Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2024 – 05:21 pm BST

PDB ID	:	9F3X
Title	:	CutC choline lyase in complex with cyclopropylcholine
Authors	:	Kalnins, G.
Deposited on	:	2024-04-26
Resolution	:	2.70 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:

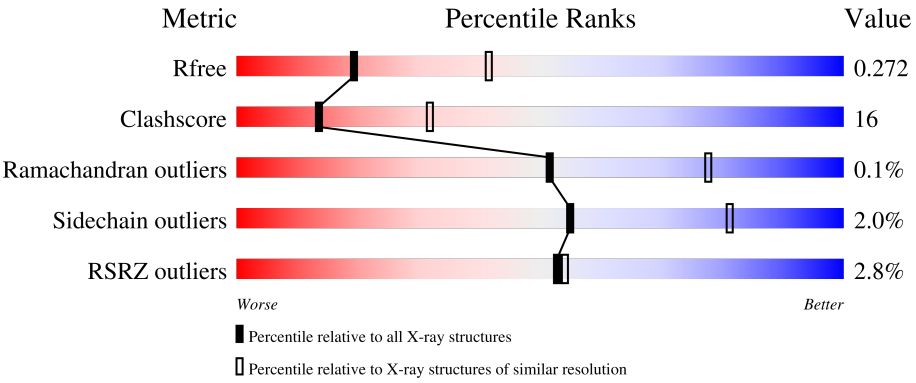
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	1150	52% 16% · 31%
1	B	1150	53% 15% 31%
1	C	1150	% 50% 18% · 31%
1	D	1150	% 45% 23% · 31%
1	E	1150	2% 45% 23% · 31%

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Mol	Chain	Length	Quality of chain
1	F	1150	3% 42% 26% 31%
1	G	1150	4% 41% 26% 31%
1	H	1150	5% 38% 30% 31%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 50434 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 Choline trimethylamine-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	B	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	C	791	Total	C	N	O	S	0	0	0
			6246	3949	1076	1180	41			
1	D	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	E	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	F	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	G	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	H	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP A0A486V7R5
A	-20	GLY	-	expression tag	UNP A0A486V7R5
A	-19	SER	-	expression tag	UNP A0A486V7R5
A	-18	SER	-	expression tag	UNP A0A486V7R5
A	-17	HIS	-	expression tag	UNP A0A486V7R5
A	-16	HIS	-	expression tag	UNP A0A486V7R5
A	-15	HIS	-	expression tag	UNP A0A486V7R5
A	-14	HIS	-	expression tag	UNP A0A486V7R5
A	-13	HIS	-	expression tag	UNP A0A486V7R5
A	-12	HIS	-	expression tag	UNP A0A486V7R5
A	-11	SER	-	expression tag	UNP A0A486V7R5
A	-10	GLN	-	expression tag	UNP A0A486V7R5
A	-9	ASP	-	expression tag	UNP A0A486V7R5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	expression tag	UNP A0A486V7R5
A	-7	GLU	-	expression tag	UNP A0A486V7R5
A	-6	ASN	-	expression tag	UNP A0A486V7R5
A	-5	LEU	-	expression tag	UNP A0A486V7R5
A	-4	TYR	-	expression tag	UNP A0A486V7R5
A	-3	PHE	-	expression tag	UNP A0A486V7R5
A	-2	GLN	-	expression tag	UNP A0A486V7R5
A	-1	GLY	-	expression tag	UNP A0A486V7R5
A	0	SER	-	expression tag	UNP A0A486V7R5
B	-21	MET	-	initiating methionine	UNP A0A486V7R5
B	-20	GLY	-	expression tag	UNP A0A486V7R5
B	-19	SER	-	expression tag	UNP A0A486V7R5
B	-18	SER	-	expression tag	UNP A0A486V7R5
B	-17	HIS	-	expression tag	UNP A0A486V7R5
B	-16	HIS	-	expression tag	UNP A0A486V7R5
B	-15	HIS	-	expression tag	UNP A0A486V7R5
B	-14	HIS	-	expression tag	UNP A0A486V7R5
B	-13	HIS	-	expression tag	UNP A0A486V7R5
B	-12	HIS	-	expression tag	UNP A0A486V7R5
B	-11	SER	-	expression tag	UNP A0A486V7R5
B	-10	GLN	-	expression tag	UNP A0A486V7R5
B	-9	ASP	-	expression tag	UNP A0A486V7R5
B	-8	HIS	-	expression tag	UNP A0A486V7R5
B	-7	GLU	-	expression tag	UNP A0A486V7R5
B	-6	ASN	-	expression tag	UNP A0A486V7R5
B	-5	LEU	-	expression tag	UNP A0A486V7R5
B	-4	TYR	-	expression tag	UNP A0A486V7R5
B	-3	PHE	-	expression tag	UNP A0A486V7R5
B	-2	GLN	-	expression tag	UNP A0A486V7R5
B	-1	GLY	-	expression tag	UNP A0A486V7R5
B	0	SER	-	expression tag	UNP A0A486V7R5
C	-21	MET	-	initiating methionine	UNP A0A486V7R5
C	-20	GLY	-	expression tag	UNP A0A486V7R5
C	-19	SER	-	expression tag	UNP A0A486V7R5
C	-18	SER	-	expression tag	UNP A0A486V7R5
C	-17	HIS	-	expression tag	UNP A0A486V7R5
C	-16	HIS	-	expression tag	UNP A0A486V7R5
C	-15	HIS	-	expression tag	UNP A0A486V7R5
C	-14	HIS	-	expression tag	UNP A0A486V7R5
C	-13	HIS	-	expression tag	UNP A0A486V7R5
C	-12	HIS	-	expression tag	UNP A0A486V7R5
C	-11	SER	-	expression tag	UNP A0A486V7R5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	GLN	-	expression tag	UNP A0A486V7R5
C	-9	ASP	-	expression tag	UNP A0A486V7R5
C	-8	HIS	-	expression tag	UNP A0A486V7R5
C	-7	GLU	-	expression tag	UNP A0A486V7R5
C	-6	ASN	-	expression tag	UNP A0A486V7R5
C	-5	LEU	-	expression tag	UNP A0A486V7R5
C	-4	TYR	-	expression tag	UNP A0A486V7R5
C	-3	PHE	-	expression tag	UNP A0A486V7R5
C	-2	GLN	-	expression tag	UNP A0A486V7R5
C	-1	GLY	-	expression tag	UNP A0A486V7R5
C	0	SER	-	expression tag	UNP A0A486V7R5
D	-21	MET	-	initiating methionine	UNP A0A486V7R5
D	-20	GLY	-	expression tag	UNP A0A486V7R5
D	-19	SER	-	expression tag	UNP A0A486V7R5
D	-18	SER	-	expression tag	UNP A0A486V7R5
D	-17	HIS	-	expression tag	UNP A0A486V7R5
D	-16	HIS	-	expression tag	UNP A0A486V7R5
D	-15	HIS	-	expression tag	UNP A0A486V7R5
D	-14	HIS	-	expression tag	UNP A0A486V7R5
D	-13	HIS	-	expression tag	UNP A0A486V7R5
D	-12	HIS	-	expression tag	UNP A0A486V7R5
D	-11	SER	-	expression tag	UNP A0A486V7R5
D	-10	GLN	-	expression tag	UNP A0A486V7R5
D	-9	ASP	-	expression tag	UNP A0A486V7R5
D	-8	HIS	-	expression tag	UNP A0A486V7R5
D	-7	GLU	-	expression tag	UNP A0A486V7R5
D	-6	ASN	-	expression tag	UNP A0A486V7R5
D	-5	LEU	-	expression tag	UNP A0A486V7R5
D	-4	TYR	-	expression tag	UNP A0A486V7R5
D	-3	PHE	-	expression tag	UNP A0A486V7R5
D	-2	GLN	-	expression tag	UNP A0A486V7R5
D	-1	GLY	-	expression tag	UNP A0A486V7R5
D	0	SER	-	expression tag	UNP A0A486V7R5
E	-21	MET	-	initiating methionine	UNP A0A486V7R5
E	-20	GLY	-	expression tag	UNP A0A486V7R5
E	-19	SER	-	expression tag	UNP A0A486V7R5
E	-18	SER	-	expression tag	UNP A0A486V7R5
E	-17	HIS	-	expression tag	UNP A0A486V7R5
E	-16	HIS	-	expression tag	UNP A0A486V7R5
E	-15	HIS	-	expression tag	UNP A0A486V7R5
E	-14	HIS	-	expression tag	UNP A0A486V7R5
E	-13	HIS	-	expression tag	UNP A0A486V7R5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-12	HIS	-	expression tag	UNP A0A486V7R5
E	-11	SER	-	expression tag	UNP A0A486V7R5
E	-10	GLN	-	expression tag	UNP A0A486V7R5
E	-9	ASP	-	expression tag	UNP A0A486V7R5
E	-8	HIS	-	expression tag	UNP A0A486V7R5
E	-7	GLU	-	expression tag	UNP A0A486V7R5
E	-6	ASN	-	expression tag	UNP A0A486V7R5
E	-5	LEU	-	expression tag	UNP A0A486V7R5
E	-4	TYR	-	expression tag	UNP A0A486V7R5
E	-3	PHE	-	expression tag	UNP A0A486V7R5
E	-2	GLN	-	expression tag	UNP A0A486V7R5
E	-1	GLY	-	expression tag	UNP A0A486V7R5
E	0	SER	-	expression tag	UNP A0A486V7R5
F	-21	MET	-	initiating methionine	UNP A0A486V7R5
F	-20	GLY	-	expression tag	UNP A0A486V7R5
F	-19	SER	-	expression tag	UNP A0A486V7R5
F	-18	SER	-	expression tag	UNP A0A486V7R5
F	-17	HIS	-	expression tag	UNP A0A486V7R5
F	-16	HIS	-	expression tag	UNP A0A486V7R5
F	-15	HIS	-	expression tag	UNP A0A486V7R5
F	-14	HIS	-	expression tag	UNP A0A486V7R5
F	-13	HIS	-	expression tag	UNP A0A486V7R5
F	-12	HIS	-	expression tag	UNP A0A486V7R5
F	-11	SER	-	expression tag	UNP A0A486V7R5
F	-10	GLN	-	expression tag	UNP A0A486V7R5
F	-9	ASP	-	expression tag	UNP A0A486V7R5
F	-8	HIS	-	expression tag	UNP A0A486V7R5
F	-7	GLU	-	expression tag	UNP A0A486V7R5
F	-6	ASN	-	expression tag	UNP A0A486V7R5
F	-5	LEU	-	expression tag	UNP A0A486V7R5
F	-4	TYR	-	expression tag	UNP A0A486V7R5
F	-3	PHE	-	expression tag	UNP A0A486V7R5
F	-2	GLN	-	expression tag	UNP A0A486V7R5
F	-1	GLY	-	expression tag	UNP A0A486V7R5
F	0	SER	-	expression tag	UNP A0A486V7R5
G	-21	MET	-	initiating methionine	UNP A0A486V7R5
G	-20	GLY	-	expression tag	UNP A0A486V7R5
G	-19	SER	-	expression tag	UNP A0A486V7R5
G	-18	SER	-	expression tag	UNP A0A486V7R5
G	-17	HIS	-	expression tag	UNP A0A486V7R5
G	-16	HIS	-	expression tag	UNP A0A486V7R5
G	-15	HIS	-	expression tag	UNP A0A486V7R5

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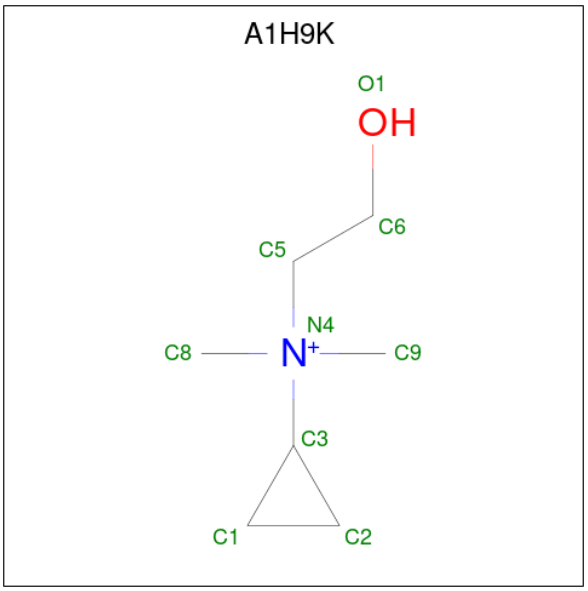
Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	HIS	-	expression tag	UNP A0A486V7R5
G	-13	HIS	-	expression tag	UNP A0A486V7R5
G	-12	HIS	-	expression tag	UNP A0A486V7R5
G	-11	SER	-	expression tag	UNP A0A486V7R5
G	-10	GLN	-	expression tag	UNP A0A486V7R5
G	-9	ASP	-	expression tag	UNP A0A486V7R5
G	-8	HIS	-	expression tag	UNP A0A486V7R5
G	-7	GLU	-	expression tag	UNP A0A486V7R5
G	-6	ASN	-	expression tag	UNP A0A486V7R5
G	-5	LEU	-	expression tag	UNP A0A486V7R5
G	-4	TYR	-	expression tag	UNP A0A486V7R5
G	-3	PHE	-	expression tag	UNP A0A486V7R5
G	-2	GLN	-	expression tag	UNP A0A486V7R5
G	-1	GLY	-	expression tag	UNP A0A486V7R5
G	0	SER	-	expression tag	UNP A0A486V7R5
H	-21	MET	-	initiating methionine	UNP A0A486V7R5
H	-20	GLY	-	expression tag	UNP A0A486V7R5
H	-19	SER	-	expression tag	UNP A0A486V7R5
H	-18	SER	-	expression tag	UNP A0A486V7R5
H	-17	HIS	-	expression tag	UNP A0A486V7R5
H	-16	HIS	-	expression tag	UNP A0A486V7R5
H	-15	HIS	-	expression tag	UNP A0A486V7R5
H	-14	HIS	-	expression tag	UNP A0A486V7R5
H	-13	HIS	-	expression tag	UNP A0A486V7R5
H	-12	HIS	-	expression tag	UNP A0A486V7R5
H	-11	SER	-	expression tag	UNP A0A486V7R5
H	-10	GLN	-	expression tag	UNP A0A486V7R5
H	-9	ASP	-	expression tag	UNP A0A486V7R5
H	-8	HIS	-	expression tag	UNP A0A486V7R5
H	-7	GLU	-	expression tag	UNP A0A486V7R5
H	-6	ASN	-	expression tag	UNP A0A486V7R5
H	-5	LEU	-	expression tag	UNP A0A486V7R5
H	-4	TYR	-	expression tag	UNP A0A486V7R5
H	-3	PHE	-	expression tag	UNP A0A486V7R5
H	-2	GLN	-	expression tag	UNP A0A486V7R5
H	-1	GLY	-	expression tag	UNP A0A486V7R5
H	0	SER	-	expression tag	UNP A0A486V7R5

- Molecule 2 is cyclopropylcholine (three-letter code: A1H9K) (formula: $C_7H_{16}NO$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 9 7 1 1	0	0
2	B	1	Total C N O 9 7 1 1	0	0
2	C	1	Total C N O 9 7 1 1	0	0
2	D	1	Total C N O 9 7 1 1	0	0
2	E	1	Total C N O 9 7 1 1	0	0
2	F	1	Total C N O 9 7 1 1	0	0
2	G	1	Total C N O 9 7 1 1	0	0
2	H	1	Total C N O 9 7 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	87	Total O 87 87	0	0
3	B	71	Total O 71 71	0	0
3	C	65	Total O 65 65	0	0
3	D	31	Total O 31 31	0	0

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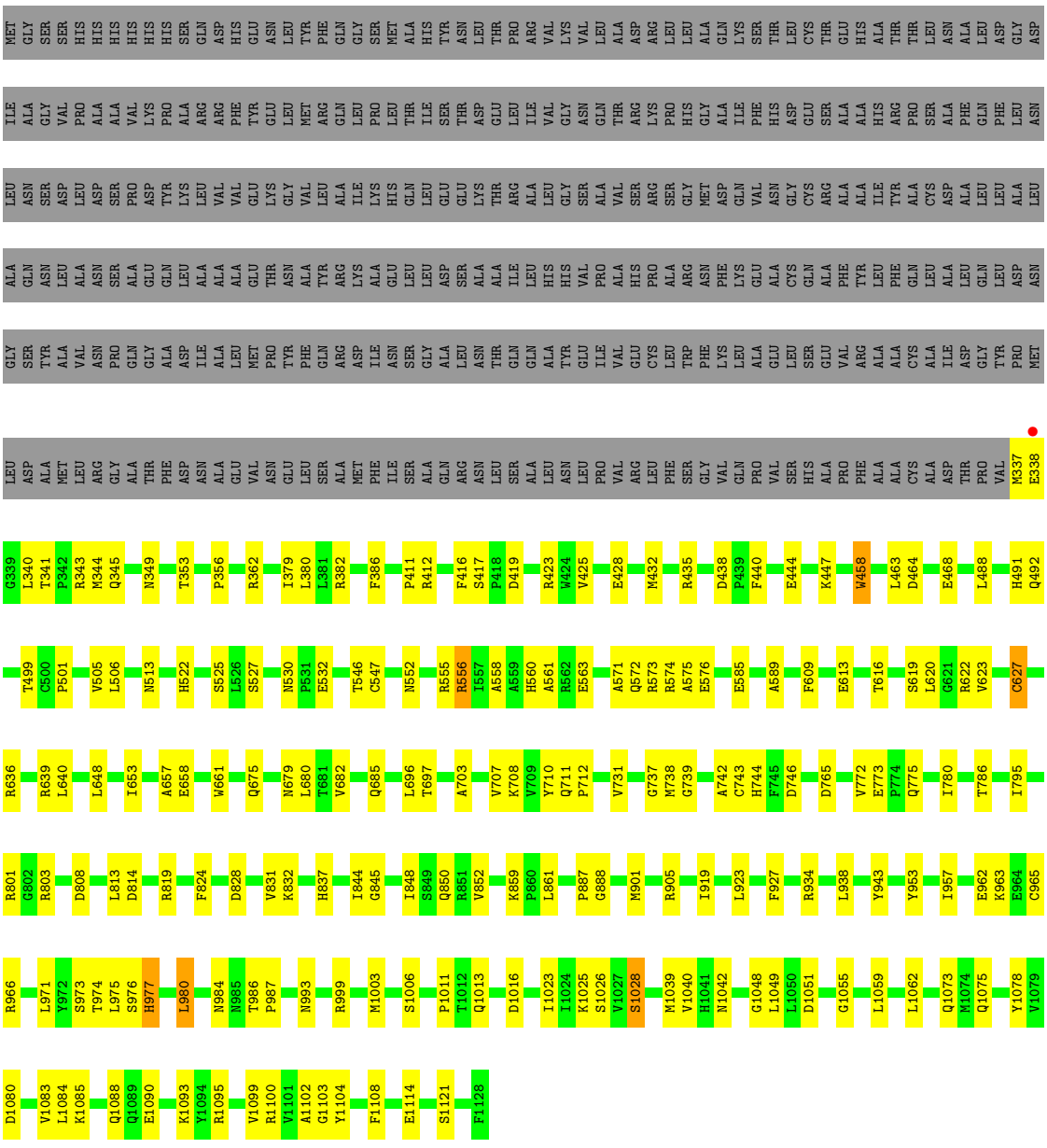
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	29	Total O 29 29	0	0
3	F	24	Total O 24 24	0	0
3	G	20	Total O 20 20	0	0
3	H	11	Total O 11 11	0	0

3 Residue-property plots (i)

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

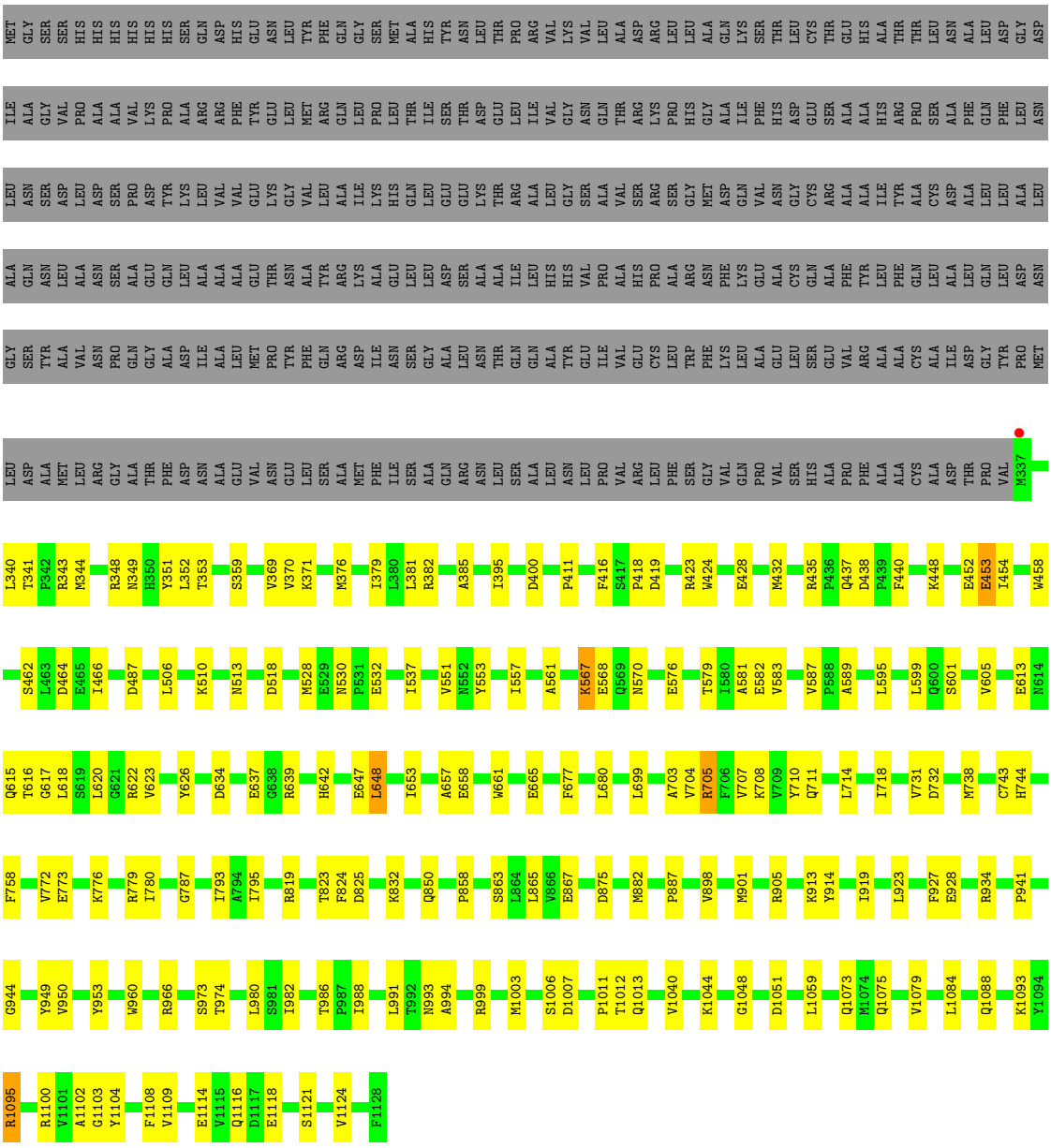
- Molecule 1: Choline trimethylamine-lyase

Chain A:



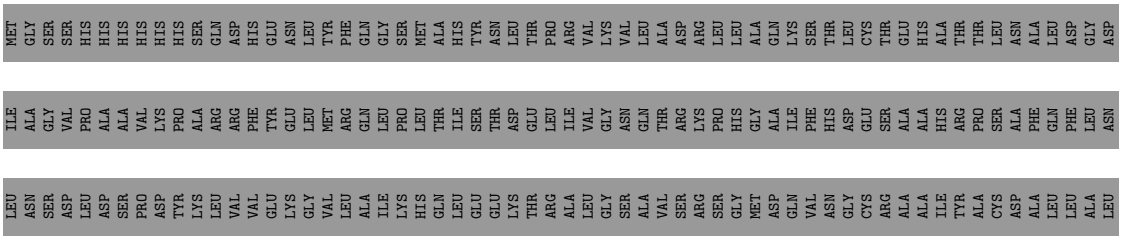
• Molecule 1: Choline trimethylamine-lyase

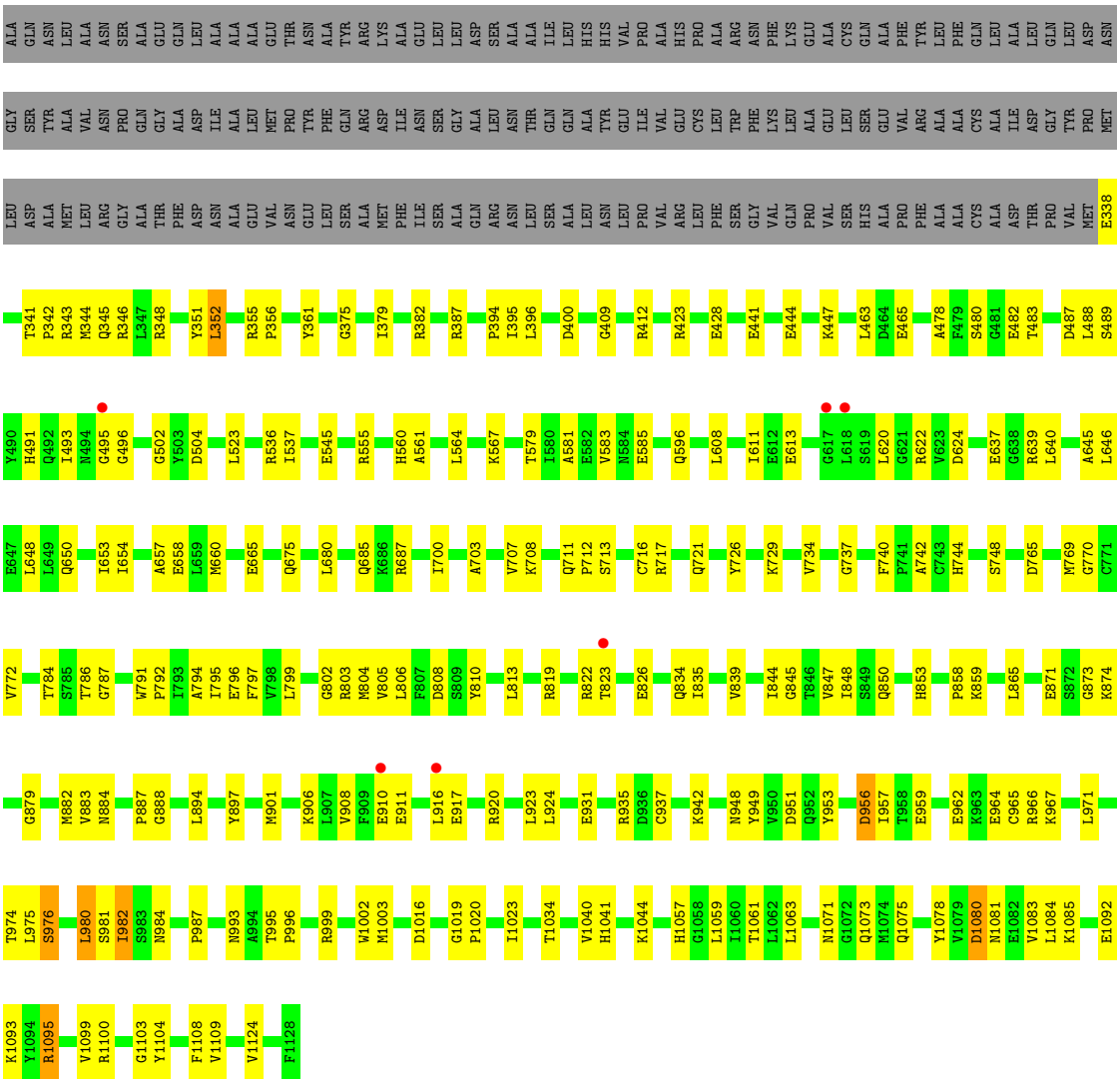
Chain B:



• Molecule 1: Choline trimethylamine-lyase

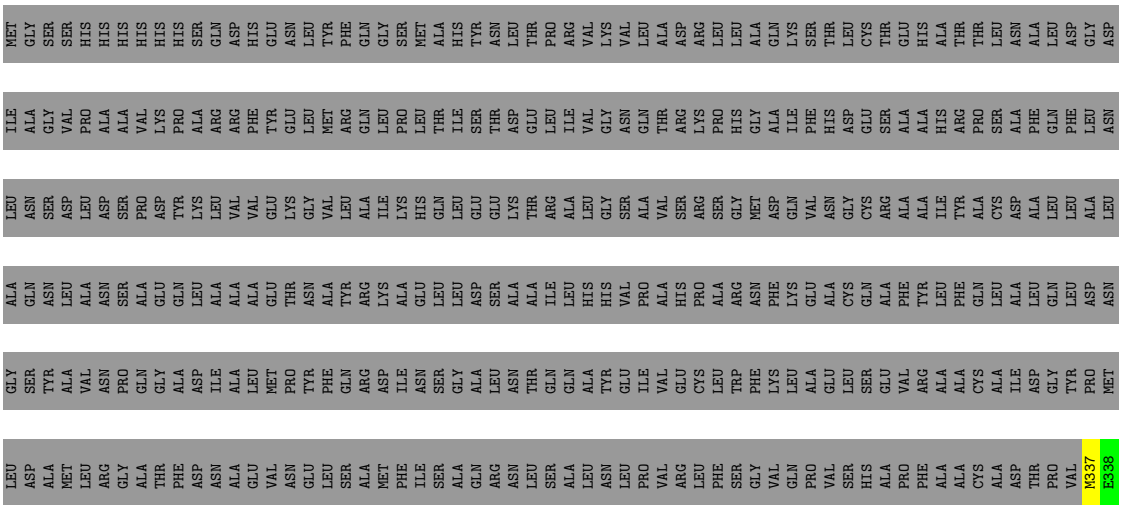
Chain C:

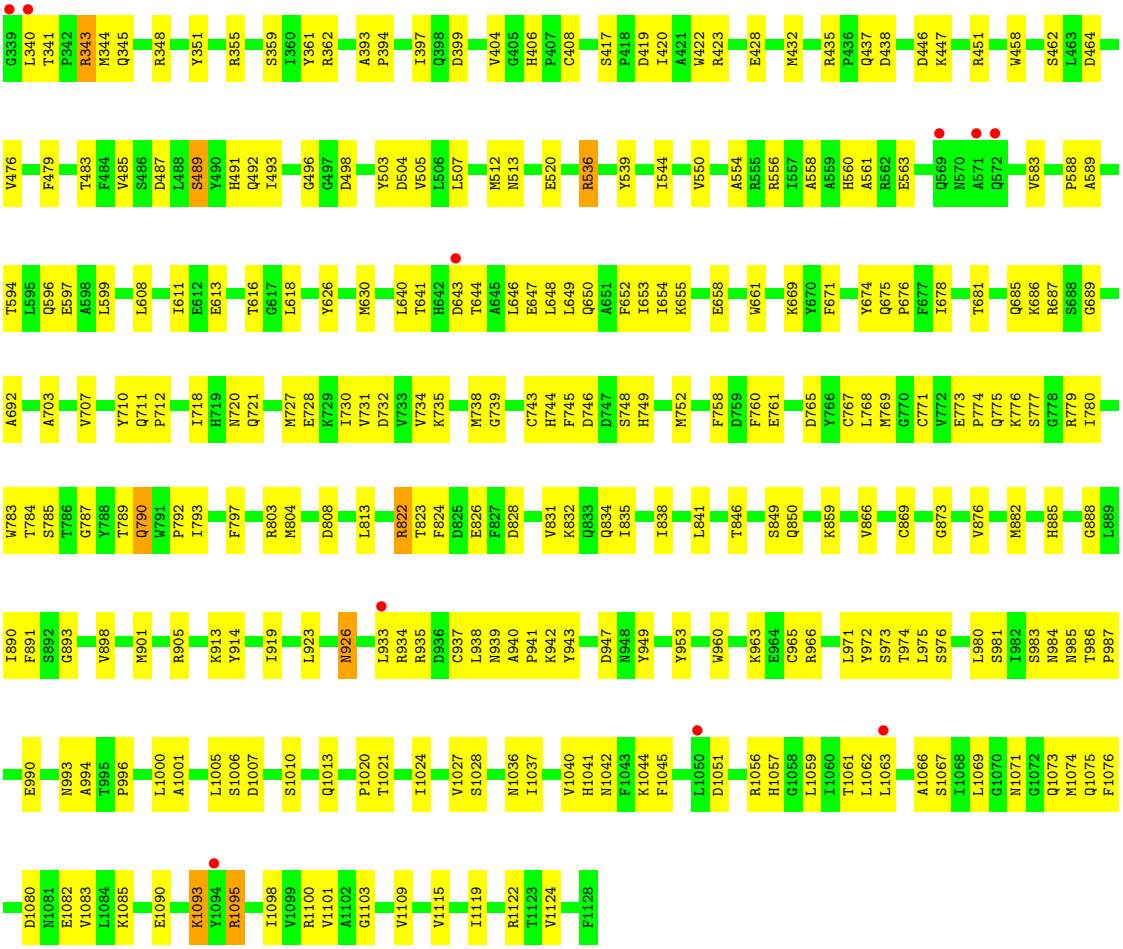




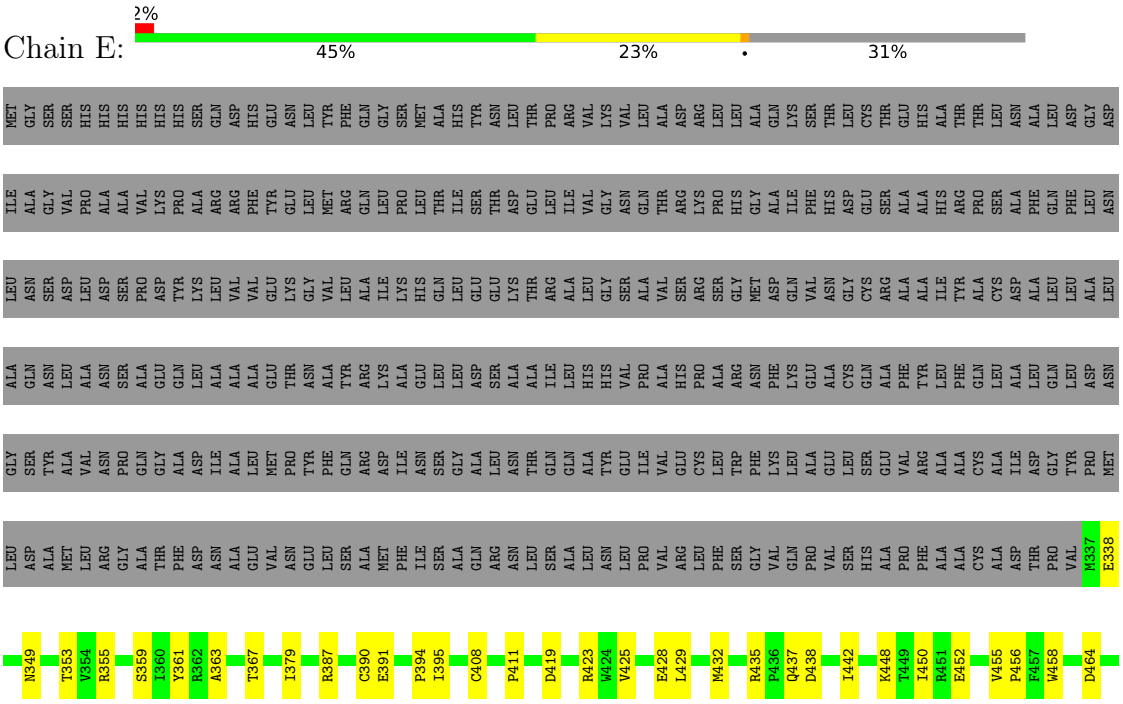
• Molecule 1: Choline trimethylamine-lyase

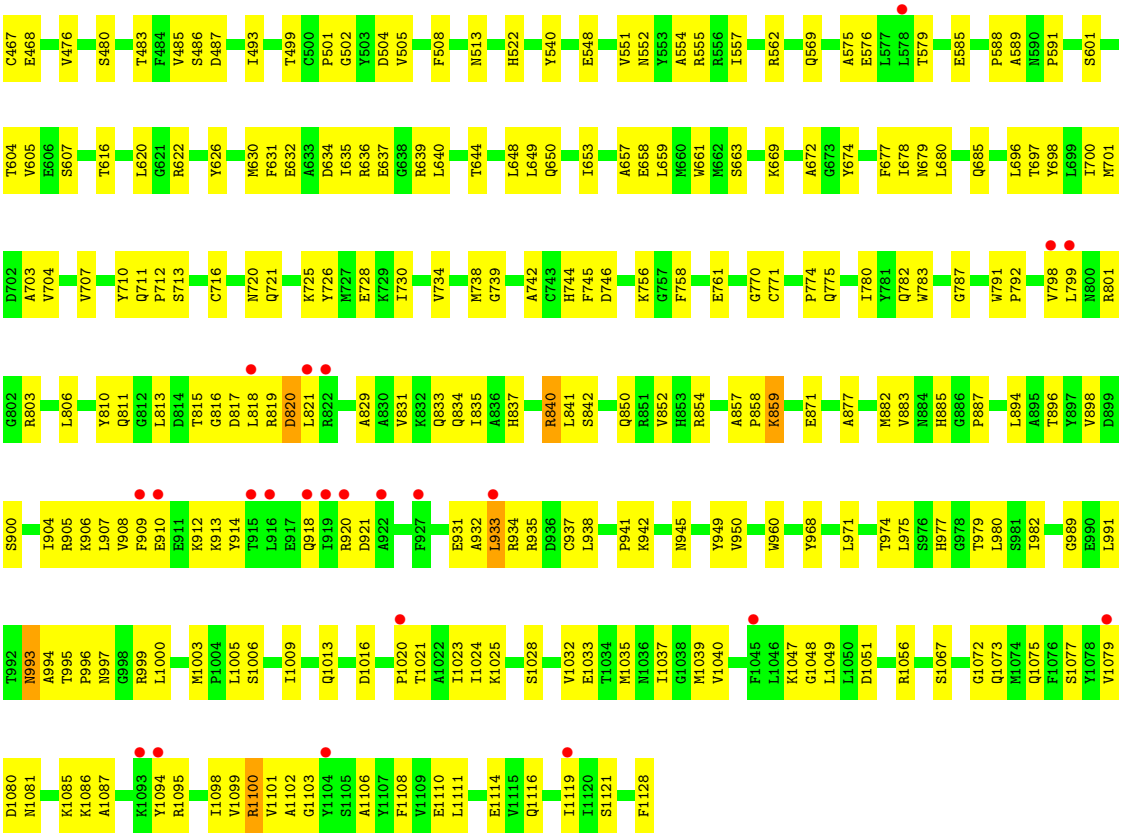
Chain D:





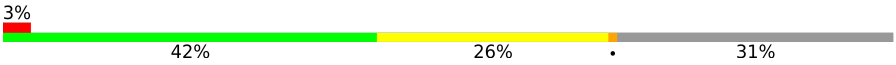
• Molecule 1: Choline trimethylamine-lyase

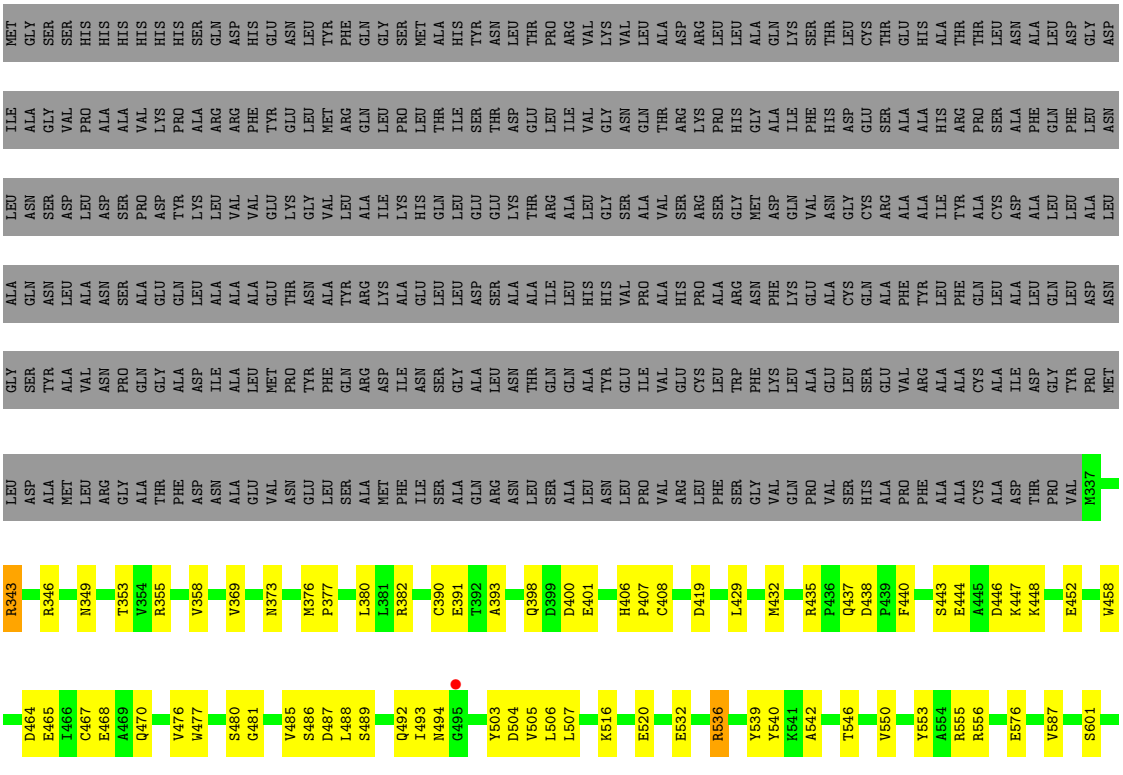


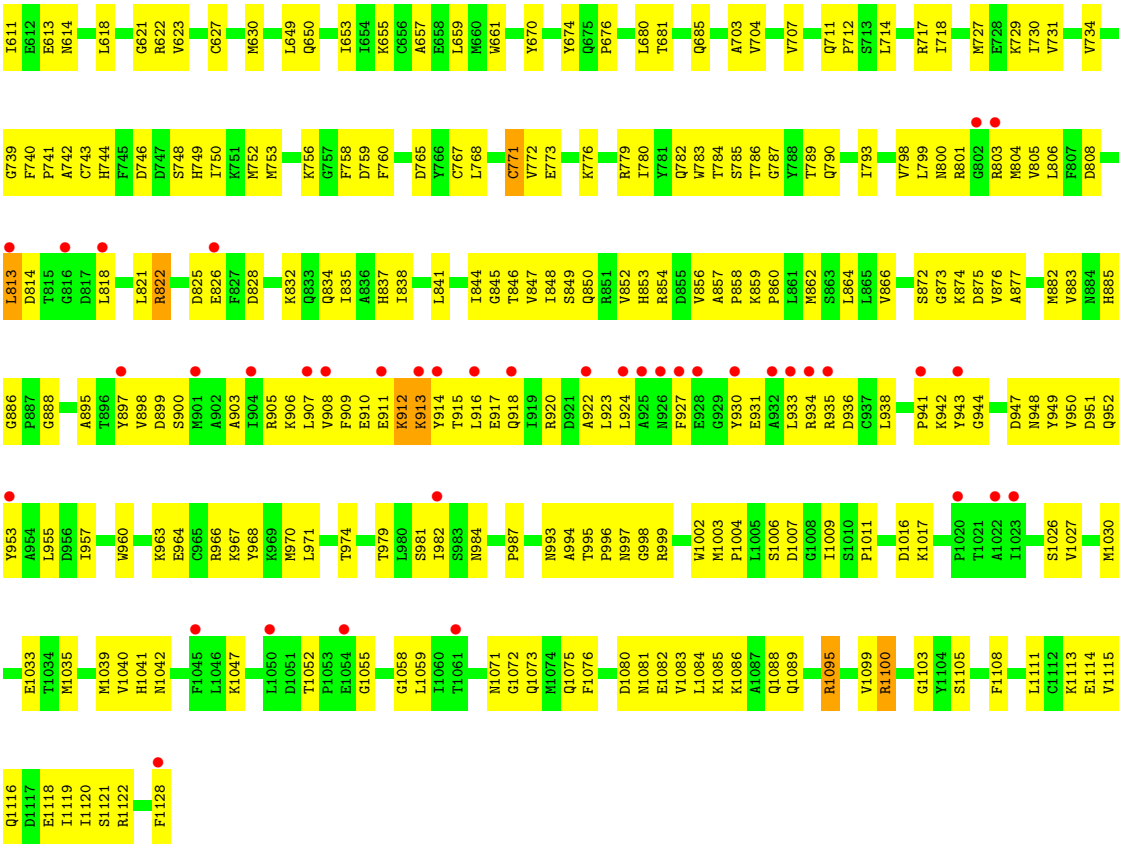


• Molecule 1: Choline trimethylamine-lyase

Chain F:

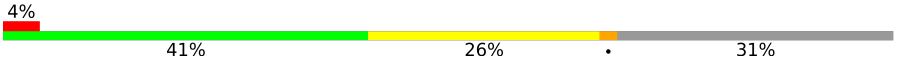


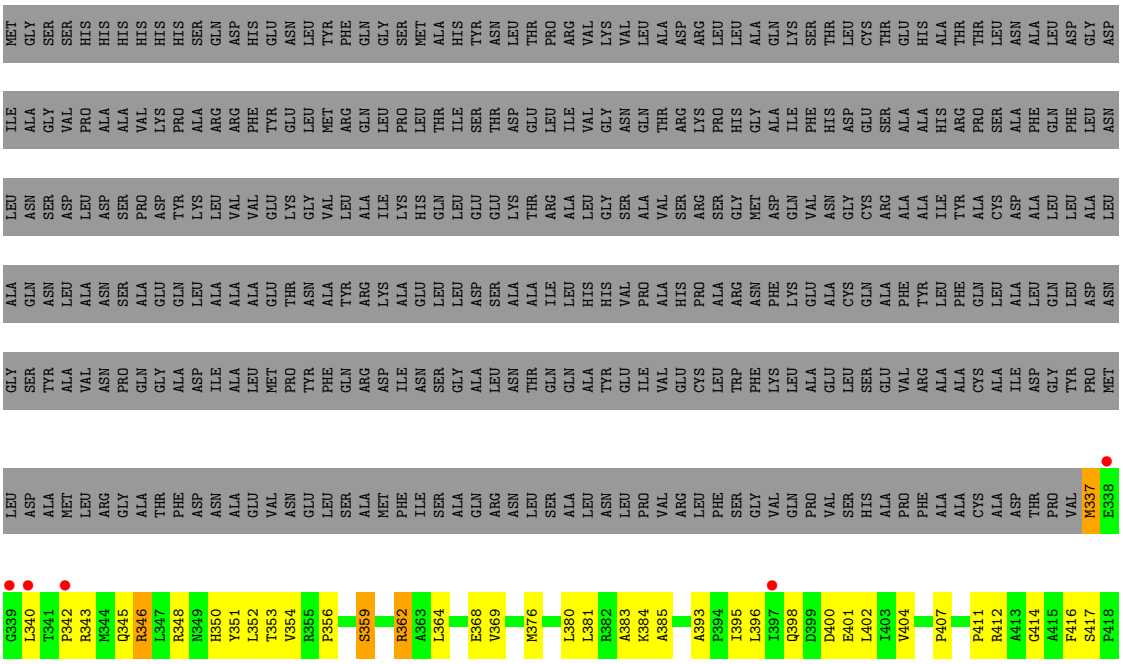


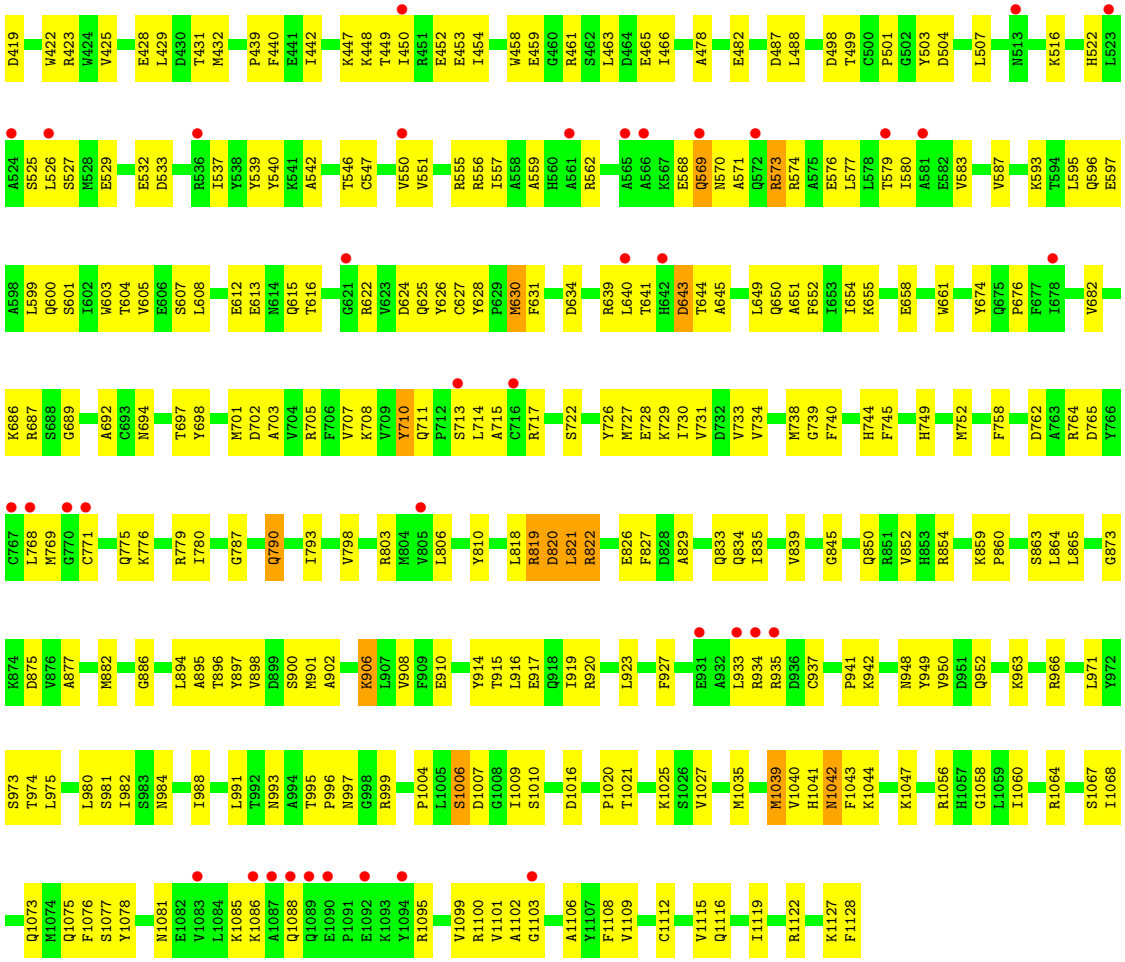


- Molecule 1: Choline trimethylamine-lyase

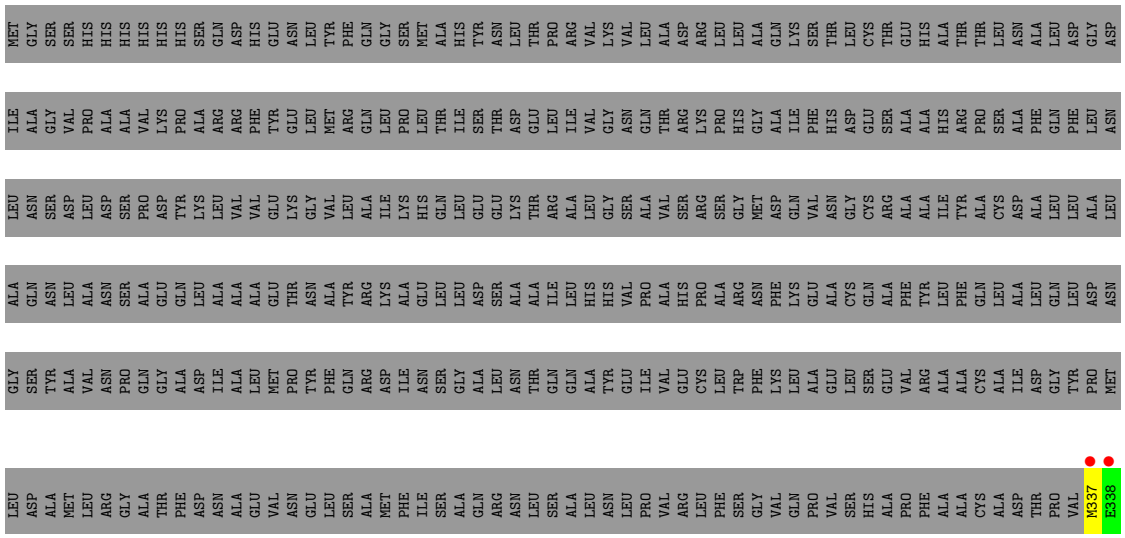
Chain G:

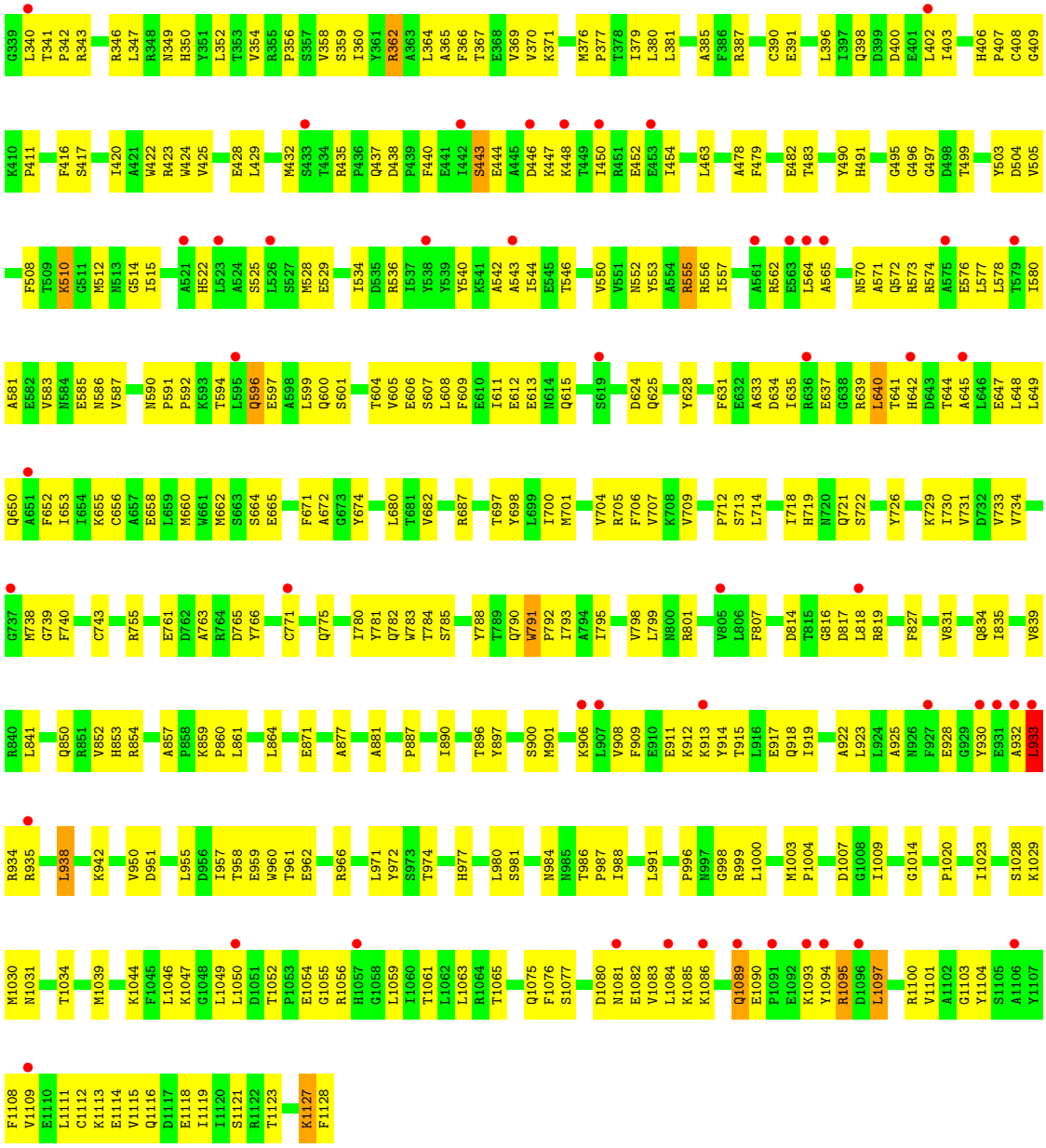






• Molecule 1: Choline trimethylamine-lyase




G339 L340 T341 P342 R343 R346 L347 R348 N349 H350 Y351 L352 T353 V354 R355 P356 S357 V358 S359 I360 Y361 R362 A363 L364 A365 F366 T367 E368 V369 V370 K371 M376 P377 T378 I379 L380 L381 A385 F386 R387 C390 E391 L396 I397 Q398 D399 D400 E401 L402 I403 H406 P407 C408 G409
K410 P411 F416 S417 I420 A421 W422 R423 W424 V425 E428 L429 M432 S433 T434 R435 P436 Q437 D438 P439 F440 E441 I442 S443 E444 A445 D446 K447 K448 T449 I450 R451 E452 E453 I454 L463 A478 F479 E482 T483 Y490 H491 G495 G496 G497 D498 T499 Y503 D504 V505
F508 T509 K510 G511 M512 N513 G514 I515 A521 H522 L523 A524 S525 L526 S527 M528 E529 I534 D535 R536 I537 Y538 Y539 Y540 K541 A542 A543 I544 E545 T546 V550 V551 N552 Y553 A554 R555 R556 I557 A561 R562 E563 L564 A565 N570 A571 Q572 R573 R574 A575 E576 L577 L578 T579 I580
A581 E582 V583 N584 E585 N586 V587 N590 P591 P592 K593 T594 L595 Q596 E597 A598 L599 Q600 S601 T604 V605 E606 S607 L608 F609 E610 I611 E612 E613 N614 Q615 S619 D624 Q625 Y628 F631 E632 A633 D634 I635 R636 E637 G638 R639 L640 T641 H642 D643 T644 A645 L646 E647 L648 L649
Q650 A651 F652 I653 I654 K655 C656 A657 E658 L659 M660 W661 M662 S663 S664 E665 F671 A672 G673 Y674 L680 T681 V682 R687 T697 Y698 L699 I700 M701 V704 R705 F706 V707 K708 V709 P712 S713 L714 I718 H719 N720 Q721 S722 Y726 K729 I730 V731 D732 V733 V734
G737 M738 G739 F740 C743 R755 E761 D762 A763 R764 D765 Y766 C771 Q775 I780 Y781 Q782 W783 T784 S785 Y788 T789 Q790 W791 P792 I793 A794 I795 V798 L799 N800 R801 V805 L806 F807 D814 T815 G816 D817 L818 R819 F827 V831 Q834 I835 V839
R840 L841 Q850 R851 V852 H853 R854 A857 P858 K859 P860 L861 L864 E871 A877 A881 P887 I890 T896 Y897 S900 M901 K906 L907 V908 F909 E910 E911 K912 K913 Y914 T915 L916 E917 Q918 I919 A922 L923 L924 A925 N926 F927 E928 G929 Y930 E931 A932 L933
R934 R935 L938 K942 V950 D951 L955 D956 I957 T958 E959 W960 T961 E962 R966 L971 Y972 S973 T974 H977 L980 S981 N984 N985 T986 P987 I988 L991 P996 N997 G998 R999 L1000 M1003 P1004 D1007 G1008 I1009 G1014 P1020 I1023 S1028 K1029
M1030 N1031 T1034 M1039 K1044 F1045 L1046 K1047 G1048 L1049 L1050 D1051 T1052 P1053 E1054 G1055 R1056 H1057 G1058 L1059 I1060 T1061 L1062 L1063 R1064 T1065 Q1075 F1076 S1077 D1080 N1081 E1082 V1083 L1084 K1085 K1086 Q1089 E1090 P1091 E1092 K1093 Y1094 R1095 D1096 L1097 R1100 V1101 A1102 G1103 Y1104 S1105 A1106 Y1107
F1108 V1109 E1110 L1111 C1112 K1113 E1114 V1115 Q1116 D1117 E1118 I1119 I1120 S1121 R1122 T1123 K1127 F1128

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	89.27Å 119.66Å 214.70Å 77.86° 85.18° 69.32°	Depositor
Resolution (Å)	44.64 – 2.70 49.41 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.5 (44.64-2.70) 95.7 (49.41-2.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.218 , 0.273 0.218 , 0.272	Depositor DCC
R_{free} test set	10756 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	50434	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: A1H9K

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	0.58	2/6385 (0.0%)	0.71	2/8640 (0.0%)
1	B	0.56	0/6385	0.71	1/8640 (0.0%)
1	C	0.51	0/6377	0.66	2/8630 (0.0%)
1	D	0.51	0/6385	0.69	0/8640
1	E	0.50	2/6385 (0.0%)	0.67	2/8640 (0.0%)
1	F	0.55	2/6385 (0.0%)	0.88	8/8640 (0.1%)
1	G	0.52	4/6385 (0.1%)	0.73	8/8640 (0.1%)
1	H	0.46	0/6385	0.68	3/8640 (0.0%)
All	All	0.52	10/51072 (0.0%)	0.72	26/69110 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
1	F	0	2
1	G	0	2
1	H	0	2
All	All	0	9

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	820	ASP	CB-CG	-13.68	1.23	1.51
1	F	822	ARG	CZ-NH1	11.02	1.47	1.33
1	G	820	ASP	CG-OD2	7.90	1.43	1.25
1	G	1127	LYS	CD-CE	6.70	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	627	CYS	CB-SG	-6.27	1.71	1.82
1	A	547	CYS	CB-SG	-5.99	1.72	1.82
1	F	822	ARG	CB-CG	-5.93	1.36	1.52
1	E	569	GLN	CG-CD	5.51	1.63	1.51
1	E	390	CYS	CB-SG	-5.51	1.72	1.81
1	G	820	ASP	CG-OD1	-5.34	1.13	1.25

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	822	ARG	NE-CZ-NH2	41.08	140.84	120.30
1	F	822	ARG	NH1-CZ-NH2	-22.28	94.89	119.40
1	G	820	ASP	CB-CG-OD1	-17.86	102.22	118.30
1	G	820	ASP	CB-CG-OD2	12.06	129.16	118.30
1	G	822	ARG	NE-CZ-NH2	-9.60	115.50	120.30
1	G	821	LEU	CA-CB-CG	-8.06	96.76	115.30
1	F	822	ARG	CB-CG-CD	-7.97	90.87	111.60
1	F	822	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	F	822	ARG	CG-CD-NE	-7.30	96.47	111.80
1	F	912	LYS	CD-CE-NZ	-7.07	95.44	111.70
1	H	640	LEU	CA-CB-CG	6.91	131.20	115.30
1	B	567	LYS	CD-CE-NZ	-6.86	95.93	111.70
1	G	820	ASP	CB-CA-C	-6.22	97.96	110.40
1	F	822	ARG	N-CA-CB	-6.19	99.46	110.60
1	G	819	ARG	CA-C-O	-6.07	107.35	120.10
1	E	933	LEU	CA-CB-CG	5.80	128.65	115.30
1	G	821	LEU	CB-CA-C	5.54	120.72	110.20
1	A	458	TRP	CA-CB-CG	-5.31	103.61	113.70
1	C	1080	ASP	CB-CG-OD1	5.31	123.08	118.30
1	H	933	LEU	CA-CB-CG	5.24	127.36	115.30
1	E	626	TYR	CA-CB-CG	5.23	123.33	113.40
1	A	1062	LEU	CA-CB-CG	5.21	127.29	115.30
1	G	821	LEU	N-CA-C	-5.07	97.31	111.00
1	H	1097	LEU	CA-CB-CG	5.06	126.94	115.30
1	F	813	LEU	CB-CG-CD1	-5.02	102.47	111.00
1	C	352	LEU	CA-CB-CG	-5.01	103.77	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	338	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	C	981	SER	Peptide
1	E	338	GLU	Peptide
1	F	826	GLU	Peptide
1	F	981	SER	Peptide
1	G	569	GLN	Peptide
1	G	981	SER	Peptide
1	H	1089	GLN	Peptide
1	H	443	SER	Peptide

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	6254	0	6171	125	0
1	B	6254	0	6171	127	0
1	C	6246	0	6162	145	0
1	D	6254	0	6171	206	1
1	E	6254	0	6171	190	1
1	F	6254	0	6171	266	1
1	G	6254	0	6171	238	1
1	H	6254	0	6171	303	0
2	A	9	0	0	0	0
2	B	9	0	0	0	0
2	C	9	0	0	0	0
2	D	9	0	0	1	0
2	E	9	0	0	0	0
2	F	9	0	0	1	0
2	G	9	0	0	2	0
2	H	9	0	0	0	0
3	A	87	0	0	5	0
3	B	71	0	0	3	0
3	C	65	0	0	3	0
3	D	31	0	0	5	0
3	E	29	0	0	0	0
3	F	24	0	0	1	0
3	G	20	0	0	0	0
3	H	11	0	0	1	0
All	All	50434	0	49359	1591	2

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 16.

All (1591) 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:979:THR:HG21	1:E:1035:MET:CE	1.53	1.35
1:E:979:THR:CG2	1:E:1035:MET:HE2	1.58	1.34
1:F:803:ARG:NH1	1:F:808:ASP:OD1	1.85	1.08
1:B:435:ARG:NH2	1:B:438:ASP:HB2	1.69	1.07
1:D:343:ARG:NE	1:D:647:GLU:OE2	1.89	1.05
1:F:908:VAL:O	1:F:912:LYS:HE3	1.57	1.04
1:H:791:TRP:HE1	1:H:961:THR:HG21	1.23	1.01
1:G:728:GLU:HG3	1:G:1056:ARG:HH21	1.24	1.01
1:E:1075:GLN:HE22	1:E:1103:GLY:H	1.06	0.97
1:F:1075:GLN:HE22	1:F:1103:GLY:HA2	1.29	0.96
1:E:979:THR:HG21	1:E:1035:MET:HE2	1.09	0.96
1:G:821:LEU:HB3	1:G:827:PHE:HB2	1.44	0.95
1:G:1056:ARG:O	1:G:1060:ILE:HD12	1.65	0.95
1:D:935:ARG:O	1:D:939:ASN:HB2	1.68	0.93
1:E:979:THR:HG21	1:E:1035:MET:HE3	1.48	0.92
1:D:343:ARG:NH2	1:D:647:GLU:OE1	2.06	0.89
1:F:906:LYS:HB2	1:F:949:TYR:OH	1.72	0.89
1:H:999:ARG:NH1	1:H:1003:MET:O	2.05	0.88
1:D:341:THR:O	1:D:345:GLN:OE1	1.92	0.88
1:F:1073:GLN:HE22	1:F:1075:GLN:HG3	1.39	0.87
1:F:915:THR:HG22	1:F:917:GLU:H	1.38	0.87
1:C:910:GLU:OE1	1:C:949:TYR:OH	1.92	0.86
1:H:713:SER:HA	1:H:740:PHE:HE1	1.39	0.84
1:E:906:LYS:HA	1:E:910:GLU:HB2	1.59	0.84
1:E:771:CYS:HB3	1:E:1103:GLY:HA3	1.59	0.84
1:B:435:ARG:HH22	1:B:438:ASP:HB2	1.42	0.84
1:H:587:VAL:HB	1:H:601:SER:HB2	1.59	0.84
1:F:739:GLY:HA3	1:F:1100:ARG:HG2	1.60	0.84
1:F:993:ASN:OD1	1:F:994:ALA:N	2.10	0.83
1:G:352:LEU:HD23	1:G:1095:ARG:HH21	1.42	0.83
1:G:429:LEU:HD21	1:G:450:ILE:HD11	1.58	0.83
1:E:979:THR:HG23	1:E:1035:MET:HE2	1.56	0.83
1:F:938:LEU:HD21	1:F:998:GLY:HA3	1.61	0.83
1:C:850:GLN:HB3	1:C:971:LEU:HD22	1.57	0.82
1:E:857:ALA:O	1:E:859:LYS:NZ	2.12	0.82
1:E:999:ARG:NH1	1:E:1003:MET:O	2.13	0.82
1:H:934:ARG:O	1:H:938:LEU:HD12	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:THR:HB	1:C:804:MET:HE1	1.59	0.81
1:F:1082:GLU:CD	1:F:1085:LYS:HE3	2.00	0.81
1:D:393:ALA:O	1:D:556:ARG:NH2	2.13	0.80
1:H:1052:THR:HG22	1:H:1054:GLU:H	1.46	0.80
1:G:546:THR:HG21	1:G:860:PRO:HB2	1.63	0.80
1:G:350:HIS:O	1:G:353:THR:OG1	2.00	0.79
1:E:1020:PRO:HA	1:E:1023:ILE:HD12	1.64	0.79
1:G:702:ASP:OD1	1:G:705:ARG:NH2	2.15	0.79
1:G:995:THR:HG23	1:G:999:ARG:HH21	1.47	0.79
1:B:435:ARG:NH2	1:B:437:GLN:O	2.16	0.79
1:F:789:THR:HG22	1:F:790:GLN:H	1.46	0.79
1:G:775:GLN:HG3	1:G:780:ILE:HG21	1.64	0.79
1:G:587:VAL:HB	1:G:601:SER:HB2	1.63	0.79
1:G:906:LYS:HB3	1:G:949:TYR:OH	1.82	0.79
1:G:850:GLN:HB3	1:G:971:LEU:HD22	1.65	0.79
1:C:823:THR:HG1	1:C:826:GLU:H	1.30	0.78
1:F:847:VAL:HG23	1:F:970:MET:CE	2.13	0.78
1:D:813:LEU:O	1:D:834:GLN:NE2	2.16	0.78
1:H:403:ILE:HA	1:H:600:GLN:HE22	1.49	0.78
1:F:906:LYS:HG3	1:F:910:GLU:HB3	1.64	0.78
1:F:847:VAL:CG2	1:F:970:MET:HE2	2.13	0.78
1:H:801:ARG:HH11	1:H:801:ARG:HG2	1.48	0.78
1:F:1052:THR:HG23	1:F:1055:GLY:H	1.49	0.78
1:D:640:LEU:HD22	1:D:644:THR:HB	1.65	0.77
1:H:396:LEU:HD21	1:H:398:GLN:HG2	1.66	0.77
1:A:962:GLU:HB2	1:A:977:HIS:CE1	2.19	0.77
1:A:491:HIS:HB2	1:A:786:THR:HG23	1.67	0.76
1:B:424:TRP:O	1:B:428:GLU:HB2	1.85	0.76
1:H:771:CYS:HB3	1:H:1103:GLY:HA3	1.68	0.76
1:D:1020:PRO:HB2	1:D:1062:LEU:HD21	1.68	0.76
1:H:337:MET:HB3	1:H:340:LEU:HD12	1.67	0.76
1:E:818:LEU:HA	1:E:821:LEU:HD23	1.67	0.75
1:E:640:LEU:HD22	1:E:644:THR:HB	1.67	0.75
1:H:1112:CYS:O	1:H:1116:GLN:NE2	2.15	0.75
1:G:771:CYS:HB3	1:G:1103:GLY:HA3	1.68	0.75
1:B:395:ILE:HG23	1:B:557:ILE:HD13	1.67	0.74
1:H:951:ASP:HB3	1:H:1029:LYS:HG3	1.68	0.74
1:E:653:ILE:HG23	1:E:712:PRO:HD2	1.66	0.74
1:H:785:SER:HB3	1:H:890:ILE:HD12	1.69	0.74
1:E:1009:ILE:HG21	1:E:1035:MET:HE1	1.69	0.74
1:G:859:LYS:O	1:G:863:SER:OG	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:962:GLU:OE1	1:A:977:HIS:ND1	2.20	0.74
1:B:1075:GLN:HE22	1:B:1103:GLY:HA2	1.53	0.74
1:G:980:LEU:HD12	1:G:980:LEU:O	1.88	0.73
1:E:813:LEU:HD11	1:E:837:HIS:HB2	1.68	0.73
1:C:653:ILE:HG23	1:C:712:PRO:HD2	1.70	0.73
1:C:948:ASN:HA	1:C:951:ASP:HB2	1.71	0.73
1:G:376:MET:HB3	1:G:381:LEU:HD13	1.69	0.73
1:G:966:ARG:HH11	1:G:974:THR:HG23	1.52	0.73
1:H:546:THR:HG23	1:H:864:LEU:HD11	1.71	0.73
1:F:480:SER:HB3	1:F:486:SER:O	1.87	0.73
1:F:813:LEU:HD11	1:F:837:HIS:HB2	1.70	0.73
1:D:1063:LEU:HD23	1:D:1074:MET:HE3	1.71	0.73
1:F:505:VAL:HG12	1:F:506:LEU:HD12	1.71	0.73
1:H:352:LEU:HD21	1:H:1095:ARG:HG3	1.69	0.73
1:G:337:MET:HG3	1:G:340:LEU:HD12	1.70	0.73
1:G:550:VAL:HG23	1:G:608:LEU:HD12	1.71	0.73
1:D:773:GLU:OE2	1:D:980:LEU:HD22	1.89	0.72
1:H:1081:ASN:HA	1:H:1084:LEU:HD12	1.71	0.72
1:C:428:GLU:HG2	3:C:1311:HOH:O	1.89	0.72
1:F:948:ASN:HB3	1:F:952:GLN:HE22	1.54	0.72
1:H:738:MET:HB2	1:H:740:PHE:HD2	1.53	0.72
1:A:1075:GLN:HE22	1:A:1103:GLY:H	1.34	0.72
1:D:739:GLY:HA3	1:D:1100:ARG:HB2	1.71	0.72
1:F:857:ALA:O	1:F:859:LYS:NZ	2.22	0.72
1:D:776:LYS:HD2	1:D:779:ARG:HD2	1.71	0.72
1:G:1108:PHE:CZ	1:G:1116:GLN:HB2	2.24	0.72
1:B:823:THR:HG22	1:B:825:ASP:H	1.55	0.72
1:G:900:SER:HB2	1:G:996:PRO:HG2	1.72	0.71
1:H:713:SER:OG	1:H:1100:ARG:NH1	2.22	0.71
1:G:631:PHE:HE2	1:G:645:ALA:CB	2.03	0.71
1:B:999:ARG:NH1	1:B:1003:MET:O	2.23	0.71
1:A:703:ALA:O	1:A:707:VAL:HG23	1.90	0.71
1:F:813:LEU:O	1:F:834:GLN:NE2	2.20	0.71
1:G:1099:VAL:HG11	1:G:1108:PHE:HD1	1.55	0.71
1:C:823:THR:OG1	1:C:826:GLU:N	2.15	0.71
1:E:882:MET:HG2	1:E:883:VAL:HG23	1.72	0.71
1:H:1101:VAL:HG13	1:H:1119:ILE:HD11	1.71	0.71
1:F:704:VAL:HG21	1:F:714:LEU:HD22	1.70	0.71
1:H:1075:GLN:HE22	1:H:1103:GLY:H	1.39	0.71
1:F:943:TYR:CE1	1:F:1026:SER:HB3	2.26	0.70
1:B:435:ARG:NH2	1:B:438:ASP:CB	2.53	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:749:HIS:HA	1:D:752:MET:HG2	1.74	0.70
1:G:516:LYS:HB3	1:G:547:CYS:SG	2.32	0.70
1:G:1101:VAL:HG13	1:G:1119:ILE:HD11	1.74	0.70
1:H:801:ARG:NH1	1:H:814:ASP:OD1	2.25	0.70
1:C:343:ARG:HG3	1:C:400:ASP:HB3	1.74	0.70
1:D:793:ILE:HD11	1:D:804:MET:HG3	1.73	0.70
1:G:604:THR:O	1:G:607:SER:OG	2.10	0.70
1:G:634:ASP:HB3	1:G:640:LEU:HD13	1.73	0.70
1:F:382:ARG:NH2	1:F:613:GLU:OE1	2.25	0.70
1:G:937:CYS:O	1:G:942:LYS:NZ	2.24	0.70
1:C:703:ALA:O	1:C:707:VAL:HG23	1.92	0.69
1:A:343:ARG:NH2	1:A:576:GLU:OE2	2.25	0.69
1:G:569:GLN:HA	1:G:574:ARG:NH1	2.07	0.69
1:D:428:GLU:HB3	1:D:432:MET:HG3	1.73	0.69
1:G:599:LEU:HD23	1:G:652:PHE:HB2	1.74	0.69
1:G:730:ILE:O	1:G:734:VAL:HG23	1.91	0.69
1:G:771:CYS:SG	2:G:1201:A1H9K:O1	2.50	0.69
1:C:937:CYS:O	1:C:942:LYS:NZ	2.26	0.69
1:B:448:LYS:HG3	1:B:452:GLU:OE1	1.92	0.68
1:C:488:LEU:HD23	1:C:787:GLY:HA3	1.74	0.68
1:E:935:ARG:HA	1:E:938:LEU:HB2	1.75	0.68
1:B:772:VAL:N	1:B:773:GLU:OE2	2.16	0.68
1:F:805:VAL:HG21	1:F:993:ASN:HD22	1.57	0.68
1:H:594:THR:HG23	1:H:597:GLU:H	1.59	0.68
1:A:432:MET:HE3	1:A:440:PHE:HB2	1.75	0.68
1:B:432:MET:HE3	1:B:440:PHE:HB2	1.74	0.68
1:H:416:PHE:HE1	1:H:425:VAL:HG21	1.59	0.68
1:H:429:LEU:HD11	1:H:450:ILE:HD11	1.76	0.68
1:C:920:ARG:O	1:C:924:LEU:HD23	1.93	0.68
1:D:731:VAL:HG22	1:D:1059:LEU:HD23	1.74	0.68
1:D:980:LEU:O	1:D:980:LEU:HD12	1.94	0.68
1:D:681:THR:HG21	1:D:768:LEU:H	1.59	0.68
1:D:985:ASN:ND2	3:D:1303:HOH:O	2.26	0.68
1:H:913:LYS:HD2	1:H:914:TYR:CZ	2.28	0.68
1:E:1047:LYS:HD2	1:E:1080:ASP:HB2	1.76	0.68
1:G:731:VAL:HG21	1:G:1060:ILE:HD11	1.75	0.67
1:E:739:GLY:HA3	1:E:1100:ARG:HG3	1.77	0.67
1:D:446:ASP:OD2	3:D:1301:HOH:O	2.12	0.67
1:D:850:GLN:HB3	1:D:971:LEU:HD22	1.76	0.67
1:C:361:TYR:CE1	1:C:394:PRO:HG3	2.29	0.67
1:G:771:CYS:N	2:G:1201:A1H9K:O1	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:873:GLY:O	1:C:874:LYS:HE2	1.94	0.67
1:G:703:ALA:O	1:G:707:VAL:HG23	1.95	0.67
1:G:1085:LYS:HA	1:G:1088:GLN:HG3	1.76	0.67
1:H:400:ASP:H	1:H:573:ARG:HH12	1.43	0.67
1:C:908:VAL:HG11	1:C:916:LEU:HD23	1.75	0.67
1:F:1075:GLN:HE22	1:F:1103:GLY:CA	2.07	0.67
1:G:442:ILE:HG23	1:G:447:LYS:NZ	2.10	0.67
1:F:488:LEU:HD13	1:F:845:GLY:HA3	1.77	0.67
1:F:911:GLU:HG3	1:F:913:LYS:NZ	2.10	0.67
1:A:382:ARG:NH2	1:A:613:GLU:OE1	2.27	0.66
1:C:341:THR:O	1:C:345:GLN:HG3	1.95	0.66
1:F:467:CYS:HB3	1:F:492:GLN:HG3	1.78	0.66
1:D:428:GLU:OE2	1:D:435:ARG:NH1	2.26	0.66
1:H:396:LEU:HD23	1:H:396:LEU:O	1.96	0.66
1:H:396:LEU:CD2	1:H:398:GLN:HG2	2.26	0.66
1:D:355:ARG:HH11	1:H:1052:THR:HG21	1.60	0.66
1:E:745:PHE:HD2	1:E:1067:SER:HB2	1.60	0.66
1:A:349:ASN:O	1:A:353:THR:HG23	1.95	0.66
1:F:783:TRP:HH2	1:F:853:HIS:CD2	2.13	0.66
1:H:358:VAL:HG21	1:H:432:MET:HE1	1.77	0.66
1:H:1000:LEU:HB2	1:H:1003:MET:HE2	1.77	0.66
1:H:1050:LEU:HD21	1:H:1059:LEU:HD22	1.78	0.66
1:D:355:ARG:NH1	1:H:1052:THR:HG21	2.11	0.65
1:E:395:ILE:HG23	1:E:557:ILE:HD13	1.78	0.65
1:F:915:THR:HG22	1:F:917:GLU:N	2.08	0.65
1:F:739:GLY:HA3	1:F:1100:ARG:CG	2.26	0.65
1:D:641:THR:N	1:D:644:THR:OG1	2.29	0.65
1:E:803:ARG:HB2	1:E:810:TYR:CZ	2.31	0.65
1:G:499:THR:HA	1:G:775:GLN:HE22	1.62	0.65
1:D:1075:GLN:HE22	1:D:1103:GLY:H	1.45	0.65
1:E:980:LEU:HD12	1:E:982:ILE:HG13	1.78	0.65
1:F:848:ILE:O	1:F:852:VAL:HG23	1.97	0.65
1:B:462:SER:O	1:B:466:ILE:HG13	1.97	0.65
1:G:713:SER:HG	1:G:740:PHE:HE2	1.45	0.65
1:G:1064:ARG:O	1:G:1068:ILE:HG12	1.96	0.65
1:E:674:TYR:HE2	1:E:1110:GLU:HG2	1.62	0.65
1:F:882:MET:HG2	1:F:883:VAL:HG23	1.79	0.65
1:H:366:PHE:O	1:H:370:VAL:HG22	1.97	0.64
1:H:857:ALA:O	1:H:859:LYS:NZ	2.29	0.64
1:D:926:ASN:HD21	1:D:1000:LEU:HB3	1.61	0.64
1:D:1115:VAL:O	1:D:1119:ILE:HG13	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:395:ILE:HG23	1:G:557:ILE:HD13	1.80	0.64
1:H:784:THR:HG22	1:H:890:ILE:HD11	1.78	0.64
1:H:1014:GLY:H	1:H:1123:THR:HG23	1.62	0.64
1:D:640:LEU:HB3	1:D:644:THR:OG1	1.98	0.64
1:F:847:VAL:HG23	1:F:970:MET:HE2	1.76	0.64
1:H:634:ASP:OD1	1:H:639:ARG:NE	2.30	0.64
1:C:348:ARG:HH21	1:C:708:LYS:HB2	1.63	0.64
1:G:917:GLU:HB3	1:G:920:ARG:HH12	1.61	0.64
1:H:437:GLN:NE2	1:H:1111:LEU:HA	2.12	0.64
1:D:599:LEU:HD22	1:D:652:PHE:CD1	2.32	0.64
1:F:1116:GLN:O	1:F:1120:ILE:HG13	1.98	0.64
1:G:993:ASN:O	1:G:999:ARG:NH2	2.30	0.64
1:G:450:ILE:HG22	1:G:454:ILE:HG13	1.80	0.64
1:H:350:HIS:NE2	1:H:398:GLN:OE1	2.31	0.64
1:B:435:ARG:HH21	1:B:438:ASP:HB2	1.58	0.64
1:D:914:TYR:CD1	1:D:933:LEU:HD12	2.33	0.64
1:F:905:ARG:HD2	1:F:953:TYR:OH	1.97	0.64
1:H:416:PHE:CE1	1:H:425:VAL:HG21	2.32	0.64
1:H:450:ILE:HA	1:H:454:ILE:HB	1.80	0.64
1:A:682:VAL:HB	1:A:697:THR:HG23	1.78	0.64
1:D:893:GLY:HA3	1:D:1005:LEU:HD23	1.78	0.64
1:E:942:LYS:O	1:E:945:ASN:ND2	2.31	0.64
1:E:995:THR:OG1	1:E:997:ASN:OD1	2.16	0.64
1:H:403:ILE:HG22	1:H:655:LYS:HD2	1.79	0.63
1:F:489:SER:O	1:F:493:ILE:HG12	1.98	0.63
1:F:960:TRP:CH2	1:F:964:GLU:HG3	2.33	0.63
1:G:354:VAL:HG11	1:G:411:PRO:HB2	1.79	0.63
1:H:596:GLN:HB3	1:H:648:LEU:HD21	1.79	0.63
1:E:487:ASP:O	1:E:787:GLY:HA2	1.98	0.63
1:A:505:VAL:HG23	1:A:506:LEU:HG	1.81	0.63
1:F:837:HIS:CE1	1:F:841:LEU:HD21	2.34	0.63
1:H:962:GLU:HB2	1:H:977:HIS:CE1	2.33	0.63
1:G:651:ALA:O	1:G:654:ILE:HG22	1.98	0.63
1:G:906:LYS:HE2	1:G:941:PRO:HD3	1.80	0.63
1:B:599:LEU:HD12	1:B:648:LEU:HD23	1.80	0.63
1:E:700:ILE:O	1:E:704:VAL:HG23	1.98	0.63
1:E:904:ILE:O	1:E:908:VAL:HG22	1.98	0.63
1:H:698:TYR:HD2	1:H:729:LYS:HE3	1.64	0.63
1:E:1099:VAL:HG11	1:E:1108:PHE:HD1	1.64	0.63
1:D:730:ILE:O	1:D:734:VAL:HG23	1.99	0.62
1:F:730:ILE:O	1:F:734:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:806:LEU:HD22	1:E:991:LEU:HA	1.80	0.62
1:H:775:GLN:HB3	1:H:780:ILE:HG21	1.82	0.62
1:C:382:ARG:NH2	1:C:613:GLU:OE1	2.33	0.62
1:F:789:THR:HG21	1:F:838:ILE:CG2	2.29	0.62
1:F:1058:GLY:HA3	1:F:1128:PHE:CD1	2.34	0.62
1:F:852:VAL:O	1:F:856:VAL:HG22	1.99	0.62
1:D:775:GLN:HB3	1:D:780:ILE:HG21	1.82	0.62
1:H:790:GLN:HG3	1:H:792:PRO:HD2	1.79	0.62
1:D:940:ALA:O	1:D:942:LYS:NZ	2.32	0.62
1:D:980:LEU:HA	1:D:1040:VAL:HG12	1.82	0.62
1:H:411:PRO:HB3	1:H:658:GLU:HG2	1.81	0.62
1:H:573:ARG:HE	1:H:577:LEU:CD2	2.13	0.62
1:D:685:GLN:HG3	1:D:746:ASP:OD2	2.00	0.61
1:D:758:PHE:HZ	1:D:780:ILE:HB	1.63	0.61
1:F:744:HIS:HE1	1:F:772:VAL:HB	1.66	0.61
1:A:653:ILE:HG23	1:A:712:PRO:HD2	1.82	0.61
1:E:411:PRO:HB3	1:E:658:GLU:HG2	1.83	0.61
1:F:837:HIS:O	1:F:841:LEU:HD23	2.00	0.61
1:F:587:VAL:HB	1:F:601:SER:HB2	1.81	0.61
1:G:863:SER:OG	1:G:875:ASP:HB2	2.00	0.61
1:E:775:GLN:HB3	1:E:780:ILE:HG21	1.82	0.61
1:F:899:ASP:HB3	1:F:942:LYS:HE3	1.81	0.61
1:A:435:ARG:NH2	1:A:438:ASP:O	2.33	0.61
1:B:428:GLU:OE2	1:B:665:GLU:HB2	2.01	0.61
1:D:943:TYR:OH	1:D:1027:VAL:HG22	2.01	0.61
1:F:488:LEU:HD23	1:F:787:GLY:HA3	1.83	0.61
1:A:1042:ASN:O	3:A:1301:HOH:O	2.16	0.61
1:E:432:MET:HE1	1:E:442:ILE:HB	1.83	0.61
1:E:1101:VAL:HG22	1:E:1119:ILE:HD11	1.82	0.61
1:F:487:ASP:O	1:F:787:GLY:HA2	2.01	0.61
1:A:999:ARG:NH1	1:A:1003:MET:O	2.34	0.61
1:E:738:MET:HG2	1:E:1098:ILE:HB	1.82	0.61
1:E:941:PRO:HB2	1:E:950:VAL:HB	1.82	0.61
1:E:1013:GLN:HG2	1:E:1121:SER:OG	2.01	0.61
1:F:911:GLU:HG3	1:F:913:LYS:HZ2	1.66	0.61
1:F:1114:GLU:OE1	1:F:1114:GLU:N	2.34	0.61
1:E:467:CYS:HB2	1:E:852:VAL:HG21	1.83	0.61
1:G:595:LEU:HD13	1:G:631:PHE:HB2	1.82	0.61
1:G:895:ALA:HB3	1:G:1006:SER:HB2	1.83	0.61
1:B:795:ILE:HG12	1:B:901:MET:HE1	1.82	0.60
1:C:423:ARG:HD2	1:C:465:GLU:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:943:TYR:HE1	1:F:1026:SER:HB3	1.66	0.60
1:H:791:TRP:NE1	1:H:961:THR:HG21	2.05	0.60
1:D:599:LEU:HD22	1:D:652:PHE:CG	2.36	0.60
1:F:406:HIS:CE1	1:F:408:CYS:HB2	2.36	0.60
1:G:806:LEU:HD23	1:G:991:LEU:HD23	1.82	0.60
1:H:528:MET:HG3	1:H:534:ILE:HG12	1.83	0.60
1:E:908:VAL:HG23	1:E:909:PHE:CD2	2.37	0.60
1:B:579:THR:O	1:B:582:GLU:HG2	2.01	0.60
1:E:674:TYR:CE2	1:E:1110:GLU:HG2	2.36	0.60
1:E:620:LEU:HD12	1:E:680:LEU:HD12	1.84	0.60
1:G:343:ARG:HG3	1:G:400:ASP:HB3	1.83	0.60
1:C:964:GLU:HA	1:C:967:LYS:HD2	1.84	0.60
1:A:444:GLU:OE2	1:C:342:PRO:HB3	2.02	0.60
1:E:1009:ILE:CG2	1:E:1035:MET:HE1	2.31	0.60
1:F:927:PHE:CD2	1:F:934:ARG:HB2	2.37	0.60
1:H:422:TRP:CE3	1:H:423:ARG:HA	2.36	0.60
1:D:790:GLN:HB2	1:D:792:PRO:HD2	1.84	0.60
1:F:955:LEU:HD13	1:F:1030:MET:HA	1.84	0.60
1:D:1073:GLN:HE22	1:D:1075:GLN:NE2	2.00	0.60
1:H:341:THR:HG22	1:H:343:ARG:H	1.67	0.60
1:H:364:LEU:HD23	1:H:454:ILE:HD11	1.84	0.60
1:H:396:LEU:HD13	1:H:409:GLY:O	2.01	0.60
1:E:428:GLU:O	1:E:432:MET:HG3	2.01	0.60
1:F:944:GLY:HA3	1:F:1011:PRO:HG3	1.84	0.60
1:B:1095:ARG:HA	1:B:1109:VAL:HG21	1.84	0.59
1:A:341:THR:HG22	1:A:343:ARG:H	1.66	0.59
1:H:407:PRO:HD3	1:H:607:SER:HB2	1.83	0.59
1:F:756:LYS:NZ	1:F:782:GLN:OE1	2.33	0.59
1:G:340:LEU:HB2	1:G:345:GLN:HE22	1.67	0.59
1:F:744:HIS:CE1	1:F:772:VAL:HB	2.38	0.59
1:F:999:ARG:NH1	1:F:1003:MET:O	2.35	0.59
1:C:823:THR:HG1	1:C:826:GLU:N	1.97	0.59
1:D:487:ASP:O	1:D:787:GLY:HA2	2.02	0.59
1:F:536:ARG:HG3	1:F:873:GLY:HA3	1.85	0.59
1:G:1060:ILE:O	1:G:1064:ARG:HG3	2.02	0.59
1:H:801:ARG:NH1	1:H:816:GLY:C	2.56	0.59
1:A:795:ILE:HG12	1:A:901:MET:HE3	1.83	0.59
1:B:744:HIS:CE1	1:B:1073:GLN:HG3	2.37	0.59
1:C:496:GLY:HA3	1:C:859:LYS:HE3	1.83	0.59
1:G:595:LEU:HG	1:G:599:LEU:HD13	1.84	0.59
1:H:478:ALA:HA	1:H:482:GLU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:622:ARG:NH2	1:F:685:GLN:O	2.27	0.59
1:H:424:TRP:O	1:H:428:GLU:HG3	2.02	0.59
1:H:570:ASN:O	1:H:573:ARG:N	2.36	0.59
1:C:1075:GLN:HE22	1:C:1103:GLY:HA2	1.67	0.59
1:D:1075:GLN:HE22	1:D:1103:GLY:N	2.00	0.59
1:E:419:ASP:HB3	1:E:458:TRP:CH2	2.38	0.59
1:F:429:LEU:HD13	1:F:447:LYS:HB2	1.84	0.59
1:H:390:CYS:HB3	1:H:553:TYR:HB2	1.85	0.59
1:E:696:LEU:O	1:E:700:ILE:HG12	2.03	0.59
1:H:416:PHE:HE2	1:H:454:ILE:HG21	1.68	0.59
1:D:479:PHE:HZ	1:D:838:ILE:HD13	1.67	0.58
1:G:407:PRO:HG3	1:G:608:LEU:HD23	1.85	0.58
1:H:570:ASN:O	1:H:572:GLN:N	2.36	0.58
1:H:573:ARG:HH21	1:H:577:LEU:HD21	1.67	0.58
1:D:1095:ARG:HA	1:D:1109:VAL:HG21	1.86	0.58
1:E:713:SER:HB3	1:E:1100:ARG:NH2	2.18	0.58
1:E:1075:GLN:HE22	1:E:1103:GLY:N	1.90	0.58
1:G:687:ARG:HD2	1:G:765:ASP:OD2	2.04	0.58
1:E:792:PRO:HG2	1:E:1005:LEU:HD13	1.83	0.58
1:E:913:LYS:HE2	1:E:914:TYR:OH	2.03	0.58
1:F:748:SER:OG	1:F:1071:ASN:O	2.17	0.58
1:H:416:PHE:CE1	1:H:425:VAL:HG11	2.38	0.58
1:C:1084:LEU:HD21	1:C:1099:VAL:HG21	1.85	0.58
1:E:817:ASP:OD1	1:E:819:ARG:HG2	2.03	0.58
1:F:742:ALA:HB2	1:F:1100:ARG:NH2	2.19	0.58
1:H:400:ASP:HA	1:H:573:ARG:HH12	1.69	0.58
1:A:337:MET:O	1:A:345:GLN:NE2	2.37	0.58
1:A:966:ARG:HH11	1:A:974:THR:CG2	2.16	0.58
1:D:337:MET:HG3	1:D:340:LEU:HD22	1.85	0.58
1:E:634:ASP:OD1	1:E:639:ARG:HD2	2.04	0.58
1:E:703:ALA:O	1:E:707:VAL:HG22	2.04	0.58
1:E:730:ILE:O	1:E:734:VAL:HG23	2.04	0.58
1:F:1055:GLY:HA2	1:F:1128:PHE:HE1	1.68	0.58
1:B:966:ARG:HH11	1:B:974:THR:HG23	1.68	0.58
1:C:966:ARG:HH11	1:C:974:THR:HG23	1.68	0.58
1:F:432:MET:HA	1:F:435:ARG:HG3	1.84	0.58
1:F:657:ALA:HA	1:F:711:GLN:HB2	1.86	0.58
1:H:739:GLY:HA3	1:H:1100:ARG:HB2	1.85	0.58
1:H:640:LEU:HB2	1:H:644:THR:OG1	2.04	0.58
1:D:728:GLU:OE2	1:D:1056:ARG:NH2	2.35	0.57
1:H:555:ARG:HG3	1:H:585:GLU:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:VAL:HG21	1:B:714:LEU:HD22	1.86	0.57
1:D:640:LEU:HD11	1:D:648:LEU:HD22	1.85	0.57
1:F:1108:PHE:CZ	1:F:1116:GLN:HG2	2.39	0.57
1:H:432:MET:CE	1:H:440:PHE:HB2	2.34	0.57
1:H:553:TYR:O	1:H:557:ILE:HG12	2.04	0.57
1:H:633:ALA:O	1:H:637:GLU:HG3	2.04	0.57
1:D:803:ARG:NH1	1:D:808:ASP:OD1	2.37	0.57
1:H:705:ARG:HD3	1:H:733:VAL:HG22	1.86	0.57
1:A:423:ARG:HH21	1:A:464:ASP:CG	2.07	0.57
1:B:898:VAL:HG13	1:B:953:TYR:HB2	1.86	0.57
1:D:905:ARG:HD2	1:D:953:TYR:OH	2.04	0.57
1:H:713:SER:HA	1:H:740:PHE:CE1	2.28	0.57
1:G:342:PRO:O	1:G:346:ARG:HG2	2.05	0.57
1:G:895:ALA:HA	1:G:898:VAL:HG22	1.85	0.57
1:F:835:ILE:HA	1:F:838:ILE:HD12	1.85	0.57
1:D:419:ASP:OD1	1:D:419:ASP:N	2.38	0.57
1:F:938:LEU:CD2	1:F:998:GLY:HA3	2.35	0.57
1:G:568:GLU:HG2	1:G:573:ARG:HD3	1.87	0.57
1:A:973:SER:OG	1:A:974:THR:N	2.37	0.57
1:C:1092:GLU:HG2	1:C:1093:LYS:H	1.70	0.57
1:E:745:PHE:CD2	1:E:1067:SER:HB2	2.40	0.57
1:F:822:ARG:O	1:F:909:PHE:HE1	1.88	0.57
1:H:962:GLU:OE1	1:H:977:HIS:ND1	2.30	0.57
1:A:813:LEU:HD11	1:A:837:HIS:HB2	1.86	0.57
1:B:966:ARG:HH11	1:B:974:THR:CG2	2.18	0.57
1:D:743:CYS:O	1:D:1073:GLN:HA	2.05	0.57
1:F:343:ARG:NH2	1:F:576:GLU:OE2	2.31	0.57
1:F:685:GLN:HG3	1:F:746:ASP:OD2	2.05	0.57
1:F:783:TRP:CH2	1:F:853:HIS:CD2	2.93	0.57
1:G:348:ARG:O	1:G:352:LEU:HD12	2.05	0.57
1:B:731:VAL:HG22	1:B:1059:LEU:HD23	1.86	0.57
1:G:616:THR:HB	1:G:661:TRP:CG	2.40	0.57
1:H:831:VAL:HG21	1:H:901:MET:HE1	1.87	0.57
1:H:871:GLU:OE1	1:H:871:GLU:N	2.35	0.57
1:D:650:GLN:HB3	1:D:707:VAL:HG21	1.87	0.56
1:D:1010:SER:HA	1:D:1041:HIS:CE1	2.39	0.56
1:H:367:THR:O	1:H:371:LYS:HB3	2.05	0.56
1:A:744:HIS:CE1	1:A:1073:GLN:HG3	2.41	0.56
1:B:530:ASN:HB3	1:B:532:GLU:OE1	2.05	0.56
1:H:403:ILE:HA	1:H:600:GLN:NE2	2.20	0.56
1:B:1100:ARG:NH2	3:B:1303:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1080:ASP:O	1:D:1083:VAL:HG22	2.05	0.56
1:E:640:LEU:HD11	1:E:648:LEU:HD12	1.86	0.56
1:F:907:LEU:O	1:F:912:LYS:HA	2.04	0.56
1:F:931:GLU:O	1:F:935:ARG:HG3	2.06	0.56
1:G:599:LEU:HD21	1:G:649:LEU:HD23	1.87	0.56
1:H:400:ASP:CA	1:H:573:ARG:HH12	2.18	0.56
1:H:650:GLN:HB3	1:H:707:VAL:HG21	1.87	0.56
1:B:382:ARG:NH2	1:B:613:GLU:OE1	2.39	0.56
1:E:894:LEU:O	1:E:898:VAL:HG22	2.05	0.56
1:G:710:TYR:HD2	1:G:1106:ALA:HA	1.69	0.56
1:H:788:TYR:CE2	1:H:890:ILE:HD13	2.40	0.56
1:H:1020:PRO:HA	1:H:1023:ILE:HD12	1.88	0.56
1:A:775:GLN:HB3	1:A:780:ILE:HG21	1.88	0.56
1:D:608:LEU:O	1:D:611:ILE:N	2.36	0.56
1:G:902:ALA:HB2	1:G:950:VAL:HG23	1.88	0.56
1:H:934:ARG:HG2	1:H:938:LEU:CD1	2.35	0.56
1:D:905:ARG:HD3	1:D:949:TYR:OH	2.05	0.56
1:H:906:LYS:HE2	1:H:911:GLU:OE2	2.06	0.56
1:H:1052:THR:HG22	1:H:1054:GLU:N	2.19	0.56
1:H:835:ILE:O	1:H:839:VAL:HG23	2.05	0.56
1:C:637:GLU:OE1	1:C:639:ARG:NH1	2.34	0.56
1:D:774:PRO:HD2	1:D:1037:ILE:O	2.06	0.56
1:D:1100:ARG:HG3	1:D:1101:VAL:N	2.21	0.56
1:E:993:ASN:ND2	1:E:994:ALA:H	2.03	0.56
1:E:756:LYS:NZ	1:E:782:GLN:OE1	2.37	0.56
1:F:914:TYR:OH	1:F:936:ASP:OD1	2.18	0.56
1:G:919:ILE:HD13	1:G:933:LEU:HD11	1.87	0.56
1:C:894:LEU:N	3:C:1302:HOH:O	2.23	0.56
1:C:959:GLU:OE2	1:C:1034:THR:HG21	2.06	0.56
1:F:465:GLU:O	1:F:468:GLU:HB3	2.06	0.56
1:G:631:PHE:HE2	1:G:645:ALA:HB1	1.71	0.56
1:G:744:HIS:HD2	1:G:749:HIS:HE1	1.55	0.56
1:A:428:GLU:HB3	1:A:432:MET:HG3	1.89	0.55
1:B:528:MET:CE	1:B:537:ILE:HG21	2.36	0.55
1:E:840:ARG:HG3	1:E:968:TYR:OH	2.05	0.55
1:A:560:HIS:HA	1:A:563:GLU:HG2	1.89	0.55
1:B:927:PHE:CD1	1:B:934:ARG:HB2	2.41	0.55
1:E:637:GLU:OE1	1:E:639:ARG:NH2	2.38	0.55
1:F:346:ARG:NH1	1:F:400:ASP:OD1	2.38	0.55
1:F:382:ARG:HD3	1:F:858:PRO:HD2	1.87	0.55
1:F:1059:LEU:HD11	1:F:1076:PHE:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:896:THR:HA	1:G:997:ASN:ND2	2.21	0.55
1:H:360:ILE:HG22	1:H:364:LEU:HG	1.87	0.55
1:H:416:PHE:HA	1:H:662:MET:HE1	1.89	0.55
1:H:599:LEU:HB3	1:H:652:PHE:CD2	2.41	0.55
1:H:1112:CYS:O	1:H:1116:GLN:HG2	2.07	0.55
1:C:346:ARG:NH1	1:C:400:ASP:OD1	2.39	0.55
1:C:685:GLN:H	1:C:717:ARG:NH2	2.04	0.55
1:E:554:ALA:HB2	1:E:588:PRO:HD2	1.87	0.55
1:H:1089:GLN:HB2	1:H:1090:GLU:HG3	1.88	0.55
1:C:797:PHE:O	1:C:802:GLY:N	2.31	0.55
1:G:546:THR:OG1	1:G:864:LEU:HD11	2.06	0.55
1:H:400:ASP:N	1:H:573:ARG:HH12	2.04	0.55
1:A:613:GLU:OE2	1:A:859:LYS:NZ	2.35	0.55
1:A:1114:GLU:OE1	1:A:1114:GLU:N	2.40	0.55
1:E:945:ASN:OD1	1:E:1016:ASP:HA	2.07	0.55
1:G:1088:GLN:OE1	1:G:1116:GLN:HG3	2.06	0.55
1:H:400:ASP:H	1:H:573:ARG:NH1	2.04	0.55
1:C:491:HIS:HB2	1:C:786:THR:HG23	1.89	0.55
1:E:905:ARG:HH11	1:E:949:TYR:HE2	1.55	0.55
1:F:776:LYS:HD2	1:F:779:ARG:HD2	1.87	0.55
1:H:1108:PHE:CZ	1:H:1116:GLN:HB2	2.42	0.55
1:C:355:ARG:HD2	1:C:441:GLU:OE2	2.05	0.55
1:D:583:VAL:HG21	1:D:596:GLN:OE1	2.07	0.55
1:C:1080:ASP:HB3	1:C:1083:VAL:HG23	1.88	0.55
1:E:480:SER:HB3	1:E:486:SER:O	2.07	0.55
1:F:844:ILE:HG22	1:F:848:ILE:HD11	1.89	0.55
1:A:558:ALA:O	1:A:561:ALA:HB3	2.06	0.55
1:B:973:SER:OG	1:B:974:THR:N	2.39	0.55
1:F:923:LEU:HD11	1:F:996:PRO:HG3	1.88	0.55
1:H:343:ARG:NH1	1:H:402:LEU:HD11	2.22	0.55
1:C:646:LEU:O	1:C:650:GLN:HG3	2.07	0.55
1:A:993:ASN:O	1:A:999:ARG:NH2	2.40	0.54
1:B:349:ASN:O	1:B:353:THR:HG23	2.07	0.54
1:D:1044:LYS:HE3	1:D:1124:VAL:HG22	1.88	0.54
1:D:437:GLN:HE21	1:D:437:GLN:HA	1.73	0.54
1:F:539:TYR:O	1:F:542:ALA:HB3	2.06	0.54
1:C:982:ILE:HG23	1:C:1104:TYR:CE1	2.42	0.54
1:C:999:ARG:NH1	1:C:1003:MET:O	2.39	0.54
1:F:432:MET:HA	1:F:435:ARG:CG	2.38	0.54
1:H:687:ARG:NH1	1:H:765:ASP:OD2	2.35	0.54
1:H:984:ASN:HB2	1:H:988:ILE:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:803:ARG:HD2	1:C:808:ASP:OD1	2.07	0.54
1:E:817:ASP:OD1	1:E:818:LEU:N	2.39	0.54
1:E:1021:THR:HA	1:E:1024:ILE:HG12	1.89	0.54
1:E:1075:GLN:NE2	1:E:1103:GLY:H	1.89	0.54
1:F:789:THR:HG21	1:F:838:ILE:HG23	1.88	0.54
1:G:422:TRP:CZ2	1:G:459:GLU:HA	2.42	0.54
1:G:790:GLN:NE2	1:G:793:ILE:HB	2.22	0.54
1:A:1084:LEU:HD22	1:A:1108:PHE:CE1	2.42	0.54
1:B:1044:LYS:HE3	1:B:1124:VAL:HG22	1.89	0.54
1:G:682:VAL:HG22	1:G:714:LEU:HD11	1.88	0.54
1:G:917:GLU:HB3	1:G:920:ARG:NH1	2.21	0.54
1:G:1095:ARG:HA	1:G:1109:VAL:HG21	1.88	0.54
1:B:618:LEU:HB2	3:B:1356:HOH:O	2.08	0.54
1:G:886:GLY:O	1:G:973:SER:HB3	2.07	0.54
1:C:654:ILE:O	1:C:658:GLU:HG3	2.08	0.54
1:E:982:ILE:O	1:E:1102:ALA:HB3	2.08	0.54
1:B:513:ASN:OD1	1:B:589:ALA:HB1	2.07	0.54
1:D:520:GLU:HG3	1:D:544:ILE:HD11	1.90	0.54
1:F:914:TYR:CD1	1:F:933:LEU:HD12	2.43	0.54
1:C:908:VAL:HG11	1:C:916:LEU:CD2	2.38	0.54
1:F:653:ILE:HG23	1:F:712:PRO:HD2	1.90	0.54
1:G:487:ASP:O	1:G:787:GLY:HA2	2.08	0.54
1:H:680:LEU:HD23	1:H:714:LEU:HD12	1.90	0.54
1:D:941:PRO:HB3	1:D:947:ASP:OD2	2.08	0.53
1:E:562:ARG:HH12	1:E:585:GLU:HG3	1.73	0.53
1:E:1111:LEU:O	1:E:1116:GLN:NE2	2.40	0.53
1:F:744:HIS:HD1	1:F:749:HIS:CE1	2.26	0.53
1:D:905:ARG:HD3	1:D:949:TYR:CZ	2.43	0.53
1:G:593:LYS:N	1:G:597:GLU:OE1	2.40	0.53
1:G:726:TYR:CE2	1:G:730:ILE:HD11	2.43	0.53
1:H:522:HIS:O	1:H:525:SER:HB3	2.08	0.53
1:H:609:PHE:CD1	1:H:861:LEU:HD23	2.43	0.53
1:D:669:LYS:O	1:D:983:SER:OG	2.26	0.53
1:F:432:MET:HA	1:F:435:ARG:HD3	1.90	0.53
1:F:622:ARG:NH1	1:F:765:ASP:HA	2.23	0.53
1:F:1039:MET:SD	1:F:1072:GLY:HA3	2.48	0.53
1:H:738:MET:HB2	1:H:740:PHE:CD2	2.40	0.53
1:C:375:GLY:HA3	1:G:466:ILE:HA	1.89	0.53
1:E:713:SER:HB3	1:E:1100:ARG:HH21	1.74	0.53
1:G:380:LEU:HA	1:G:542:ALA:HB2	1.89	0.53
1:H:739:GLY:HA2	1:H:1076:PHE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:ARG:NH1	1:B:732:ASP:HB3	2.23	0.53
1:C:962:GLU:OE2	1:C:976:SER:OG	2.26	0.53
1:D:744:HIS:NE2	1:D:1073:GLN:HG3	2.24	0.53
1:E:739:GLY:HA3	1:E:1100:ARG:CG	2.38	0.53
1:G:1044:LYS:NZ	1:G:1081:ASN:HD21	2.07	0.53
1:H:463:LEU:HG	1:H:852:VAL:HG12	1.91	0.53
1:G:442:ILE:HG23	1:G:447:LYS:HZ2	1.72	0.53
1:G:682:VAL:CG2	1:G:714:LEU:HD11	2.39	0.53
1:H:443:SER:CB	1:H:446:ASP:H	2.22	0.53
1:C:478:ALA:HA	1:C:482:GLU:HB2	1.91	0.53
1:D:790:GLN:OE1	1:D:792:PRO:HD2	2.09	0.53
1:F:407:PRO:HB2	1:F:611:ILE:HD11	1.89	0.53
1:F:818:LEU:HD23	1:F:821:LEU:HD12	1.89	0.53
1:G:999:ARG:HD2	1:G:1004:PRO:O	2.09	0.53
1:E:639:ARG:O	1:E:640:LEU:HD23	2.09	0.53
1:F:752:MET:O	1:F:756:LYS:HG3	2.09	0.53
1:F:773:GLU:OE1	1:F:784:THR:HG21	2.07	0.53
1:A:685:GLN:HG3	1:A:746:ASP:OD2	2.09	0.53
1:B:379:ILE:HD13	1:B:858:PRO:HB2	1.91	0.53
1:E:803:ARG:HB2	1:E:810:TYR:CE1	2.44	0.53
1:E:1106:ALA:HB3	1:E:1111:LEU:HD11	1.91	0.53
1:H:641:THR:N	1:H:644:THR:OG1	2.37	0.53
1:C:504:ASP:OD1	1:C:504:ASP:N	2.42	0.52
1:E:1049:LEU:HD21	1:E:1128:PHE:CE2	2.43	0.52
1:F:464:ASP:OD1	1:F:492:GLN:NE2	2.42	0.52
1:H:550:VAL:CG1	1:H:608:LEU:HD13	2.38	0.52
1:H:553:TYR:CZ	1:H:557:ILE:HD11	2.44	0.52
1:C:344:MET:HG2	1:C:650:GLN:OE1	2.09	0.52
1:E:774:PRO:HD2	1:E:1037:ILE:O	2.09	0.52
1:H:612:GLU:OE1	1:H:615:GLN:NE2	2.34	0.52
1:H:986:THR:HA	1:H:1004:PRO:HB3	1.91	0.52
1:A:513:ASN:OD1	1:A:589:ALA:HB1	2.09	0.52
1:D:487:ASP:OD1	1:D:489:SER:HB3	2.08	0.52
1:D:937:CYS:C	1:D:939:ASN:H	2.12	0.52
1:E:1048:GLY:HA2	1:E:1051:ASP:OD2	2.08	0.52
1:H:578:LEU:HD12	1:H:578:LEU:O	2.09	0.52
1:G:686:LYS:N	1:G:692:ALA:HB2	2.25	0.52
1:H:370:VAL:HG12	1:H:381:LEU:HD21	1.91	0.52
1:A:657:ALA:HA	1:A:711:GLN:HB2	1.92	0.52
1:C:737:GLY:HA2	1:C:1078:TYR:HB3	1.89	0.52
1:C:888:GLY:HA2	1:C:976:SER:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1032:VAL:HB	1:E:1039:MET:SD	2.50	0.52
1:F:803:ARG:NH2	1:F:924:LEU:HD21	2.24	0.52
1:F:927:PHE:CE2	1:F:933:LEU:HD23	2.45	0.52
1:F:1073:GLN:HE22	1:F:1075:GLN:CG	2.18	0.52
1:H:819:ARG:HG3	1:H:917:GLU:OE1	2.08	0.52
1:B:1075:GLN:CD	1:B:1100:ARG:HE	2.12	0.52
1:C:1092:GLU:HG2	1:C:1093:LYS:N	2.24	0.52
1:D:343:ARG:CZ	1:D:647:GLU:OE1	2.58	0.52
1:F:828:ASP:OD1	1:F:832:LYS:HE2	2.10	0.52
1:F:970:MET:HE2	1:F:970:MET:HA	1.91	0.52
1:G:790:GLN:HE21	1:G:793:ILE:H	1.57	0.52
1:H:491:HIS:CE1	1:H:783:TRP:CG	2.97	0.52
1:H:1003:MET:HG2	1:H:1004:PRO:HD2	1.92	0.52
1:A:1006:SER:O	3:A:1302:HOH:O	2.18	0.52
1:C:564:LEU:HD23	1:C:567:LYS:NZ	2.24	0.52
1:D:653:ILE:HG23	1:D:712:PRO:HD2	1.92	0.52
1:F:355:ARG:NH2	1:F:1095:ARG:HE	2.06	0.52
1:C:488:LEU:HD13	1:C:845:GLY:HA3	1.90	0.52
1:C:805:VAL:HG21	1:C:993:ASN:ND2	2.25	0.52
1:D:735:LYS:NZ	1:D:1051:ASP:HA	2.25	0.52
1:D:965:CYS:O	1:D:975:LEU:HB3	2.10	0.52
1:F:930:TYR:O	1:F:933:LEU:N	2.42	0.52
1:G:624:ASP:OD1	1:G:625:GLN:HG2	2.09	0.52
1:H:1009:ILE:HD13	1:H:1039:MET:HG3	1.91	0.52
1:H:1101:VAL:HB	1:H:1104:TYR:CE1	2.44	0.52
1:B:1075:GLN:HE22	1:B:1103:GLY:CA	2.21	0.52
1:D:362:ARG:NH1	1:D:417:SER:HA	2.25	0.52
1:D:681:THR:HG21	1:D:768:LEU:N	2.25	0.52
1:D:923:LEU:HD11	1:D:996:PRO:HG3	1.91	0.52
1:G:641:THR:O	1:G:643:ASP:N	2.43	0.52
1:A:639:ARG:O	1:A:640:LEU:HD12	2.09	0.52
1:B:341:THR:HG21	1:B:647:GLU:CD	2.31	0.52
1:E:728:GLU:OE2	1:E:1056:ARG:NE	2.42	0.52
1:G:429:LEU:O	1:G:447:LYS:HE3	2.10	0.52
1:H:785:SER:HB3	1:H:890:ILE:CD1	2.37	0.52
1:B:988:ILE:O	1:B:991:LEU:HB2	2.09	0.51
1:C:744:HIS:CE1	1:C:772:VAL:HG12	2.46	0.51
1:C:993:ASN:O	1:C:999:ARG:NH2	2.42	0.51
1:D:503:TYR:HA	1:D:507:LEU:HB3	1.92	0.51
1:D:1073:GLN:NE2	1:D:1075:GLN:HE21	2.08	0.51
1:D:1082:GLU:HA	1:D:1085:LYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:448:LYS:O	1:E:452:GLU:HG3	2.10	0.51
1:F:934:ARG:O	1:F:938:LEU:HG	2.10	0.51
1:G:798:VAL:HG23	1:G:834:GLN:HG3	1.92	0.51
1:B:718:ILE:HD12	1:B:743:CYS:HB3	1.91	0.51
1:B:832:LYS:HD3	1:B:960:TRP:CE2	2.45	0.51
1:C:769:MET:SD	1:C:770:GLY:N	2.83	0.51
1:C:1041:HIS:HB3	1:C:1073:GLN:O	2.11	0.51
1:F:676:PRO:HD2	1:F:711:GLN:NE2	2.25	0.51
1:F:800:ASN:HD21	1:F:924:LEU:HD11	1.75	0.51
1:D:785:SER:HA	1:D:888:GLY:O	2.10	0.51
1:F:801:ARG:HG2	1:F:801:ARG:O	2.10	0.51
1:G:779:ARG:HG2	1:G:882:MET:SD	2.50	0.51
1:G:1043:PHE:HB2	1:G:1076:PHE:CD2	2.45	0.51
1:B:428:GLU:HG2	1:B:432:MET:HG3	1.92	0.51
1:C:805:VAL:HG21	1:C:993:ASN:HD22	1.74	0.51
1:E:979:THR:CG2	1:E:1035:MET:CE	2.35	0.51
1:G:432:MET:HE3	1:G:440:PHE:HB2	1.92	0.51
1:G:820:ASP:OD2	1:G:822:ARG:NH2	2.43	0.51
1:A:801:ARG:HG2	1:A:814:ASP:OD1	2.10	0.51
1:B:487:ASP:O	1:B:787:GLY:HA2	2.11	0.51
1:C:346:ARG:HD2	1:C:400:ASP:OD2	2.09	0.51
1:D:986:THR:O	1:D:990:GLU:HG3	2.11	0.51
1:E:486:SER:HG	1:E:842:SER:HG	1.56	0.51
1:G:722:SER:O	1:G:1064:ARG:NH2	2.44	0.51
1:H:1086:LYS:HE3	1:H:1086:LYS:HA	1.92	0.51
1:A:708:LYS:HA	1:A:738:MET:SD	2.51	0.51
1:E:508:PHE:O	1:E:591:PRO:HB3	2.09	0.51
1:E:937:CYS:O	1:E:942:LYS:NZ	2.44	0.51
1:F:1084:LEU:HD22	1:F:1108:PHE:CE1	2.45	0.51
1:H:437:GLN:NE2	1:H:672:ALA:HB1	2.25	0.51
1:D:790:GLN:NE2	1:D:793:ILE:HB	2.26	0.51
1:F:369:VAL:O	1:F:373:ASN:ND2	2.44	0.51
1:F:1084:LEU:HD21	1:F:1099:VAL:HG21	1.93	0.51
1:G:605:VAL:HG11	1:G:865:LEU:HD11	1.93	0.51
1:H:352:LEU:HD21	1:H:1095:ARG:HE	1.76	0.51
1:A:773:GLU:OE2	1:A:980:LEU:HD13	2.11	0.51
1:A:965:CYS:O	1:A:975:LEU:HB3	2.11	0.51
1:D:771:CYS:O	3:D:1302:HOH:O	2.19	0.51
1:F:448:LYS:HE2	1:F:452:GLU:CD	2.31	0.51
1:F:845:GLY:HA2	1:F:848:ILE:HD12	1.93	0.51
1:F:995:THR:HB	1:F:997:ASN:OD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:348:ARG:HH21	1:G:708:LYS:HB2	1.76	0.51
1:H:564:LEU:HD23	1:H:564:LEU:O	2.10	0.51
1:A:522:HIS:O	1:A:525:SER:OG	2.26	0.51
1:D:785:SER:HB3	1:D:890:ILE:HG12	1.92	0.51
1:E:980:LEU:HA	1:E:1040:VAL:HG12	1.92	0.51
1:G:498:ASP:HA	1:G:769:MET:SD	2.50	0.51
1:H:342:PRO:O	1:H:346:ARG:HG3	2.10	0.51
1:H:510:LYS:HB2	1:H:514:GLY:HA3	1.92	0.51
1:C:523:LEU:HD11	1:C:537:ILE:HG23	1.93	0.51
1:D:337:MET:HB3	1:D:340:LEU:HB2	1.92	0.51
1:F:393:ALA:O	1:F:556:ARG:NH2	2.44	0.51
1:H:719:HIS:CD2	1:H:721:GLN:H	2.29	0.51
1:F:872:SER:HB3	1:F:874:LYS:HG2	1.93	0.50
1:H:522:HIS:HB3	1:H:540:TYR:CE2	2.46	0.50
1:G:343:ARG:NH1	1:G:402:LEU:HD11	2.26	0.50
1:H:379:ILE:HG23	1:H:380:LEU:H	1.76	0.50
1:H:583:VAL:HG22	1:H:597:GLU:HG3	1.92	0.50
1:H:850:GLN:CD	1:H:971:LEU:HB2	2.32	0.50
1:A:962:GLU:HB2	1:A:977:HIS:HE1	1.74	0.50
1:C:882:MET:HG2	1:C:883:VAL:HG23	1.93	0.50
1:E:783:TRP:HB2	1:E:887:PRO:HB3	1.93	0.50
1:F:920:ARG:HD2	1:F:924:LEU:HD12	1.93	0.50
1:F:999:ARG:HD2	1:F:1004:PRO:O	2.11	0.50
1:G:739:GLY:HA3	1:G:1100:ARG:HD3	1.93	0.50
1:B:416:PHE:HE2	1:B:454:ILE:HG21	1.77	0.50
1:C:965:CYS:O	1:C:975:LEU:HB3	2.10	0.50
1:D:1080:ASP:HB3	1:D:1083:VAL:HG13	1.93	0.50
1:F:1088:GLN:HE21	1:F:1113:LYS:HG3	1.77	0.50
1:G:728:GLU:HG3	1:G:1056:ARG:NH2	2.08	0.50
1:G:1027:VAL:HG21	1:G:1041:HIS:CD2	2.47	0.50
1:H:915:THR:OG1	1:H:918:GLN:HG3	2.11	0.50
1:B:568:GLU:HG3	1:B:570:ASN:H	1.76	0.50
1:F:825:ASP:O	1:F:828:ASP:HB3	2.11	0.50
1:F:915:THR:HB	1:F:918:GLN:HG2	1.93	0.50
1:H:680:LEU:HD23	1:H:714:LEU:CD1	2.42	0.50
1:H:962:GLU:HB2	1:H:977:HIS:HE1	1.74	0.50
1:B:637:GLU:OE1	1:B:639:ARG:NH1	2.43	0.50
1:E:464:ASP:OD1	1:E:493:ILE:HG22	2.10	0.50
1:F:443:SER:O	1:F:447:LYS:HD2	2.12	0.50
1:F:546:THR:HG21	1:F:860:PRO:HB2	1.94	0.50
1:F:1080:ASP:HB3	1:F:1083:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1082:GLU:HA	1:F:1085:LYS:CG	2.42	0.50
1:H:573:ARG:O	1:H:577:LEU:HD23	2.10	0.50
1:H:586:ASN:O	1:H:590:ASN:HB2	2.10	0.50
1:A:499:THR:O	1:A:501:PRO:HD3	2.12	0.50
1:B:528:MET:HE3	1:B:537:ILE:HG21	1.93	0.50
1:B:595:LEU:N	1:B:634:ASP:OD2	2.38	0.50
1:C:1073:GLN:HE22	1:C:1075:GLN:HG3	1.76	0.50
1:D:779:ARG:HG2	1:D:882:MET:SD	2.51	0.50
1:E:435:ARG:NH1	1:E:663:SER:O	2.45	0.50
1:F:546:THR:OG1	1:F:864:LEU:HD11	2.12	0.50
1:F:771:CYS:HB3	1:F:1103:GLY:HA3	1.92	0.50
1:F:906:LYS:HG3	1:F:910:GLU:CB	2.40	0.50
1:H:387:ARG:HG2	1:H:391:GLU:OE1	2.10	0.50
1:A:572:GLN:O	1:A:575:ALA:N	2.45	0.50
1:F:349:ASN:O	1:F:353:THR:HG23	2.10	0.50
1:G:499:THR:O	1:G:501:PRO:HD3	2.12	0.50
1:G:984:ASN:HB2	1:G:988:ILE:HG13	1.94	0.50
1:H:799:LEU:HA	1:H:818:LEU:HD21	1.94	0.50
1:A:850:GLN:NE2	1:A:887:PRO:HD3	2.27	0.50
1:C:387:ARG:NH1	1:C:545:GLU:OE2	2.44	0.50
1:C:657:ALA:HA	1:C:711:GLN:HB2	1.94	0.50
1:F:504:ASP:OD2	1:F:505:VAL:HG23	2.12	0.50
1:G:351:TYR:HB2	1:G:654:ILE:HD11	1.94	0.50
1:H:900:SER:HB3	1:H:996:PRO:HD2	1.94	0.50
1:A:980:LEU:HD23	1:A:980:LEU:H	1.76	0.49
1:D:745:PHE:CD1	1:D:1067:SER:HB2	2.46	0.49
1:E:435:ARG:NH2	1:E:438:ASP:O	2.45	0.49
1:F:670:TYR:CD2	1:F:984:ASN:HB3	2.48	0.49
1:H:914:TYR:CZ	1:H:933:LEU:HB3	2.47	0.49
1:B:370:VAL:HA	1:B:381:LEU:HD11	1.94	0.49
1:B:1079:VAL:HG11	1:B:1084:LEU:HD21	1.94	0.49
1:E:669:LYS:HA	1:E:672:ALA:HB2	1.93	0.49
1:F:943:TYR:OH	1:F:1027:VAL:HA	2.11	0.49
1:H:450:ILE:HG22	1:H:454:ILE:HG13	1.94	0.49
1:A:966:ARG:HH11	1:A:974:THR:HG23	1.76	0.49
1:D:554:ALA:HB2	1:D:588:PRO:HD2	1.94	0.49
1:H:490:TYR:HE2	1:H:491:HIS:CE1	2.30	0.49
1:H:1046:LEU:HD12	1:H:1047:LYS:H	1.77	0.49
1:B:623:VAL:HG21	1:B:680:LEU:HD11	1.93	0.49
1:D:504:ASP:OD1	1:D:504:ASP:N	2.45	0.49
1:E:483:THR:HG21	1:E:811:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:773:GLU:OE2	2:F:1201:A1H9K:O1	2.31	0.49
1:F:835:ILE:O	1:F:838:ILE:HB	2.12	0.49
1:G:359:SER:HB3	1:G:414:GLY:O	2.12	0.49
1:H:955:LEU:HD13	1:H:1030:MET:HA	1.95	0.49
1:H:1085:LYS:HD2	1:H:1085:LYS:O	2.13	0.49
1:A:636:ARG:HG2	1:A:636:ARG:HH11	1.78	0.49
1:B:708:LYS:HA	1:B:738:MET:SD	2.53	0.49
1:D:720:ASN:OD1	1:D:1067:SER:OG	2.24	0.49
1:D:749:HIS:HA	1:D:752:MET:CG	2.41	0.49
1:H:573:ARG:HE	1:H:577:LEU:HD23	1.77	0.49
1:H:790:GLN:OE1	1:H:793:ILE:HB	2.13	0.49
1:H:795:ILE:HG12	1:H:901:MET:HE3	1.93	0.49
1:A:737:GLY:HA2	1:A:1078:TYR:HB3	1.94	0.49
1:C:396:LEU:HD22	1:C:409:GLY:O	2.12	0.49
1:D:735:LYS:HE2	1:D:1056:ARG:NH1	2.27	0.49
1:F:786:THR:HG21	1:F:849:SER:HB3	1.94	0.49
1:H:540:TYR:O	1:H:544:ILE:HG13	2.13	0.49
1:H:986:THR:HG21	1:H:1115:VAL:HA	1.93	0.49
1:H:1114:GLU:CD	1:H:1114:GLU:H	2.15	0.49
1:D:866:VAL:HG11	1:D:876:VAL:CG1	2.42	0.49
1:F:847:VAL:HG23	1:F:970:MET:HE1	1.89	0.49
1:F:898:VAL:HG12	1:F:950:VAL:HG22	1.94	0.49
1:F:966:ARG:HH11	1:F:974:THR:HG23	1.77	0.49
1:C:1075:GLN:NE2	1:C:1103:GLY:HA2	2.27	0.49
1:D:732:ASP:O	1:D:735:LYS:HB2	2.12	0.49
1:F:1082:GLU:OE2	1:F:1085:LYS:HE3	2.12	0.49
1:H:346:ARG:HE	1:H:400:ASP:CG	2.16	0.49
1:H:407:PRO:HB2	1:H:611:ILE:CG1	2.43	0.49
1:H:1127:LYS:HD3	1:H:1127:LYS:N	2.27	0.49
1:B:993:ASN:HB3	3:B:1364:HOH:O	2.13	0.49
1:C:640:LEU:HD13	1:C:645:ALA:HB2	1.95	0.49
1:C:931:GLU:O	1:C:935:ARG:HG3	2.13	0.49
1:E:758:PHE:HZ	1:E:780:ILE:HD12	1.78	0.49
1:G:573:ARG:O	1:G:577:LEU:HG	2.12	0.49
1:B:743:CYS:O	1:B:1073:GLN:HA	2.12	0.49
1:F:622:ARG:HH11	1:F:765:ASP:HA	1.78	0.49
1:F:805:VAL:HG11	1:F:993:ASN:ND2	2.28	0.49
1:G:488:LEU:HD13	1:G:845:GLY:HA3	1.94	0.49
1:G:603:TRP:CZ2	1:G:655:LYS:HG2	2.48	0.49
1:G:948:ASN:O	1:G:952:GLN:HG2	2.12	0.49
1:H:635:ILE:HD13	1:H:642:HIS:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:850:GLN:HB3	1:H:971:LEU:HD22	1.94	0.49
1:H:1063:LEU:HD21	1:H:1076:PHE:HZ	1.78	0.49
1:A:919:ILE:O	1:A:923:LEU:HG	2.13	0.48
1:D:934:ARG:HE	1:D:938:LEU:HD11	1.77	0.48
1:F:419:ASP:HB3	1:F:458:TRP:CZ3	2.48	0.48
1:F:742:ALA:HB2	1:F:1100:ARG:HH22	1.76	0.48
1:G:1016:ASP:OD1	1:G:1016:ASP:N	2.43	0.48
1:H:437:GLN:HG3	1:H:438:ASP:H	1.77	0.48
1:H:543:ALA:O	1:H:546:THR:HG22	2.12	0.48
1:H:573:ARG:HH21	1:H:577:LEU:CD2	2.26	0.48
1:C:917:GLU:HB3	1:C:920:ARG:NH2	2.28	0.48
1:D:993:ASN:OD1	1:D:994:ALA:N	2.46	0.48
1:D:1075:GLN:OE1	1:D:1100:ARG:HD3	2.13	0.48
1:E:906:LYS:HB2	1:E:949:TYR:OH	2.14	0.48
1:F:844:ILE:O	1:F:848:ILE:HG13	2.13	0.48
1:G:1027:VAL:HG21	1:G:1041:HIS:HD2	1.78	0.48
1:H:761:GLU:O	1:H:765:ASP:HB2	2.12	0.48
1:H:790:GLN:CG	1:H:792:PRO:HD2	2.43	0.48
1:D:397:ILE:HG12	1:D:404:VAL:HB	1.94	0.48
1:D:599:LEU:HD11	1:D:649:LEU:HD23	1.94	0.48
1:E:934:ARG:NH1	1:E:1000:LEU:HD21	2.27	0.48
1:H:512:MET:CE	1:H:605:VAL:HG11	2.43	0.48
1:A:574:ARG:HD2	3:A:1361:HOH:O	2.12	0.48
1:H:562:ARG:O	1:H:565:ALA:HB3	2.14	0.48
1:H:790:GLN:CD	1:H:793:ILE:HB	2.34	0.48
1:H:971:LEU:HB3	1:H:972:TYR:CD2	2.48	0.48
1:A:386:PHE:CE2	1:A:546:THR:HG23	2.48	0.48
1:B:435:ARG:NE	1:B:437:GLN:O	2.47	0.48
1:C:1044:LYS:HE3	1:C:1124:VAL:HG12	1.96	0.48
1:G:364:LEU:O	1:G:368:GLU:HG3	2.13	0.48
1:G:559:ALA:HA	1:G:562:ARG:NH1	2.28	0.48
1:H:1094:TYR:HB3	1:H:1097:LEU:HB2	1.95	0.48
1:A:1090:GLU:OE1	1:A:1093:LYS:NZ	2.38	0.48
1:G:927:PHE:CD2	1:G:934:ARG:HD2	2.49	0.48
1:A:468:GLU:HB2	1:A:492:GLN:NE2	2.28	0.48
1:D:616:THR:HB	1:D:661:TRP:CG	2.48	0.48
1:G:906:LYS:HE2	1:G:941:PRO:CD	2.43	0.48
1:G:1020:PRO:HG3	1:G:1128:PHE:HD1	1.79	0.48
1:A:340:LEU:HB3	1:A:344:MET:HB3	1.94	0.48
1:A:828:ASP:CG	1:A:832:LYS:HZ3	2.16	0.48
1:C:871:GLU:OE1	1:C:871:GLU:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:823:THR:OG1	1:D:824:PHE:N	2.46	0.48
1:D:1042:ASN:ND2	1:D:1101:VAL:O	2.46	0.48
1:D:1042:ASN:ND2	1:D:1122:ARG:NH1	2.61	0.48
1:D:1066:ALA:CB	1:D:1074:MET:HE2	2.44	0.48
1:F:798:VAL:HG12	1:F:799:LEU:HD23	1.95	0.48
1:F:908:VAL:O	1:F:912:LYS:CE	2.46	0.48
1:G:369:VAL:HG21	1:G:385:ALA:HA	1.95	0.48
1:H:503:TYR:OH	1:H:606:GLU:OE1	2.23	0.48
1:H:573:ARG:HE	1:H:577:LEU:HD21	1.79	0.48
1:A:1080:ASP:HB3	1:A:1083:VAL:HG23	1.96	0.48
1:B:776:LYS:HD2	1:B:779:ARG:HD2	1.96	0.48
1:C:742:ALA:HB2	1:C:1100:ARG:NH2	2.29	0.48
1:C:806:LEU:HB2	1:C:1002:TRP:CH2	2.48	0.48
1:C:995:THR:HG23	1:C:999:ARG:HH21	1.78	0.48
1:H:428:GLU:OE1	1:H:665:GLU:HB2	2.14	0.48
1:H:508:PHE:O	1:H:591:PRO:HB3	2.13	0.48
1:H:908:VAL:O	1:H:912:LYS:HE2	2.13	0.48
1:H:1093:LYS:N	1:H:1093:LYS:HD2	2.29	0.48
1:B:343:ARG:HH12	1:B:576:GLU:CD	2.17	0.48
1:B:376:MET:HB3	1:B:381:LEU:HB2	1.95	0.48
1:D:483:THR:OG1	1:D:485:VAL:HG23	2.14	0.48
1:D:1095:ARG:HG2	1:D:1095:ARG:HH11	1.78	0.48
1:H:653:ILE:HG23	1:H:712:PRO:HD2	1.96	0.48
1:H:1108:PHE:CE1	1:H:1116:GLN:HB2	2.49	0.48
1:C:1095:ARG:HA	1:C:1109:VAL:HG21	1.95	0.47
1:D:654:ILE:O	1:D:658:GLU:HG3	2.13	0.47
1:D:898:VAL:HG13	1:D:953:TYR:HB2	1.96	0.47
1:E:934:ARG:CZ	1:E:1000:LEU:HD21	2.44	0.47
1:F:391:GLU:O	1:F:556:ARG:NH1	2.47	0.47
1:G:708:LYS:HA	1:G:738:MET:SD	2.54	0.47
1:B:941:PRO:HG2	1:B:949:TYR:CD2	2.49	0.47
1:D:491:HIS:CE1	1:D:783:TRP:CD2	3.02	0.47
1:D:594:THR:O	1:D:597:GLU:N	2.47	0.47
1:E:968:TYR:O	1:E:974:THR:OG1	2.27	0.47
1:F:832:LYS:HD3	1:F:960:TRP:CE2	2.49	0.47
1:G:458:TRP:O	1:G:461:ARG:N	2.46	0.47
1:H:859:LYS:HD2	3:H:1307:HOH:O	2.15	0.47
1:D:420:ILE:HD11	1:D:613:GLU:OE1	2.14	0.47
1:D:1095:ARG:HD3	1:D:1095:ARG:C	2.34	0.47
1:E:854:ARG:HA	1:E:877:ALA:HB1	1.96	0.47
1:F:503:TYR:HA	1:F:507:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:746:ASP:O	1:F:750:ILE:HG13	2.15	0.47
1:H:600:GLN:O	1:H:604:THR:OG1	2.24	0.47
1:H:981:SER:O	1:H:981:SER:OG	2.26	0.47
1:C:822:ARG:HD2	1:C:822:ARG:HA	1.65	0.47
1:F:785:SER:HA	1:F:888:GLY:O	2.14	0.47
1:G:717:ARG:NH2	1:G:764:ARG:O	2.47	0.47
1:H:925:ALA:O	1:H:928:GLU:HG3	2.14	0.47
1:A:343:ARG:HH22	1:A:576:GLU:CD	2.18	0.47
1:C:346:ARG:HH11	1:C:400:ASP:CG	2.18	0.47
1:C:620:LEU:HD12	1:C:680:LEU:HD12	1.96	0.47
1:D:343:ARG:NE	1:D:647:GLU:CD	2.65	0.47
1:D:953:TYR:N	1:D:953:TYR:CD2	2.81	0.47
1:E:744:HIS:NE2	1:E:1073:GLN:HG3	2.30	0.47
1:E:979:THR:OG1	1:E:1039:MET:HA	2.14	0.47
1:G:579:THR:HG22	1:G:596:GLN:HE22	1.78	0.47
1:G:906:LYS:HA	1:G:910:GLU:HB2	1.96	0.47
1:H:573:ARG:NH2	1:H:577:LEU:HD21	2.29	0.47
1:H:613:GLU:HG2	1:H:615:GLN:NE2	2.29	0.47
1:H:1090:GLU:HB3	1:H:1093:LYS:HD3	1.95	0.47
1:A:984:ASN:HA	1:A:987:PRO:HD2	1.96	0.47
1:C:716:CYS:HB3	1:C:726:TYR:OH	2.15	0.47
1:H:341:THR:HG21	1:H:647:GLU:OE2	2.15	0.47
1:H:599:LEU:O	1:H:652:PHE:HE2	1.97	0.47
1:A:824:PHE:CG	1:A:905:ARG:HD2	2.50	0.47
1:A:1048:GLY:HA2	1:A:1051:ASP:OD2	2.15	0.47
1:B:423:ARG:HD3	1:B:464:ASP:OD2	2.15	0.47
1:B:1084:LEU:HD22	1:B:1108:PHE:CD1	2.50	0.47
1:C:395:ILE:HA	3:C:1306:HOH:O	2.14	0.47
1:E:419:ASP:HB3	1:E:458:TRP:CZ3	2.49	0.47
1:E:551:VAL:O	1:E:555:ARG:HG2	2.15	0.47
1:E:815:THR:HG23	1:E:834:GLN:HE21	1.79	0.47
1:E:914:TYR:HB3	1:E:918:GLN:OE1	2.15	0.47
1:E:941:PRO:HG2	1:E:949:TYR:CD1	2.50	0.47
1:E:1099:VAL:HG11	1:E:1108:PHE:CD1	2.47	0.47
1:E:1106:ALA:CB	1:E:1111:LEU:HD11	2.44	0.47
1:F:488:LEU:HD23	1:F:787:GLY:CA	2.44	0.47
1:F:1084:LEU:HD22	1:F:1108:PHE:CZ	2.50	0.47
1:G:393:ALA:O	1:G:556:ARG:NH2	2.48	0.47
1:G:550:VAL:HG23	1:G:608:LEU:CD1	2.43	0.47
1:H:497:GLY:O	1:H:499:THR:OG1	2.28	0.47
1:B:599:LEU:HD12	1:B:648:LEU:CD2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:TYR:CE1	1:C:412:ARG:HD3	2.50	0.47
1:C:596:GLN:HB2	1:C:648:LEU:HD11	1.96	0.47
1:E:483:THR:OG1	1:E:485:VAL:HG23	2.15	0.47
1:F:849:SER:OG	1:F:850:GLN:N	2.48	0.47
1:G:569:GLN:HA	1:G:574:ARG:HH12	1.78	0.47
1:G:710:TYR:CD2	1:G:1106:ALA:HA	2.50	0.47
1:A:555:ARG:NH1	1:A:585:GLU:O	2.48	0.47
1:B:510:LYS:NZ	1:B:518:ASP:OD2	2.35	0.47
1:E:363:ALA:O	1:E:367:THR:OG1	2.26	0.47
1:F:875:ASP:OD2	1:F:877:ALA:HB3	2.14	0.47
1:G:396:LEU:HD21	1:G:398:GLN:HG2	1.97	0.47
1:A:552:ASN:O	1:A:556:ARG:HG2	2.14	0.47
1:C:487:ASP:O	1:C:787:GLY:HA2	2.14	0.47
1:D:846:THR:O	1:D:849:SER:OG	2.24	0.47
1:E:476:VAL:HG12	1:E:841:LEU:HG	1.95	0.47
1:E:742:ALA:HB2	1:E:1100:ARG:HH12	1.80	0.47
1:F:759:ASP:OD1	1:F:760:PHE:N	2.41	0.47
1:F:905:ARG:HG3	1:F:906:LYS:N	2.30	0.47
1:G:758:PHE:HZ	1:G:780:ILE:HB	1.79	0.47
1:G:803:ARG:HA	1:G:810:TYR:HA	1.96	0.47
1:H:354:VAL:HG11	1:H:411:PRO:O	2.15	0.47
1:C:931:GLU:OE1	1:C:931:GLU:N	2.47	0.46
1:B:1118:GLU:O	1:B:1121:SER:OG	2.31	0.46
1:C:984:ASN:HA	1:C:987:PRO:HD2	1.97	0.46
1:E:758:PHE:CZ	1:E:780:ILE:HD12	2.51	0.46
1:F:437:GLN:HE22	1:F:1111:LEU:HA	1.79	0.46
1:F:485:VAL:O	1:F:789:THR:HG23	2.15	0.46
1:F:850:GLN:HB3	1:F:971:LEU:HD22	1.97	0.46
1:F:866:VAL:HG11	1:F:876:VAL:CG1	2.44	0.46
1:F:906:LYS:HB3	1:F:906:LYS:HE2	1.57	0.46
1:H:406:HIS:CE1	1:H:408:CYS:HB2	2.49	0.46
1:H:1003:MET:HG2	1:H:1004:PRO:CD	2.45	0.46
1:C:463:LEU:HD11	1:C:853:HIS:CD2	2.51	0.46
1:D:735:LYS:HZ1	1:D:1051:ASP:HA	1.79	0.46
1:E:601:SER:O	1:E:605:VAL:HG22	2.15	0.46
1:E:716:CYS:HB3	1:E:726:TYR:OH	2.15	0.46
1:F:906:LYS:O	1:F:906:LYS:HG2	2.15	0.46
1:F:1033:GLU:CD	1:F:1033:GLU:H	2.19	0.46
1:G:627:CYS:HA	1:G:630:MET:SD	2.55	0.46
1:G:1047:LYS:HA	1:G:1078:TYR:CE1	2.51	0.46
1:H:512:MET:HE1	1:H:605:VAL:HG11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:ALA:N	3:A:1304:HOH:O	2.27	0.46
1:B:343:ARG:HG2	1:B:400:ASP:HB3	1.98	0.46
1:B:343:ARG:CG	1:B:400:ASP:HB3	2.45	0.46
1:C:483:THR:HB	1:C:804:MET:CE	2.38	0.46
1:C:1124:VAL:HG23	1:C:1124:VAL:O	2.15	0.46
1:E:355:ARG:HA	1:E:355:ARG:HD3	1.74	0.46
1:E:1077:SER:OG	1:E:1079:VAL:HG12	2.16	0.46
1:F:801:ARG:HG3	1:F:814:ASP:OD1	2.16	0.46
1:D:447:LYS:O	1:D:451:ARG:HG3	2.16	0.46
1:D:675:GLN:HE22	1:D:711:GLN:HE22	1.64	0.46
1:E:698:TYR:CE2	1:E:725:LYS:HE2	2.50	0.46
1:F:818:LEU:HA	1:F:821:LEU:HG	1.96	0.46
1:F:1118:GLU:O	1:F:1121:SER:HB2	2.16	0.46
1:G:351:TYR:CB	1:G:654:ILE:HD11	2.46	0.46
1:G:354:VAL:HG21	1:G:411:PRO:HB2	1.97	0.46
1:H:365:ALA:O	1:H:369:VAL:HG23	2.15	0.46
1:A:435:ARG:HH21	1:A:438:ASP:HB2	1.81	0.46
1:B:371:LYS:NZ	1:B:453:GLU:OE2	2.49	0.46
1:C:784:THR:HG21	1:C:980:LEU:HD11	1.97	0.46
1:G:422:TRP:HZ2	1:G:459:GLU:HA	1.80	0.46
1:H:707:VAL:HG12	1:H:709:VAL:HG13	1.97	0.46
1:B:435:ARG:CZ	1:B:438:ASP:O	2.64	0.46
1:D:437:GLN:HA	1:D:437:GLN:NE2	2.30	0.46
1:D:492:GLN:HG2	1:D:493:ILE:HG23	1.98	0.46
1:D:655:LYS:HD2	1:D:658:GLU:OE2	2.16	0.46
1:F:670:TYR:CD2	1:F:984:ASN:CB	2.99	0.46
1:F:813:LEU:CD1	1:F:837:HIS:HB2	2.44	0.46
1:G:762:ASP:OD1	1:G:779:ARG:NH1	2.49	0.46
1:G:894:LEU:O	1:G:898:VAL:HG13	2.15	0.46
1:D:419:ASP:HB3	1:D:458:TRP:CH2	2.51	0.46
1:F:376:MET:SD	1:F:380:LEU:HD23	2.55	0.46
1:F:650:GLN:HB3	1:F:707:VAL:HG11	1.97	0.46
1:F:1082:GLU:HA	1:F:1085:LYS:CE	2.45	0.46
1:G:539:TYR:CD2	1:G:873:GLY:HA2	2.50	0.46
1:H:358:VAL:CG2	1:H:432:MET:HE1	2.46	0.46
1:H:763:ALA:O	1:H:766:TYR:HD2	1.98	0.46
1:H:938:LEU:HG	1:H:998:GLY:HA3	1.98	0.46
1:B:703:ALA:O	1:B:707:VAL:HG22	2.15	0.46
1:D:738:MET:HB3	1:D:1098:ILE:CG2	2.46	0.46
1:G:383:ALA:HB2	1:G:542:ALA:HB1	1.98	0.46
1:A:432:MET:HE3	1:A:440:PHE:CB	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:TYR:O	1:B:557:ILE:HG12	2.16	0.46
1:D:718:ILE:O	1:D:745:PHE:HA	2.16	0.46
1:E:435:ARG:HG2	1:E:437:GLN:H	1.81	0.46
1:F:674:TYR:O	1:F:676:PRO:HD3	2.16	0.46
1:F:858:PRO:O	1:F:860:PRO:HD3	2.16	0.46
1:H:909:PHE:O	1:H:912:LYS:HE3	2.15	0.46
1:A:731:VAL:HG22	1:A:1059:LEU:HD23	1.97	0.45
1:A:1099:VAL:HG21	1:A:1108:PHE:CD1	2.51	0.45
1:C:844:ILE:O	1:C:848:ILE:HG13	2.16	0.45
1:D:344:MET:CE	1:D:647:GLU:HG2	2.47	0.45
1:D:641:THR:O	1:D:644:THR:OG1	2.24	0.45
1:F:476:VAL:HG12	1:F:841:LEU:HD12	1.97	0.45
1:F:968:TYR:HE2	1:H:529:GLU:HG2	1.81	0.45
1:G:686:LYS:HE3	1:G:689:GLY:O	2.16	0.45
1:G:829:ALA:O	1:G:833:GLN:HG3	2.15	0.45
1:H:347:LEU:HD21	1:H:400:ASP:HB2	1.97	0.45
1:H:356:PRO:HG2	1:H:674:TYR:CE1	2.51	0.45
1:H:448:LYS:NZ	1:H:452:GLU:OE2	2.46	0.45
1:H:635:ILE:HD13	1:H:642:HIS:HD2	1.80	0.45
1:H:897:TYR:CE2	1:H:957:ILE:HG21	2.51	0.45
1:H:960:TRP:HE3	1:H:961:THR:HG22	1.79	0.45
1:A:1084:LEU:HD22	1:A:1108:PHE:CD1	2.52	0.45
1:B:340:LEU:HD22	1:B:344:MET:CG	2.46	0.45
1:B:622:ARG:O	1:B:626:TYR:HD2	1.98	0.45
1:D:422:TRP:CD1	1:D:462:SER:HB3	2.51	0.45
1:E:631:PHE:O	1:E:635:ILE:HG12	2.16	0.45
1:E:1047:LYS:CD	1:E:1080:ASP:HB2	2.44	0.45
1:F:532:GLU:H	1:F:532:GLU:CD	2.20	0.45
1:F:906:LYS:CG	1:F:910:GLU:HB3	2.40	0.45
1:H:367:THR:O	1:H:371:LYS:CB	2.65	0.45
1:A:362:ARG:HH11	1:A:417:SER:HA	1.81	0.45
1:A:527:SER:HB3	1:A:530:ASN:OD1	2.17	0.45
1:B:980:LEU:HD12	1:B:980:LEU:O	2.16	0.45
1:B:1048:GLY:HA2	1:B:1051:ASP:OD2	2.15	0.45
1:C:622:ARG:HH11	1:C:765:ASP:HA	1.81	0.45
1:F:536:ARG:HG2	1:F:540:TYR:HE2	1.81	0.45
1:F:1082:GLU:HA	1:F:1085:LYS:HE3	1.98	0.45
1:H:546:THR:CG2	1:H:864:LEU:HD11	2.41	0.45
1:C:906:LYS:NZ	1:C:911:GLU:OE2	2.49	0.45
1:D:498:ASP:HA	1:D:769:MET:SD	2.57	0.45
1:D:618:LEU:HD13	1:D:618:LEU:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1075:GLN:NE2	1:D:1103:GLY:H	2.12	0.45
1:E:391:GLU:OE2	1:E:552:ASN:ND2	2.50	0.45
1:F:758:PHE:CE2	1:F:780:ILE:HD12	2.51	0.45
1:F:850:GLN:HG2	3:F:1320:HOH:O	2.16	0.45
1:G:818:LEU:HD23	1:G:818:LEU:HA	1.79	0.45
1:H:352:LEU:HD23	1:H:352:LEU:O	2.17	0.45
1:H:479:PHE:CG	1:H:841:LEU:HD23	2.51	0.45
1:H:957:ILE:HD12	1:H:958:THR:N	2.32	0.45
1:H:966:ARG:HD3	1:H:974:THR:HG23	1.98	0.45
1:E:387:ARG:NH1	1:E:548:GLU:HG3	2.32	0.45
1:F:614:ASN:OD1	1:F:661:TRP:HD1	1.99	0.45
1:F:618:LEU:H	1:F:618:LEU:HD22	1.82	0.45
1:F:979:THR:HG21	1:F:1035:MET:CE	2.47	0.45
1:F:1016:ASP:OD1	1:F:1016:ASP:N	2.48	0.45
1:G:803:ARG:HB2	1:G:810:TYR:CE1	2.51	0.45
1:G:984:ASN:O	1:G:988:ILE:HG13	2.17	0.45
1:H:984:ASN:HA	1:H:987:PRO:HG2	1.98	0.45
1:B:506:LEU:HD23	1:B:510:LYS:HE3	1.99	0.45
1:B:758:PHE:CE2	1:B:780:ILE:HD12	2.51	0.45
1:C:561:ALA:HB3	1:C:581:ALA:HB2	1.99	0.45
1:C:608:LEU:O	1:C:611:ILE:N	2.49	0.45
1:F:542:ALA:O	1:F:546:THR:HG23	2.17	0.45
1:G:526:LEU:HB3	1:G:533:ASP:HB3	1.99	0.45
1:G:980:LEU:HD12	1:G:982:ILE:HG13	1.98	0.45
1:G:1099:VAL:HG11	1:G:1108:PHE:CD1	2.44	0.45
1:H:437:GLN:OE1	1:H:1112:CYS:HB3	2.16	0.45
1:H:942:LYS:C	1:H:950:VAL:HG11	2.37	0.45
1:A:623:VAL:HG13	1:A:627:CYS:SG	2.56	0.45
1:C:1040:VAL:HG23	1:C:1075:GLN:NE2	2.32	0.45
1:E:650:GLN:HB3	1:E:707:VAL:HG11	1.99	0.45
1:E:871:GLU:H	1:E:871:GLU:CD	2.19	0.45
1:G:356:PRO:HA	1:G:412:ARG:O	2.16	0.45
1:G:729:LYS:O	1:G:733:VAL:HG23	2.16	0.45
1:B:913:LYS:HD3	1:B:914:TYR:CZ	2.52	0.45
1:E:799:LEU:HA	1:E:818:LEU:HD21	1.99	0.45
1:F:398:GLN:HB2	1:F:401:GLU:CD	2.38	0.45
1:G:917:GLU:H	1:G:917:GLU:HG3	1.39	0.45
1:A:573:ARG:HD2	1:A:576:GLU:OE1	2.16	0.45
1:C:560:HIS:CE1	1:C:564:LEU:HD11	2.52	0.45
1:C:795:ILE:HD11	1:C:897:TYR:CD2	2.52	0.45
1:D:646:LEU:O	1:D:650:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:971:LEU:HB3	1:D:972:TYR:CD2	2.52	0.45
1:D:1073:GLN:HE22	1:D:1075:GLN:HE21	1.62	0.45
1:E:450:ILE:O	1:E:455:VAL:HG23	2.17	0.45
1:G:776:LYS:HD2	1:G:776:LYS:HA	1.66	0.45
1:G:919:ILE:O	1:G:923:LEU:HG	2.16	0.45
1:G:1042:ASN:OD1	1:G:1122:ARG:NH1	2.50	0.45
1:H:515:ILE:HG21	1:H:864:LEU:HB3	1.99	0.45
1:H:934:ARG:HG2	1:H:938:LEU:HD11	1.98	0.45
1:H:1082:GLU:O	1:H:1086:LYS:HG2	2.17	0.45
1:A:416:PHE:CE1	1:A:425:VAL:HG21	2.52	0.44
1:A:419:ASP:HB3	1:A:458:TRP:CH2	2.53	0.44
1:C:624:ASP:HB3	1:C:700:ILE:HD12	1.98	0.44
1:D:1090:GLU:OE2	1:D:1093:LYS:HD3	2.17	0.44
1:F:621:GLY:HA2	1:F:767:CYS:HB2	1.99	0.44
1:F:832:LYS:HD3	1:F:960:TRP:NE1	2.31	0.44
1:F:872:SER:HB3	1:F:874:LYS:CG	2.47	0.44
1:G:577:LEU:HD23	1:G:580:ILE:HD12	1.99	0.44
1:G:628:TYR:CD1	1:G:694:ASN:ND2	2.84	0.44
1:G:641:THR:O	1:G:644:THR:N	2.50	0.44
1:G:744:HIS:HD2	1:G:749:HIS:CE1	2.34	0.44
1:G:900:SER:N	1:G:997:ASN:HB3	2.32	0.44
1:G:966:ARG:NH1	1:G:974:THR:HG23	2.26	0.44
1:G:1035:MET:HE3	1:G:1039:MET:HE2	1.99	0.44
1:H:406:HIS:HE1	1:H:408:CYS:HB2	1.82	0.44
1:H:443:SER:O	1:H:447:LYS:HG3	2.18	0.44
1:H:504:ASP:CG	1:H:505:VAL:HG13	2.38	0.44
1:H:682:VAL:HB	1:H:697:THR:HG23	1.99	0.44
1:H:986:THR:HG22	1:H:1004:PRO:CG	2.48	0.44
1:H:1063:LEU:HD21	1:H:1076:PHE:CZ	2.51	0.44
1:H:1090:GLU:HB3	1:H:1093:LYS:CE	2.47	0.44
1:A:362:ARG:NH1	1:A:417:SER:HA	2.32	0.44
1:A:966:ARG:HD3	1:A:975:LEU:O	2.17	0.44
1:B:583:VAL:O	1:B:587:VAL:HG22	2.18	0.44
1:D:686:LYS:N	1:D:692:ALA:HB2	2.33	0.44
1:D:1057:HIS:O	1:D:1061:THR:OG1	2.21	0.44
1:F:885:HIS:ND1	1:F:886:GLY:N	2.65	0.44
1:G:439:PRO:O	1:G:674:TYR:OH	2.22	0.44
1:G:573:ARG:O	1:G:576:GLU:HB3	2.17	0.44
1:G:715:ALA:HB1	1:G:768:LEU:HD12	1.99	0.44
1:G:1044:LYS:HZ2	1:G:1081:ASN:HD21	1.63	0.44
1:H:483:THR:HG22	1:H:807:PHE:CD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:896:THR:O	1:H:900:SER:OG	2.22	0.44
1:A:739:GLY:HA3	1:A:1100:ARG:HD3	1.99	0.44
1:B:824:PHE:CE1	1:B:905:ARG:HB2	2.52	0.44
1:C:1057:HIS:O	1:C:1061:THR:OG1	2.29	0.44
1:F:476:VAL:HG12	1:F:841:LEU:CD1	2.47	0.44
1:F:806:LEU:HB2	1:F:1002:TRP:CZ3	2.53	0.44
1:G:634:ASP:CB	1:G:640:LEU:HD22	2.47	0.44
1:H:352:LEU:HD11	1:H:1095:ARG:O	2.17	0.44
1:A:850:GLN:HE22	1:A:887:PRO:HD3	1.81	0.44
1:B:867:GLU:HB3	1:B:882:MET:HE3	2.00	0.44
1:F:614:ASN:OD1	1:F:661:TRP:CD1	2.70	0.44
1:F:703:ALA:O	1:F:707:VAL:HG22	2.17	0.44
1:F:793:ILE:HD11	1:F:804:MET:SD	2.58	0.44
1:F:915:THR:HG22	1:F:916:LEU:N	2.33	0.44
1:F:1100:ARG:HD3	1:F:1105:SER:OG	2.17	0.44
1:H:1090:GLU:HB3	1:H:1093:LYS:CD	2.47	0.44
1:A:675:GLN:CD	1:A:1104:TYR:CD2	2.91	0.44
1:A:888:GLY:HA2	1:A:976:SER:O	2.18	0.44
1:B:776:LYS:HD3	1:B:776:LYS:C	2.37	0.44
1:B:1013:GLN:CD	1:B:1013:GLN:H	2.21	0.44
1:D:348:ARG:O	1:D:351:TYR:HB3	2.18	0.44
1:D:504:ASP:HB3	1:D:626:TYR:CG	2.53	0.44
1:E:379:ILE:HD13	1:E:858:PRO:HB2	1.99	0.44
1:E:685:GLN:HG3	1:E:746:ASP:OD2	2.17	0.44
1:E:887:PRO:O	1:E:975:LEU:HD12	2.17	0.44
1:F:727:MET:O	1:F:731:VAL:HG23	2.18	0.44
1:F:913:LYS:HB2	1:F:914:TYR:CE2	2.51	0.44
1:G:595:LEU:HG	1:G:595:LEU:O	2.17	0.44
1:D:406:HIS:CE1	1:D:408:CYS:HB2	2.52	0.44
1:E:932:ALA:HA	1:E:935:ARG:NH1	2.32	0.44
1:F:922:ALA:HA	1:F:930:TYR:CE1	2.52	0.44
1:G:915:THR:O	1:G:919:ILE:HG12	2.18	0.44
1:H:362:ARG:NH1	1:H:417:SER:HA	2.33	0.44
1:H:416:PHE:HA	1:H:662:MET:CE	2.47	0.44
1:A:824:PHE:CD1	1:A:905:ARG:HD2	2.53	0.44
1:B:1040:VAL:HG11	1:B:1102:ALA:HB1	2.00	0.44
1:E:679:ASN:HB2	1:E:770:GLY:O	2.17	0.44
1:E:900:SER:HB3	1:E:996:PRO:HB2	2.00	0.44
1:F:789:THR:HG22	1:F:790:GLN:N	2.24	0.44
1:G:727:MET:HG3	1:G:1064:ARG:NH1	2.32	0.44
1:H:624:ASP:OD1	1:H:625:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:782:GLN:O	1:H:782:GLN:HG2	2.17	0.44
1:H:959:GLU:OE2	1:H:1034:THR:HG21	2.18	0.44
1:B:428:GLU:OE2	1:B:435:ARG:HD2	2.18	0.44
1:B:653:ILE:HG21	1:B:707:VAL:HG21	1.99	0.44
1:C:1075:GLN:NE2	1:C:1100:ARG:HH21	2.15	0.44
1:D:1069:LEU:HD23	1:E:721:GLN:NE2	2.32	0.44
1:E:1040:VAL:HA	1:E:1073:GLN:OE1	2.17	0.44
1:F:516:LYS:O	1:F:520:GLU:HG2	2.17	0.44
1:F:1082:GLU:HA	1:F:1085:LYS:HG3	1.99	0.44
1:H:360:ILE:HD12	1:H:360:ILE:HG23	1.76	0.44
1:H:443:SER:HB3	1:H:446:ASP:H	1.83	0.44
1:H:444:GLU:HA	1:H:447:LYS:HG3	2.00	0.44
1:A:772:VAL:HG11	1:A:1039:MET:O	2.18	0.44
1:A:963:LYS:HD2	1:A:963:LYS:HA	1.66	0.44
1:B:561:ALA:HB3	1:B:581:ALA:HB2	1.98	0.44
1:C:555:ARG:HG3	1:C:555:ARG:HH11	1.83	0.44
1:C:847:VAL:HG13	1:C:971:LEU:HD13	1.99	0.44
1:C:923:LEU:HD11	1:C:996:PRO:HD3	2.00	0.44
1:D:953:TYR:N	1:D:953:TYR:HD2	2.16	0.44
1:D:1045:PHE:CE2	1:D:1059:LEU:HD13	2.53	0.44
1:E:575:ALA:O	1:E:579:THR:HG23	2.17	0.44
1:F:435:ARG:NH2	1:F:438:ASP:O	2.51	0.44
1:F:1108:PHE:CE2	1:F:1116:GLN:HG2	2.52	0.44
1:G:640:LEU:HA	1:G:644:THR:HG21	1.99	0.44
1:G:854:ARG:HA	1:G:877:ALA:HB1	1.99	0.44
1:H:350:HIS:ND1	1:H:350:HIS:O	2.51	0.44
1:H:817:ASP:OD1	1:H:818:LEU:N	2.51	0.44
1:B:411:PRO:HB3	1:B:658:GLU:HG2	2.00	0.43
1:D:769:MET:HB3	1:D:769:MET:HE3	1.71	0.43
1:D:919:ILE:O	1:D:923:LEU:HG	2.18	0.43
1:E:1009:ILE:CG2	1:E:1035:MET:CE	2.96	0.43
1:F:659:LEU:O	1:F:676:PRO:HG3	2.18	0.43
1:F:895:ALA:HB3	1:F:1006:SER:OG	2.18	0.43
1:G:419:ASP:OD1	1:G:419:ASP:N	2.51	0.43
1:H:440:PHE:HE1	1:H:660:MET:SD	2.41	0.43
1:C:734:VAL:HG11	1:C:1059:LEU:HD21	2.00	0.43
1:C:966:ARG:HD3	1:C:975:LEU:O	2.18	0.43
1:D:748:SER:OG	1:D:1071:ASN:O	2.28	0.43
1:G:790:GLN:HE21	1:G:793:ILE:N	2.16	0.43
1:G:908:VAL:HG11	1:G:916:LEU:HG	2.00	0.43
1:G:1112:CYS:HB3	1:G:1115:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:417:SER:O	1:H:420:ILE:HG13	2.18	0.43
1:H:495:GLY:HA3	1:H:613:GLU:HG3	2.00	0.43
1:H:496:GLY:N	1:H:613:GLU:OE2	2.47	0.43
1:A:1025:LYS:O	1:A:1028:SER:HB3	2.18	0.43
1:A:1049:LEU:O	1:A:1055:GLY:HA3	2.18	0.43
1:B:993:ASN:O	1:B:999:ARG:NH2	2.50	0.43
1:C:1016:ASP:OD1	1:C:1016:ASP:N	2.49	0.43
1:D:504:ASP:CG	1:D:777:SER:HG	2.21	0.43
1:E:425:VAL:O	1:E:429:LEU:HG	2.18	0.43
1:G:533:ASP:O	1:G:537:ILE:HG12	2.18	0.43
1:G:698:TYR:HE1	1:G:726:TYR:HA	1.82	0.43
1:G:1058:GLY:HA3	1:G:1128:PHE:CD2	2.53	0.43
1:H:971:LEU:HD12	1:H:971:LEU:HA	1.72	0.43
1:A:444:GLU:OE1	1:A:447:LYS:HD2	2.18	0.43
1:B:528:MET:HE2	1:B:537:ILE:HG21	2.00	0.43
1:C:953:TYR:O	1:C:957:ILE:HG22	2.18	0.43
1:C:1081:ASN:O	1:C:1085:LYS:HG3	2.19	0.43
1:E:632:GLU:O	1:E:636:ARG:HB2	2.17	0.43
1:F:1086:LYS:HA	1:F:1089:GLN:HG3	1.99	0.43
1:G:522:HIS:O	1:G:525:SER:OG	2.26	0.43
1:G:527:SER:HB3	1:G:529:GLU:HG3	2.00	0.43
1:G:613:GLU:O	1:G:615:GLN:HG2	2.18	0.43
1:G:914:TYR:CD1	1:G:933:LEU:HD12	2.53	0.43
1:G:941:PRO:HG2	1:G:949:TYR:CD2	2.53	0.43
1:H:850:GLN:NE2	1:H:887:PRO:HD3	2.33	0.43
1:A:488:LEU:HD13	1:A:845:GLY:HA3	2.00	0.43
1:A:1040:VAL:HG11	1:A:1102:ALA:HB1	2.00	0.43
1:A:1080:ASP:HB3	1:A:1083:VAL:CG2	2.48	0.43
1:B:419:ASP:OD1	1:B:419:ASP:N	2.51	0.43
1:D:773:GLU:OE1	1:D:784:THR:HG21	2.19	0.43
1:E:649:LEU:HD13	1:E:700:ILE:HD13	2.00	0.43
1:E:756:LYS:HG2	1:E:885:HIS:CD2	2.54	0.43
1:E:771:CYS:HA	1:E:1103:GLY:O	2.18	0.43
1:F:655:LYS:HD2	1:F:655:LYS:HA	1.79	0.43
1:F:1084:LEU:CD2	1:F:1099:VAL:HG21	2.48	0.43
1:G:352:LEU:HD12	1:G:352:LEU:H	1.84	0.43
1:G:401:GLU:HG3	1:G:404:VAL:HG12	2.01	0.43
1:G:745:PHE:CD1	1:G:1067:SER:HB2	2.54	0.43
1:H:406:HIS:ND1	1:H:407:PRO:HD2	2.33	0.43
1:H:1031:ASN:O	1:H:1034:THR:HG23	2.18	0.43
1:A:463:LEU:HG	1:A:852:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:ARG:NH1	1:A:808:ASP:OD1	2.46	0.43
1:C:555:ARG:HD2	1:C:585:GLU:OE2	2.19	0.43
1:D:823:THR:HG23	1:D:826:GLU:H	1.84	0.43
1:D:1013:GLN:HA	3:D:1325:HOH:O	2.19	0.43
1:E:1114:GLU:OE1	1:E:1114:GLU:N	2.45	0.43
1:F:685:GLN:H	1:F:717:ARG:NH2	2.17	0.43
1:F:911:GLU:HG3	1:F:913:LYS:HZ1	1.83	0.43
1:G:423:ARG:HH11	1:G:465:GLU:HG3	1.83	0.43
1:G:478:ALA:HA	1:G:482:GLU:HB2	2.00	0.43
1:H:599:LEU:HD22	1:H:652:PHE:CD2	2.54	0.43
1:A:411:PRO:HB3	1:A:658:GLU:HG2	2.00	0.43
1:A:572:GLN:HG3	1:A:573:ARG:N	2.33	0.43
1:B:824:PHE:CD1	1:B:905:ARG:HB2	2.53	0.43
1:C:379:ILE:HD13	1:C:858:PRO:HB2	2.00	0.43
1:C:1020:PRO:HA	1:C:1023:ILE:HD12	2.00	0.43
1:D:348:ARG:NH1	1:D:348:ARG:HG2	2.34	0.43
1:D:760:PHE:CZ	1:E:1033:GLU:HB3	2.54	0.43
1:D:1045:PHE:HE2	1:D:1059:LEU:HD13	1.84	0.43
1:E:435:ARG:HG2	1:E:437:GLN:O	2.19	0.43
1:E:1047:LYS:HD2	1:E:1080:ASP:N	2.33	0.43
1:F:358:VAL:HG23	1:F:440:PHE:HB3	2.01	0.43
1:F:753:MET:HE3	1:F:753:MET:HB3	1.74	0.43
1:F:767:CYS:C	1:F:768:LEU:HD22	2.39	0.43
1:H:1112:CYS:SG	1:H:1115:VAL:HG12	2.59	0.43
1:B:832:LYS:HD3	1:B:960:TRP:NE1	2.34	0.43
1:D:963:LYS:NZ	1:E:761:GLU:OE2	2.40	0.43
1:F:649:LEU:O	1:F:653:ILE:HG13	2.18	0.43
1:F:846:THR:O	1:F:849:SER:OG	2.22	0.43
1:F:1007:ASP:OD1	1:F:1042:ASN:HB2	2.19	0.43
1:F:1082:GLU:CG	1:F:1085:LYS:HE3	2.48	0.43
1:G:982:ILE:O	1:G:1102:ALA:HB3	2.18	0.43
1:H:583:VAL:HG13	1:H:597:GLU:HG2	2.01	0.43
1:C:802:GLY:O	1:C:810:TYR:HA	2.19	0.43
1:D:489:SER:O	1:D:492:GLN:HB3	2.19	0.43
1:D:512:MET:HG3	1:D:550:VAL:HG11	2.00	0.43
1:D:703:ALA:O	1:D:707:VAL:HG23	2.18	0.43
1:F:960:TRP:CZ3	1:F:964:GLU:HG3	2.53	0.43
1:H:1109:VAL:C	1:H:1111:LEU:H	2.21	0.43
1:B:913:LYS:HD3	1:B:914:TYR:CE2	2.54	0.43
1:B:1073:GLN:HE22	1:B:1075:GLN:NE2	2.16	0.43
1:C:795:ILE:CD1	1:C:901:MET:HE3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:ARG:HG2	1:D:348:ARG:HH11	1.84	0.43
1:D:423:ARG:HH21	1:D:464:ASP:CG	2.22	0.43
1:D:752:MET:HB2	1:D:1036:ASN:ND2	2.33	0.43
1:D:1028:SER:HB3	1:D:1069:LEU:HD13	2.01	0.43
1:E:908:VAL:O	1:E:912:LYS:HA	2.18	0.43
1:E:1081:ASN:O	1:E:1085:LYS:HG3	2.19	0.43
1:F:854:ARG:HA	1:F:877:ALA:HB1	2.01	0.43
1:H:700:ILE:O	1:H:704:VAL:HG12	2.19	0.43
1:H:790:GLN:HE21	1:H:792:PRO:HB2	1.84	0.43
1:B:616:THR:HB	1:B:661:TRP:CG	2.54	0.42
1:B:657:ALA:HA	1:B:711:GLN:HB2	2.01	0.42
1:C:444:GLU:OE2	1:C:447:LYS:NZ	2.37	0.42
1:D:361:TYR:CE2	1:D:394:PRO:HG3	2.54	0.42
1:D:438:ASP:HA	1:D:674:TYR:CZ	2.54	0.42
1:E:604:THR:O	1:E:607:SER:OG	2.33	0.42
1:E:1021:THR:HG22	1:E:1025:LYS:HE2	2.00	0.42
1:G:1075:GLN:HE22	1:G:1103:GLY:H	1.67	0.42
1:H:612:GLU:OE2	1:H:860:PRO:HD2	2.19	0.42
1:H:1007:ASP:OD1	1:H:1007:ASP:N	2.52	0.42
1:B:435:ARG:NH2	1:B:438:ASP:O	2.52	0.42
1:C:748:SER:OG	1:C:1071:ASN:O	2.25	0.42
1:D:686:LYS:HB2	1:D:689:GLY:O	2.19	0.42
1:D:832:LYS:HB3	1:D:960:TRP:CZ2	2.54	0.42
1:D:986:THR:HB	1:D:987:PRO:HD3	2.00	0.42
1:E:452:GLU:O	1:E:456:PRO:HG2	2.19	0.42
1:E:989:GLY:HA2	1:E:1005:LEU:HD21	2.01	0.42
1:F:915:THR:CG2	1:F:916:LEU:N	2.82	0.42
1:F:1085:LYS:H	1:F:1085:LYS:HG2	1.59	0.42
1:H:360:ILE:HG13	1:H:446:ASP:HB3	2.01	0.42
1:H:734:VAL:HA	1:H:740:PHE:O	2.19	0.42
1:D:496:GLY:HA3	1:D:859:LYS:HE3	2.01	0.42
1:D:513:ASN:ND2	1:D:589:ALA:HB1	2.34	0.42
1:E:576:GLU:O	1:E:579:THR:OG1	2.24	0.42
1:E:697:THR:O	1:E:701:MET:HG3	2.19	0.42
1:E:1039:MET:SD	1:E:1072:GLY:HA3	2.59	0.42
1:F:1047:LYS:HG3	1:F:1080:ASP:HB2	2.00	0.42
1:G:362:ARG:NH1	1:G:417:SER:HA	2.34	0.42
1:G:380:LEU:O	1:G:384:LYS:HG3	2.19	0.42
1:G:694:ASN:OD1	1:G:697:THR:N	2.37	0.42
1:H:604:THR:O	1:H:607:SER:OG	2.23	0.42
1:B:1093:LYS:O	1:B:1093:LYS:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:579:THR:O	1:C:583:VAL:HG23	2.19	0.42
1:C:1063:LEU:HD23	1:C:1063:LEU:HA	1.86	0.42
1:D:343:ARG:HG2	1:D:647:GLU:OE2	2.20	0.42
1:D:685:GLN:NE2	1:D:746:ASP:OD2	2.45	0.42
1:D:835:ILE:O	1:D:838:ILE:HB	2.19	0.42
1:F:862:MET:HB2	1:F:862:MET:HE2	1.80	0.42
1:H:680:LEU:HD21	1:H:700:ILE:HG21	2.02	0.42
1:A:337:MET:HB3	1:A:340:LEU:HD12	2.00	0.42
1:A:986:THR:HB	1:A:987:PRO:CD	2.49	0.42
1:B:435:ARG:CZ	1:B:437:GLN:O	2.66	0.42
1:B:623:VAL:HA	1:B:626:TYR:CE2	2.55	0.42
1:C:835:ILE:HD13	1:C:957:ILE:HD11	2.01	0.42
1:D:539:TYR:OH	1:D:869:CYS:HB3	2.20	0.42
1:D:937:CYS:C	1:D:939:ASN:N	2.72	0.42
1:D:1063:LEU:HD21	1:D:1076:PHE:CZ	2.55	0.42
1:F:443:SER:HB3	1:F:446:ASP:HB2	2.01	0.42
1:F:718:ILE:HD12	1:F:743:CYS:HB3	2.01	0.42
1:G:579:THR:O	1:G:583:VAL:HG22	2.19	0.42
1:G:1009:ILE:HD13	1:G:1039:MET:HG3	2.01	0.42
1:H:576:GLU:O	1:H:580:ILE:HG13	2.19	0.42
1:C:799:LEU:O	1:C:920:ARG:HD3	2.20	0.42
1:C:839:VAL:HG11	1:C:964:GLU:HG3	2.02	0.42
1:D:476:VAL:HG12	1:D:841:LEU:HG	2.01	0.42
1:D:671:PHE:CE2	2:D:1201:A1H9K:C1	3.03	0.42
1:E:659:LEU:HD23	1:E:678:ILE:HD11	2.01	0.42
1:F:803:ARG:HH22	1:F:924:LEU:HD21	1.85	0.42
1:G:676:PRO:HG2	1:G:711:GLN:OE1	2.19	0.42
1:C:489:SER:O	1:C:493:ILE:HG12	2.20	0.42
1:C:687:ARG:HD2	1:C:765:ASP:OD2	2.20	0.42
1:C:879:GLY:O	1:C:884:ASN:ND2	2.51	0.42
1:C:953:TYR:HA	1:C:956:ASP:OD1	2.20	0.42
1:D:359:SER:OG	1:D:408:CYS:HB3	2.20	0.42
1:D:560:HIS:HA	1:D:563:GLU:HG2	2.01	0.42
1:D:1040:VAL:HA	1:D:1073:GLN:OE1	2.19	0.42
1:F:444:GLU:HA	1:F:447:LYS:CD	2.48	0.42
1:F:1115:VAL:O	1:F:1119:ILE:HG13	2.20	0.42
1:G:655:LYS:HA	1:G:658:GLU:HG3	2.00	0.42
1:G:865:LEU:HA	1:G:865:LEU:HD23	1.85	0.42
1:G:1007:ASP:O	1:G:1010:SER:HB2	2.20	0.42
1:H:552:ASN:O	1:H:556:ARG:HB2	2.19	0.42
1:H:781:TYR:HB2	1:H:881:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1061:THR:O	1:H:1065:THR:HG23	2.19	0.42
1:C:428:GLU:OE2	1:C:665:GLU:HB2	2.20	0.42
1:C:502:GLY:H	1:C:865:LEU:HB3	1.84	0.42
1:C:850:GLN:NE2	1:C:887:PRO:HD3	2.35	0.42
1:C:1095:ARG:O	1:C:1095:ARG:HD3	2.19	0.42
1:D:504:ASP:OD2	1:D:505:VAL:HG13	2.20	0.42
1:D:981:SER:O	1:D:981:SER:OG	2.36	0.42
1:F:390:CYS:HB3	1:F:553:TYR:HB2	2.01	0.42
1:F:943:TYR:HD1	1:F:951:ASP:OD1	2.02	0.42
1:F:1080:ASP:OD1	1:F:1082:GLU:N	2.53	0.42
1:G:428:GLU:HG2	1:G:431:THR:OG1	2.20	0.42
1:G:906:LYS:CE	1:G:941:PRO:HD3	2.49	0.42
1:A:530:ASN:HB3	1:A:532:GLU:OE1	2.20	0.42
1:B:369:VAL:HG21	1:B:385:ALA:HA	2.01	0.42
1:B:779:ARG:HG2	1:B:882:MET:SD	2.60	0.42
1:D:971:LEU:HD12	1:D:971:LEU:HA	1.66	0.42
1:E:359:SER:HB3	1:E:408:CYS:HB3	2.02	0.42
1:E:657:ALA:HA	1:E:711:GLN:HB2	2.02	0.42
1:E:850:GLN:HB3	1:E:971:LEU:HD22	2.02	0.42
1:F:470:GLN:HG2	1:H:377:PRO:HD3	2.01	0.42
1:F:900:SER:O	1:F:903:ALA:HB3	2.20	0.42
1:H:1080:ASP:O	1:H:1084:LEU:HD12	2.20	0.42
1:A:850:GLN:HB3	1:A:971:LEU:HD22	2.02	0.42
1:B:599:LEU:HA	1:B:599:LEU:HD23	1.67	0.42
1:B:620:LEU:HD12	1:B:680:LEU:HD13	2.01	0.42
1:B:898:VAL:HG12	1:B:950:VAL:HG22	2.01	0.42
1:D:789:THR:O	1:D:891:PHE:HA	2.20	0.42
1:E:798:VAL:HG21	1:E:831:VAL:HA	2.02	0.42
1:E:835:ILE:HG22	1:E:960:TRP:HZ3	1.85	0.42
1:G:463:LEU:HG	1:G:852:VAL:HG12	2.01	0.42
1:G:1021:THR:O	1:G:1025:LYS:HG3	2.20	0.42
1:H:988:ILE:O	1:H:991:LEU:HB2	2.20	0.42
1:H:1046:LEU:HD12	1:H:1047:LYS:N	2.35	0.42
1:H:1118:GLU:O	1:H:1121:SER:OG	2.25	0.42
1:A:739:GLY:HA3	1:A:1100:ARG:HB2	2.01	0.41
1:A:1016:ASP:OD1	1:A:1016:ASP:N	2.37	0.41
1:B:850:GLN:NE2	1:B:887:PRO:HD3	2.35	0.41
1:D:976:SER:HB3	1:D:1037:ILE:HD11	2.02	0.41
1:E:423:ARG:NH1	1:E:468:GLU:OE1	2.53	0.41
1:E:428:GLU:HB3	1:E:432:MET:HG2	2.02	0.41
1:F:1007:ASP:OD2	1:F:1122:ARG:HD3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1113:LYS:HB3	1:F:1113:LYS:HE2	1.62	0.41
1:G:504:ASP:HB3	1:G:626:TYR:CG	2.55	0.41
1:H:798:VAL:HG23	1:H:834:GLN:HG3	2.01	0.41
1:H:919:ILE:HG22	1:H:923:LEU:HD11	2.01	0.41
1:C:356:PRO:HB3	1:C:660:MET:HE3	2.03	0.41
1:C:813:LEU:O	1:C:834:GLN:NE2	2.34	0.41
1:D:984:ASN:C	1:D:987:PRO:HD2	2.40	0.41
1:E:504:ASP:OD1	1:E:504:ASP:N	2.48	0.41
1:F:493:ILE:O	1:F:494:ASN:ND2	2.54	0.41
1:F:550:VAL:O	1:F:553:TYR:HB3	2.21	0.41
1:F:804:MET:O	1:F:808:ASP:HA	2.21	0.41
1:F:941:PRO:HB3	1:F:947:ASP:OD2	2.20	0.41
1:G:350:HIS:HA	1:G:353:THR:HG23	2.02	0.41
1:G:532:GLU:CD	1:G:532:GLU:H	2.23	0.41
1:H:435:ARG:HH21	1:H:438:ASP:HB2	1.84	0.41
1:H:565:ALA:HB1	1:H:574:ARG:HG3	2.01	0.41
1:A:648:LEU:HA	1:A:648:LEU:HD23	1.78	0.41
1:E:361:TYR:CE2	1:E:394:PRO:HG3	2.55	0.41
1:E:896:THR:N	1:E:1006:SER:OG	2.52	0.41
1:F:477:TRP:CD2	1:F:481:GLY:HA3	2.56	0.41
1:F:623:VAL:HG22	1:F:680:LEU:HD21	2.02	0.41
1:G:362:ARG:NH2	1:G:612:GLU:O	2.44	0.41
1:G:448:LYS:HE2	1:G:452:GLU:OE2	2.20	0.41
1:G:551:VAL:O	1:G:555:ARG:HG2	2.20	0.41
1:H:1077:SER:HB2	1:H:1100:ARG:HB3	2.01	0.41
1:A:609:PHE:CD1	1:A:861:LEU:HD23	2.55	0.41
1:A:957:ILE:HD12	1:A:957:ILE:HA	1.83	0.41
1:B:613:GLU:O	1:B:615:GLN:HG2	2.20	0.41
1:C:675:GLN:CD	1:C:1104:TYR:CD2	2.94	0.41
1:C:1019:GLY:O	1:C:1023:ILE:HG13	2.20	0.41
1:E:914:TYR:CZ	1:E:933:LEU:HB3	2.55	0.41
1:G:450:ILE:HA	1:G:454:ILE:HB	2.01	0.41
1:G:522:HIS:HB3	1:G:540:TYR:CE2	2.56	0.41
1:G:1077:SER:HB2	1:G:1100:ARG:HB3	2.03	0.41
1:H:827:PHE:CE2	1:H:901:MET:HE1	2.56	0.41
1:A:356:PRO:HA	1:A:412:ARG:O	2.21	0.41
1:A:622:ARG:HH11	1:A:765:ASP:HA	1.84	0.41
1:A:743:CYS:O	1:A:1073:GLN:HG2	2.20	0.41
1:B:605:VAL:HG11	1:B:865:LEU:HD11	2.02	0.41
1:D:676:PRO:HB2	1:D:678:ILE:HG13	2.02	0.41
1:D:797:PHE:HE1	1:D:804:MET:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:934:ARG:NE	1:D:938:LEU:HD11	2.35	0.41
1:E:349:ASN:O	1:E:353:THR:HG23	2.21	0.41
1:E:502:GLY:HA3	1:E:505:VAL:HG12	2.03	0.41
1:E:720:ASN:OD1	1:E:1067:SER:OG	2.38	0.41
1:F:927:PHE:HE2	1:F:933:LEU:HD23	1.86	0.41
1:F:984:ASN:HA	1:F:987:PRO:HD2	2.02	0.41
1:G:775:GLN:CG	1:G:780:ILE:HG21	2.42	0.41
1:G:1086:LYS:O	1:G:1086:LYS:HG3	2.21	0.41
1:H:359:SER:O	1:H:360:ILE:HD13	2.20	0.41
1:H:628:TYR:O	1:H:631:PHE:N	2.54	0.41
1:H:1052:THR:O	1:H:1056:ARG:HG3	2.20	0.41
1:A:696:LEU:HD12	1:A:696:LEU:HA	1.85	0.41
1:A:844:ILE:O	1:A:848:ILE:HG13	2.20	0.41
1:A:938:LEU:HD23	1:A:938:LEU:HA	1.86	0.41
1:B:905:ARG:CZ	1:B:949:TYR:CE1	3.03	0.41
1:C:796:GLU:OE2	1:C:805:VAL:HG23	2.19	0.41
1:C:953:TYR:O	1:C:956:ASP:OD1	2.38	0.41
1:D:913:LYS:HA	1:D:913:LYS:HD3	1.77	0.41
1:D:973:SER:OG	1:D:974:THR:N	2.48	0.41
1:F:740:PHE:HA	1:F:741:PRO:HA	1.83	0.41
1:F:1009:ILE:HG12	1:F:1040:VAL:O	2.20	0.41
1:F:1075:GLN:NE2	1:F:1103:GLY:HA2	2.12	0.41
1:G:650:GLN:HG2	1:G:707:VAL:HG22	2.01	0.41
1:G:897:TYR:CE1	1:G:901:MET:HE1	2.56	0.41
1:H:656:CYS:HB2	1:H:712:PRO:HD3	2.03	0.41
1:H:932:ALA:O	1:H:935:ARG:HB2	2.21	0.41
1:A:379:ILE:HG23	1:A:380:LEU:N	2.36	0.41
1:A:1013:GLN:HB3	1:A:1121:SER:O	2.20	0.41
1:B:927:PHE:CG	1:B:934:ARG:HD2	2.55	0.41
1:D:558:ALA:O	1:D:561:ALA:HB3	2.21	0.41
1:F:1081:ASN:O	1:F:1085:LYS:HG2	2.20	0.41
1:G:727:MET:O	1:G:731:VAL:HG23	2.20	0.41
1:G:821:LEU:H	1:G:821:LEU:HG	1.50	0.41
1:H:697:THR:HG22	1:H:701:MET:SD	2.61	0.41
1:B:617:GLY:HA2	1:B:677:PHE:HB2	2.03	0.41
1:B:863:SER:OG	1:B:875:ASP:HB2	2.21	0.41
1:C:622:ARG:NH1	1:C:765:ASP:HA	2.36	0.41
1:D:761:GLU:H	1:D:761:GLU:HG2	1.72	0.41
1:D:901:MET:HB3	1:D:953:TYR:HD1	1.85	0.41
1:E:622:ARG:NH2	1:E:685:GLN:O	2.52	0.41
1:E:931:GLU:OE1	1:E:931:GLU:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:913:LYS:HB2	1:F:914:TYR:CD2	2.56	0.41
1:G:393:ALA:N	1:G:556:ARG:HH22	2.18	0.41
1:G:449:THR:O	1:G:453:GLU:HB2	2.21	0.41
1:G:622:ARG:HG3	1:G:622:ARG:HH11	1.86	0.41
1:G:820:ASP:O	1:G:826:GLU:OE1	2.39	0.41
1:H:379:ILE:HG23	1:H:380:LEU:N	2.35	0.41
1:H:550:VAL:HG11	1:H:608:LEU:HD13	2.01	0.41
1:H:587:VAL:HG11	1:H:592:PRO:HB3	2.03	0.41
1:H:635:ILE:HG12	1:H:640:LEU:O	2.21	0.41
1:H:645:ALA:O	1:H:649:LEU:HG	2.21	0.41
1:H:706:PHE:HD1	1:H:706:PHE:HA	1.79	0.41
1:H:726:TYR:CE2	1:H:730:ILE:HD11	2.55	0.41
1:H:734:VAL:HG21	1:H:1076:PHE:HB2	2.03	0.41
1:H:1049:LEU:O	1:H:1055:GLY:HA3	2.21	0.41
1:A:571:ALA:HA	3:A:1361:HOH:O	2.21	0.41
1:A:616:THR:HB	1:A:661:TRP:CG	2.56	0.41
1:A:905:ARG:NH1	1:A:953:TYR:OH	2.48	0.41
1:A:927:PHE:CG	1:A:934:ARG:HD2	2.55	0.41
1:A:943:TYR:O	1:A:1011:PRO:HB3	2.21	0.41
1:A:1085:LYS:O	1:A:1088:GLN:HB2	2.21	0.41
1:B:348:ARG:O	1:B:351:TYR:HB3	2.21	0.41
1:B:944:GLY:HA3	1:B:1011:PRO:HG3	2.03	0.41
1:B:1100:ARG:HG3	1:B:1104:TYR:O	2.20	0.41
1:C:352:LEU:HD23	1:C:352:LEU:HA	1.94	0.41
1:C:495:GLY:HA3	1:C:613:GLU:HG3	2.03	0.41
1:C:794:ALA:CB	1:C:835:ILE:HG13	2.51	0.41
1:C:797:PHE:HD1	1:C:797:PHE:HA	1.79	0.41
1:C:1084:LEU:HD22	1:C:1108:PHE:CE1	2.56	0.41
1:E:904:ILE:HD11	1:E:996:PRO:HG2	2.03	0.41
1:E:906:LYS:HE3	1:E:907:LEU:CD2	2.51	0.41
1:E:971:LEU:HD12	1:E:971:LEU:HA	1.68	0.41
1:E:1094:TYR:HD1	1:E:1094:TYR:N	2.18	0.41
1:F:1017:LYS:HE2	1:F:1017:LYS:HB3	1.93	0.41
1:G:550:VAL:CG2	1:G:608:LEU:HD12	2.46	0.41
1:G:583:VAL:HG21	1:G:596:GLN:HE21	1.86	0.41
1:G:587:VAL:HG21	1:G:597:GLU:HA	2.03	0.41
1:G:749:HIS:HA	1:G:752:MET:SD	2.60	0.41
1:G:966:ARG:HD3	1:G:975:LEU:O	2.21	0.41
1:G:1035:MET:CE	1:G:1039:MET:HE2	2.51	0.41
1:H:613:GLU:O	1:H:615:GLN:HG2	2.20	0.41
1:H:971:LEU:HB3	1:H:972:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:VAL:HG21	1:A:901:MET:HE1	2.03	0.41
1:A:1023:ILE:HD13	1:A:1023:ILE:HG21	1.86	0.41
1:B:793:ILE:HD12	1:B:793:ILE:HA	1.79	0.41
1:B:923:LEU:HD13	1:B:994:ALA:O	2.21	0.41
1:B:986:THR:HG21	1:B:1114:GLU:HB3	2.03	0.41
1:B:1006:SER:HB3	1:B:1012:THR:HG22	2.03	0.41
1:D:520:GLU:HG3	1:D:544:ILE:CD1	2.51	0.41
1:D:1021:THR:HA	1:D:1024:ILE:HG12	2.03	0.41
1:E:522:HIS:HB3	1:E:540:TYR:CE2	2.56	0.41
1:E:616:THR:HB	1:E:661:TRP:CG	2.56	0.41
1:E:791:TRP:HD1	1:E:835:ILE:HD13	1.85	0.41
1:E:1025:LYS:O	1:E:1028:SER:HB3	2.20	0.41
1:F:376:MET:SD	1:F:377:PRO:HD2	2.61	0.41
1:F:905:ARG:O	1:F:909:PHE:HB2	2.20	0.41
1:F:1088:GLN:NE2	1:F:1113:LYS:HG3	2.35	0.41
1:G:404:VAL:H	1:G:600:GLN:HE22	1.69	0.41
1:G:416:PHE:CE1	1:G:425:VAL:HG21	2.56	0.41
1:G:1040:VAL:HA	1:G:1073:GLN:OE1	2.21	0.41
1:B:551:VAL:HG22	1:B:589:ALA:HB2	2.04	0.40
1:B:919:ILE:O	1:B:923:LEU:HG	2.21	0.40
1:D:646:LEU:HA	1:D:646:LEU:HD12	1.82	0.40
1:D:994:ALA:N	1:D:1001:ALA:HA	2.36	0.40
1:E:499:THR:O	1:E:501:PRO:HD3	2.21	0.40
1:E:677:PHE:O	1:E:770:GLY:HA2	2.21	0.40
1:E:829:ALA:O	1:E:833:GLN:HG3	2.20	0.40
1:E:1087:ALA:HB2	1:E:1094:TYR:CD2	2.56	0.40
1:F:1055:GLY:HA2	1:F:1128:PHE:CE1	2.53	0.40
1:H:366:PHE:CD1	1:H:385:ALA:HB1	2.56	0.40
1:H:731:VAL:HA	1:H:734:VAL:HG12	2.04	0.40
1:H:850:GLN:OE1	1:H:971:LEU:HB2	2.21	0.40
1:A:619:SER:HB3	1:A:679:ASN:HB3	2.02	0.40
1:B:699:LEU:HA	1:B:699:LEU:HD23	1.84	0.40
1:D:727:MET:O	1:D:730:ILE:HB	2.22	0.40
1:D:1063:LEU:HD23	1:D:1074:MET:CE	2.45	0.40
1:E:801:ARG:HG2	1:E:816:GLY:O	2.21	0.40
1:F:627:CYS:HA	1:F:630:MET:CE	2.51	0.40
1:F:650:GLN:HB3	1:F:707:VAL:CG1	2.51	0.40
1:F:1052:THR:CG2	1:F:1055:GLY:H	2.26	0.40
1:G:701:MET:HG2	1:G:714:LEU:HD21	2.02	0.40
1:H:400:ASP:HA	1:H:573:ARG:NH1	2.34	0.40
1:H:653:ILE:O	1:H:656:CYS:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:783:TRP:HH2	1:H:853:HIS:HB2	1.86	0.40
1:A:622:ARG:NH1	1:A:765:ASP:HA	2.36	0.40
1:B:1088:GLN:HG2	1:B:1116:GLN:OE1	2.21	0.40
1:C:653:ILE:HG23	1:C:712:PRO:CD	2.46	0.40
1:C:713:SER:HA	1:C:740:PHE:CE1	2.56	0.40
1:C:791:TRP:HB2	1:C:792:PRO:HD3	2.03	0.40
1:D:536:ARG:HG2	1:D:873:GLY:HA3	2.02	0.40
1:D:885:HIS:CE1	1:D:966:ARG:HH22	2.40	0.40
1:D:1122:ARG:HA	3:D:1325:HOH:O	2.21	0.40
1:E:1075:GLN:OE1	1:E:1100:ARG:NH1	2.54	0.40
1:E:1094:TYR:N	1:E:1094:TYR:CD1	2.87	0.40
1:G:503:TYR:O	1:G:507:LEU:HB3	2.22	0.40
1:H:341:THR:OG1	1:H:647:GLU:HG3	2.21	0.40
1:H:739:GLY:HA2	1:H:1077:SER:HA	2.03	0.40
1:H:854:ARG:HA	1:H:877:ALA:HB1	2.02	0.40
1:A:419:ASP:OD1	1:A:419:ASP:N	2.50	0.40
1:A:742:ALA:HB1	1:A:1073:GLN:HE21	1.87	0.40
1:D:828:ASP:HA	1:D:831:VAL:HG22	2.04	0.40
1:E:513:ASN:ND2	1:E:589:ALA:HB1	2.36	0.40
1:F:681:THR:CG2	1:F:768:LEU:HD23	2.52	0.40
1:F:957:ILE:HD12	1:F:957:ILE:HA	1.89	0.40
1:G:571:ALA:HA	1:G:574:ARG:CZ	2.52	0.40
1:G:655:LYS:HG3	1:G:658:GLU:OE1	2.21	0.40
1:G:835:ILE:O	1:G:839:VAL:HG23	2.20	0.40
1:H:718:ILE:HD12	1:H:743:CYS:HB3	2.03	0.40
1:A:620:LEU:HD12	1:A:680:LEU:HD12	2.03	0.40
1:B:348:ARG:O	1:B:352:LEU:HD12	2.21	0.40
1:B:418:PRO:HB2	1:B:458:TRP:CG	2.56	0.40
1:D:687:ARG:HD2	1:D:765:ASP:OD2	2.22	0.40
1:F:419:ASP:HB3	1:F:458:TRP:CH2	2.56	0.40
1:F:963:LYS:HB2	1:F:963:LYS:HE2	1.68	0.40
1:H:380:LEU:HA	1:H:542:ALA:HB2	2.04	0.40
1:H:402:LEU:HA	1:H:580:ILE:HD11	2.03	0.40
1:H:562:ARG:HG3	1:H:581:ALA:HB1	2.04	0.40
1:H:801:ARG:HG2	1:H:801:ARG:NH1	2.27	0.40
1:H:922:ALA:HA	1:H:930:TYR:CE2	2.57	0.40
1:H:1080:ASP:HB3	1:H:1083:VAL:HG23	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:912:LYS:NZ	1:G:822:ARG:NH1[1_455]	1.92	0.28
1:D:822:ARG:NH1	1:E:820:ASP:OD2[1_455]	2.02	0.18

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	790/1150 (69%)	749 (95%)	41 (5%)	0	100	100
1	B	790/1150 (69%)	750 (95%)	39 (5%)	1 (0%)	51	78
1	C	789/1150 (69%)	753 (95%)	35 (4%)	1 (0%)	51	78
1	D	790/1150 (69%)	736 (93%)	54 (7%)	0	100	100
1	E	790/1150 (69%)	741 (94%)	49 (6%)	0	100	100
1	F	790/1150 (69%)	725 (92%)	63 (8%)	2 (0%)	41	66
1	G	790/1150 (69%)	734 (93%)	55 (7%)	1 (0%)	51	78
1	H	790/1150 (69%)	716 (91%)	73 (9%)	1 (0%)	51	78
All	All	6319/9200 (69%)	5904 (93%)	409 (6%)	6 (0%)	51	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	982	ILE
1	F	982	ILE
1	F	771	CYS
1	G	819	ARG
1	H	571	ALA
1	B	982	ILE

5.3.2 Protein sidechains (i)

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	668/955 (70%)	660 (99%)	8 (1%)	71	88
1	B	668/955 (70%)	656 (98%)	12 (2%)	59	83
1	C	667/955 (70%)	657 (98%)	10 (2%)	65	86
1	D	668/955 (70%)	652 (98%)	16 (2%)	49	77
1	E	668/955 (70%)	656 (98%)	12 (2%)	59	83
1	F	668/955 (70%)	658 (98%)	10 (2%)	65	86
1	G	668/955 (70%)	651 (98%)	17 (2%)	47	76
1	H	668/955 (70%)	647 (97%)	21 (3%)	40	69
All	All	5343/7640 (70%)	5237 (98%)	106 (2%)	55	81

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	556	ARG
1	A	710	TYR
1	A	819	ARG
1	A	977	HIS
1	A	980	LEU
1	A	1026	SER
1	A	1028	SER
1	A	1095	ARG
1	B	359	SER
1	B	453	GLU
1	B	567	LYS
1	B	601	SER
1	B	642	HIS
1	B	648	LEU
1	B	705	ARG
1	B	710	TYR
1	B	819	ARG
1	B	928	GLU
1	B	1007	ASP
1	B	1095	ARG
1	C	338	GLU
1	C	480	SER
1	C	536	ARG

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Mol	Chain	Res	Type
1	C	721	GLN
1	C	729	LYS
1	C	819	ARG
1	C	956	ASP
1	C	976	SER
1	C	980	LEU
1	C	1095	ARG
1	D	343	ARG
1	D	399	ASP
1	D	489	SER
1	D	536	ARG
1	D	630	MET
1	D	643	ASP
1	D	710	TYR
1	D	721	GLN
1	D	767	CYS
1	D	790	GLN
1	D	822	ARG
1	D	926	ASN
1	D	1006	SER
1	D	1007	ASP
1	D	1093	LYS
1	D	1095	ARG
1	E	630	MET
1	E	710	TYR
1	E	820	ASP
1	E	840	ARG
1	E	859	LYS
1	E	920	ARG
1	E	921	ASP
1	E	977	HIS
1	E	993	ASN
1	E	1086	LYS
1	E	1095	ARG
1	E	1100	ARG
1	F	343	ARG
1	F	536	ARG
1	F	555	ARG
1	F	729	LYS
1	F	897	TYR
1	F	913	LYS
1	F	967	LYS

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Mol	Chain	Res	Type
1	F	1041	HIS
1	F	1095	ARG
1	F	1100	ARG
1	G	337	MET
1	G	346	ARG
1	G	359	SER
1	G	362	ARG
1	G	570	ASN
1	G	573	ARG
1	G	630	MET
1	G	639	ARG
1	G	643	ASP
1	G	710	TYR
1	G	790	GLN
1	G	906	LYS
1	G	935	ARG
1	G	963	LYS
1	G	1006	SER
1	G	1039	MET
1	G	1042	ASN
1	H	349	ASN
1	H	362	ARG
1	H	376	MET
1	H	510	LYS
1	H	536	ARG
1	H	555	ARG
1	H	596	GLN
1	H	664	SER
1	H	671	PHE
1	H	722	SER
1	H	755	ARG
1	H	791	TRP
1	H	933	LEU
1	H	938	LEU
1	H	980	LEU
1	H	1028	SER
1	H	1044	LYS
1	H	1095	ARG
1	H	1113	LYS
1	H	1127	LYS
1	H	1128	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	513	ASN
1	A	572	GLN
1	B	1042	ASN
1	B	1075	GLN
1	C	711	GLN
1	C	1036	ASN
1	C	1075	GLN
1	D	675	GLN
1	D	926	ASN
1	D	1075	GLN
1	D	1088	GLN
1	E	569	GLN
1	E	993	ASN
1	E	1075	GLN
1	F	494	ASN
1	F	569	GLN
1	F	800	ASN
1	F	837	HIS
1	F	948	ASN
1	F	952	GLN
1	F	1036	ASN
1	F	1075	GLN
1	G	570	ASN
1	G	596	GLN
1	G	724	GLN
1	G	749	HIS
1	G	775	GLN
1	G	790	GLN
1	G	833	GLN
1	G	1081	ASN
1	H	570	ASN
1	H	642	HIS
1	H	719	HIS
1	H	790	GLN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
2	A1H9K	F	1201	-	7,9,9	1.33	1 (14%)	5,13,13	0.66	0
2	A1H9K	H	1201	-	7,9,9	1.38	1 (14%)	5,13,13	0.88	0
2	A1H9K	D	1201	-	7,9,9	1.46	2 (28%)	5,13,13	1.03	0
2	A1H9K	G	1201	-	7,9,9	1.27	1 (14%)	5,13,13	0.81	0
2	A1H9K	B	1201	-	7,9,9	1.36	1 (14%)	5,13,13	0.88	0
2	A1H9K	C	1201	-	7,9,9	1.57	2 (28%)	5,13,13	0.62	0
2	A1H9K	E	1201	-	7,9,9	1.29	1 (14%)	5,13,13	0.59	0
2	A1H9K	A	1201	-	7,9,9	1.25	1 (14%)	5,13,13	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1H9K	F	1201	-	-	4/4/12/12	0/1/1/1
2	A1H9K	H	1201	-	-	1/4/12/12	0/1/1/1
2	A1H9K	D	1201	-	-	1/4/12/12	0/1/1/1
2	A1H9K	G	1201	-	-	4/4/12/12	0/1/1/1
2	A1H9K	B	1201	-	-	1/4/12/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1H9K	C	1201	-	-	0/4/12/12	0/1/1/1
2	A1H9K	E	1201	-	-	4/4/12/12	0/1/1/1
2	A1H9K	A	1201	-	-	2/4/12/12	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1201	A1H9K	C2-C3	2.59	1.53	1.47
2	C	1201	A1H9K	C2-C3	2.51	1.53	1.47
2	C	1201	A1H9K	C1-C3	2.45	1.53	1.47
2	F	1201	A1H9K	C1-C3	2.28	1.53	1.47
2	H	1201	A1H9K	C1-C3	2.28	1.53	1.47
2	B	1201	A1H9K	C2-C3	2.26	1.52	1.47
2	G	1201	A1H9K	C1-C3	2.22	1.52	1.47
2	A	1201	A1H9K	C1-C3	2.16	1.52	1.47
2	D	1201	A1H9K	C1-C3	2.13	1.52	1.47
2	E	1201	A1H9K	C1-C3	2.09	1.52	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1201	A1H9K	N4-C5-C6-O1
2	E	1201	A1H9K	C6-C5-N4-C9
2	E	1201	A1H9K	N4-C5-C6-O1
2	G	1201	A1H9K	N4-C5-C6-O1
2	E	1201	A1H9K	C6-C5-N4-C8
2	G	1201	A1H9K	C6-C5-N4-C8
2	G	1201	A1H9K	C6-C5-N4-C9
2	E	1201	A1H9K	C6-C5-N4-C3
2	F	1201	A1H9K	C6-C5-N4-C9
2	F	1201	A1H9K	C6-C5-N4-C8
2	H	1201	A1H9K	N4-C5-C6-O1
2	F	1201	A1H9K	C6-C5-N4-C3
2	G	1201	A1H9K	C6-C5-N4-C3
2	F	1201	A1H9K	N4-C5-C6-O1
2	D	1201	A1H9K	N4-C5-C6-O1
2	A	1201	A1H9K	C6-C5-N4-C8
2	A	1201	A1H9K	C6-C5-N4-C9

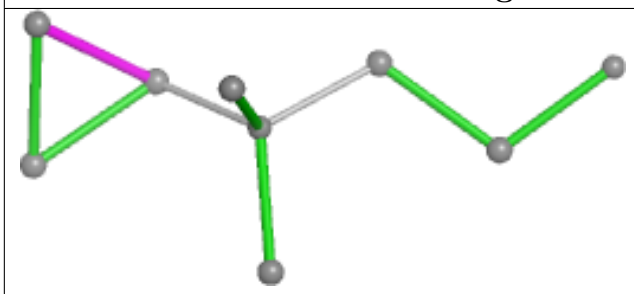
There are no ring outliers.

3 monomers are involved in 4 short contacts:

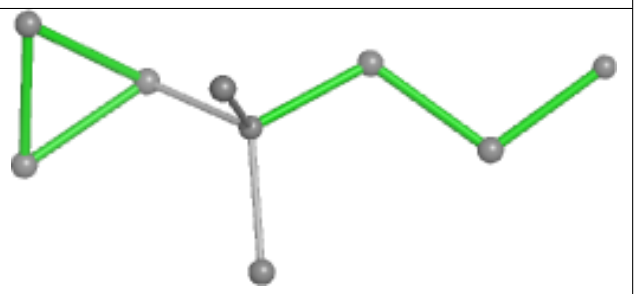
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1201	A1H9K	1	0
2	D	1201	A1H9K	1	0
2	G	1201	A1H9K	2	0

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 then 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.

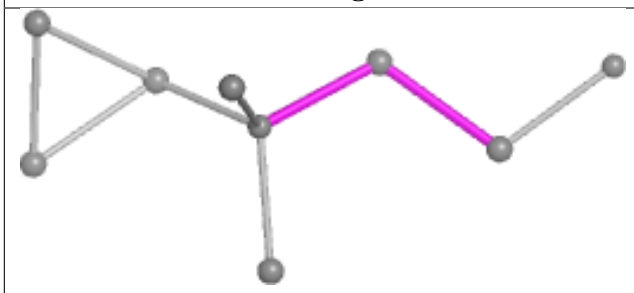
Ligand A1H9K F 1201



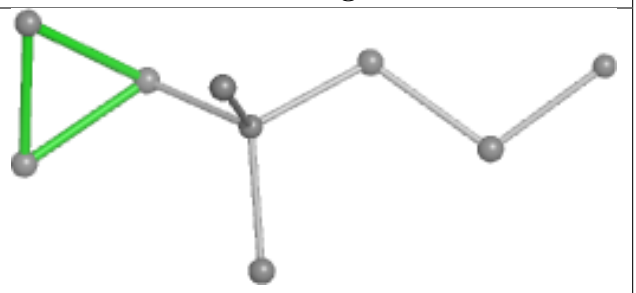
Bond lengths



Bond angles

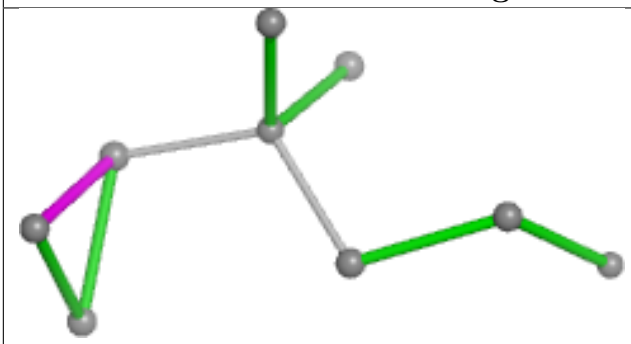


Torsions

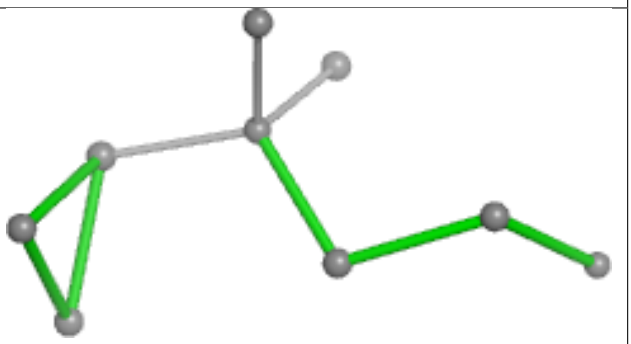


Rings

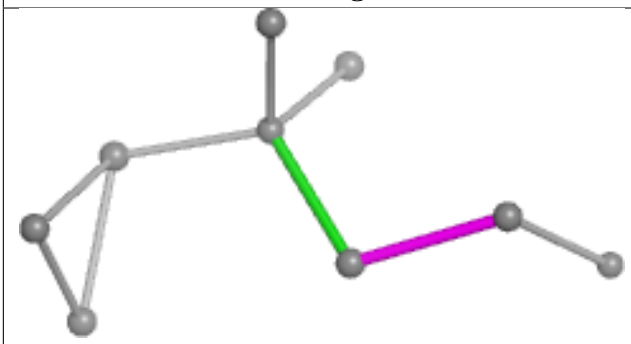
Ligand A1H9K H 1201



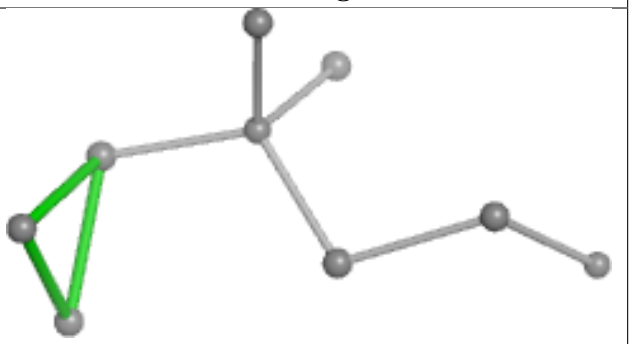
Bond lengths



Bond angles

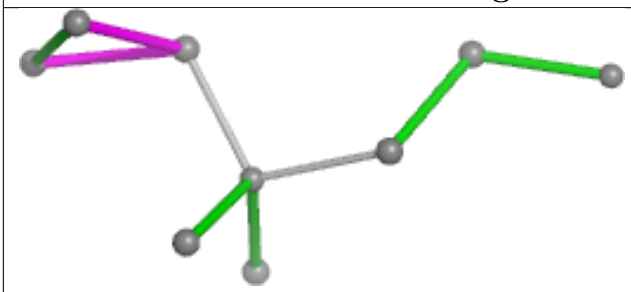


Torsions

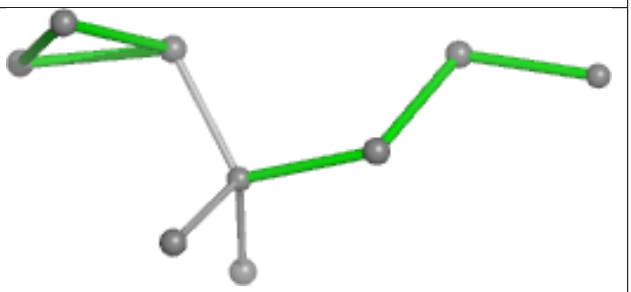


Rings

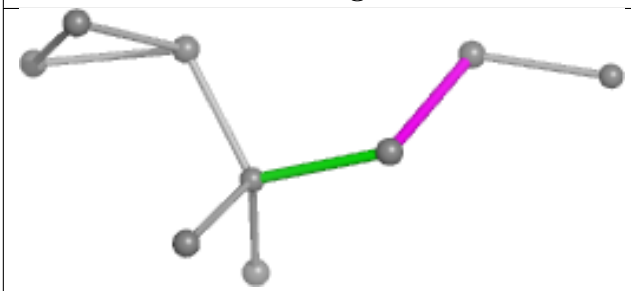
Ligand A1H9K D 1201



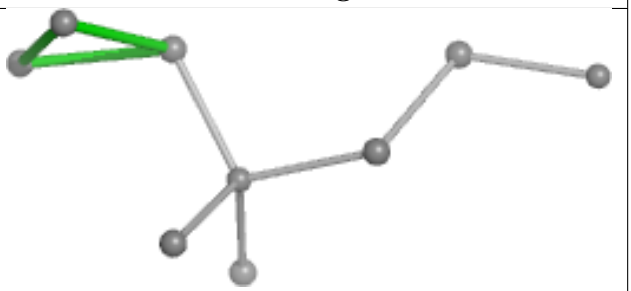
Bond lengths



Bond angles

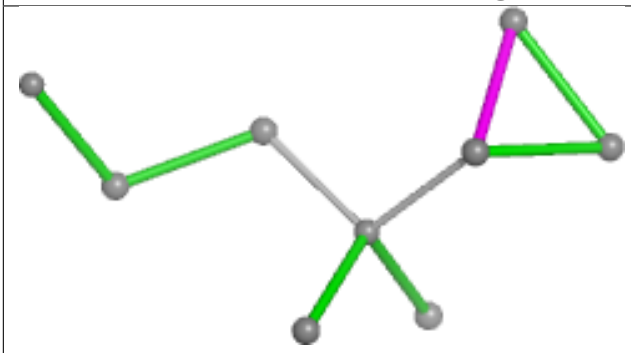


Torsions

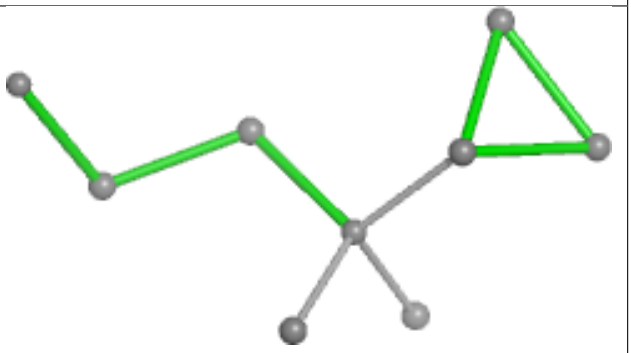


Rings

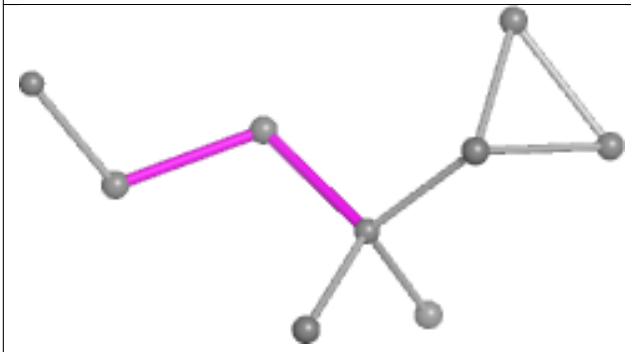
Ligand A1H9K G 1201



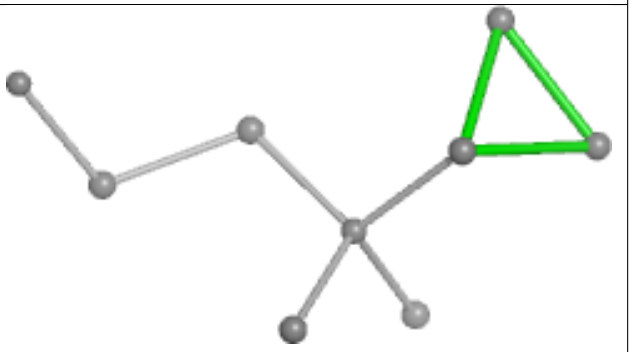
Bond lengths



Bond angles

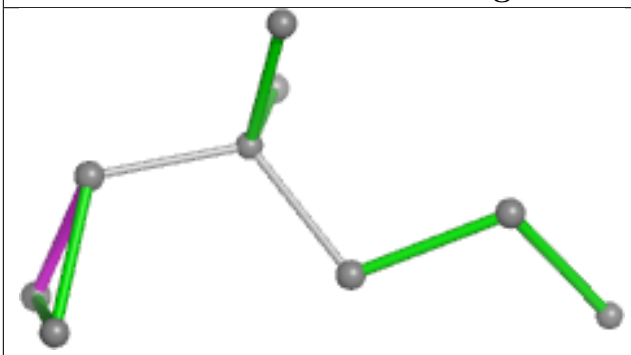


Torsions

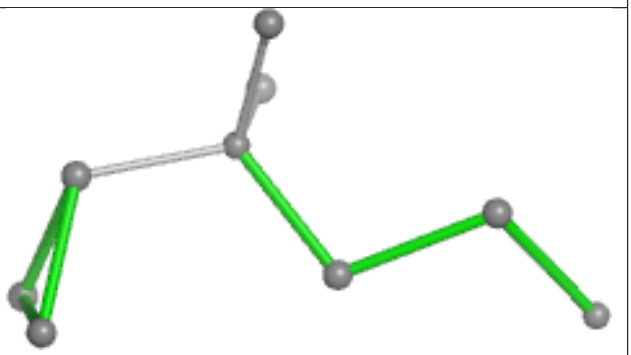


Rings

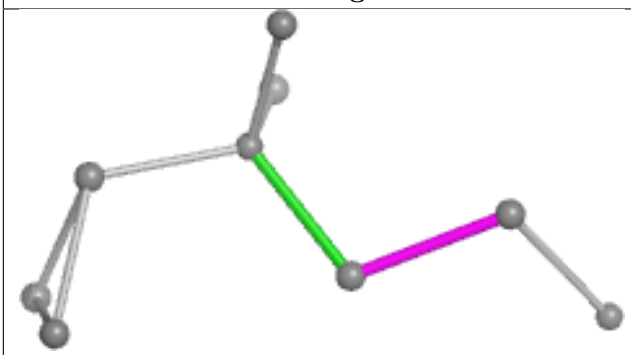
Ligand A1H9K B 1201



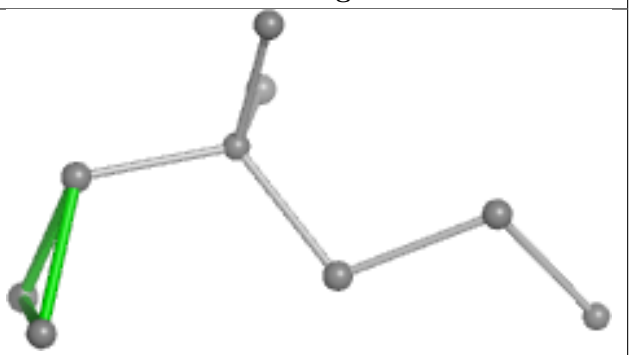
Bond lengths



Bond angles

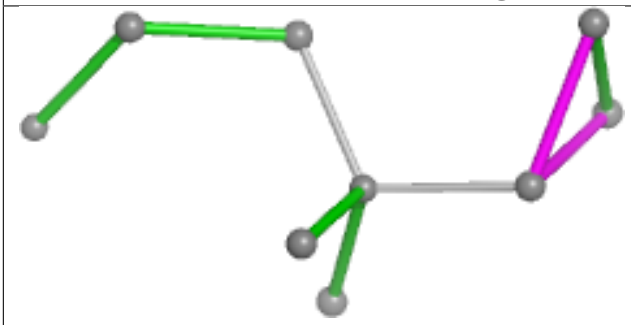


Torsions

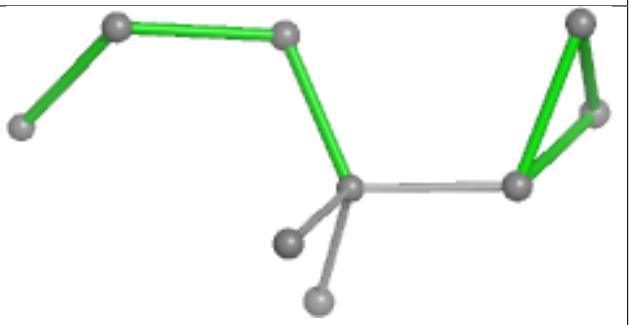


Rings

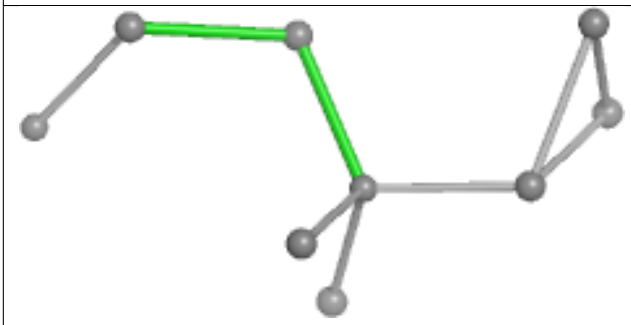
Ligand A1H9K C 1201



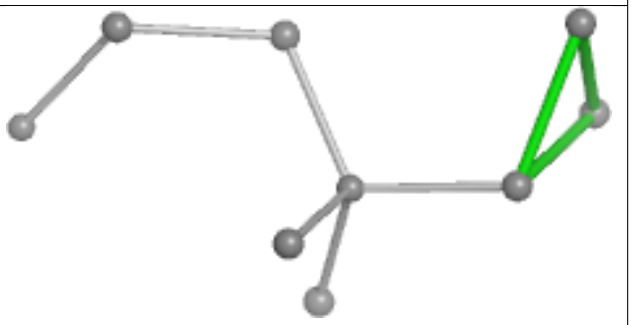
Bond lengths



Bond angles

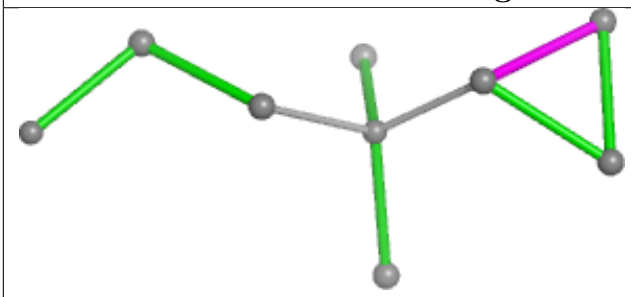


Torsions

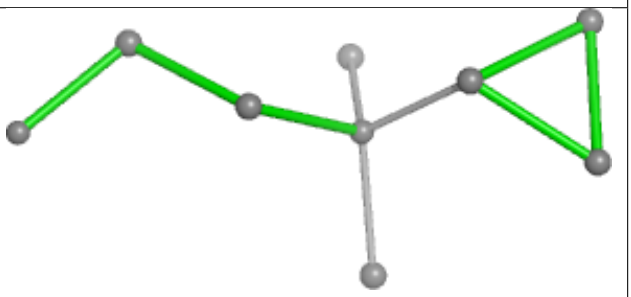


Rings

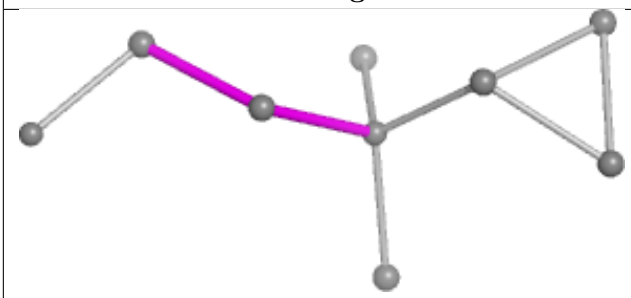
Ligand A1H9K E 1201



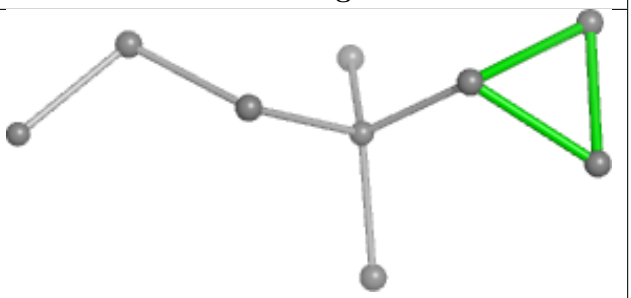
Bond lengths



Bond angles

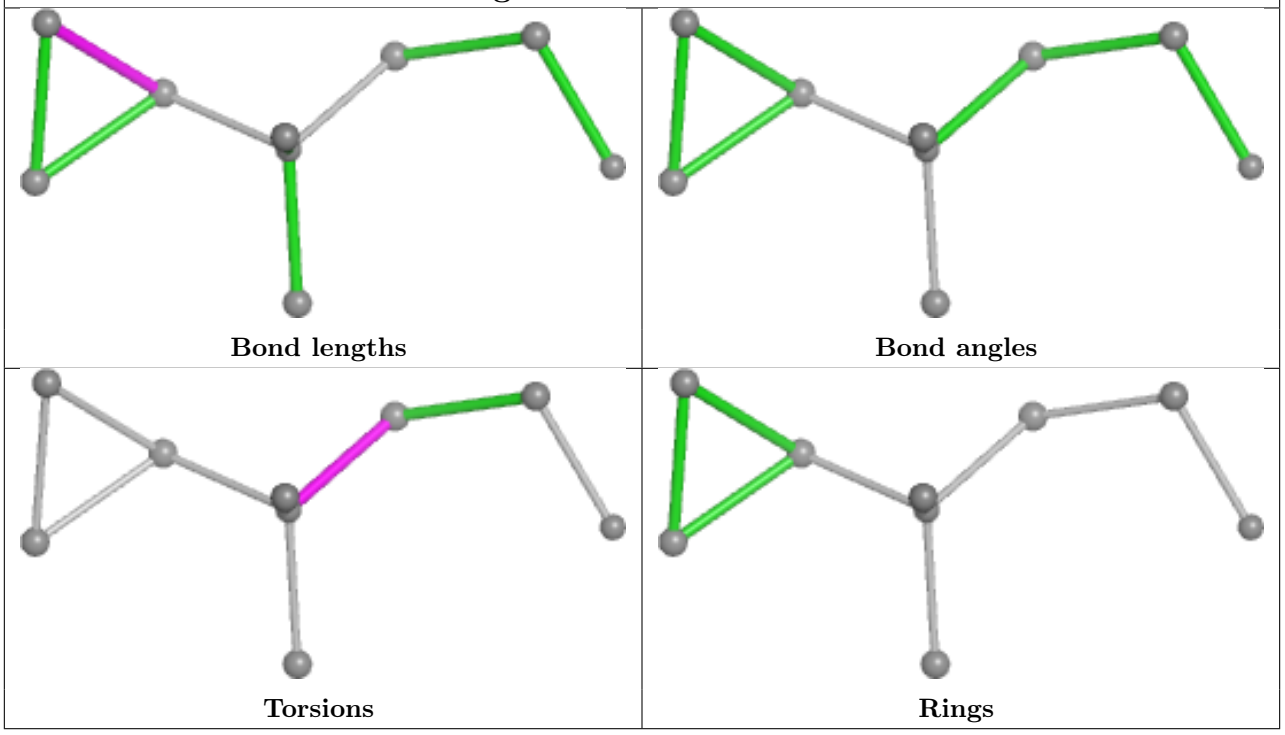


Torsions



Rings

Ligand A1H9K A 1201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	792/1150 (68%)	-0.51	1 (0%)	95	96	15, 26, 47, 74	0
1	B	792/1150 (68%)	-0.46	1 (0%)	95	96	13, 29, 44, 71	0
1	C	791/1150 (68%)	-0.22	6 (0%)	86	87	21, 36, 53, 74	0
1	D	792/1150 (68%)	-0.06	10 (1%)	77	78	19, 46, 63, 83	0
1	E	792/1150 (68%)	0.06	23 (2%)	51	52	20, 48, 77, 93	0
1	F	792/1150 (68%)	0.18	40 (5%)	28	26	23, 48, 74, 94	0
1	G	792/1150 (68%)	0.32	43 (5%)	25	24	29, 53, 79, 106	0
1	H	792/1150 (68%)	0.40	52 (6%)	18	16	35, 62, 86, 103	0
All	All	6335/9200 (68%)	-0.04	176 (2%)	53	54	13, 43, 75, 106	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	916	LEU	6.2
1	E	922	ALA	5.0
1	G	561	ALA	4.9
1	G	339	GLY	4.5
1	G	572	GLN	4.3
1	F	907	LEU	4.3
1	F	904	ILE	4.1
1	H	1093	LYS	4.1
1	E	821	LEU	3.9
1	E	915	THR	3.9
1	D	933	LEU	3.8
1	F	916	LEU	3.6
1	G	338	GLU	3.6
1	H	932	ALA	3.6
1	H	575	ALA	3.5
1	G	1087	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	561	ALA	3.4
1	F	924	LEU	3.4
1	E	818	LEU	3.4
1	G	1086	LYS	3.4
1	H	565	ALA	3.3
1	G	1089	GLN	3.3
1	G	642	HIS	3.3
1	G	1083	VAL	3.3
1	D	569	GLN	3.2
1	F	802	GLY	3.2
1	H	805	VAL	3.2
1	H	450	ILE	3.2
1	H	1081	ASN	3.2
1	E	909	PHE	3.1
1	E	910	GLU	3.1
1	F	913	LYS	3.1
1	H	737	GLY	3.0
1	D	643	ASP	3.0
1	F	933	LEU	3.0
1	F	925	ALA	3.0
1	E	1119	ILE	3.0
1	F	826	GLU	3.0
1	H	338	GLU	3.0
1	H	337	MET	3.0
1	E	919	ILE	3.0
1	F	943	TYR	3.0
1	D	340	LEU	3.0
1	H	1091	PRO	3.0
1	F	818	LEU	2.9
1	F	1020	PRO	2.9
1	F	953	TYR	2.9
1	H	442	ILE	2.9
1	F	914	TYR	2.8
1	G	581	ALA	2.8
1	H	642	HIS	2.8
1	G	579	THR	2.8
1	E	1104	TYR	2.8
1	F	1022	ALA	2.8
1	H	636	ARG	2.8
1	G	342	PRO	2.8
1	D	572	GLN	2.8
1	H	1089	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	771	CYS	2.7
1	H	651	ALA	2.7
1	F	908	VAL	2.7
1	G	805	VAL	2.7
1	F	803	ARG	2.7
1	F	1128	PHE	2.7
1	F	930	TYR	2.7
1	B	337	MET	2.6
1	F	1050	LEU	2.6
1	H	933	LEU	2.6
1	F	928	GLU	2.6
1	F	1045	PHE	2.6
1	H	935	ARG	2.6
1	F	1054	GLU	2.6
1	G	550	VAL	2.6
1	F	941	PRO	2.6
1	E	920	ARG	2.6
1	H	1096	ASP	2.6
1	F	1023	ILE	2.6
1	G	931	GLU	2.5
1	D	571	ALA	2.5
1	G	526	LEU	2.5
1	G	767	CYS	2.5
1	H	931	GLU	2.5
1	G	565	ALA	2.5
1	G	935	ARG	2.5
1	F	927	PHE	2.5
1	G	1090	GLU	2.5
1	G	1094	TYR	2.5
1	G	768	LEU	2.5
1	H	453	GLU	2.5
1	G	771	CYS	2.5
1	H	521	ALA	2.4
1	D	1050	LEU	2.4
1	H	1109	VAL	2.4
1	E	1045	PHE	2.4
1	H	1084	LEU	2.4
1	H	1106	ALA	2.4
1	G	450	ILE	2.4
1	C	910	GLU	2.4
1	F	935	ARG	2.4
1	E	822	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	523	LEU	2.3
1	H	523	LEU	2.3
1	E	1020	PRO	2.3
1	E	799	LEU	2.3
1	E	1094	TYR	2.3
1	H	619	SER	2.3
1	G	566	ALA	2.3
1	E	927	PHE	2.3
1	C	495	GLY	2.3
1	G	933	LEU	2.3
1	H	448	LYS	2.3
1	D	1063	LEU	2.3
1	F	982	ILE	2.3
1	G	569	GLN	2.3
1	H	433	SER	2.3
1	H	818	LEU	2.3
1	H	538	TYR	2.3
1	H	927	PHE	2.3
1	H	1086	LYS	2.3
1	E	1079	VAL	2.3
1	E	918	GLN	2.2
1	G	713	SER	2.2
1	H	563	GLU	2.2
1	C	823	THR	2.2
1	F	1061	THR	2.2
1	A	338	GLU	2.2
1	F	911	GLU	2.2
1	D	1094	TYR	2.2
1	G	513	ASN	2.2
1	H	340	LEU	2.2
1	H	595	LEU	2.2
1	H	645	ALA	2.2
1	G	1103	GLY	2.2
1	F	926	ASN	2.2
1	H	906	LYS	2.2
1	G	934	ARG	2.2
1	H	526	LEU	2.2
1	F	901	MET	2.2
1	G	1088	GLN	2.2
1	E	933	LEU	2.2
1	H	564	LEU	2.2
1	F	816	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	618	LEU	2.2
1	H	543	ALA	2.2
1	C	916	LEU	2.1
1	G	340	LEU	2.1
1	G	536	ARG	2.1
1	D	339	GLY	2.1
1	F	897	TYR	2.1
1	E	578	LEU	2.1
1	F	813	LEU	2.1
1	E	1093	LYS	2.1
1	F	934	ARG	2.1
1	H	402	LEU	2.1
1	H	1057	HIS	2.1
1	F	932	ALA	2.1
1	G	770	GLY	2.1
1	H	930	TYR	2.1
1	H	579	THR	2.1
1	F	495	GLY	2.1
1	G	640	LEU	2.1
1	G	621	GLY	2.1
1	H	1050	LEU	2.1
1	F	918	GLN	2.1
1	G	397	ILE	2.0
1	H	1094	TYR	2.0
1	F	922	ALA	2.0
1	H	913	LYS	2.0
1	E	798	VAL	2.0
1	G	678	ILE	2.0
1	H	907	LEU	2.0
1	C	617	GLY	2.0
1	G	524	ALA	2.0
1	H	446	ASP	2.0
1	G	716	CYS	2.0
1	G	1092	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

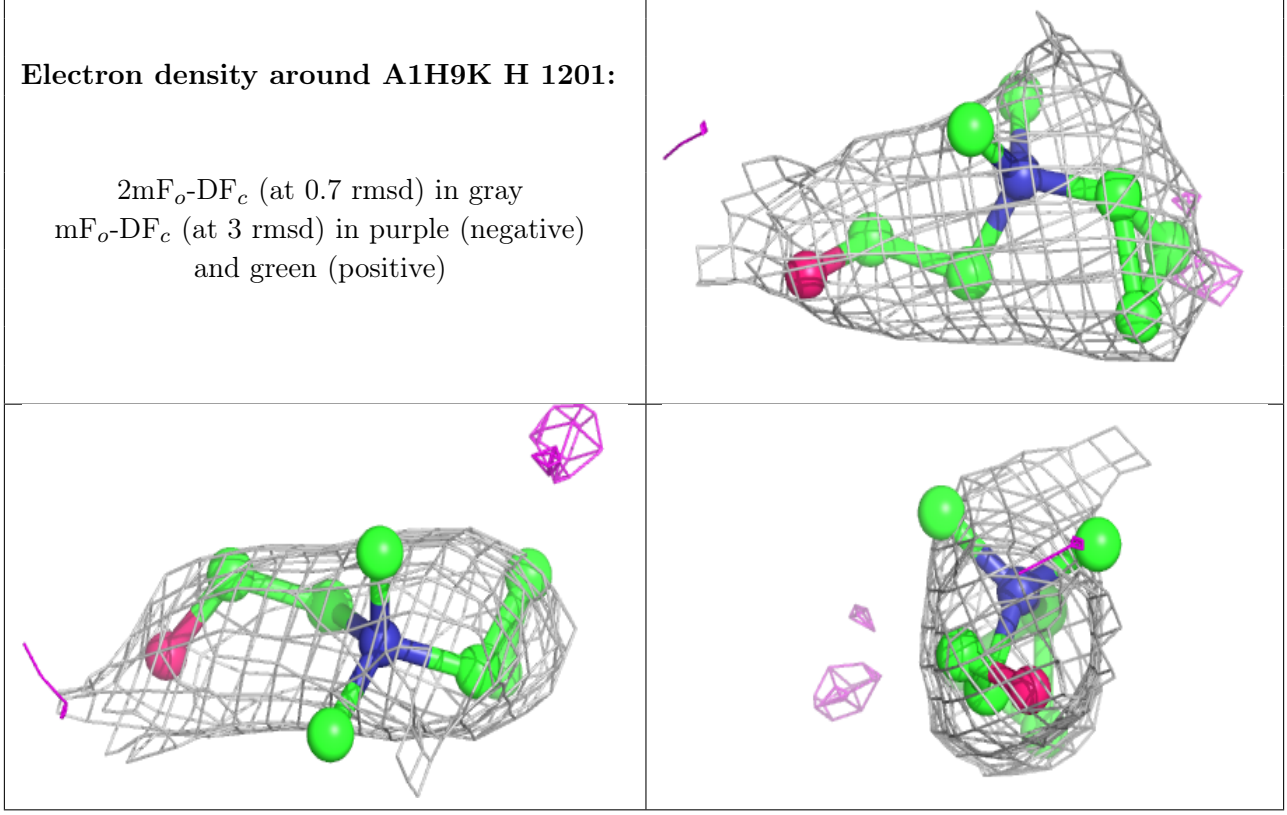
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1H9K	H	1201	9/9	0.92	0.31	55,58,61,64	0
2	A1H9K	E	1201	9/9	0.94	0.30	33,38,44,45	0
2	A1H9K	G	1201	9/9	0.95	0.30	38,42,51,51	0
2	A1H9K	F	1201	9/9	0.96	0.30	41,44,49,52	0
2	A1H9K	C	1201	9/9	0.96	0.28	24,30,33,36	0
2	A1H9K	A	1201	9/9	0.96	0.20	17,19,23,24	0
2	A1H9K	B	1201	9/9	0.97	0.23	16,20,24,26	0
2	A1H9K	D	1201	9/9	0.97	0.25	25,34,36,41	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.

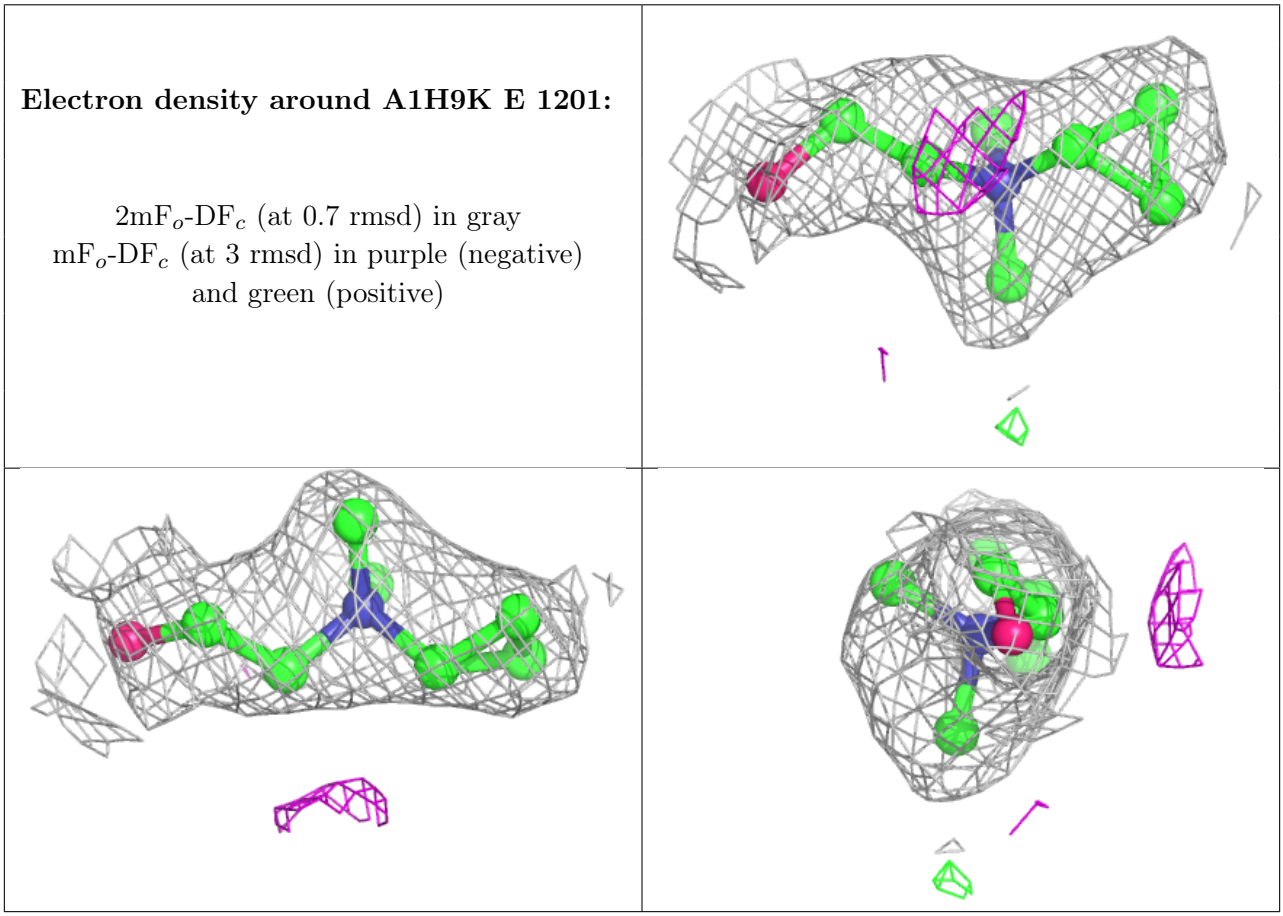
Electron density around A1H9K H 1201:

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



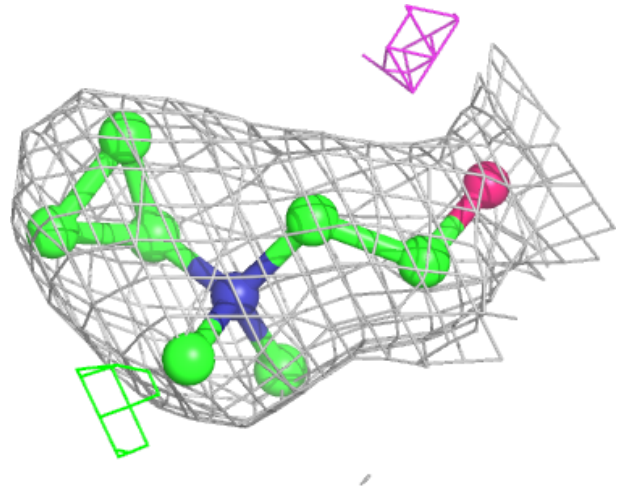
Electron density around A1H9K E 1201:

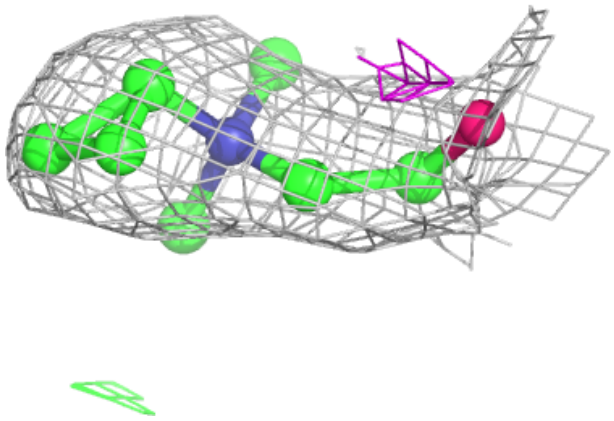
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

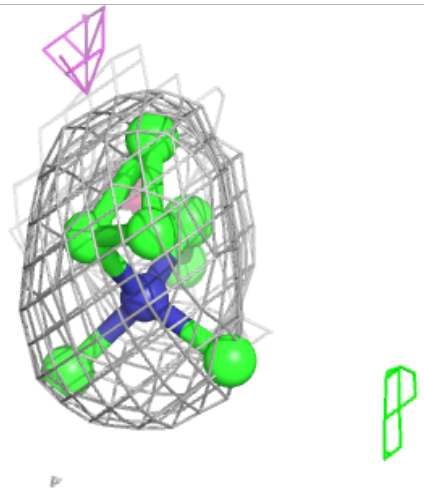


Electron density around A1H9K G 1201:

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

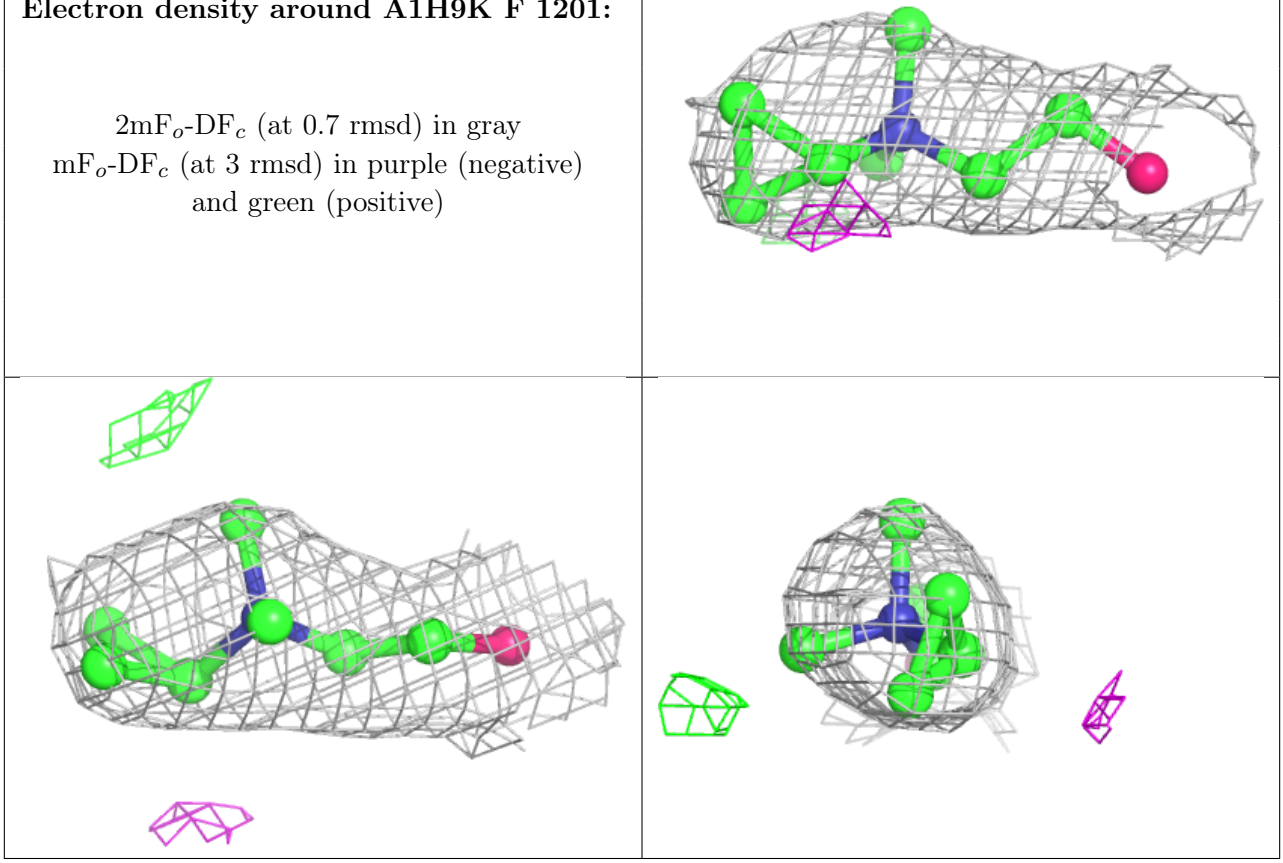






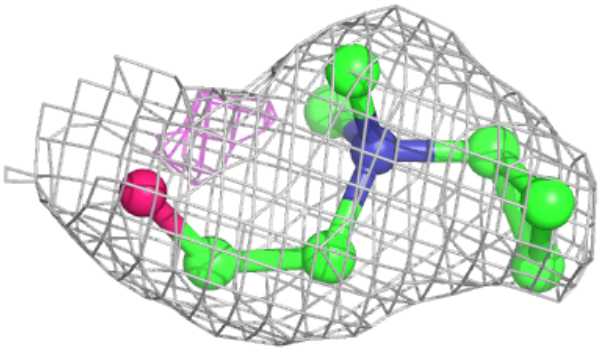
Electron density around A1H9K F 1201:

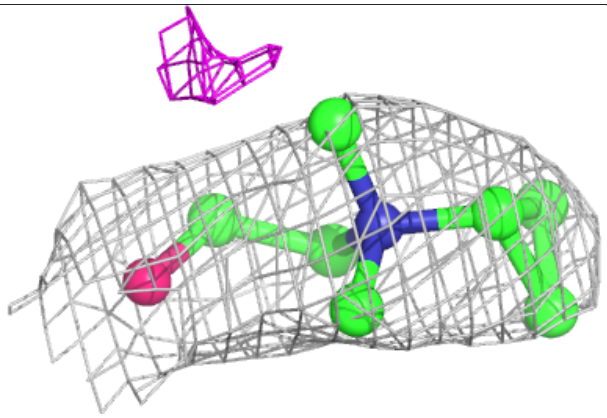
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

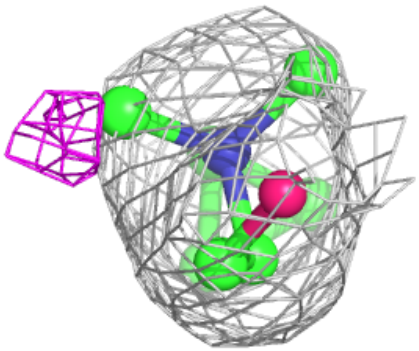


Electron density around A1H9K C 1201:

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

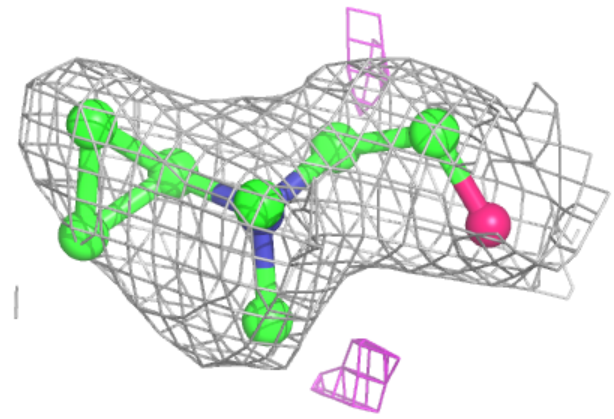


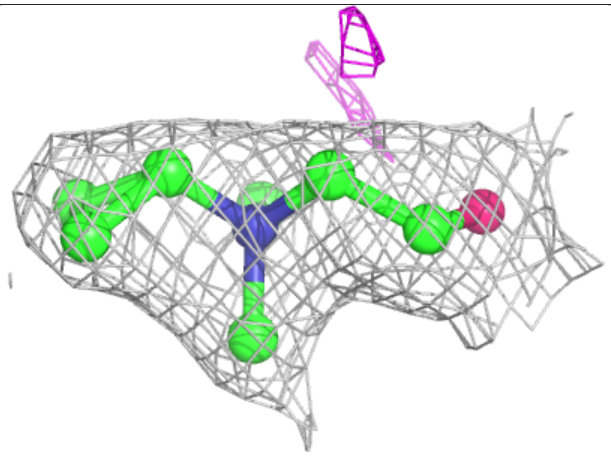


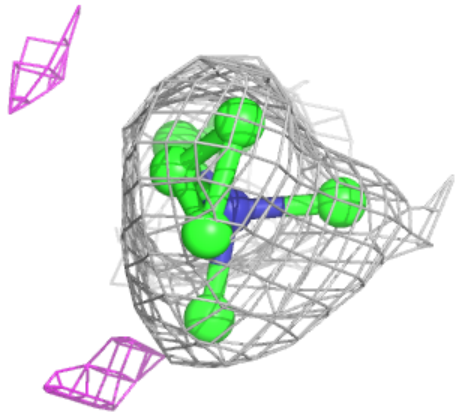


Electron density around A1H9K A 1201:

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

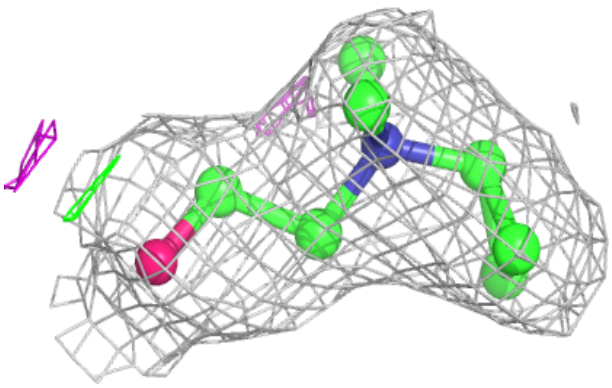


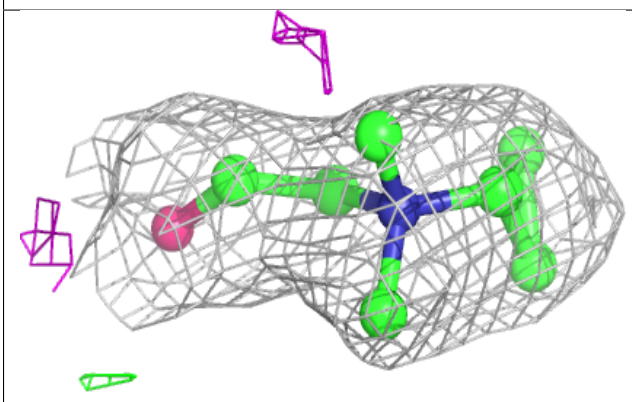


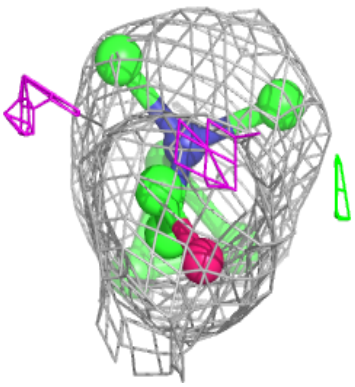


Electron density around A1H9K B 1201:

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

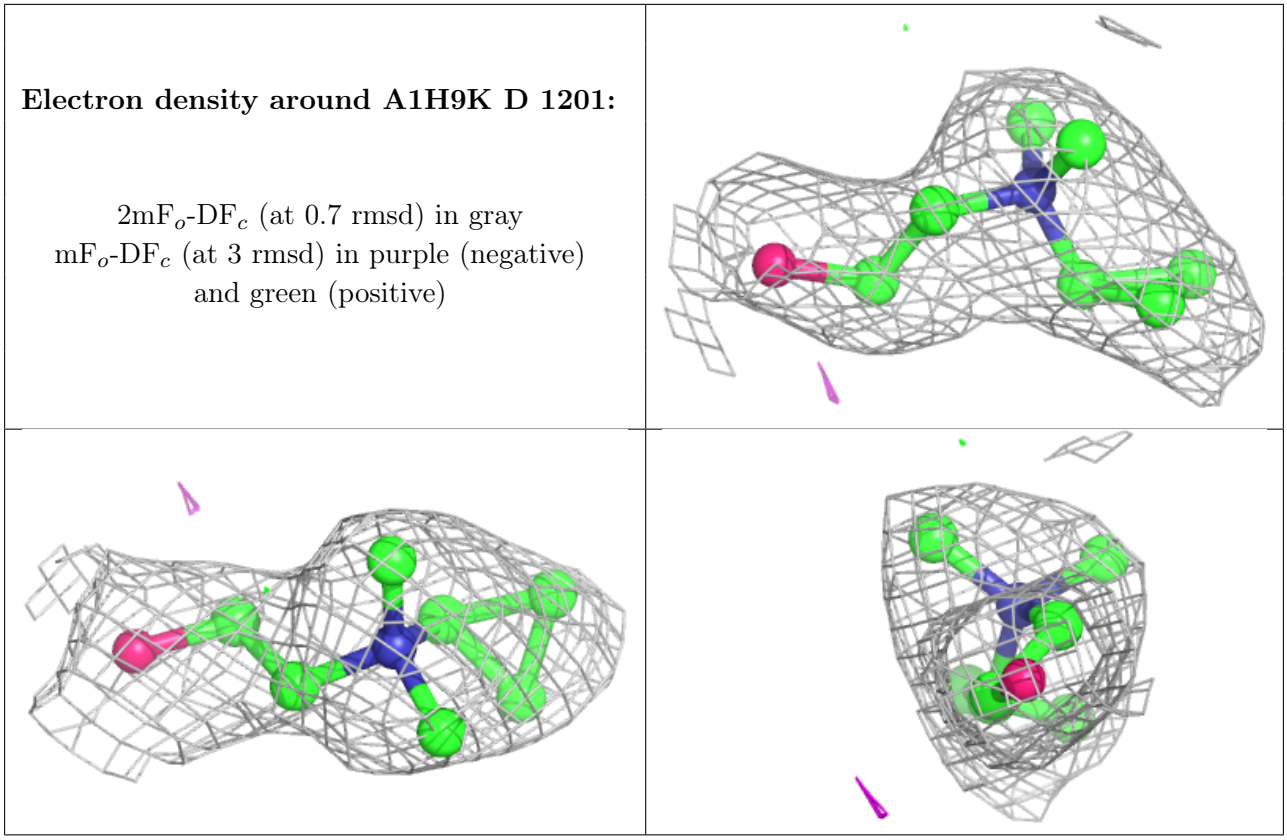






Electron density around A1H9K D 1201:

$2mF_o$-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.