:B:260:LEU:CD2	2:B:298:ALA:CA	2.94	0.42
2:B:307:VAL:HG13	2:B:334:HIS:ND1	2.35	0.42
1:D:868:VAL:O	1:D:869:HIS:HB2	2.18	0.42
1:D:876:MET:SD	1:D:884:LEU:HD23	2.59	0.42
1:H:730:PHE:CE2	1:H:751:PHE:HB2	2.54	0.42
1:A:727:PHE:CE1	1:A:765:ILE:HG23	2.54	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
2:F:267:LEU:HD13	2:F:267:LEU:C	2.39	0.42
1:H:720:TYR:CD1	1:H:720:TYR:N	2.87	0.42
1:A:783:ALA:O	1:A:826:VAL:HG22	2.20	0.42
2:C:279:PRO:CB	2:C:281:PHE:HE1	2.32	0.42
1:D:862:ARG:NH1	1:D:868:VAL:HG21	2.33	0.42
2:G:326:ASN:ND2	2:G:326:ASN:H	2.18	0.42
1:H:632:VAL:CG1	1:H:633:LEU:N	2.82	0.42
1:H:730:PHE:CZ	1:H:734:LEU:HD12	2.54	0.42
1:A:775:MET:HE1	1:A:787:ALA:HB1	2.01	0.42
1:E:687:THR:O	1:E:690:HIS:N	2.53	0.42
1:H:692:GLN:N	1:H:692:GLN:OE1	2.52	0.42
1:H:786:ARG:NH1	1:H:864:PHE:CE2	2.88	0.42
1:H:904:TYR:C	1:H:905:PHE:CD1	2.92	0.42
1:A:632:VAL:CG1	1:A:633:LEU:N	2.82	0.42
1:A:880:ALA:O	1:A:881:ARG:C	2.58	0.42
2:B:230:LYS:N	2:B:230:LYS:HD2	2.35	0.42
1:D:819:ARG:HH21	1:D:859:GLU:CD	2.21	0.42
2:F:257:SER:O	2:F:260:LEU:N	2.53	0.42
2:F:372:ARG:CD	2:F:377:TYR:HB2	2.50	0.42
2:G:363:LEU:CD2	2:G:363:LEU:H	2.28	0.42
1:H:883:ARG:HD3	1:H:887:ARG:HH22	1.85	0.42
1:A:691:ILE:HG21	1:A:736:ASP:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:342:GLU:O	2:B:345:LEU:HB3	2.19	0.42
1:D:699:LEU:HG	1:D:701:ILE:HG23	2.02	0.42
1:E:876:MET:CG	1:E:880:ALA:HB3	2.50	0.42
2:G:245:THR:HB	2:G:289:VAL:HG11	2.02	0.42
1:A:683:VAL:HG23	1:A:684:ARG:H	1.85	0.42
1:A:849:ASN:O	1:A:850:GLU:CB	2.68	0.42
2:B:267:LEU:HD22	2:B:267:LEU:O	2.20	0.42
1:D:815:LEU:CD1	1:D:846:VAL:HG12	2.50	0.42
1:D:778:ALA:HB2	1:D:893:VAL:HG21	2.02	0.42
1:E:639:ILE:O	1:E:870:TYR:OH	2.28	0.42
1:E:690:HIS:O	1:E:694:TRP:N	2.49	0.42
1:E:878:ARG:O	1:E:882:GLN:HB2	2.20	0.42
1:H:630:ILE:HG13	1:H:905:PHE:CE2	2.55	0.42
2:G:300:ARG:NH1	1:H:729:GLU:OE2	2.48	0.42
1:H:728:PHE:HA	1:H:731:TYR:HB3	2.02	0.42
1:A:632:VAL:HG12	1:A:633:LEU:N	2.33	0.42
1:A:779:LYS:HA	1:A:784:ALA:O	2.20	0.42
1:A:856:TRP:HB2	1:A:859:GLU:CG	2.47	0.42
1:D:657:ILE:CG2	1:D:680:VAL:HG23	2.50	0.42
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:E:699:LEU:HA	1:E:748:PHE:O	2.20	0.42
1:H:871:THR:HB	1:H:881:ARG:CG	2.50	0.42
1:E:881:ARG:NH2	1:H:872:ASP:OD2	2.49	0.42
1:A:627:ARG:HH12	1:A:903:GLU:HA	1.85	0.42
1:A:706:CYS:HB2	1:A:754:VAL:HG13	2.00	0.42
1:A:730:PHE:CE2	1:A:751:PHE:HB2	2.54	0.42
2:B:243:GLY:O	2:B:284:PHE:HA	2.20	0.42
2:C:368:PHE:CD2	2:C:368:PHE:N	2.86	0.42
1:D:773:PRO:HB2	1:D:789:TYR:HD1	1.84	0.42
1:D:848:MET:O	1:D:849:ASN:C	2.59	0.42
1:E:786:ARG:HB3	1:E:788:ARG:NH1	2.35	0.42
1:E:888:SER:HA	3:E:5:SAH:C	2.49	0.42
2:F:247:PRO:HA	2:F:287:ASN:HD22	1.85	0.42
2:F:273:LYS:CB	2:F:274:PRO:HD2	2.42	0.42
2:F:187:ARG:HB3	2:F:375:PHE:HA	2.01	0.42
1:H:898:PHE:N	1:H:898:PHE:CD2	2.86	0.42
1:D:694:TRP:CE3	1:D:694:TRP:HA	2.55	0.41
1:D:898:PHE:O	1:D:901:LEU:HB2	2.20	0.41
2:F:260:LEU:HD21	2:F:298:ALA:HA	2.02	0.41
2:G:346:LEU:HD23	2:G:346:LEU:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:811:LEU:CD2	1:H:826:VAL:HG13	2.50	0.41
2:C:229:ARG:HA	2:C:269:TYR:CD1	2.55	0.41
1:D:755:VAL:HG13	1:D:756:ALA:N	2.35	0.41
2:F:271:ARG:HG3	2:F:271:ARG:HH11	1.85	0.41
2:F:282:TRP:H	2:F:326:ASN:ND2	2.15	0.41
2:G:184:VAL:HG13	2:G:185:TRP:N	2.34	0.41
2:G:196:PHE:O	2:G:197:GLU:HG2	2.20	0.41
2:B:208:PHE:C	2:B:209:LEU:HD12	2.41	0.41
2:B:224:VAL:O	2:B:225:THR:C	2.59	0.41
2:C:229:ARG:HB2	1:D:770:GLU:OE1	2.21	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
1:D:683:VAL:HG23	1:D:684:ARG:H	1.83	0.41
1:E:876:MET:SD	1:E:884:LEU:HD22	2.60	0.41
2:F:224:VAL:HB	2:F:266:LEU:HD11	2.01	0.41
1:A:633:LEU:CD2	1:A:635:LEU:HD21	2.50	0.41
2:B:248:LEU:HD11	2:B:288:LEU:HB2	2.02	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:683:VAL:HG23	1:A:684:ARG:HD3	2.02	0.41
1:A:796:GLY:O	1:A:799:ARG:HG2	2.20	0.41
1:A:815:LEU:HD11	1:A:821:ALA:HB2	2.02	0.41
2:B:327:ILE:HA	2:B:328:PRO:HD3	1.93	0.41
1:E:898:PHE:O	1:E:900:PRO:N	2.53	0.41
2:F:224:VAL:CG1	2:F:266:LEU:HD11	2.50	0.41
2:G:199:ILE:CG2	2:G:203:LEU:HB2	2.47	0.41
1:A:691:ILE:HD12	1:A:691:ILE:HA	1.81	0.41
1:A:702:GLY:O	1:A:751:PHE:HA	2.21	0.41
1:A:799:ARG:NH2	1:A:900:PRO:CD	2.84	0.41
1:A:804:THR:CG2	1:A:805:VAL:N	2.83	0.41
1:A:811:LEU:HD23	1:A:821:ALA:HB1	2.01	0.41
1:A:872:ASP:CG	1:D:881:ARG:HH22	2.24	0.41
1:D:627:ARG:HG3	1:D:627:ARG:H	1.71	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:E:874:SER:C	1:E:876:MET:N	2.74	0.41
1:E:896:HIS:O	1:E:898:PHE:N	2.53	0.41
2:F:311:ASP:HB2	2:F:363:LEU:HD11	2.01	0.41
2:G:262:GLN:NE2	2:G:265:ARG:HE	2.12	0.41
1:H:801:LEU:N	1:H:801:LEU:CD1	2.83	0.41
1:A:799:ARG:HA	1:A:800:PRO:HD3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:LEU:HD11	2:B:208:PHE:CD1	2.53	0.41
2:C:294:ASP:OD2	1:D:725:ARG:NH2	2.54	0.41
1:D:669:GLY:HA3	1:D:679:TYR:OH	2.21	0.41
1:E:811:LEU:HD12	1:E:821:ALA:HB1	2.02	0.41
1:H:672:ARG:HA	1:H:672:ARG:HD3	1.84	0.41
1:A:898:PHE:O	1:A:899:ALA:C	2.58	0.41
2:C:241:VAL:O	2:C:282:TRP:HA	2.20	0.41
1:D:891:VAL:N	1:D:892:PRO:CD	2.84	0.41
1:E:876:MET:HG3	1:E:880:ALA:CB	2.51	0.41
2:G:203:LEU:HD23	2:G:209:LEU:HD11	2.02	0.41
1:H:804:THR:HG22	1:H:805:VAL:N	2.36	0.41
1:A:699:LEU:HA	1:A:748:PHE:O	2.20	0.41
1:A:752:GLU:O	1:A:753:ASN:HB2	2.21	0.41
2:B:346:LEU:C	2:B:346:LEU:HD23	2.41	0.41
1:E:788:ARG:NH1	1:E:788:ARG:CG	2.84	0.41
2:F:339:SER:O	2:F:343:LEU:HB2	2.21	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:C:297:VAL:O	2:C:301:PHE:HB2	2.20	0.41
1:D:810:GLU:OE2	1:D:810:GLU:N	2.53	0.41
1:D:899:ALA:HB3	1:D:900:PRO:CD	2.51	0.41
1:H:643:LEU:HG	1:H:647:LYS:HE3	2.02	0.41
1:H:727:PHE:CZ	1:H:765:ILE:HG23	2.55	0.41
1:A:801:LEU:HD12	1:A:801:LEU:H	1.85	0.41
1:A:873:VAL:O	1:A:874:SER:OG	2.26	0.41
2:B:241:VAL:O	2:B:282:TRP:HA	2.21	0.41
1:D:860:MET:O	1:D:863:VAL:HB	2.21	0.41
1:D:898:PHE:O	1:D:899:ALA:C	2.59	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:752:GLU:HG2	1:H:753:ASN:N	2.36	0.41
1:H:783:ALA:O	1:H:826:VAL:HG22	2.21	0.41
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:717:LYS:HB3	1:A:721:GLU:HB2	2.02	0.40
1:A:817:HIS:CD2	1:D:674:GLN:HA	2.56	0.40
2:C:189:PRO:HB3	2:C:378:PHE:HZ	1.86	0.40
1:D:632:VAL:HG13	1:D:699:LEU:HB3	2.03	0.40
1:D:808:LYS:HG2	1:D:808:LYS:H	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:LEU:CG	2:B:209:LEU:HD11	2.50	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
1:E:684:ARG:HB2	2:F:300:ARG:CZ	2.52	0.40
2:F:202:GLU:OE1	2:F:202:GLU:N	2.45	0.40
1:E:729:GLU:OE2	2:F:300:ARG:NH1	2.55	0.40
1:H:632:VAL:HG22	1:H:699:LEU:HB3	2.03	0.40
1:H:732:ARG:CZ	1:H:733:LEU:HD21	2.51	0.40
1:H:816:GLU:CD	1:H:862:ARG:NH2	2.75	0.40
2:B:179:PHE:CE2	2:B:279:PRO:HA	2.56	0.40
1:E:794:LEU:HA	1:E:795:PRO:HD2	1.95	0.40
1:E:804:THR:HB	1:E:806:ASN:O	2.21	0.40
1:H:745:ARG:HA	1:H:746:PRO:HD3	1.93	0.40
1:H:770:GLU:O	1:H:771:SER:HB3	2.22	0.40
1:H:801:LEU:CD1	1:H:801:LEU:H	2.35	0.40
2:B:246:PRO:HA	2:B:247:PRO:HD3	1.91	0.40
1:D:632:VAL:HG12	1:D:633:LEU:N	2.37	0.40
1:D:706:CYS:CB	1:D:754:VAL:HG13	2.52	0.40
2:F:248:LEU:N	2:F:287:ASN:HD22	2.16	0.40
1:H:637:ASP:CB	1:H:658:ALA:HB1	2.51	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:873:VAL:C	1:H:874:SER:O	2.60	0.40
2:C:258:TRP:CE2	2:C:262:GLN:HG3	2.57	0.40
2:C:265:ARG:HG2	2:C:265:ARG:HH11	1.87	0.40
1:D:799:ARG:CZ	1:D:896:HIS:CE1	3.05	0.40
2:F:257:SER:O	2:F:258:TRP:C	2.60	0.40
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

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%)	3	13
1	D	263/295 (89%)	221 (84%)	35 (13%)	7 (3%)	5	19
1	E	266/295 (90%)	223 (84%)	34 (13%)	9 (3%)	3	15
1	H	263/295 (89%)	226 (86%)	29 (11%)	8 (3%)	4	17
2	B	178/230 (77%)	135 (76%)	34 (19%)	9 (5%)	2	7
2	C	178/230 (77%)	138 (78%)	32 (18%)	8 (4%)	2	9
2	F	178/230 (77%)	136 (76%)	36 (20%)	6 (3%)	3	15
2	G	178/230 (77%)	138 (78%)	33 (18%)	7 (4%)	3	12
All	All	1772/2100 (84%)	1445 (82%)	263 (15%)	64 (4%)	3	14

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
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

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Mol	Chain	Res	Type
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
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%)	4	14
1	D	222/259 (86%)	194 (87%)	28 (13%)	4	13
1	E	223/259 (86%)	188 (84%)	35 (16%)	2	8
1	H	222/259 (86%)	203 (91%)	19 (9%)	10	30
2	B	166/210 (79%)	153 (92%)	13 (8%)	12	34
2	C	166/210 (79%)	154 (93%)	12 (7%)	14	39
2	F	166/210 (79%)	155 (93%)	11 (7%)	16	44
2	G	166/210 (79%)	157 (95%)	9 (5%)	22	54
All	All	1555/1876 (83%)	1400 (90%)	155 (10%)	7	23

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

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	H	882	GLN
1	H	896	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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	H	8	-	21,28,28	1.78	4 (19%)	20,40,40	2.35	8 (40%)
3	SAH	D	4	-	21,28,28	1.62	4 (19%)	20,40,40	2.76	9 (45%)
3	SAH	A	1	-	21,28,28	1.92	5 (23%)	20,40,40	2.98	7 (35%)
3	SAH	E	5	-	21,28,28	1.87	4 (19%)	20,40,40	2.26	10 (50%)

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	H	8	-	-	1/7/31/31	0/3/3/3
3	SAH	D	4	-	-	1/7/31/31	0/3/3/3
3	SAH	A	1	-	-	0/7/31/31	0/3/3/3
3	SAH	E	5	-	-	0/7/31/31	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5	SAH	C2-N3	4.70	1.39	1.32
3	A	1	SAH	O4'-C1'	4.68	1.47	1.41
3	H	8	SAH	O4'-C1'	4.64	1.47	1.41
3	E	5	SAH	O4'-C1'	4.35	1.47	1.41
3	D	4	SAH	C2-N3	4.05	1.38	1.32
3	A	1	SAH	C2-N3	4.04	1.38	1.32
3	H	8	SAH	C2-N3	3.74	1.38	1.32
3	D	4	SAH	CA-N	2.98	1.53	1.47
3	H	8	SAH	CA-N	2.98	1.53	1.47
3	A	1	SAH	CA-N	2.88	1.53	1.47
3	E	5	SAH	C8-N7	-2.78	1.29	1.34
3	A	1	SAH	C8-N7	-2.56	1.30	1.34
3	A	1	SAH	C2'-C3'	2.49	1.60	1.53
3	E	5	SAH	C2-N1	2.39	1.38	1.33
3	H	8	SAH	C8-N7	-2.27	1.30	1.34
3	D	4	SAH	O4'-C1'	2.05	1.43	1.41
3	D	4	SAH	C2'-C3'	2.04	1.58	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	SAH	O4'-C1'-C2'	-9.78	92.63	106.93
3	D	4	SAH	O4'-C4'-C5'	-6.51	92.07	108.83
3	D	4	SAH	O4'-C1'-C2'	-6.48	97.45	106.93
3	H	8	SAH	CB-CG-SD	-5.49	100.99	113.31
3	E	5	SAH	N3-C2-N1	-4.46	121.71	128.68
3	H	8	SAH	O4'-C1'-C2'	-4.26	100.69	106.93
3	A	1	SAH	N3-C2-N1	-4.07	122.31	128.68
3	H	8	SAH	N3-C2-N1	-4.02	122.39	128.68
3	E	5	SAH	C1'-N9-C4	-3.89	119.81	126.64
3	D	4	SAH	C1'-N9-C4	-3.76	120.03	126.64
3	D	4	SAH	N3-C2-N1	-3.75	122.82	128.68
3	A	1	SAH	CB-CG-SD	-3.62	105.18	113.31
3	A	1	SAH	C1'-N9-C4	-3.50	120.48	126.64
3	H	8	SAH	C1'-N9-C4	-3.47	120.54	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	SAH	C5-C6-N6	3.37	125.48	120.35
3	D	4	SAH	CB-CG-SD	-3.30	105.91	113.31
3	E	5	SAH	CB-CG-SD	-3.24	106.03	113.31
3	E	5	SAH	O4'-C1'-C2'	-3.16	102.31	106.93
3	E	5	SAH	C2-N1-C6	3.07	124.01	118.75
3	H	8	SAH	C2-N1-C6	2.97	123.83	118.75
3	A	1	SAH	C2-N1-C6	2.62	123.24	118.75
3	E	5	SAH	C5-C6-N6	2.60	124.30	120.35
3	D	4	SAH	C2-N1-C6	2.60	123.20	118.75
3	E	5	SAH	C3'-C2'-C1'	2.56	104.84	100.98
3	H	8	SAH	O4'-C4'-C3'	2.52	110.10	105.11
3	E	5	SAH	C5-C6-N1	-2.50	114.69	120.35
3	A	1	SAH	C3'-C2'-C1'	2.47	104.70	100.98
3	E	5	SAH	C4'-C5'-SD	-2.15	106.08	113.78
3	H	8	SAH	C5-C6-N1	-2.14	115.51	120.35
3	E	5	SAH	O4'-C4'-C5'	-2.08	103.47	108.83
3	D	4	SAH	C5-C6-N6	2.07	123.50	120.35
3	D	4	SAH	C5-C6-N1	-2.06	115.67	120.35
3	H	8	SAH	C5-C6-N6	2.01	123.40	120.35
3	D	4	SAH	O3'-C3'-C2'	2.00	118.30	111.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	8	SAH	CA-CB-CG-SD
3	D	4	SAH	CA-CB-CG-SD

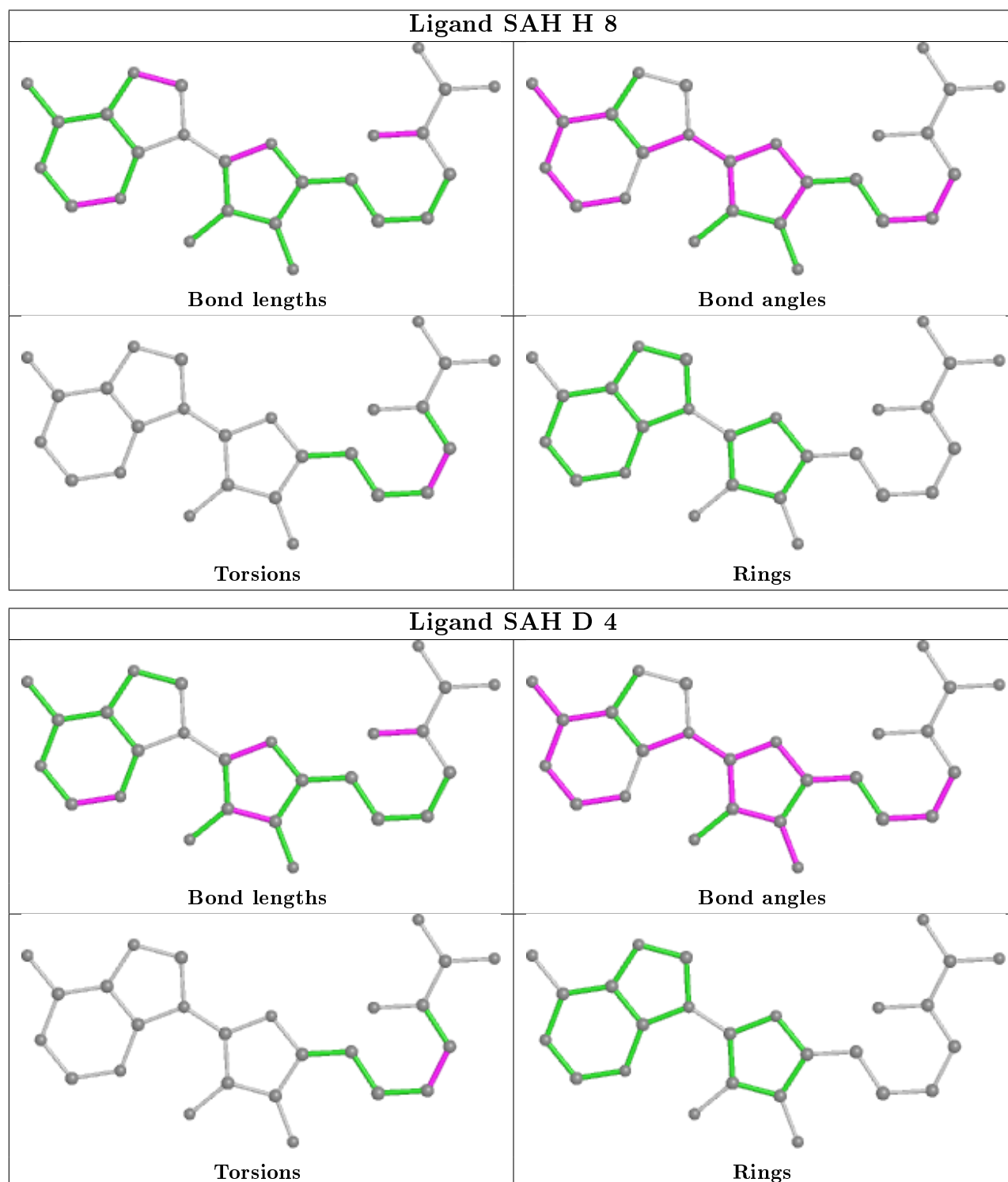
There are no ring outliers.

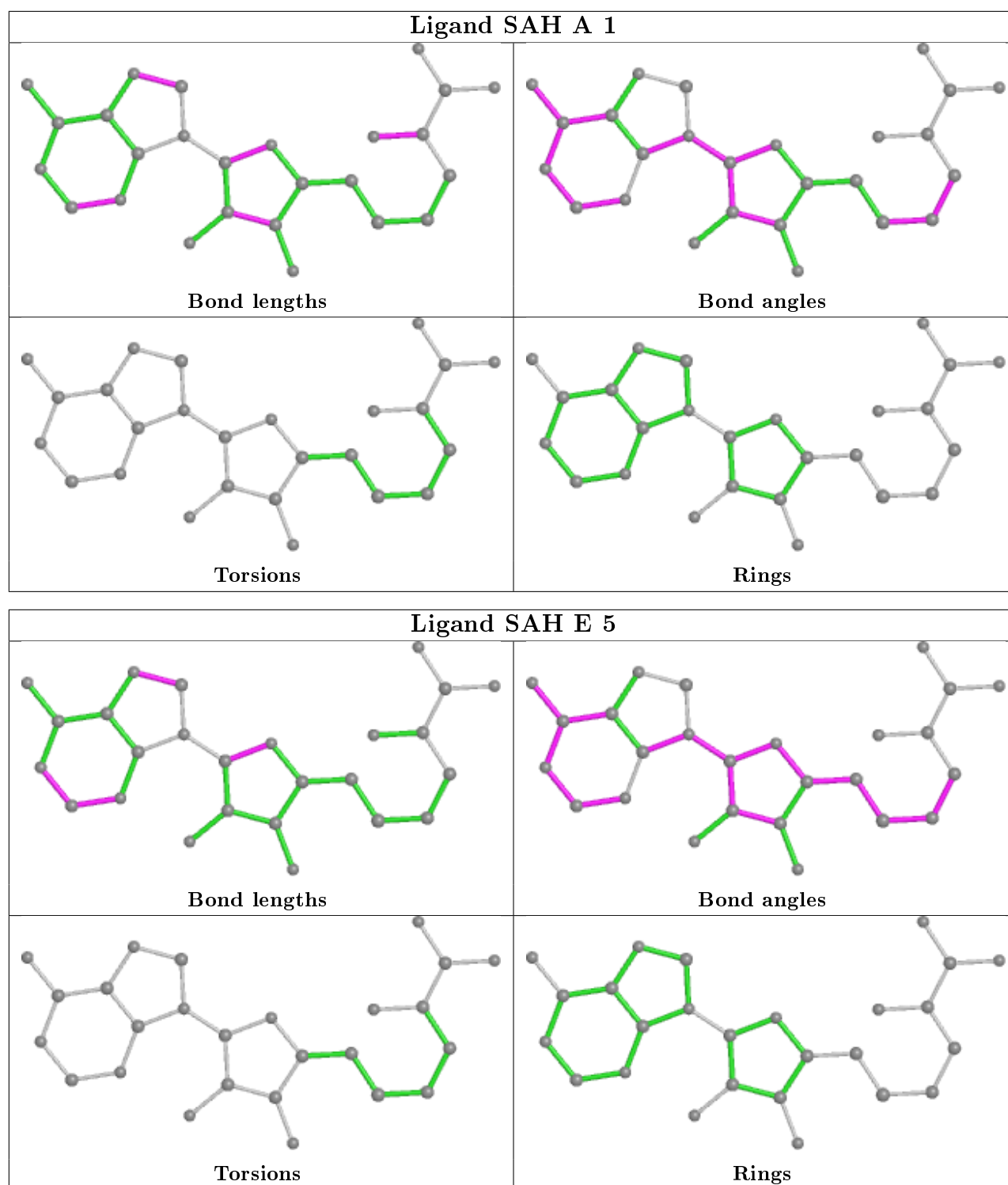
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	8	SAH	2	0
3	A	1	SAH	1	0
3	E	5	SAH	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

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%)	0.19	4 (1%) 73 73	30, 64, 106, 146	0
1	D	267/295 (90%)	0.15	5 (1%) 66 65	37, 75, 122, 157	0
1	E	270/295 (91%)	0.21	3 (1%) 80 80	27, 67, 111, 132	0
1	H	267/295 (90%)	0.54	25 (9%) 8 6	51, 101, 138, 170	0
2	B	186/230 (80%)	1.04	37 (19%) 1 0	55, 121, 187, 207	0
2	C	186/230 (80%)	1.02	36 (19%) 1 0	61, 118, 189, 206	0
2	F	186/230 (80%)	1.16	36 (19%) 1 0	66, 121, 189, 210	0
2	G	186/230 (80%)	2.73	88 (47%) 0 0	109, 163, 201, 210	0
All	All	1820/2100 (86%)	0.77	234 (12%) 3 2	27, 93, 181, 210	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	321	VAL	26.4
2	G	309	ILE	17.9
2	G	334	HIS	16.8
2	F	334	HIS	13.9
2	G	331	ARG	12.1
2	G	308	THR	11.8
2	F	310	PRO	11.5
2	F	315	GLY	11.2
2	F	331	ARG	11.1
2	G	353	SER	10.1
2	G	344	SER	10.0
2	C	361	THR	8.4
2	G	310	PRO	8.2
2	G	335	TRP	7.8
2	F	314	GLY	7.7
2	B	334	HIS	7.3

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Mol	Chain	Res	Type	RSRZ
2	F	316	SER	7.3
2	C	316	SER	7.0
2	G	222	VAL	6.9
2	B	352	SER	6.9
2	G	279	PRO	6.8
2	G	280	PHE	6.7
2	G	196	PHE	6.6
2	C	315	GLY	6.6
2	G	206	LEU	6.5
2	B	336	ALA	6.4
2	G	362	LYS	6.2
2	G	185	TRP	6.2
2	G	192	VAL	6.1
2	B	364	VAL	6.1
2	F	336	ALA	6.0
2	F	363	LEU	5.8
2	G	311	ASP	5.7
2	G	377	TYR	5.7
2	G	350	LYS	5.7
2	G	182	VAL	5.6
2	G	312	VAL	5.6
2	C	313	HIS	5.5
2	C	336	ALA	5.5
2	G	203	LEU	5.4
2	G	348	GLN	5.4
2	F	276	SER	5.4
2	B	203	LEU	5.3
2	G	216	GLY	5.3
2	C	365	LYS	5.3
2	G	364	VAL	5.3
2	G	324	TRP	5.2
2	G	307	VAL	5.2
2	G	199	ILE	5.1
2	B	242	TYR	5.1
2	G	217	GLN	5.1
2	C	334	HIS	5.0
2	G	252	CYS	5.0
2	G	343	LEU	4.9
2	G	316	SER	4.9
1	H	731	TYR	4.9
2	G	186	ARG	4.8
2	G	302	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
2	F	251	THR	4.8
2	C	314	GLY	4.8
2	F	364	VAL	4.8
2	G	270	ALA	4.8
2	G	183	PRO	4.7
2	C	310	PRO	4.7
2	C	192	VAL	4.6
2	C	341	GLU	4.6
2	G	241	VAL	4.6
2	F	333	ARG	4.4
2	G	184	VAL	4.4
2	C	349	ASN	4.3
2	G	328	PRO	4.3
2	G	340	GLU	4.3
2	G	366	ASN	4.2
2	G	284	PHE	4.2
2	B	192	VAL	4.2
2	G	363	LEU	4.2
2	G	205	SER	4.1
1	D	740	LYS	4.1
2	C	208	PHE	4.1
2	F	353	SER	4.1
2	G	289	VAL	4.0
2	B	310	PRO	4.0
2	F	343	LEU	4.0
2	G	374	TYR	3.9
2	G	282	TRP	3.9
1	H	735	HIS	3.9
2	G	323	VAL	3.9
1	H	686	VAL	3.9
1	A	806	ASN	3.8
2	C	348	GLN	3.8
2	F	309	ILE	3.8
2	C	206	LEU	3.8
2	G	229	ARG	3.8
2	B	309	ILE	3.8
2	B	332	SER	3.8
2	G	288	LEU	3.7
2	F	313	HIS	3.7
1	E	805	VAL	3.7
2	G	285	VAL	3.7
2	C	274	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
2	G	315	GLY	3.6
2	F	330	ILE	3.6
2	G	346	LEU	3.6
2	G	327	ILE	3.6
2	C	333	ARG	3.5
1	H	794	LEU	3.5
1	H	630	ILE	3.5
2	G	367	CYS	3.4
2	C	369	LEU	3.4
2	B	335	TRP	3.4
2	G	251	THR	3.4
2	G	378	PHE	3.4
1	H	734	LEU	3.4
2	C	376	LYS	3.4
2	B	285	VAL	3.4
2	C	370	PRO	3.4
2	B	353	SER	3.4
2	G	232	VAL	3.4
2	G	180	GLU	3.3
2	G	201	LYS	3.3
2	F	335	TRP	3.3
2	C	352	SER	3.3
2	G	273	LYS	3.3
1	H	683	VAL	3.3
2	B	244	ALA	3.3
2	F	182	VAL	3.3
2	G	271	ARG	3.3
2	G	368	PHE	3.2
1	H	790	PHE	3.2
2	G	259	TYR	3.2
2	B	277	PRO	3.2
1	H	805	VAL	3.2
2	G	349	ASN	3.2
2	F	279	PRO	3.2
2	B	179	PHE	3.1
2	B	252	CYS	3.1
2	C	368	PHE	3.1
2	G	190	VAL	3.1
2	C	240	LEU	3.1
2	F	203	LEU	3.1
2	F	277	PRO	3.1
2	G	314	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	844	PHE	3.1
2	B	371	LEU	3.1
2	G	178	MET	3.1
1	H	748	PHE	3.1
2	F	252	CYS	3.1
2	F	332	SER	3.0
2	F	311	ASP	3.0
2	C	209	LEU	3.0
1	H	745	ARG	3.0
2	C	251	THR	3.0
2	B	365	LYS	3.0
2	G	179	PHE	3.0
2	G	195	LEU	2.9
2	C	288	LEU	2.9
1	A	805	VAL	2.9
2	C	203	LEU	2.9
2	G	365	LYS	2.9
2	B	331	ARG	2.9
2	G	338	VAL	2.8
2	G	272	PRO	2.8
2	G	198	ASP	2.8
2	G	283	MET	2.8
1	H	636	PHE	2.8
1	H	802	ALA	2.8
2	F	352	SER	2.8
2	G	304	MET	2.8
2	F	216	GLY	2.7
2	B	185	TRP	2.7
2	F	347	ALA	2.7
1	D	741	GLU	2.7
2	C	363	LEU	2.7
2	F	209	LEU	2.7
1	H	646	LEU	2.7
2	B	363	LEU	2.7
2	B	368	PHE	2.7
2	B	330	ILE	2.7
2	F	369	LEU	2.6
2	G	276	SER	2.6
2	C	367	CYS	2.6
2	C	179	PHE	2.6
1	H	631	ARG	2.6
2	G	369	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	739	PRO	2.5
2	C	378	PHE	2.5
2	F	290	LEU	2.5
2	F	285	VAL	2.5
1	H	789	TYR	2.5
2	G	207	GLY	2.4
1	H	791	TRP	2.4
2	B	347	ALA	2.4
2	F	274	PRO	2.4
2	B	338	VAL	2.4
2	C	252	CYS	2.4
2	G	351	GLN	2.4
2	G	242	TYR	2.4
2	C	362	LYS	2.4
1	E	878	ARG	2.4
2	F	338	VAL	2.4
1	E	844	PHE	2.3
2	C	345	LEU	2.3
2	G	333	ARG	2.3
1	H	649	LEU	2.3
1	D	852	GLU	2.3
2	B	239	ASP	2.3
2	C	283	MET	2.3
1	H	757	MET	2.3
2	G	181	THR	2.2
2	B	190	VAL	2.2
2	B	316	SER	2.2
2	B	288	LEU	2.2
2	B	333	ARG	2.2
1	H	750	LEU	2.2
2	C	371	LEU	2.2
2	B	276	SER	2.1
2	G	221	VAL	2.1
2	G	301	PHE	2.1
1	H	680	VAL	2.1
1	H	741	GLU	2.1
2	F	275	GLY	2.1
1	H	746	PRO	2.1
2	B	283	MET	2.1
2	G	337	LEU	2.1
2	B	256	PRO	2.1
2	B	206	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	811	LEU	2.0
1	A	854	ILE	2.0
2	G	223	ASP	2.0
1	H	758	GLY	2.0
1	D	901	LEU	2.0
2	B	311	ASP	2.0
2	F	375	PHE	2.0
2	B	281	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

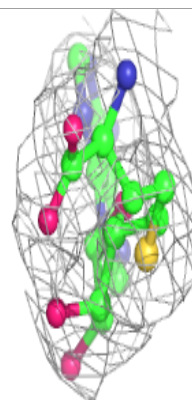
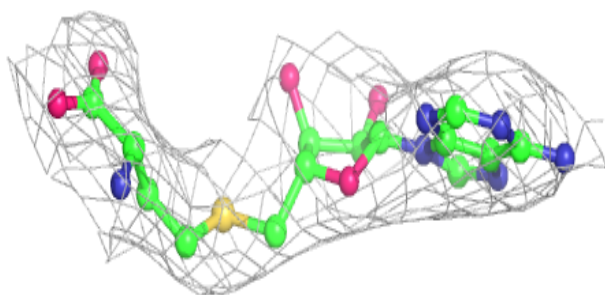
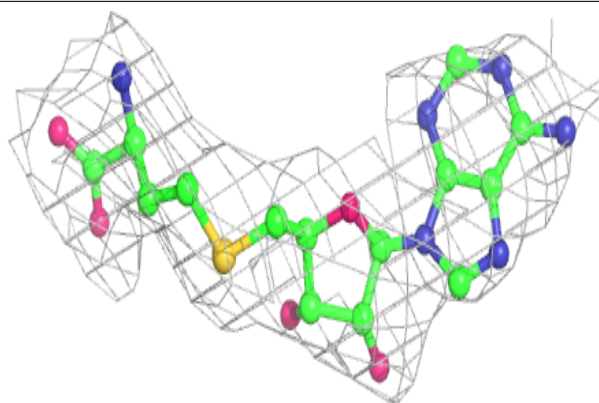
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SAH	H	8	26/26	0.90	0.18	49,104,112,114	0
3	SAH	D	4	26/26	0.91	0.21	40,59,71,73	0
3	SAH	A	1	26/26	0.93	0.23	38,67,84,95	0
3	SAH	E	5	26/26	0.96	0.19	31,56,66,69	0

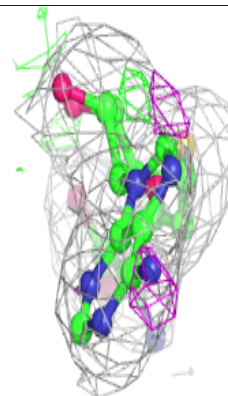
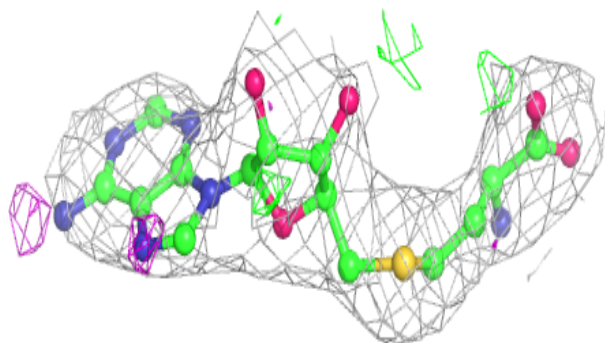
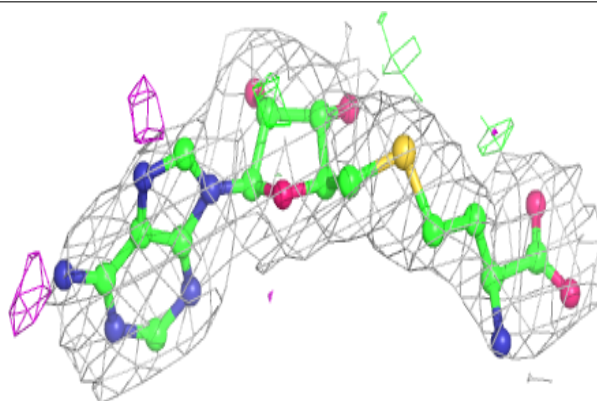
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SAH H 8:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

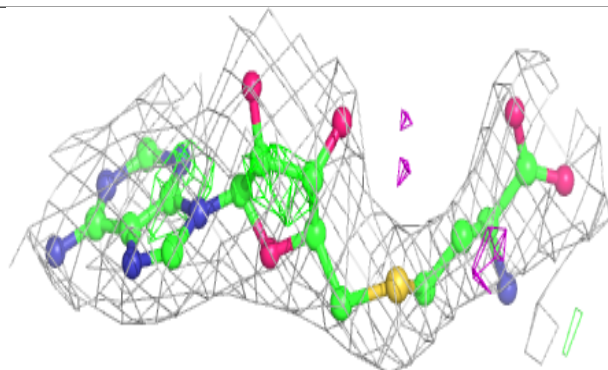
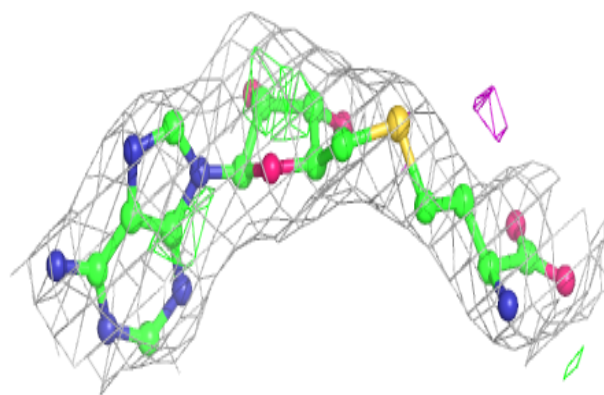
**Electron density around SAH D 4:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

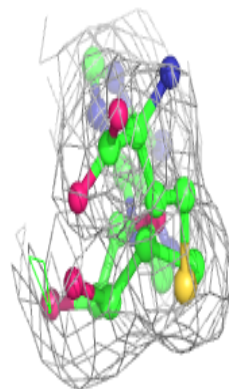
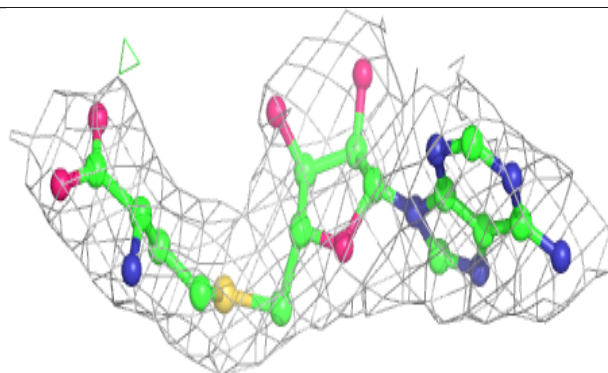
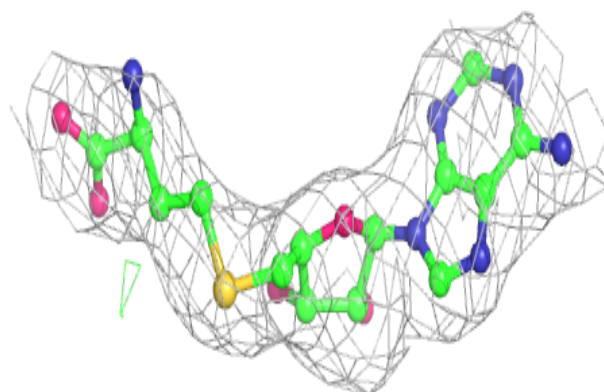


Electron density around SAH A 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around SAH E 5:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.