



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:43 PM UTC

PDB ID : 2QRV / pdb_00002qrv
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

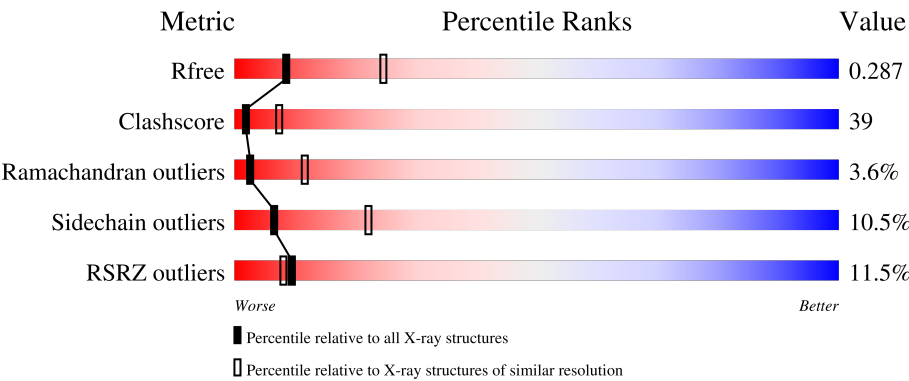
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of 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	3% 34%46%9%•8%
1	D	295	% 34%46%9%•9%
1	E	295	4% 35%43%13%•8%
1	H	295	8% 33%49%8%•9%
2	B	230	19% 37%33%10%19%

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Mol	Chain	Length	Quality of chain
2	C	230	11% 35% 40% 6% 19%
2	F	230	14% 38% 36% 7% 19%
2	G	230	28% 39% 37% 5% 19%

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:

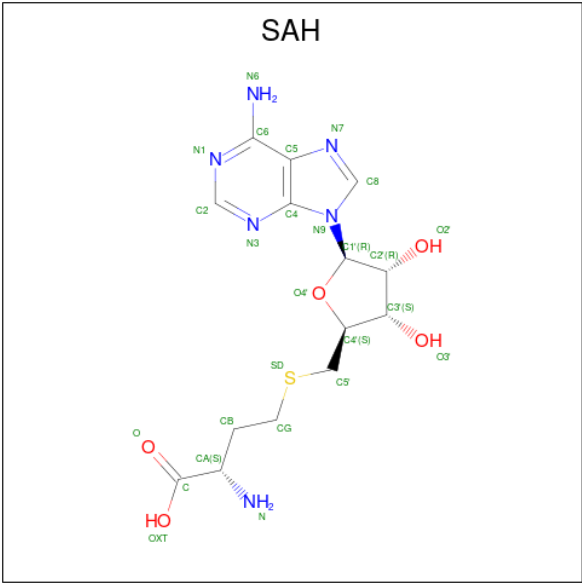
Chain	Residue	Modelled	Actual	Comment	Reference
B	157	GLY	-	expression tag	UNP Q9UJW3
B	158	SER	-	expression tag	UNP Q9UJW3
B	159	MET	-	expression tag	UNP Q9UJW3
C	157	GLY	-	expression tag	UNP Q9UJW3
C	158	SER	-	expression tag	UNP Q9UJW3
C	159	MET	-	expression tag	UNP Q9UJW3
F	157	GLY	-	expression tag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

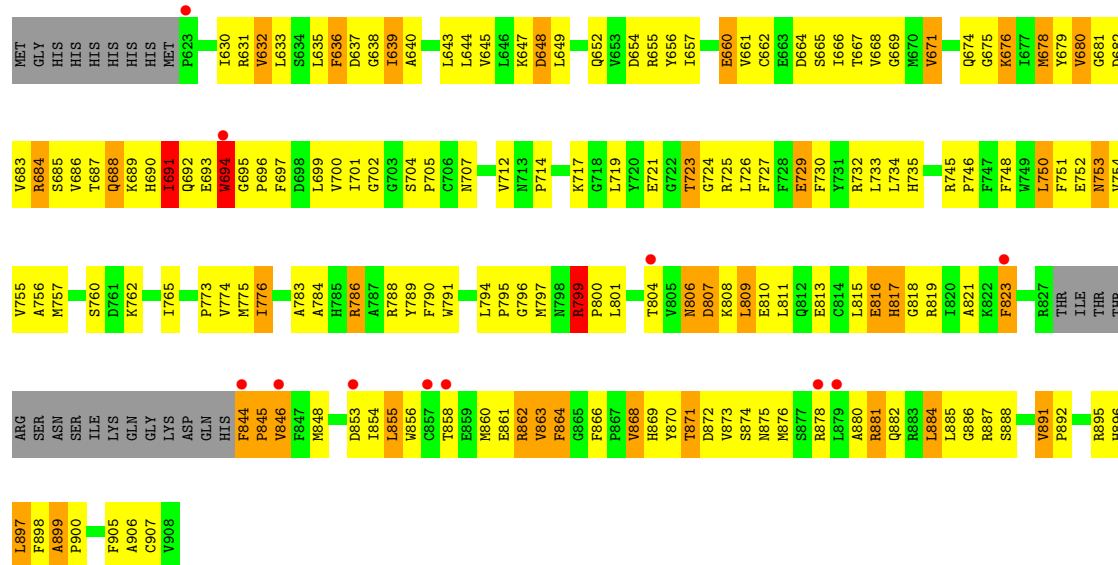
- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



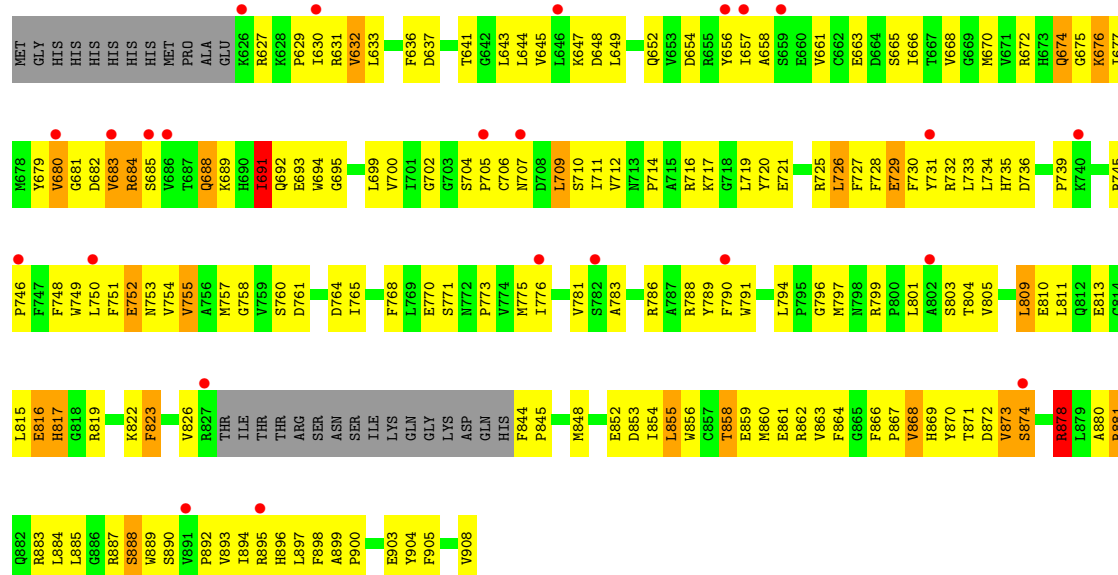
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	H	1	Total	C	N	O	S	0	0
			26	14	6	5	1		



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

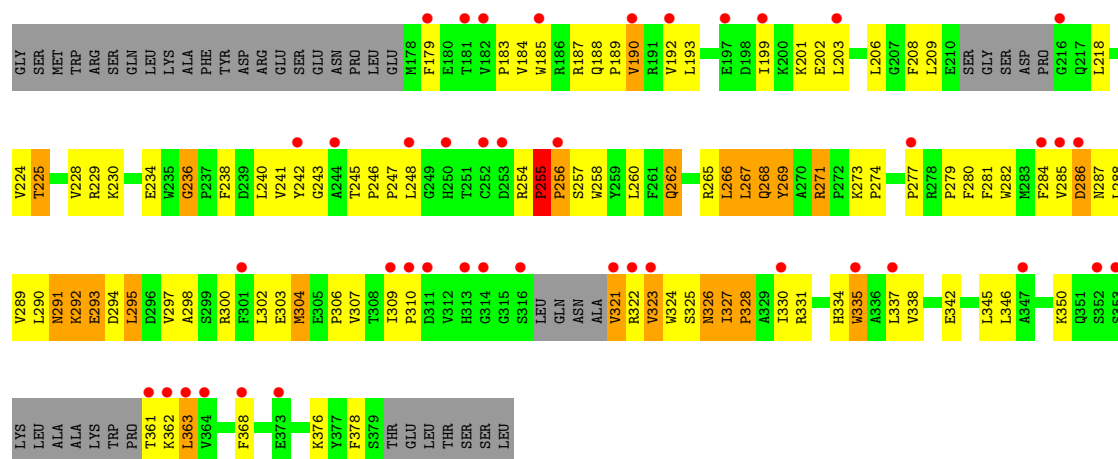


- Molecule 1: DNA (cytosine-5)-methyltransferase 3A

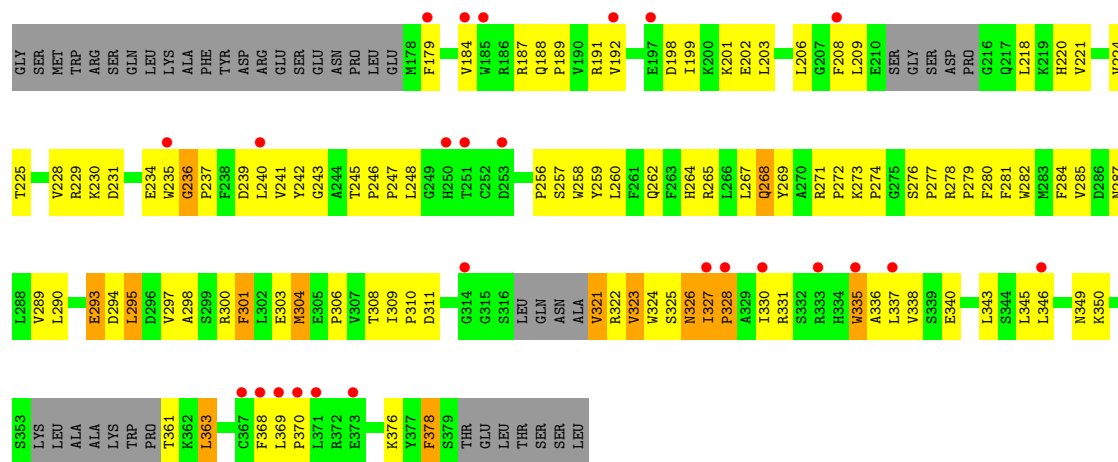


- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

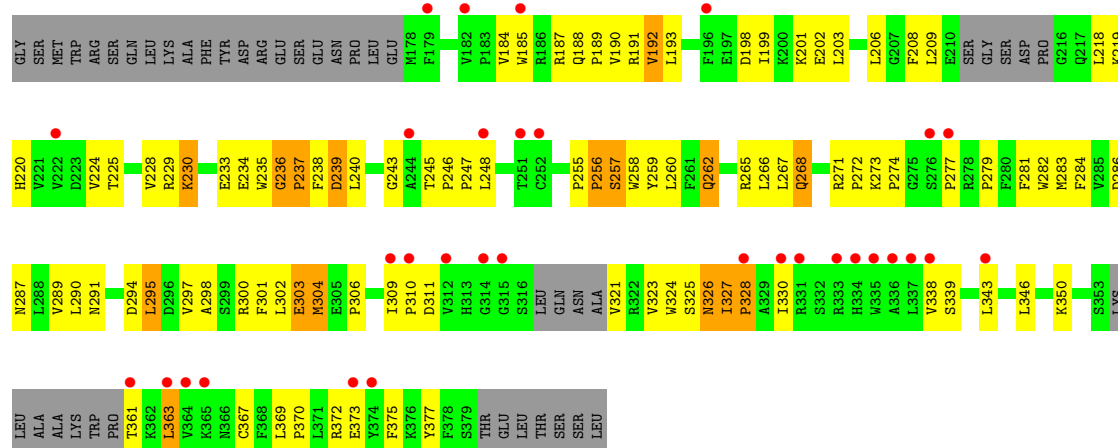




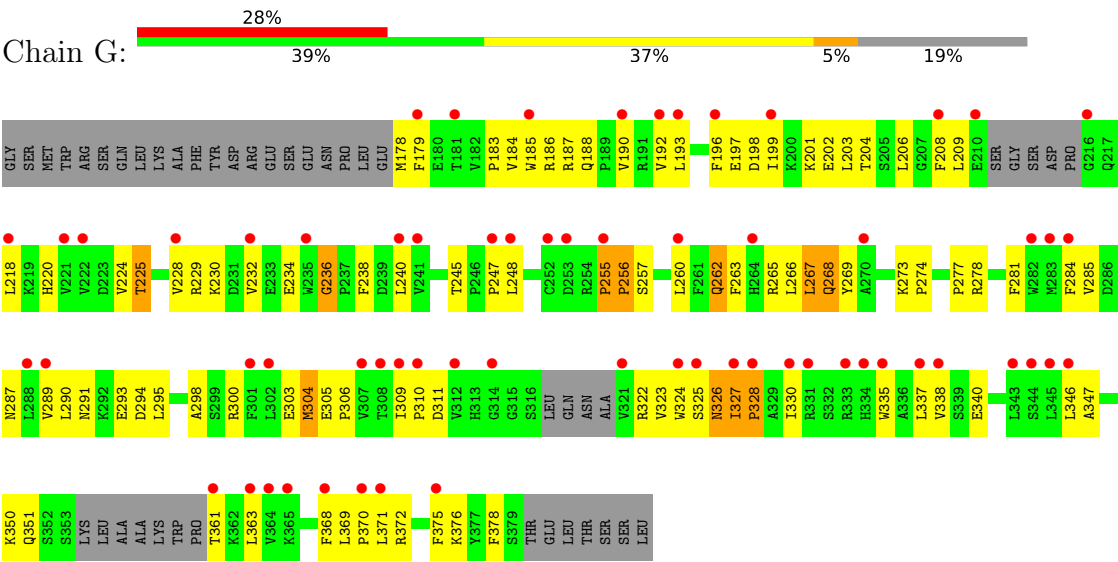
• Molecule 2: DNA (cytosine-5)-methyltransferase 3-like



• 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	401.88Å 401.88Å 49.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.90 – 2.89 38.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	81.9 (38.90-2.89) 92.7 (38.90-2.90)	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 0.271 , 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 , 77.4	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

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	0.66	1/2196 (0.0%)	1.25	25/2973 (0.8%)
1	D	0.59	0/2162	1.16	16/2926 (0.5%)
1	E	0.65	0/2180	1.18	19/2951 (0.6%)
1	H	0.50	0/2162	1.00	6/2926 (0.2%)
2	B	0.43	0/1560	0.96	8/2120 (0.4%)
2	C	0.41	0/1560	0.93	6/2120 (0.3%)
2	F	0.39	0/1560	0.91	7/2120 (0.3%)
2	G	0.41	0/1560	0.87	4/2120 (0.2%)
All	All	0.53	1/14940 (0.0%)	1.06	91/20256 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	860	MET	SD-CE	5.46	1.93	1.79

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	875	ASN	N-CA-C	-15.67	93.47	112.59
1	A	844	PHE	CA-C-N	14.91	138.48	119.84
1	A	844	PHE	C-N-CA	14.91	138.48	119.84
1	A	861	GLU	N-CA-C	-9.55	100.85	111.07
1	D	844	PHE	CA-C-N	8.69	130.70	119.84
1	D	844	PHE	C-N-CA	8.69	130.70	119.84
1	E	846	VAL	N-CA-C	8.66	119.09	108.53
1	A	844	PHE	C-N-CD	-8.29	91.00	125.00
1	E	799	ARG	CA-C-N	8.21	130.10	119.84
1	E	799	ARG	C-N-CA	8.21	130.10	119.84
1	E	685	SER	N-CA-C	-7.95	101.77	114.09
1	H	685	SER	N-CA-C	-7.73	102.11	114.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	887	ARG	N-CA-C	7.42	122.18	113.20
1	A	683	VAL	CB-CA-C	-7.39	102.25	111.70
1	D	685	SER	N-CA-C	-7.31	101.44	113.50
2	B	184	VAL	N-CA-C	7.25	118.04	110.72
1	A	685	SER	N-CA-C	-7.04	103.17	114.09
1	D	895	ARG	N-CA-C	-6.91	103.68	111.07
1	A	636	PHE	N-CA-C	-6.81	102.79	111.92
1	A	891	VAL	CA-C-N	6.76	126.71	119.28
1	A	891	VAL	C-N-CA	6.76	126.71	119.28
1	A	641	THR	N-CA-C	-6.74	104.01	111.36
1	D	873	VAL	N-CA-C	6.69	123.25	109.34
2	B	327	ILE	CA-C-N	6.62	128.12	119.84
2	B	327	ILE	C-N-CA	6.62	128.12	119.84
2	C	323	VAL	N-CA-C	6.53	118.19	108.46
1	H	636	PHE	N-CA-C	-6.43	103.31	111.92
2	B	255	PRO	CA-C-N	6.37	127.80	119.84
2	B	255	PRO	C-N-CA	6.37	127.80	119.84
1	E	858	THR	N-CA-C	-6.29	104.35	111.14
1	E	844	PHE	CA-C-N	6.29	127.70	119.84
1	E	844	PHE	C-N-CA	6.29	127.70	119.84
1	A	878	ARG	N-CA-C	-6.26	104.46	111.28
1	A	843	HIS	N-CA-C	6.23	124.08	110.80
1	A	895	ARG	N-CA-C	-6.20	104.45	111.14
2	F	327	ILE	CA-C-N	6.20	127.58	119.84
2	F	327	ILE	C-N-CA	6.20	127.58	119.84
1	D	636	PHE	N-CA-C	-6.12	103.73	111.92
1	A	844	PHE	N-CA-C	6.09	123.28	109.81
1	E	871	THR	N-CA-C	6.04	119.61	112.72
1	H	632	VAL	N-CA-C	6.02	118.52	109.20
2	B	293	GLU	N-CA-C	-5.97	103.54	111.24
2	B	323	VAL	N-CA-C	5.93	117.22	108.45
1	D	628	LYS	CA-C-N	5.81	125.72	119.85
1	D	628	LYS	C-N-CA	5.81	125.72	119.85
2	C	293	GLU	N-CA-C	-5.75	103.82	111.24
1	E	691	ILE	N-CA-C	5.75	116.21	110.23
1	D	853	ASP	N-CA-C	5.73	117.78	109.07
1	D	674	GLN	N-CA-C	5.71	119.06	111.30
1	E	632	VAL	N-CA-C	5.66	117.50	108.89
1	A	674	GLN	N-CA-C	5.66	118.99	111.30
1	A	824	SER	N-CA-C	-5.64	106.57	113.50
1	E	671	VAL	CB-CA-C	-5.60	104.80	111.97
1	A	799	ARG	CA-C-N	5.58	125.58	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	799	ARG	C-N-CA	5.58	125.58	119.89
1	A	866	PHE	N-CA-C	-5.52	102.11	110.50
1	H	817	HIS	N-CA-C	5.47	117.96	110.24
1	A	626	LYS	N-CA-C	5.46	117.78	110.35
1	D	854	ILE	N-CA-C	5.44	117.14	108.87
1	E	707	ASN	N-CA-C	5.43	120.28	111.37
1	E	704	SER	CA-C-N	5.42	126.61	119.84
1	E	704	SER	C-N-CA	5.42	126.61	119.84
2	B	292	LYS	N-CA-C	-5.41	106.64	113.18
2	F	323	VAL	N-CA-C	5.41	116.52	108.46
1	A	683	VAL	N-CA-CB	5.36	116.25	110.62
1	H	878	ARG	N-CA-C	-5.30	105.67	111.82
1	H	709	LEU	N-CA-C	-5.30	107.47	114.31
2	G	255	PRO	CA-C-N	5.29	126.45	119.84
2	G	255	PRO	C-N-CA	5.29	126.45	119.84
1	D	694	TRP	N-CA-C	-5.27	107.15	113.21
2	G	327	ILE	CA-C-N	5.26	126.42	119.84
2	G	327	ILE	C-N-CA	5.26	126.42	119.84
1	A	734	LEU	N-CA-C	-5.24	105.46	111.07
2	F	192	VAL	N-CA-C	5.21	115.46	108.17
1	E	636	PHE	N-CA-C	-5.19	104.97	111.92
1	D	632	VAL	N-CA-C	5.18	116.77	108.89
1	E	817	HIS	N-CA-C	5.18	117.98	110.42
1	D	861	GLU	N-CA-C	-5.12	104.96	111.11
1	E	891	VAL	CB-CA-C	-5.12	108.84	113.70
1	D	887	ARG	N-CA-C	5.11	118.39	112.97
2	F	255	PRO	CA-C-N	5.11	126.23	119.84
2	F	255	PRO	C-N-CA	5.11	126.23	119.84
1	A	875	ASN	N-CA-C	-5.11	104.67	111.87
2	C	378	PHE	N-CA-C	5.11	116.96	108.02
1	E	864	PHE	N-CA-C	5.11	119.27	113.19
2	C	184	VAL	N-CA-C	5.07	119.89	109.34
2	F	303	GLU	N-CA-C	5.07	118.62	111.52
2	C	327	ILE	CA-C-N	5.05	126.15	119.84
2	C	327	ILE	C-N-CA	5.05	126.15	119.84
1	A	794	LEU	CA-C-N	5.04	124.80	119.76
1	A	794	LEU	C-N-CA	5.04	124.80	119.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2143	0	2076	181	0
1	D	2111	0	2052	183	0
1	E	2128	0	2067	181	0
1	H	2111	0	2052	204	0
2	B	1515	0	1484	129	0
2	C	1515	0	1484	97	0
2	F	1515	0	1484	114	0
2	G	1515	0	1484	114	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	3	0
All	All	14657	0	14259	1135	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 39.

All (1135) 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:HH11	1:E:786:ARG:HG3	1.19	1.06
1:E:655:ARG:HH12	1:E:695:GLY:HA3	1.20	1.05
2:B:271:ARG:HG3	2:B:271:ARG:HH11	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:HE21	2:F:262:GLN:HA	1.26	0.97
2:F:363:LEU:HD22	2:F:363:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:326:ASN:HD22	2:C:326:ASN:H	1.19	0.89
1:A:878:ARG:HG2	1:A:878:ARG:HH11	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
1:A:843:HIS:C	1:A:845:PRO:HD3	1.99	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:A:775:MET:HE1	1:A:787:ALA:HB1	1.60	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:294:ASP:CG	1:D:725:ARG:HH22	1.86	0.83
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:H:704:SER:HG	1:H:751:PHE:HZ	1.24	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: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
2:G:256:PRO:HB3	2:G:290:LEU:HD23	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:ARG:HG3	2:B:271:ARG:NH1	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
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:HG3	1:E:786:ARG:NH1	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:H	2:B:326:ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HG2	1:A:878:ARG:NH1	1.99	0.73
2:C:228:VAL:HG12	2:C:229:ARG:N	2.02	0.72
1:E:788:ARG:HG2	1:E:788:ARG:HH11	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:N	2:B:268:GLN:HE21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:757:MET:HE1	1:E:765:ILE:HD12	1.72	0.70
2:F:363:LEU:H	2:F:363:LEU:CD2	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
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:N	1:H:823:PHE:CD1	2.57	0.69
1:H:666:ILE:HA	1:H:679:TYR:HE2	1.56	0.69
1:A:881:ARG:O	1:A:884:LEU:HB2	1.93	0.69
1:E:810:GLU:OE2	1:E:810:GLU:N	2.24	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
1:E:866:PHE:HE2	1:E:888:SER:HG	1.42	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:HA	2:G:262:GLN:NE2	2.09	0.68
1:E:757:MET:HE2	1:E:762:LYS:N	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:187:ARG:HH12	2:F:373:GLU:HA	1.59	0.66
2:G:363:LEU:H	2:G:363:LEU:HD22	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:H:810:GLU:CD	1:H:810:GLU:H	2.04	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
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:HD22	2:F:363:LEU:N	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
2:F:262:GLN:HA	2:F:262:GLN:NE2	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:872:ASP:HB3	1:H:869:HIS:CE1	2.33	0.63
2:F:230:LYS:HD2	2:F:230:LYS:N	2.12	0.63
2:G:228:VAL:HG12	2:G:229:ARG:N	2.13	0.63
2:B:199:ILE:HD11	2:B:242:TYR:CE2	2.33	0.63
2:G:262:GLN:HE21	2:G:262:GLN:CA	2.10	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:HG2	2:G:361:THR:HG23	1.79	0.63
2:G:202:GLU:O	2:G:206:LEU:HD23	1.99	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:HD2	2:F:230:LYS:H	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:H	2:B:363:LEU:CD2	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:D:673:HIS:C	1:D:674:GLN:HG2	2.24	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:282:TRP:CZ3	2:B:302:LEU:HD22	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:889:TRP:NE1	3:H:8:SAH:HN1	1.98	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:815:LEU:HA	1:H:859:GLU:CG	2.29	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
1:D:709:LEU:HD13	1:D:757:MET:HE3	1.84	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
1:A:853:ASP:CG	1:A:854:ILE:N	2.59	0.60
2:B:202:GLU:OE1	2:B:202:GLU:N	2.35	0.60
1:D:874:SER:C	1:D:876:MET:H	2.06	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:E:874:SER:C	1:E:876:MET:H	2.10	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:F:208:PHE:C	2:F:209:LEU:HD12	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:860:MET:HE1	1:E:882:GLN:HG2	1.85	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
1:A:843:HIS:ND1	1:A:843:HIS:N	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: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
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
2:G:185:TRP:H	2:G:185:TRP:CD1	2.21	0.58
1:D:649:LEU:HD22	1:D:899:ALA:HA	1.86	0.58
1:A:811:LEU:HG	1:A:811:LEU:O	2.02	0.58
2:B:203:LEU:HG	2:B:209:LEU:HD11	1.86	0.58
1:D:775:MET:HE1	1:D:787:ALA:HB1	1.86	0.58
1:H:817:HIS:C	1:H:817:HIS:CD2	2.82	0.58
2:C:346:LEU:O	2:C:350:LYS:HG2	2.04	0.58
2:F:372:ARG:HG2	2:F:372:ARG:HH11	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
1:A:875:ASN:CG	1:D:878:ARG:HD2	2.29	0.57
2:G:300:ARG:NH1	1:H:732:ARG:HH12	1.96	0.57
1:H:693:GLU:C	1:H:695:GLY:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:682:ASP:OD2	1:H:682:ASP:C	2.48	0.57
1:E:898:PHE:C	1:E:900:PRO:HD2	2.30	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
2:G:178:MET:HE3	2:G:179:PHE:O	2.05	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:A:872:ASP:HB3	1:D:869:HIS:CE1	2.41	0.56
2:C:230:LYS:H	2:C:230:LYS:HD2	1.70	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
2:C:309:ILE:HG13	2:C:321:VAL:HG12	1.88	0.56
1:E:823:PHE:N	1:E:823:PHE:CD1	2.72	0.56
2:F:286:ASP:OD2	2:F:290:LEU:HG	2.05	0.56
1:H:810:GLU:N	1:H:810:GLU:OE2	2.38	0.56
1:A:786:ARG:NH1	1:A:864:PHE:HE2	2.03	0.56
2:C:230:LYS:HD2	2:C:230:LYS:N	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
2:G:184:VAL:C	2:G:186:ARG:H	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:322:ARG:HH22	2:G:340:GLU:CD	2.12	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:H	2:B:326:ASN:ND2	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:711:ILE:HD11	1:D:757:MET:C	2.31	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:E:693:GLU:C	1:E:695:GLY:H	2.14	0.55
2:F:234:GLU:C	2:F:236:GLY:H	2.14	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
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:748:PHE:HB3	1:A:794:LEU:HD23	1.88	0.55
1:D:757:MET:HE1	1:D:765:ILE:HD12	1.89	0.55
2:G:372:ARG:HG2	2:G:372:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:635:LEU:HD12	1:A:730:PHE:HD1	1.70	0.54
1:A:716:ARG:HG2	1:A:716:ARG:HH11	1.70	0.54
1:D:819:ARG:NH1	1:D:853:ASP:OD1	2.40	0.54
1:E:817:HIS:C	1:E:817:HIS:CD2	2.85	0.54
1:E:848:MET:HE3	1:H:670:MET:CE	2.37	0.54
1:H:868:VAL:O	1:H:869:HIS:HB2	2.06	0.54
2:B:266:LEU:N	2:B:266:LEU:HD23	2.22	0.54
1:E:757:MET:HE2	1:E:762:LYS:CA	2.38	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
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:885:LEU:O	1:D:886:GLY:C	2.52	0.53
1:E:860:MET:HE1	1:E:882:GLN:CG	2.38	0.53
1:D:711:ILE:HD11	1:D:758:GLY:N	2.24	0.53
1:D:739:PRO:HG3	1:D:745:ARG:NH2	2.23	0.53
2:G:192:VAL:HG21	2:G:203:LEU:HD21	1.89	0.53
1:H:733:LEU:HD22	1:H:733:LEU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:694:TRP:HE3	1:E:694:TRP:HA	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:N	2:C:293:GLU:OE2	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
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
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
2:B:234:GLU:C	2:B:236:GLY:H	2.16	0.52
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: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
2:F:283:MET:HE3	2:F:327:ILE:HD12	1.91	0.52
2:G:363:LEU:HD22	2:G:363:LEU:N	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:268:GLN:HG2	1:H:735:HIS:NE2	2.25	0.52
2:G:281:PHE:CE2	2:G:328:PRO:HD3	2.40	0.52
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:D:810:GLU:H	1:D:810:GLU:CD	2.17	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:O	2:B:346:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:209:LEU:N	2:C:209:LEU:HD12	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
1:E:885:LEU:O	1:E:886:GLY:C	2.51	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:750:LEU:HD11	1:H:790:PHE:HD2	1.75	0.51
1:H:788:ARG:HG2	1:H:788:ARG:HH11	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:D:648:ASP:CG	1:D:895:ARG:HH12	2.19	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:848:MET:HE3	1:H:670:MET:HE2	1.92	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:324:TRP:O	2:G:325:SER:HB2	2.10	0.51
1:E:748:PHE:HB3	1:E:794:LEU:CD2	2.41	0.51
1:H:757:MET:HE1	1:H:765:ILE:HD12	1.92	0.51
1:A:671:VAL:CG1	1:D:816:GLU:HG2	2.41	0.51
2:C:346:LEU:HD23	2:C:346:LEU:C	2.36	0.51
1:D:693:GLU:C	1:D:695:GLY:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H:629:PRO:HB2	1:H:654:ASP:HB2	1.92	0.51
1:E:730:PHE:CE2	1:E:751:PHE:HB2	2.46	0.50
2:G:208:PHE:C	2:G:209:LEU:HD12	2.36	0.50
2:B:271:ARG:HH11	2:B:271:ARG:CG	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:HG2	1:E:788:ARG:NH1	2.21	0.50
1:E:810:GLU:H	1:E:810:GLU:CD	2.17	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:HD12	2:G:209:LEU:N	2.26	0.50
1:H:866:PHE:O	1:H:867:PRO:C	2.55	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:H	2:B:202:GLU:CD	2.20	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
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
2:F:218:LEU:HD23	2:F:218:LEU:C	2.37	0.50
1:A:693:GLU:C	1:A:695:GLY:H	2.19	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:807:ASP:O	1:E:809:LEU:HG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:234:GLU:C	2:C:236:GLY:H	2.20	0.49
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
1:E:816:GLU:CD	1:E:862:ARG:HH22	2.21	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
2:B:218:LEU:C	2:B:218:LEU:HD23	2.37	0.49
1:E:810:GLU:HG2	1:E:813:GLU:CB	2.42	0.49
2:G:346:LEU:O	2:G:346:LEU:HD23	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
2:F:326:ASN:HD22	2:F:326:ASN:N	1.92	0.49
2:F:346:LEU:C	2:F:346:LEU:HD23	2.37	0.49
1:H:754:VAL:HA	1:H:788:ARG:CD	2.42	0.49
1:A:716:ARG:HG2	1:A:716:ARG:NH1	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	1:E:786:ARG:CG	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:H:873:VAL:O	1:H:874:SER:C	2.57	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:C:208:PHE:C	2:C:209:LEU:HD12	2.38	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:B:304:MET:HE3	2:B:331:ARG:HE	1.79	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
1:E:881:ARG:HH22	1:H:872:ASP:CG	2.22	0.48
2:G:267:LEU:O	2:G:267:LEU:HD22	2.14	0.48
1:A:647:LYS:HZ1	1:A:673:HIS:HB3	1.78	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:HG22	2:F:199:ILE:O	2.14	0.48
1:H:720:TYR:HH	1:H:764:ASP:CG	2.21	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:218:LEU:C	2:C:218:LEU:HD23	2.40	0.47
2:C:327:ILE:O	2:C:330:ILE:HB	2.14	0.47
2:F:372:ARG:HD2	2:F:377:TYR:HB2	1.96	0.47
2:G:234:GLU:C	2:G:236:GLY:H	2.20	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:H:904:TYR:C	1:H:905:PHE:CD1	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:326:ASN:H	2:C:326:ASN:ND2	1.98	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:267:LEU:HD13	2:F:267:LEU:C	2.39	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:A:880:ALA:O	1:A:881:ARG:C	2.58	0.47
1:D:662:CYS:O	1:D:666:ILE:HG13	2.14	0.47
1:D:748:PHE:HB3	1:D:794:LEU:HD23	1.95	0.47
2:F:247:PRO:HA	2:F:287:ASN:ND2	2.29	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:H:663:GLU:O	1:H:666:ILE:HB	2.14	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:D:819:ARG:HH21	1:D:859:GLU:CD	2.21	0.47
1:E:702:GLY:O	1:E:751:PHE:HA	2.15	0.47
2:G:257:SER:OG	1:H:725:ARG:NH2	2.47	0.47
2:G:300:ARG:NH1	1:H:684:ARG:HB2	2.29	0.47
2:G:304:MET:HE2	2:G:305:GLU:O	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:755:VAL:HG13	1:E:756:ALA:N	2.30	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:D:699:LEU:HA	1:D:748:PHE:O	2.15	0.46
1:D:848:MET:O	1:D:849:ASN:C	2.59	0.46
1:D:871:THR:CB	1:D:881:ARG:HD3	2.46	0.46
1:D:873:VAL:HG23	1:D:874:SER:N	2.29	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:OE1	2:F:188:GLN:N	2.49	0.46
2:G:346:LEU:HD23	2:G:346:LEU:C	2.40	0.46
1:H:823:PHE:N	1:H:823:PHE:HD1	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
1:A:623:PRO:O	1:A:624:ALA:HB2	2.14	0.46
2:B:208:PHE:C	2:B:209:LEU:HD12	2.41	0.46
2:B:224:VAL:O	2:B:225:THR:C	2.59	0.46
2:C:262:GLN:CA	2:C:262:GLN:HE21	2.29	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:A:843:HIS:C	1:A:845:PRO:CD	2.82	0.46
1:D:801:LEU:H	1:D:801:LEU:CD1	2.21	0.46
1:D:819:ARG:CZ	1:D:846:VAL:HG21	2.46	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
1:H:661:VAL:O	1:H:661:VAL:HG22	2.16	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
1:A:898:PHE:O	1:A:899:ALA:C	2.58	0.46
2:B:309:ILE:HG13	2:B:309:ILE:O	2.15	0.46
1:E:757:MET:HE2	1:E:762:LYS:HA	1.96	0.46
1:A:860:MET:O	1:A:864:PHE:HD1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:346:LEU:HD23	2:B:346:LEU:C	2.41	0.45
2:F:372:ARG:HG2	2:F:372:ARG:NH1	2.31	0.45
1:H:705:PRO:HG2	1:H:726:LEU:HD12	1.97	0.45
1:A:682:ASP:OD2	1:A:682:ASP:C	2.58	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:D:898:PHE:O	1:D:899:ALA:C	2.59	0.45
1:E:643:LEU:HD22	1:E:656:TYR:CG	2.50	0.45
1:E:905:PHE:O	1:E:906:ALA:C	2.60	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: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
1:H:752:GLU:CG	1:H:753:ASN:N	2.79	0.45
1:H:794:LEU:O	1:H:797:MET:HG3	2.16	0.45
2:G:232:VAL:HG12	2:G:232:VAL:O	2.17	0.45
1:H:657:ILE:CG2	1:H:680:VAL:CG2	2.95	0.45
1:H:853:ASP:CG	1:H:854:ILE:N	2.74	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
1:D:652:GLN:CD	1:D:906:ALA:HB1	2.41	0.45
2:F:185:TRP:H	2:F:185:TRP:CD1	2.34	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:H:816:GLU:CD	1:H:862:ARG:NH2	2.75	0.45
1:A:757:MET:HE1	1:A:765:ILE:CD1	2.47	0.45
2:C:221:VAL:HG21	2:C:235:TRP:CH2	2.52	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:H:873:VAL:C	1:H:874:SER:O	2.60	0.45
1:A:773:PRO:HD3	1:A:791:TRP:NE1	2.32	0.45
1:A:872:ASP:CG	1:D:881:ARG:HH22	2.24	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
1:E:817:HIS:ND1	1:H:674:GLN:HB3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:192:VAL:HG21	2:F:203:LEU:CD2	2.42	0.45
1:D:812:GLN:OE1	1:D:821:ALA:N	2.34	0.45
2:F:257:SER:O	2:F:258:TRP:C	2.60	0.45
2:G:230:LYS:HD2	2:G:230:LYS:N	2.32	0.45
2:B:287:ASN:CG	2:B:287:ASN:O	2.60	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:HG2	2:G:372:ARG:NH1	2.31	0.45
1:A:891:VAL:N	1:A:892:PRO:CD	2.79	0.45
2:B:199:ILE:HG22	2:B:199:ILE:O	2.17	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
1:E:735:HIS:NE2	2:F:268:GLN:CG	2.80	0.45
2:G:188:GLN:N	2:G:188:GLN:OE1	2.50	0.45
1:H:711:ILE:HD11	1:H:757:MET:C	2.41	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:O	1:E:719:LEU:HG	2.16	0.44
1:E:810:GLU:HG2	1:E:813:GLU:H	1.82	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:675:GLY:O	1:A:676:LYS:C	2.60	0.44
1:A:725:ARG:HH12	2:B:297:VAL:CG2	2.17	0.44
1:A:808:LYS:H	1:A:808:LYS:HG2	1.56	0.44
1:A:875:ASN:HB3	1:D:878:ARG:CD	2.47	0.44
2:B:325:SER:OG	2:B:327:ILE:HG13	2.18	0.44
2:B:326:ASN:HD22	2:B:326:ASN:N	1.98	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:865:GLY:O	1:A:891:VAL:CB	2.66	0.44
2:C:231:ASP:OD1	2:C:231:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:203:LEU:C	2:G:209:LEU:HD13	2.42	0.44
1:A:899:ALA:HB3	1:A:900:PRO:CD	2.48	0.44
2:C:326:ASN:N	2:C:326:ASN:ND2	2.62	0.44
1:D:652:GLN:HG3	1:D:906:ALA:O	2.17	0.44
1:D:786:ARG:HH21	1:D:788:ARG:NH2	2.16	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:D:684:ARG:HB3	1:D:729:GLU:CD	2.43	0.44
1:E:675:GLY:O	1:E:676:LYS:C	2.60	0.44
1:H:670:MET:SD	1:H:670:MET:C	3.01	0.44
1:H:717:LYS:HB3	1:H:721:GLU:HB2	1.98	0.44
1:A:719:LEU:O	1:A:719:LEU:HG	2.18	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:G:248:LEU:N	2:G:287:ASN:HD22	2.15	0.44
1:H:760:SER:O	1:H:764:ASP:CG	2.61	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:684:ARG:HB3	1:A:729:GLU:CD	2.43	0.43
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:184:VAL:C	2:G:186:ARG:N	2.76	0.43
2:G:187:ARG:HB3	2:G:375:PHE:C	2.43	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
2:B:330:ILE:O	2:B:330:ILE:HG13	2.17	0.43
2:F:326:ASN:N	2:F:326:ASN:ND2	2.63	0.43
1:H:788:ARG:HG2	1:H:788:ARG:NH1	2.33	0.43
1:H:890:SER:O	1:H:893:VAL:HB	2.17	0.43
1:A:738:ARG:HA	1:A:747:PHE:CE2	2.52	0.43
1:A:739:PRO:HG3	1:A:745:ARG:CZ	2.48	0.43
1:A:750:LEU:HD11	1:A:790:PHE:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:ARG:O	1:A:887:ARG:HG2	2.18	0.43
2:B:289:VAL:HG22	2:B:289:VAL:O	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:682:ASP:CG	1:D:684:ARG:HE	2.26	0.43
1:D:706:CYS:O	1:D:707:ASN:C	2.60	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: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
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:672:ARG:CG	1:A:870:TYR:CE1	2.97	0.43
1:A:855:LEU:HD23	1:A:855:LEU:HA	1.84	0.43
1:A:857:CYS:O	1:A:858:THR:C	2.62	0.43
2:C:363:LEU:H	2:C:363:LEU:CD2	2.31	0.43
1:E:630:ILE:HD11	1:E:699:LEU:HD23	2.01	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:HD23	1:A:646:LEU:HA	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
1:E:723:THR:O	1:E:724:GLY:C	2.62	0.43
2:G:218:LEU:C	2:G:218:LEU:HD23	2.44	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:185:TRP:CD1	2:B:185:TRP:H	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:675:GLY:O	1:D:676:LYS:C	2.61	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
1:D:694:TRP:HE3	1:D:694:TRP:HA	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:HH11	1:A:878:ARG:CG	2.15	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
2:C:289:VAL:O	2:C:289:VAL:HG22	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:224:VAL:O	2:F:225:THR:C	2.61	0.43
2:F:282:TRP:CZ3	2:F:302:LEU:HD22	2.54	0.43
2:G:269:TYR:N	2:G:269:TYR:CD2	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:257:SER:O	2:B:258:TRP:C	2.62	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
1:H:720:TYR:N	1:H:720:TYR:CD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:326:ASN:H	2:G:326:ASN:ND2	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:E:687:THR:O	1:E:690:HIS:N	2.53	0.42
1:E:862:ARG:O	1:E:863:VAL:C	2.61	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:A:632:VAL:CG1	1:A:633:LEU:N	2.82	0.42
2:B:230:LYS:HD2	2:B:230:LYS:N	2.35	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:H	2:G:363:LEU:CD2	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
1:A:775:MET:SD	1:A:775:MET:C	3.03	0.42
1:A:809:LEU:O	1:A:825:LYS:NZ	2.45	0.42
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:777:ASP:C	1:A:779:LYS:H	2.27	0.42
1:A:849:ASN:O	1:A:850:GLU:CB	2.68	0.42
2:B:267:LEU:O	2:B:267:LEU:HD22	2.20	0.42
1:D:778:ALA:HB2	1:D:893:VAL:HG21	2.02	0.42
1:D:815:LEU:CD1	1:D:846:VAL:HG12	2.50	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
2:G:300:ARG:NH1	1:H:729:GLU:OE2	2.48	0.42
1:H:630:ILE:HG13	1:H:905:PHE:CE2	2.55	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:D:757:MET:HE2	1:D:761:ASP:CB	2.49	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:E:725:ARG:HH22	2:F:294:ASP:CG	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:881:ARG:NH2	1:H:872:ASP:OD2	2.49	0.42
2:G:224:VAL:O	2:G:225:THR:C	2.63	0.42
1:H:871:THR:HB	1:H:881:ARG:CG	2.50	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:N	2:C:368:PHE:CD2	2.86	0.42
1:D:773:PRO:HB2	1:D:789:TYR:HD1	1.84	0.42
1:D:816:GLU:CD	1:D:862:ARG:NH2	2.78	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:187:ARG:HB3	2:F:375:PHE:HA	2.01	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
1:H:898:PHE:N	1:H:898:PHE:CD2	2.86	0.42
1:D:694:TRP:HA	1:D:694:TRP:CE3	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
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:256:PRO:O	2:F:257:SER:C	2.63	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:C:179:PHE:HE2	2:C:280:PHE:H	1.60	0.41
2:C:229:ARG:HB2	1:D:770:GLU:OE1	2.21	0.41
2:C:343:LEU:HD12	2:C:343:LEU:HA	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:335:TRP:C	2:C:337:LEU:H	2.28	0.41
2:C:363:LEU:HD22	2:C:363:LEU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:691:ILE:HD12	1.81	0.41
1:A:702:GLY:O	1:A:751:PHE:HA	2.21	0.41
1:A:725:ARG:HH22	2:B:294:ASP:CG	2.27	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
2:C:224:VAL:O	2:C:225:THR:C	2.64	0.41
1:D:627:ARG:H	1:D:627:ARG:HG3	1.71	0.41
1:D:723:THR:O	1:D:724:GLY:C	2.62	0.41
1:D:763:ARG:O	1:D:764:ASP:C	2.63	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: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
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:691:ILE:HG22	1:E:692:GLN:N	2.32	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:H:861:GLU:OE2	1:H:871:THR:OG1	2.39	0.41
2:B:361:THR:C	2:B:363:LEU:N	2.79	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:368:PHE:N	2:B:368:PHE:CD2	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:E:788:ARG:NH1	1:E:788:ARG:CG	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:339:SER:O	2:F:343:LEU:HB2	2.21	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
2:B:256:PRO:O	2:B:257:SER:C	2.64	0.41
2:C:337:LEU:O	2:C:338:VAL:C	2.63	0.41
1:D:630:ILE:HA	1:D:905:PHE:CD2	2.56	0.41
1:D:860:MET:O	1:D:863:VAL:HB	2.21	0.41
1:E:856:TRP:CE2	1:H:874:SER:HA	2.55	0.41
2:F:234:GLU:C	2:F:236:GLY:N	2.79	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: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:H	1:D:808:LYS:HG2	1.71	0.40
2:F:325:SER:OG	2:F:327:ILE:HG13	2.21	0.40
2:B:203:LEU:CG	2:B:209:LEU:HD11	2.50	0.40
1:D:734:LEU:C	1:D:734:LEU:CD2	2.94	0.40
1:D:815:LEU:HD11	1:D:846:VAL:HG12	2.03	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
2:F:202:GLU:OE1	2:F:202:GLU:N	2.45	0.40
1:H:632:VAL:HG22	1:H:699:LEU:HB3	2.03	0.40
1:H:675:GLY:O	1:H:676:LYS:C	2.65	0.40
1:H:732:ARG:CZ	1:H:733:LEU:HD21	2.51	0.40
2:B:179:PHE:CE2	2:B:279:PRO:HA	2.56	0.40
2:C:322:ARG:HH22	2:C:340:GLU:CD	2.30	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
2:G:326:ASN:ND2	2:G:326:ASN:C	2.79	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:H	1:H:801:LEU:CD1	2.35	0.40
1:A:884:LEU:O	1:A:885:LEU:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:757:MET:HE1	1:H:765:ILE:CD1	2.50	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
1:D:853:ASP:CG	1:D:854:ILE:N	2.79	0.40
1:E:874:SER:C	1:E:876:MET:N	2.74	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%)	2	11
1	D	248/295 (84%)	208 (84%)	34 (14%)	6 (2%)	4	18
1	E	266/295 (90%)	223 (84%)	34 (13%)	9 (3%)	3	12
1	H	263/295 (89%)	226 (86%)	29 (11%)	8 (3%)	3	14
2	B	178/230 (77%)	135 (76%)	34 (19%)	9 (5%)	1	6
2	C	178/230 (77%)	138 (78%)	32 (18%)	8 (4%)	2	8
2	F	178/230 (77%)	136 (76%)	36 (20%)	6 (3%)	3	12
2	G	178/230 (77%)	138 (78%)	33 (18%)	7 (4%)	2	10
All	All	1757/2100 (84%)	1432 (82%)	262 (15%)	63 (4%)	2	11

All (63) 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
2	B	225	THR
2	B	304	MET
2	B	362	LYS
2	C	236	GLY
2	C	304	MET
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

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Mol	Chain	Res	Type
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%)	191 (85%)	33 (15%)	3	10
1	D	222/259 (86%)	195 (88%)	27 (12%)	5	16
1	E	223/259 (86%)	185 (83%)	38 (17%)	2	7
1	H	222/259 (86%)	200 (90%)	22 (10%)	7	24
2	B	166/210 (79%)	152 (92%)	14 (8%)	10	31
2	C	166/210 (79%)	153 (92%)	13 (8%)	11	35
2	F	166/210 (79%)	156 (94%)	10 (6%)	17	47
2	G	166/210 (79%)	159 (96%)	7 (4%)	26	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1555/1876 (83%)	1391 (90%)	164 (10%)	6 22

All (164) 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	668	VAL
1	A	671	VAL
1	A	674	GLN
1	A	682	ASP
1	A	683	VAL
1	A	684	ARG
1	A	688	GLN
1	A	691	ILE
1	A	701	ILE
1	A	760	SER
1	A	775	MET
1	A	776	ILE
1	A	782	SER
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	846	VAL
1	A	848	MET
1	A	858	THR
1	A	867	PRO
1	A	868	VAL
1	A	878	ARG
1	A	881	ARG
1	A	891	VAL
1	A	904	TYR
1	A	907	CYS
2	B	190	VAL
2	B	255	PRO
2	B	262	GLN
2	B	266	LEU

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Mol	Chain	Res	Type
2	B	267	LEU
2	B	268	GLN
2	B	269	TYR
2	B	271	ARG
2	B	286	ASP
2	B	295	LEU
2	B	321	VAL
2	B	326	ASN
2	B	335	TRP
2	B	363	LEU
2	C	239	ASP
2	C	256	PRO
2	C	257	SER
2	C	267	LEU
2	C	268	GLN
2	C	295	LEU
2	C	301	PHE
2	C	308	THR
2	C	321	VAL
2	C	326	ASN
2	C	328	PRO
2	C	335	TRP
2	C	363	LEU
1	D	631	ARG
1	D	644	LEU
1	D	648	ASP
1	D	665	SER
1	D	674	GLN
1	D	684	ARG
1	D	692	GLN
1	D	694	TRP
1	D	705	PRO
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

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Mol	Chain	Res	Type
1	D	816	GLU
1	D	823	PHE
1	D	826	VAL
1	D	845	PRO
1	D	853	ASP
1	D	855	LEU
1	D	881	ARG
1	D	884	LEU
1	E	639	ILE
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	678	MET
1	E	684	ARG
1	E	688	GLN
1	E	691	ILE
1	E	694	TRP
1	E	723	THR
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	853	ASP
1	E	855	LEU
1	E	862	ARG
1	E	863	VAL

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Mol	Chain	Res	Type
1	E	868	VAL
1	E	881	ARG
1	E	884	LEU
1	E	907	CYS
2	F	230	LYS
2	F	237	PRO
2	F	239	ASP
2	F	257	SER
2	F	262	GLN
2	F	268	GLN
2	F	295	LEU
2	F	326	ASN
2	F	328	PRO
2	F	363	LEU
2	G	262	GLN
2	G	267	LEU
2	G	268	GLN
2	G	295	LEU
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	688	GLN
1	H	691	ILE
1	H	694	TRP
1	H	729	GLU
1	H	752	GLU
1	H	755	VAL
1	H	803	SER
1	H	809	LEU
1	H	816	GLU
1	H	823	PHE
1	H	855	LEU
1	H	858	THR
1	H	868	VAL
1	H	878	ARG

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Mol	Chain	Res	Type
1	H	881	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	753	ASN
1	A	869	HIS
1	A	896	HIS
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	217	GLN
2	C	262	GLN
2	C	264	HIS
2	C	268	GLN
2	C	287	ASN
2	C	326	ASN
2	C	334	HIS
1	D	707	ASN
1	D	753	ASN
1	D	869	HIS
1	D	896	HIS
1	E	688	GLN
1	E	753	ASN
1	E	817	HIS
1	E	875	ASN
2	F	262	GLN
2	F	264	HIS
2	F	287	ASN
2	F	326	ASN
2	F	351	GLN
2	G	262	GLN
2	G	268	GLN
2	G	287	ASN
2	G	313	HIS
2	G	326	ASN
1	H	674	GLN
1	H	688	GLN
1	H	753	ASN

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Mol	Chain	Res	Type
1	H	785	HIS
1	H	798	ASN
1	H	817	HIS
1	H	896	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	27,28,28	1.61	6 (22%)	36,40,40	1.96	9 (25%)
3	SAH	A	1	-	27,28,28	1.66	5 (18%)	36,40,40	2.02	9 (25%)
3	SAH	D	4	-	27,28,28	1.62	5 (18%)	36,40,40	2.03	10 (27%)
3	SAH	E	5	-	27,28,28	1.68	4 (14%)	36,40,40	1.69	8 (22%)

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	SAH	C1'-N9	-4.93	1.32	1.46
3	E	5	SAH	C1'-N9	-4.88	1.32	1.46
3	A	1	SAH	C1'-N9	-4.28	1.34	1.46
3	H	8	SAH	C1'-N9	-4.23	1.34	1.46
3	E	5	SAH	C2-N3	3.23	1.39	1.33
3	H	8	SAH	C4-N9	2.79	1.43	1.37
3	D	4	SAH	C2-N3	2.64	1.38	1.33
3	A	1	SAH	C2-N3	2.63	1.38	1.33
3	D	4	SAH	C4-N9	2.62	1.43	1.37
3	A	1	SAH	C4-N9	2.57	1.43	1.37
3	A	1	SAH	C2'-C3'	2.51	1.60	1.53
3	E	5	SAH	C2-N1	2.49	1.38	1.33
3	A	1	SAH	O4'-C1'	2.43	1.47	1.42
3	H	8	SAH	O4'-C1'	2.40	1.47	1.42
3	H	8	SAH	C2-N3	2.36	1.38	1.33
3	E	5	SAH	O4'-C1'	2.22	1.47	1.42
3	H	8	SAH	C5-N7	2.17	1.43	1.39
3	D	4	SAH	C2'-C3'	2.05	1.58	1.53
3	H	8	SAH	CB-CA	-2.04	1.48	1.53
3	D	4	SAH	C2-N1	2.02	1.37	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	SAH	O4'-C1'-C2'	-6.53	92.63	106.62
3	D	4	SAH	O4'-C4'-C5'	-6.51	92.07	108.83
3	H	8	SAH	CB-CG-SD	-5.58	100.99	113.45
3	E	5	SAH	N3-C2-N1	-4.54	121.71	128.58
3	D	4	SAH	O4'-C1'-C2'	-4.28	97.45	106.62
3	H	8	SAH	O4'-C1'-N9	4.27	116.28	108.09
3	A	1	SAH	N3-C2-N1	-4.14	122.31	128.58
3	H	8	SAH	N3-C2-N1	-4.09	122.39	128.58
3	D	4	SAH	C1'-N9-C8	3.98	135.94	127.09
3	A	1	SAH	C1'-N9-C8	3.96	135.89	127.09
3	H	8	SAH	C1'-N9-C8	3.91	135.77	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	SAH	C1'-N9-C8	3.86	135.66	127.09
3	D	4	SAH	N3-C2-N1	-3.80	122.82	128.58
3	A	1	SAH	CB-CG-SD	-3.70	105.18	113.45
3	D	4	SAH	CB-CG-SD	-3.38	105.91	113.45
3	E	5	SAH	CB-CG-SD	-3.32	106.03	113.45
3	E	5	SAH	C2-N1-C6	3.22	124.01	118.73
3	A	1	SAH	CB-CA-N	3.11	118.24	110.12
3	H	8	SAH	C2-N1-C6	3.11	123.83	118.73
3	E	5	SAH	C4-N9-C1'	-2.92	119.81	126.63
3	D	4	SAH	C4-N9-C1'	-2.82	120.03	126.63
3	H	8	SAH	O4'-C1'-C2'	-2.77	100.69	106.62
3	A	1	SAH	C2-N1-C6	2.75	123.24	118.73
3	D	4	SAH	C2-N1-C6	2.72	123.20	118.73
3	A	1	SAH	C4-N9-C1'	-2.63	120.48	126.63
3	H	8	SAH	C4-N9-C1'	-2.60	120.54	126.63
3	H	8	SAH	O4'-C4'-C3'	2.49	110.10	105.15
3	A	1	SAH	C2'-C1'-N9	2.47	119.45	113.30
3	H	8	SAH	C4'-O4'-C1'	-2.17	104.68	109.47
3	D	4	SAH	C4'-O4'-C1'	-2.16	104.69	109.47
3	E	5	SAH	C4'-C5'-SD	-2.16	106.08	113.78
3	D	4	SAH	CB-CA-N	2.12	115.65	110.12
3	E	5	SAH	O4'-C4'-C5'	-2.08	103.47	108.83
3	A	1	SAH	C4-N9-C8	-2.03	103.60	105.74
3	D	4	SAH	O3'-C3'-C2'	2.02	118.30	111.82
3	E	5	SAH	O4'-C1'-C2'	-2.01	102.31	106.62

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	8	SAH	C2'-C1'-N9-C8
3	H	8	SAH	CA-CB-CG-SD
3	H	8	SAH	C2'-C1'-N9-C4
3	D	4	SAH	CA-CB-CG-SD

There are no ring outliers.

3 monomers are involved in 5 short contacts:

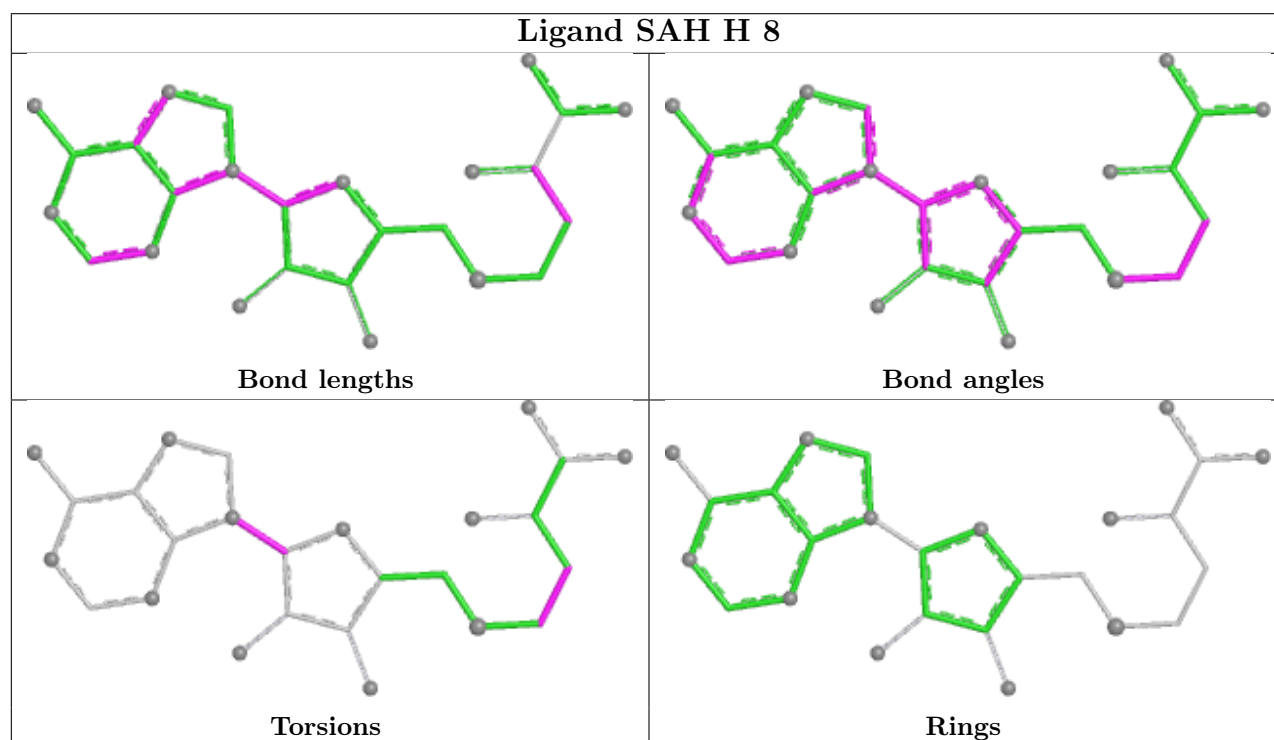
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	8	SAH	3	0
3	A	1	SAH	1	0

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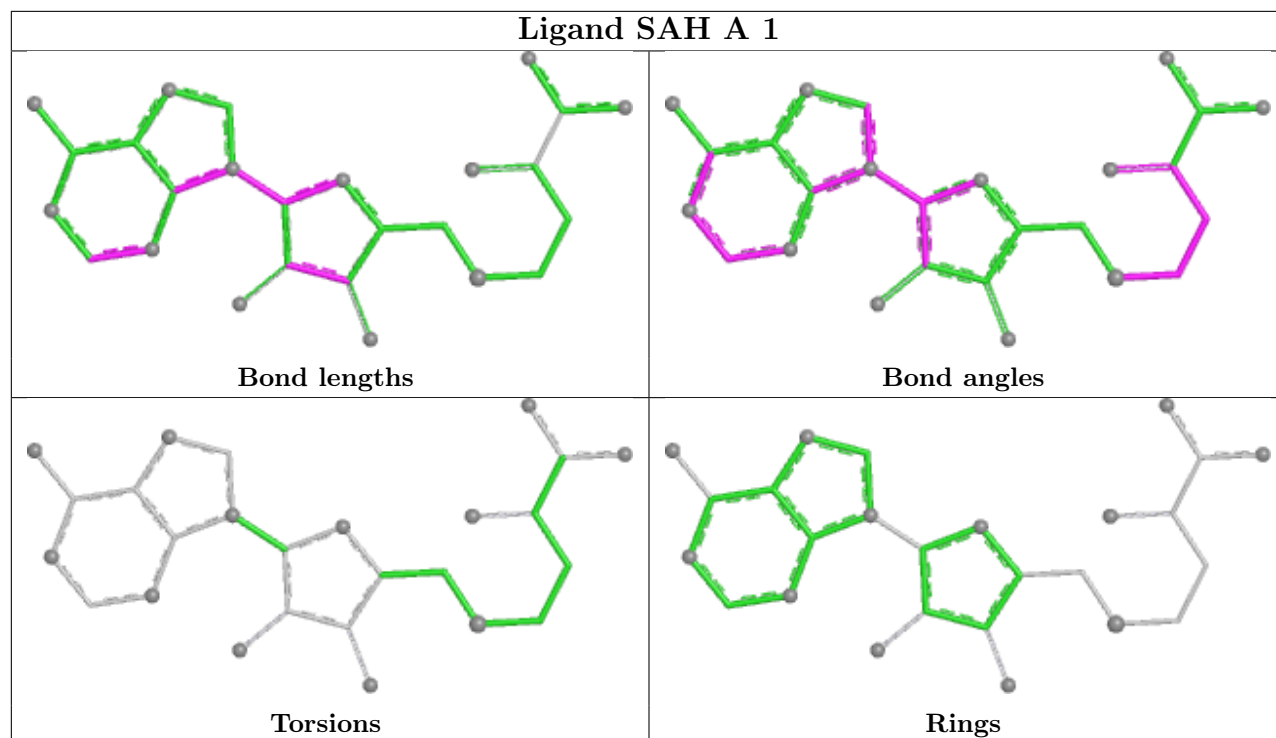
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5	SAH	1	0

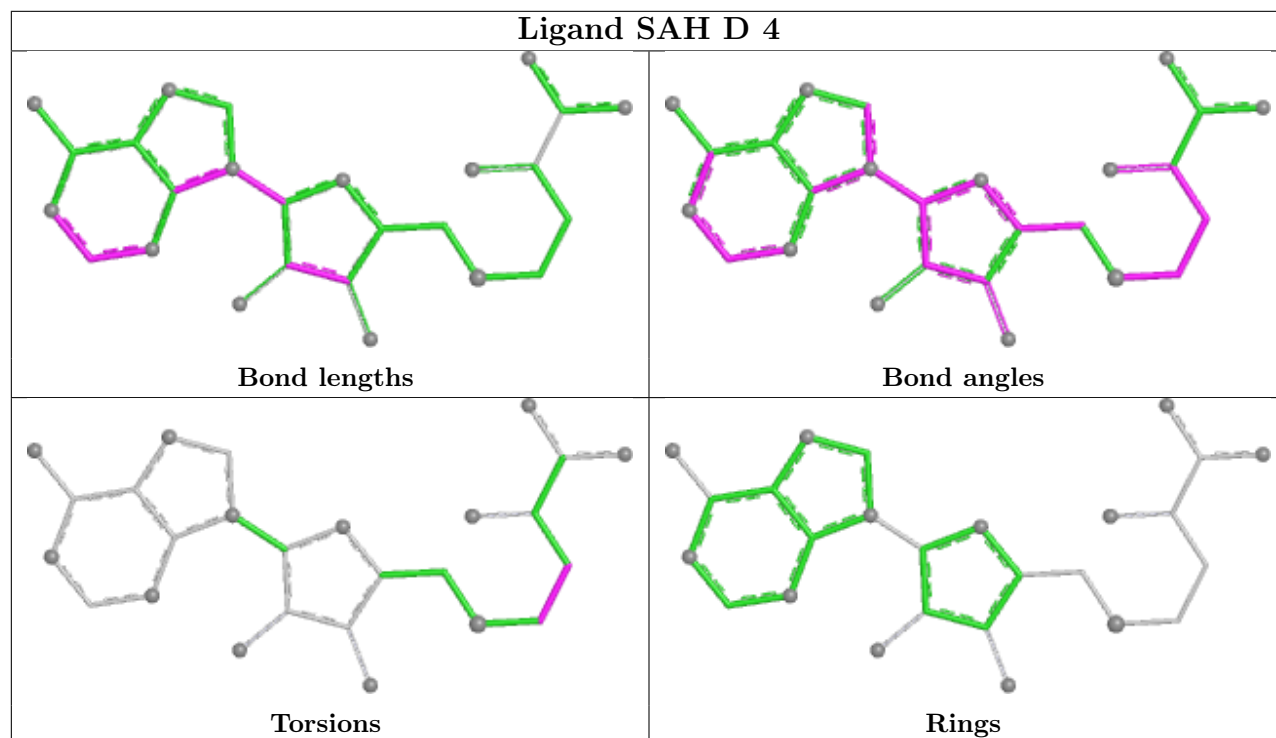
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

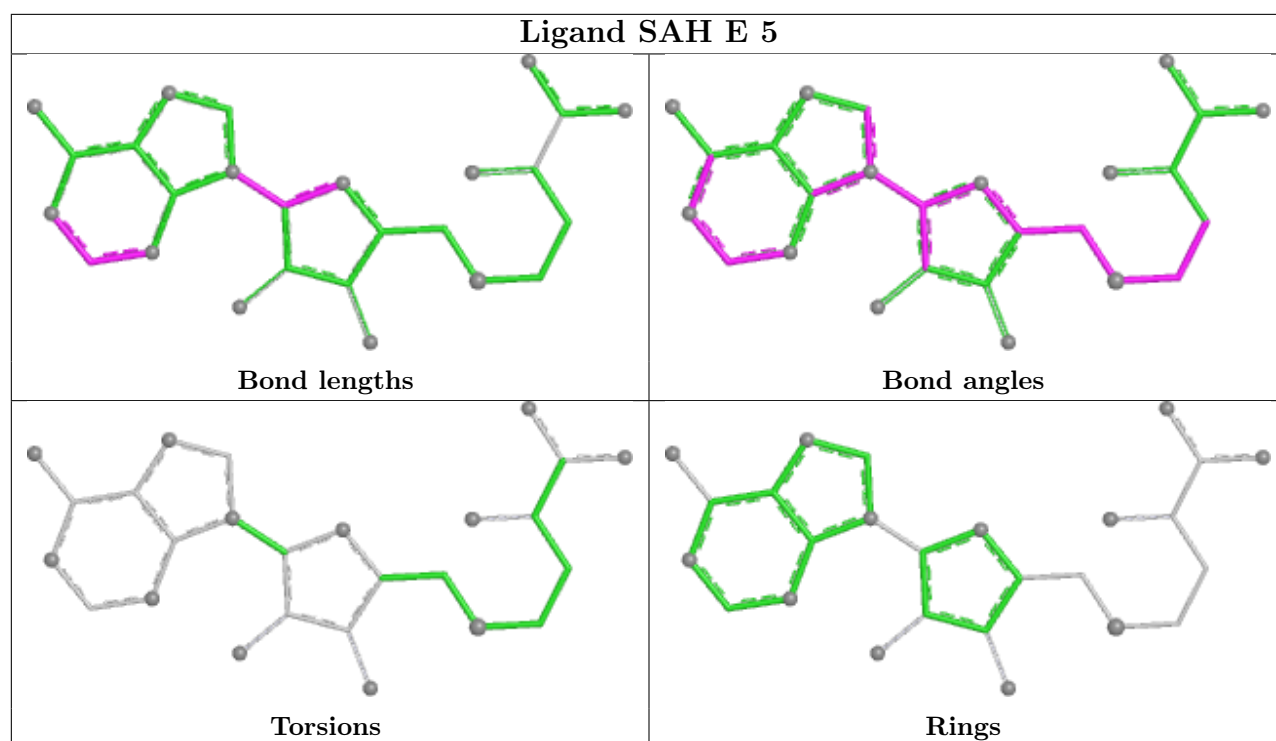


Ligand SAH A 1



Ligand SAH D 4





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.28	8 (2%)	53	45	30, 64, 106, 146	0
1	D	267/295 (90%)	0.24	3 (1%)	78	71	37, 75, 122, 157	0
1	E	270/295 (91%)	0.38	11 (4%)	41	33	27, 67, 111, 132	0
1	H	267/295 (90%)	0.79	24 (8%)	15	13	51, 101, 138, 170	0
2	B	186/230 (80%)	1.21	43 (23%)	2	2	55, 121, 187, 207	0
2	C	186/230 (80%)	0.95	25 (13%)	7	5	61, 118, 189, 206	0
2	F	186/230 (80%)	1.03	32 (17%)	4	3	62, 121, 188, 210	0
2	G	186/230 (80%)	1.69	64 (34%)	1	1	106, 163, 201, 210	0
All	All	1820/2100 (86%)	0.75	210 (11%)	9	8	27, 93, 181, 210	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	309	ILE	6.6
2	G	308	THR	5.8
1	E	878	ARG	5.6
2	F	315	GLY	5.5
2	G	221	VAL	5.2
2	C	330	ILE	4.9
2	G	321	VAL	4.9
2	B	363	LEU	4.8
2	G	302	LEU	4.7
2	B	242	TYR	4.5
2	C	185	TRP	4.4
2	G	282	TRP	4.3
2	G	330	ILE	4.3
2	G	222	VAL	4.3
2	G	196	PHE	4.3
2	F	310	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
2	F	335	TRP	4.2
2	F	182	VAL	4.1
2	F	276	SER	4.1
2	F	330	ILE	3.9
2	G	361	THR	3.9
2	B	352	SER	3.9
2	B	364	VAL	3.9
2	B	310	PRO	3.8
2	B	285	VAL	3.8
2	F	336	ALA	3.7
2	F	251	THR	3.7
2	G	375	PHE	3.7
2	C	369	LEU	3.7
2	B	203	LEU	3.6
2	G	328	PRO	3.6
2	C	367	CYS	3.6
2	C	370	PRO	3.6
2	B	330	ILE	3.6
2	G	199	ILE	3.6
2	G	241	VAL	3.5
2	B	244	ALA	3.5
2	C	192	VAL	3.4
1	H	680	VAL	3.4
2	F	363	LEU	3.4
1	A	845	PRO	3.4
2	F	337	LEU	3.3
2	B	185	TRP	3.3
2	F	277	PRO	3.3
2	G	248	LEU	3.3
2	G	334	HIS	3.3
1	H	874	SER	3.3
2	B	368	PHE	3.2
2	B	192	VAL	3.2
2	G	335	TRP	3.2
1	E	623	PRO	3.2
2	B	199	ILE	3.2
2	G	284	PHE	3.2
2	G	240	LEU	3.2
2	B	335	TRP	3.1
2	B	313	HIS	3.1
2	C	251	THR	3.1
2	G	327	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	740	LYS	3.1
2	G	371	LEU	3.1
2	G	312	VAL	3.1
2	B	314	GLY	3.1
2	F	312	VAL	3.0
2	G	190	VAL	3.0
2	G	364	VAL	3.0
2	F	343	LEU	3.0
2	G	208	PHE	3.0
2	F	334	HIS	3.0
2	G	324	TRP	3.0
2	F	185	TRP	3.0
1	A	806	ASN	3.0
2	G	310	PRO	3.0
1	A	908	VAL	3.0
1	H	782	SER	2.9
1	E	846	VAL	2.9
2	C	250	HIS	2.9
2	G	370	PRO	2.9
2	G	325	SER	2.9
2	F	244	ALA	2.9
1	A	844	PHE	2.9
2	G	228	VAL	2.9
2	F	331	ARG	2.9
2	C	240	LEU	2.9
2	B	216	GLY	2.9
2	C	335	TRP	2.9
2	F	364	VAL	2.9
2	G	192	VAL	2.9
2	B	309	ILE	2.9
2	C	235	TRP	2.8
2	C	314	GLY	2.8
2	G	301	PHE	2.8
2	G	260	LEU	2.8
1	E	857	CYS	2.8
2	B	321	VAL	2.8
1	H	790	PHE	2.8
2	F	328	PRO	2.7
2	C	368	PHE	2.7
2	B	361	THR	2.7
1	E	853	ASP	2.7
2	B	286	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	683	VAL	2.7
2	G	179	PHE	2.7
2	B	362	LYS	2.7
2	G	235	TRP	2.7
2	C	328	PRO	2.7
2	G	232	VAL	2.7
1	D	778	ALA	2.7
1	H	731	TYR	2.7
2	G	331	ARG	2.7
2	B	284	PHE	2.6
2	G	346	LEU	2.6
2	C	179	PHE	2.6
2	B	250	HIS	2.6
1	E	879	LEU	2.6
2	B	182	VAL	2.6
2	B	301	PHE	2.6
2	C	208	PHE	2.6
2	B	337	LEU	2.6
1	H	626	LYS	2.5
2	F	365	LYS	2.5
1	E	844	PHE	2.5
2	F	252	CYS	2.5
2	G	193	LEU	2.5
2	F	222	VAL	2.5
2	C	197	GLU	2.5
2	G	181	THR	2.5
2	B	316	SER	2.5
2	F	314	GLY	2.5
2	G	185	TRP	2.5
1	D	626	LYS	2.5
1	H	707	ASN	2.4
2	B	252	CYS	2.4
2	G	344	SER	2.4
2	G	210	GLU	2.4
1	H	630	ILE	2.4
2	B	190	VAL	2.4
2	B	322	ARG	2.4
1	H	776	ILE	2.4
2	F	338	VAL	2.4
2	G	289	VAL	2.4
2	G	314	GLY	2.3
2	F	179	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	656	TYR	2.3
1	E	823	PHE	2.3
2	G	218	LEU	2.3
1	E	858	THR	2.3
1	H	657	ILE	2.3
2	F	361	THR	2.3
2	G	307	VAL	2.3
1	A	850	GLU	2.3
1	E	804	THR	2.3
2	G	338	VAL	2.3
2	F	373	GLU	2.3
2	B	248	LEU	2.3
2	G	337	LEU	2.3
1	E	694	TRP	2.3
1	H	891	VAL	2.3
1	H	646	LEU	2.2
2	G	264	HIS	2.2
1	A	907	CYS	2.2
2	B	277	PRO	2.2
2	G	247	PRO	2.2
2	F	374	TYR	2.2
2	G	368	PHE	2.2
1	H	827	ARG	2.2
2	C	253	ASP	2.2
2	G	252	CYS	2.2
2	B	179	PHE	2.2
1	D	802	ALA	2.2
2	G	283	MET	2.2
1	H	685	SER	2.2
2	G	365	LYS	2.2
2	G	270	ALA	2.2
1	A	854	ILE	2.2
2	B	181	THR	2.2
2	B	353	SER	2.2
2	C	337	LEU	2.2
2	B	347	ALA	2.2
2	B	323	VAL	2.1
2	C	346	LEU	2.1
2	G	363	LEU	2.1
1	H	895	ARG	2.1
2	C	333	ARG	2.1
2	B	311	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	333	ARG	2.1
2	B	197	GLU	2.1
2	F	309	ILE	2.1
1	H	746	PRO	2.1
2	B	256	PRO	2.1
1	H	750	LEU	2.1
2	G	253	ASP	2.1
2	G	288	LEU	2.1
2	G	345	LEU	2.1
1	H	802	ALA	2.1
1	H	659	SER	2.1
1	H	705	PRO	2.1
2	G	255	PRO	2.1
2	G	343	LEU	2.1
2	C	327	ILE	2.1
2	B	373	GLU	2.1
1	A	843	HIS	2.0
2	C	184	VAL	2.0
2	C	371	LEU	2.0
2	F	248	LEU	2.0
2	G	216	GLY	2.0
2	B	253	ASP	2.0
2	C	373	GLU	2.0
2	F	333	ARG	2.0
2	F	196	PHE	2.0
1	H	686	VAL	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](#)

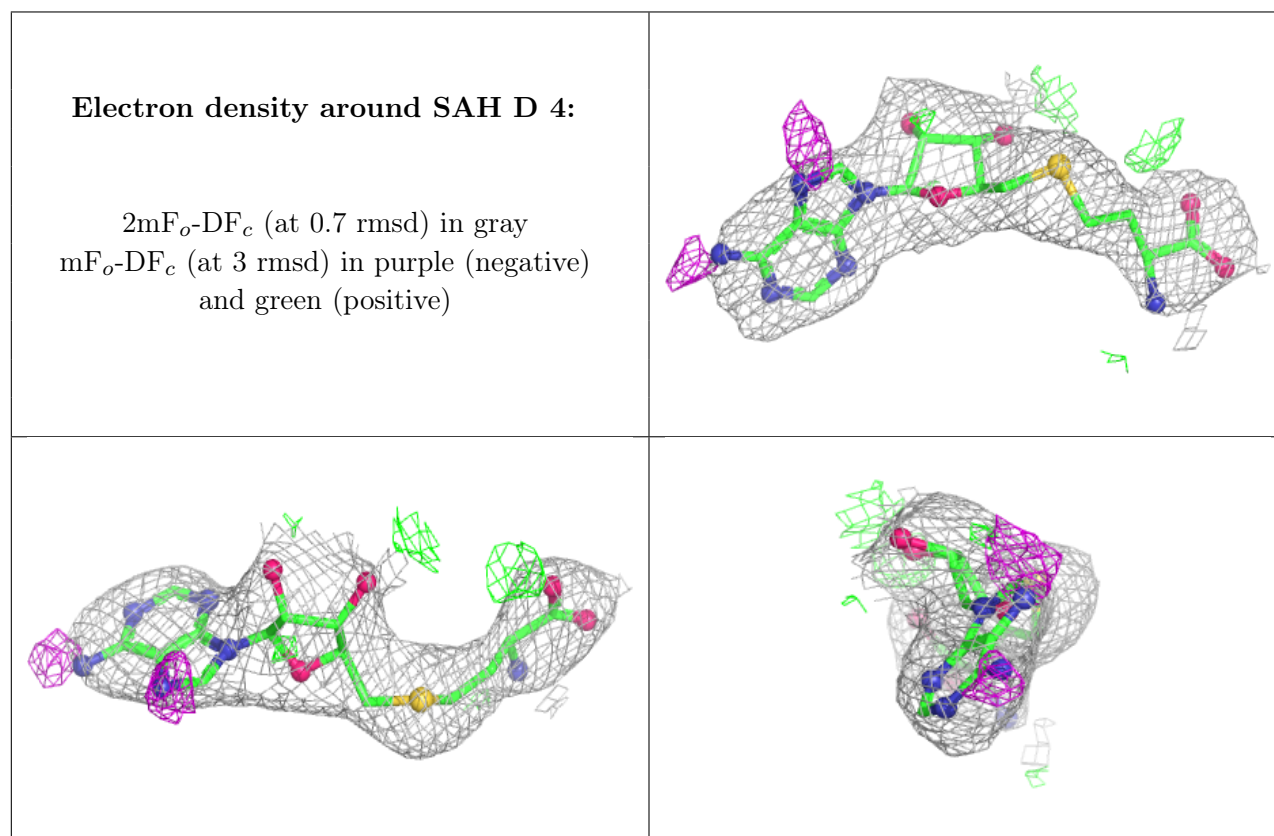
There are no oligosaccharides in this entry.

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.

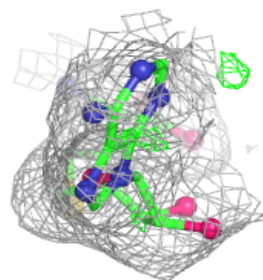
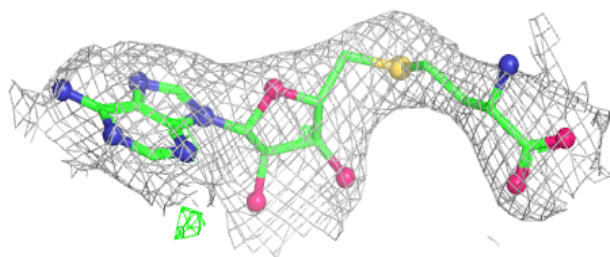
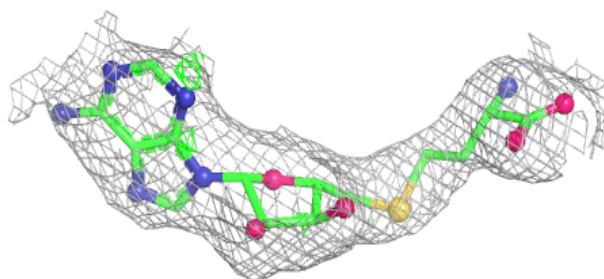
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SAH	D	4	26/26	0.89	0.11	40,59,71,73	0
3	SAH	A	1	26/26	0.90	0.13	38,67,84,95	0
3	SAH	H	8	26/26	0.90	0.12	49,104,112,114	0
3	SAH	E	5	26/26	0.93	0.09	31,56,66,69	0

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.

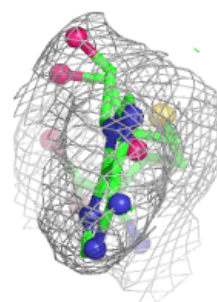
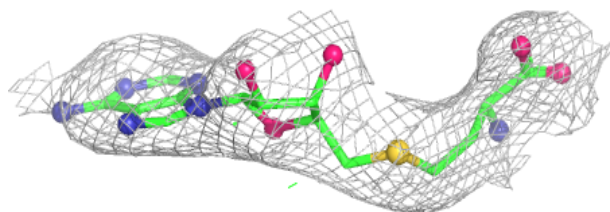
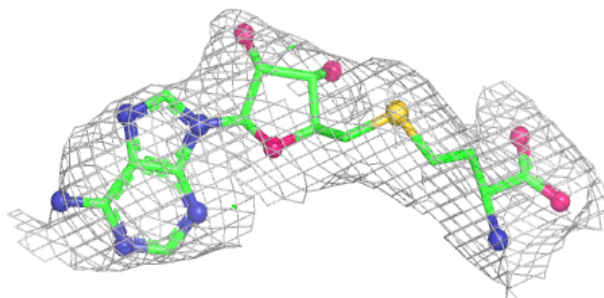


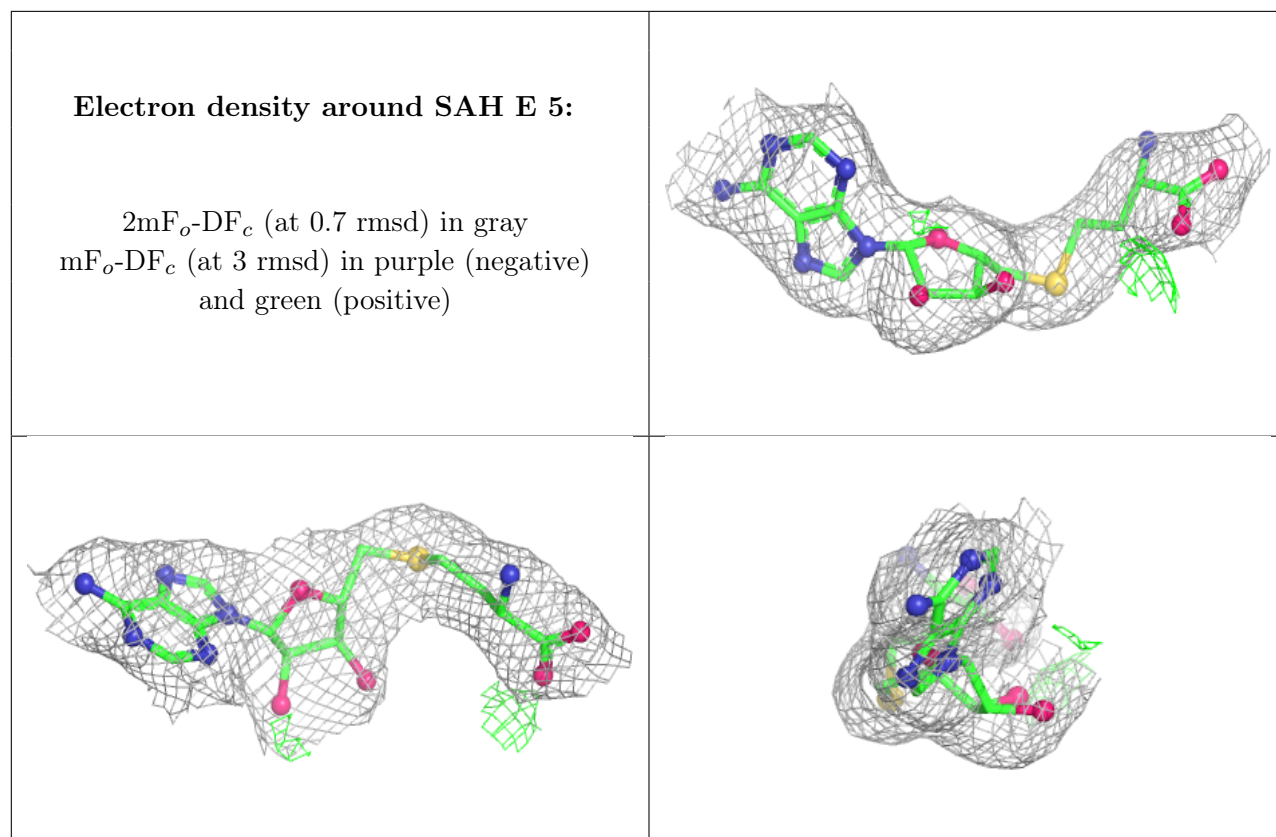
Electron density around SAH A 1:

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

**Electron density around SAH 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.