Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 12:16 pm BST

PDB ID	:	5C8S
Title	:	Crystal structure of the SARS coronavirus nsp14-nsp10 complex with functional ligands SAH and GpppA
Authors	:	Ma, Y.Y.; Wu, L.J.; Zhang, R.G.; Rao, Z.H.
Deposited on	:	2015-06-26
Resolution	:	3.33 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

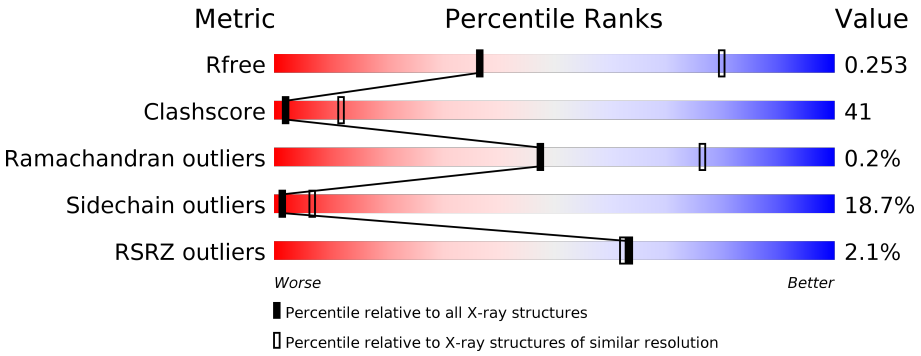
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.33 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	144	5% 38% 44% 10% 8%
1	C	144	% 36% 45% 11% 8%
2	B	527	2% 40% 46% 10%
2	D	527	2% 42% 46% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SAH	B	605	-	-	X	-
5	SAH	D	605	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10324 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 Non-structural protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			969	600	164	189	16			
1	C	133	Total	C	N	O	S	0	0	0
			969	600	164	189	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P0C6X7
A	-3	PRO	-	expression tag	UNP P0C6X7
A	-2	LEU	-	expression tag	UNP P0C6X7
A	-1	GLY	-	expression tag	UNP P0C6X7
A	0	SER	-	expression tag	UNP P0C6X7
C	-4	GLY	-	expression tag	UNP P0C6X7
C	-3	PRO	-	expression tag	UNP P0C6X7
C	-2	LEU	-	expression tag	UNP P0C6X7
C	-1	GLY	-	expression tag	UNP P0C6X7
C	0	SER	-	expression tag	UNP P0C6X7

- Molecule 2 is a protein called Guanine-N7 methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	514	Total	C	N	O	S	0	0	0
			4111	2632	704	739	36			
2	D	514	Total	C	N	O	S	0	0	0
			4111	2632	704	739	36			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Zn	0	0
			3	3		

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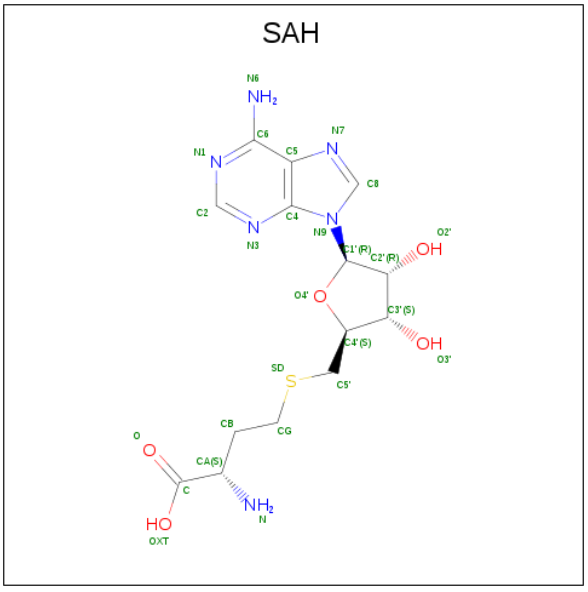
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	D	3	Total Zn 3 3	0	0
3	C	2	Total Zn 2 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

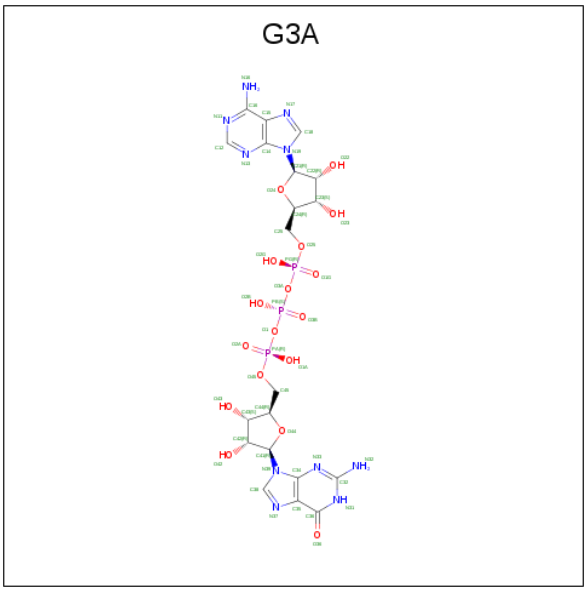
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O S 26 14 6 5 1	0	0
5	D	1	Total C N O S 26 14 6 5 1	0	0

- Molecule 6 is GUANOSINE-P3-ADENOSINE-5',5'-TRIPHOSPHATE (three-letter code: G3A) (formula: $C_{20}H_{27}N_{10}O_{17}P_3$).



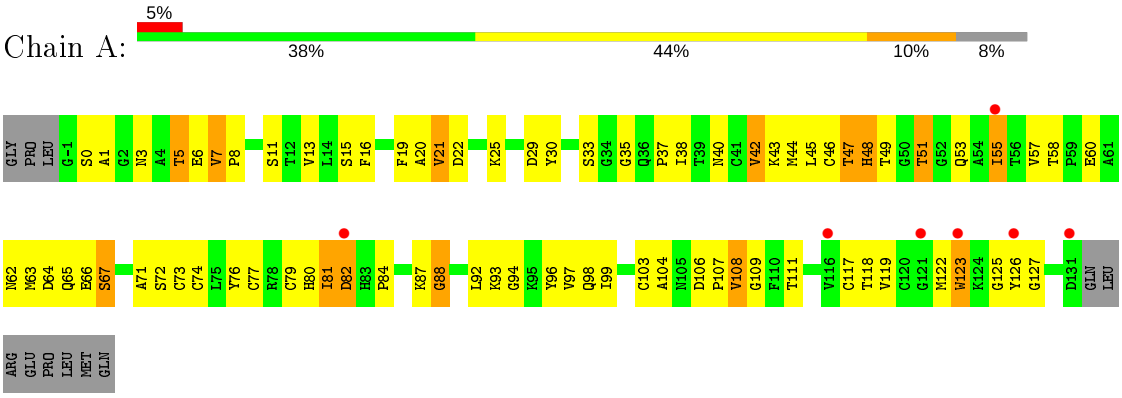
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			50	20	10	17	3		
6	D	1	Total	C	N	O	P	0	0
			50	20	10	17	3		

3 Residue-property plots (i)

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

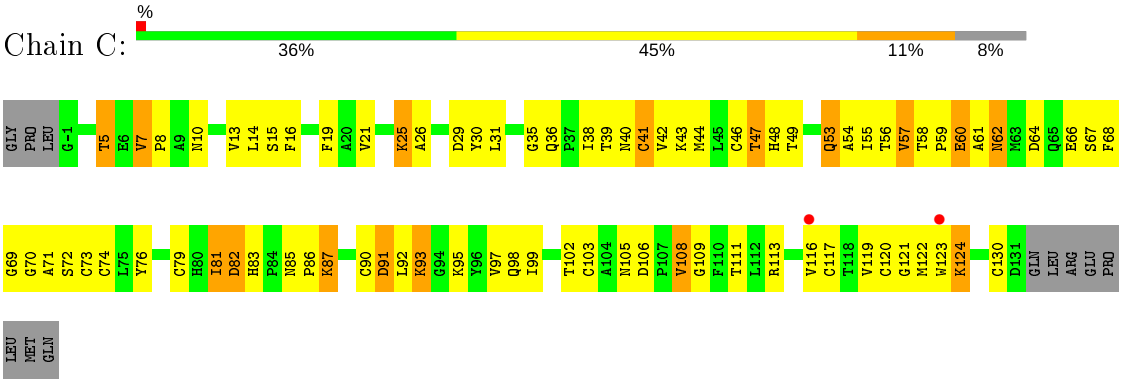
- Molecule 1: Non-structural protein 10

Chain A:



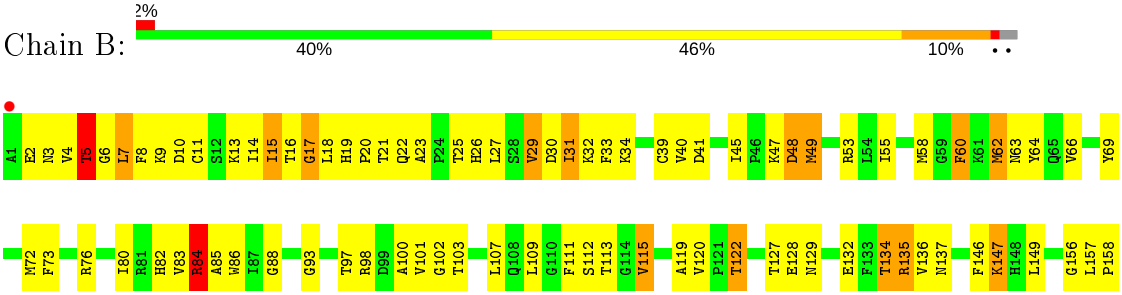
- Molecule 1: Non-structural protein 10

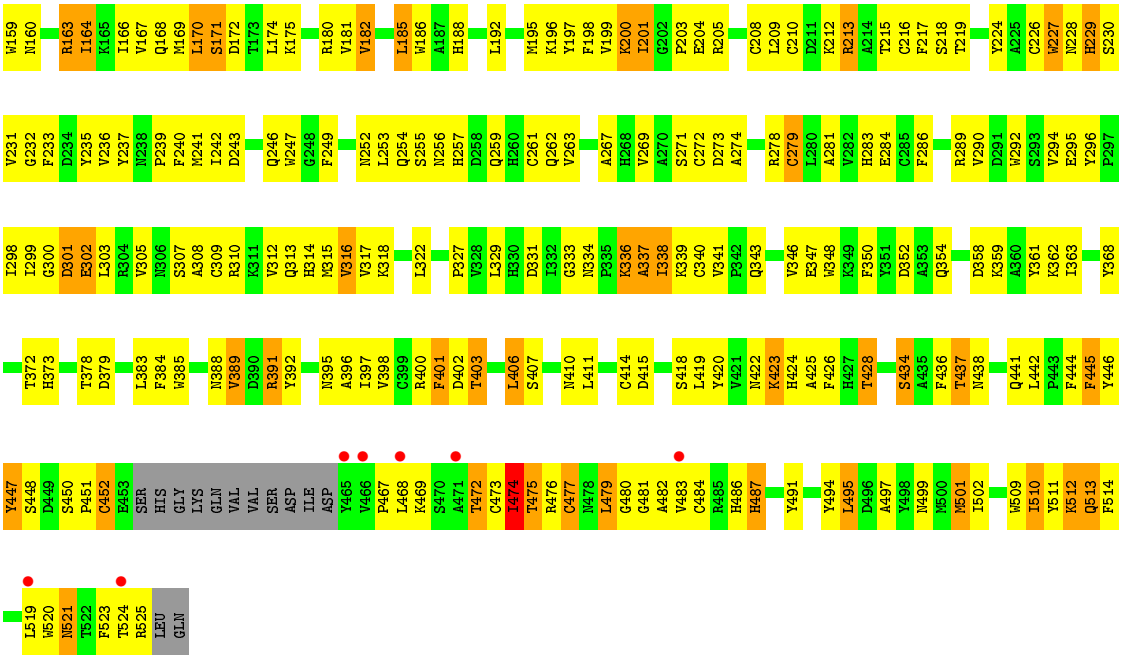
Chain C:



- Molecule 2: Guanine-N7 methyltransferase

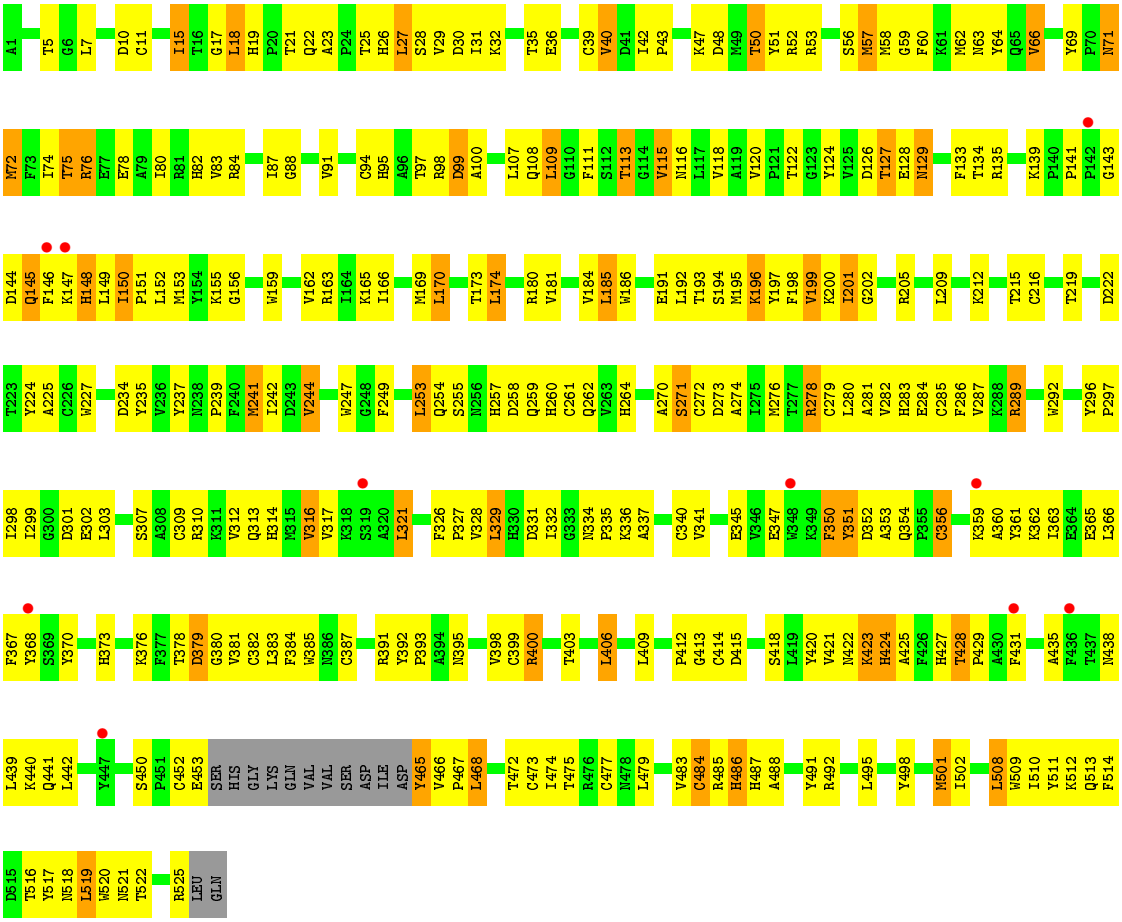
Chain B:





• Molecule 2: Guanine-N7 methyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	188.80Å 196.84Å 180.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.56 – 3.33 42.56 – 3.33	Depositor EDS
% Data completeness (in resolution range)	97.9 (42.56-3.33) 98.0 (42.56-3.33)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.217 , 0.259 0.210 , 0.253	Depositor DCC
R_{free} test set	2455 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	111.1	Xtriage
Anisotropy	0.792	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 85.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10324	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: G3A, ZN, SAH, MG

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	0.34	0/991	0.57	0/1348
1	C	0.35	0/991	0.59	0/1348
2	B	0.39	0/4228	0.67	4/5745 (0.1%)
2	D	0.37	0/4228	0.62	0/5745
All	All	0.37	0/10438	0.64	4/14186 (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
2	B	0	3
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	17	GLY	N-CA-C	-6.29	97.38	113.10
2	B	474	ILE	N-CA-C	-5.84	95.23	111.00
2	B	7	LEU	N-CA-C	-5.59	95.89	111.00
2	B	29	VAL	N-CA-C	-5.10	97.22	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	GLY	Peptide
2	B	472	THR	Peptide
2	B	5	THR	Peptide
2	B	84	ARG	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	969	0	920	75	0
1	C	969	0	920	87	0
2	B	4111	0	3981	363	0
2	D	4111	0	3981	320	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	26	0	19	9	0
5	D	26	0	19	15	0
6	B	50	0	23	19	0
6	D	50	0	23	19	0
All	All	10324	0	9886	820	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (820) 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)
2:D:477:CYS:HB2	2:D:484:CYS:SG	1.62	1.37
2:B:296:TYR:H	2:B:423:LYS:HE3	1.10	1.08
2:B:310:ARG:HA	6:B:606:G3A:H12	1.38	1.06
2:D:468:LEU:HD23	2:D:483:VAL:HG11	1.39	1.04
5:D:605:SAH:O	6:D:606:G3A:H18	1.57	1.03
5:D:605:SAH:C	6:D:606:G3A:H18	1.89	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:476:ARG:HD2	2:B:487:HIS:CD2	1.95	1.01
2:B:296:TYR:H	2:B:423:LYS:CE	1.75	1.00
2:B:296:TYR:N	2:B:423:LYS:HE3	1.78	0.98
2:D:336:LYS:HZ3	6:D:606:G3A:H23	1.26	0.98
2:D:215:THR:HG21	2:D:227:TRP:CE2	1.99	0.97
2:B:294:VAL:O	2:B:423:LYS:NZ	1.97	0.96
1:A:40:ASN:ND2	2:B:25:THR:OG1	1.98	0.96
2:D:328:VAL:HG12	2:D:347:GLU:HB3	1.47	0.96
2:D:428:THR:HG21	6:D:606:G3A:H321	1.29	0.95
2:B:447:TYR:HD2	2:B:519:LEU:HD13	1.30	0.95
2:B:5:THR:HB	2:B:7:LEU:N	1.82	0.94
2:B:476:ARG:HB2	2:B:487:HIS:CE1	2.04	0.93
1:A:38:ILE:HB	1:A:108:VAL:HG21	1.49	0.93
2:D:82:HIS:CD2	2:D:180:ARG:HD2	2.04	0.93
1:A:5:THR:O	2:B:25:THR:HG21	1.68	0.92
2:B:181:VAL:HG22	2:B:227:TRP:HZ2	1.31	0.92
2:B:298:ILE:HG12	2:B:302:GLU:HB3	1.50	0.92
2:B:423:LYS:HE2	2:B:423:LYS:HA	1.49	0.92
2:D:35:THR:HG22	2:D:36:GLU:HG2	1.53	0.91
2:D:83:VAL:HG21	2:D:286:PHE:CZ	2.07	0.90
1:A:126:TYR:N	1:A:127:GLY:HA2	1.85	0.90
2:D:83:VAL:HG21	2:D:286:PHE:HZ	1.34	0.89
2:B:181:VAL:CG2	2:B:227:TRP:HZ2	1.85	0.88
1:A:92:LEU:HD13	1:A:97:VAL:HG21	1.53	0.88
2:B:163:ARG:HE	2:B:235:TYR:HE1	1.21	0.87
1:C:56:THR:HG21	1:C:60:GLU:HG3	1.56	0.87
2:D:517:TYR:HA	2:D:520:TRP:HD1	1.40	0.87
2:B:295:GLU:HA	2:B:423:LYS:NZ	1.90	0.86
1:C:54:ALA:HB2	1:C:98:GLN:HB2	1.53	0.86
1:A:47:THR:OG1	1:A:49:THR:HG22	1.74	0.86
2:B:5:THR:HB	2:B:7:LEU:H	1.36	0.86
2:D:370:TYR:HE2	2:D:391:ARG:HH21	1.21	0.86
2:B:49:MET:H	2:B:49:MET:CE	1.88	0.85
2:B:317:VAL:HG11	2:B:340:CYS:SG	2.16	0.85
2:B:310:ARG:HA	6:B:606:G3A:C12	2.07	0.85
1:C:55:ILE:HG22	1:C:97:VAL:HA	1.58	0.85
2:B:476:ARG:HD2	2:B:487:HIS:CG	2.11	0.84
1:A:15:SER:OG	2:B:60:PHE:O	1.96	0.84
2:B:395:ASN:ND2	2:B:395:ASN:O	2.11	0.84
2:D:309:CYS:HA	2:D:501:MET:HE3	1.59	0.84
2:D:80:ILE:O	2:D:83:VAL:HG23	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:452:CYS:SG	2:D:484:CYS:HB2	2.17	0.84
1:C:38:ILE:HB	1:C:108:VAL:HG21	1.57	0.83
1:C:117:CYS:SG	1:C:119:VAL:HB	2.19	0.83
2:D:253:LEU:HD13	2:D:254:GLN:H	1.42	0.83
2:B:283:HIS:HB2	2:B:414:CYS:SG	2.18	0.83
2:B:228:ASN:HB2	2:B:229:HIS:ND1	1.94	0.82
2:B:88:GLY:N	2:B:112:SER:OG	2.10	0.82
2:D:335:PRO:HG3	2:D:352:ASP:OD2	1.79	0.82
2:B:84:ARG:HB2	2:B:411:LEU:HD13	1.60	0.81
2:B:82:HIS:CD2	2:B:180:ARG:HD2	2.14	0.81
2:B:171:SER:HA	2:B:227:TRP:CE3	2.15	0.81
2:D:279:CYS:SG	2:D:414:CYS:HB3	2.21	0.81
1:C:76:TYR:HB2	1:C:83:HIS:CE1	2.16	0.81
1:A:0:SER:N	1:A:1:ALA:HB3	1.96	0.80
2:B:29:VAL:HG23	2:B:34:LYS:HE3	1.62	0.80
2:D:391:ARG:HG3	2:D:435:ALA:HA	1.61	0.80
1:C:40:ASN:ND2	2:D:25:THR:OG1	2.15	0.79
2:B:80:ILE:O	2:B:83:VAL:HG23	1.83	0.79
2:D:260:HIS:CD2	2:D:283:HIS:HE1	2.00	0.79
2:B:423:LYS:HZ3	2:B:424:HIS:H	1.29	0.79
1:A:51:THR:OG1	1:A:60:GLU:OE2	1.99	0.79
1:C:13:VAL:HG22	1:C:30:TYR:CE2	2.18	0.79
2:B:286:PHE:HD2	2:B:419:LEU:HD13	1.46	0.79
2:D:50:THR:HA	2:D:128:GLU:CG	2.14	0.78
1:C:5:THR:O	2:D:25:THR:HG21	1.83	0.78
2:B:83:VAL:HG21	2:B:286:PHE:CZ	2.20	0.77
2:D:518:ASN:O	2:D:525:ARG:NH2	2.18	0.77
2:B:423:LYS:CA	2:B:423:LYS:HE2	2.13	0.77
2:B:49:MET:HE2	2:B:49:MET:H	1.49	0.77
1:C:55:ILE:HG21	1:C:97:VAL:HG22	1.67	0.77
1:C:83:HIS:CD2	1:C:90:CYS:HB2	2.19	0.77
2:D:385:TRP:O	5:D:605:SAH:N	2.17	0.76
2:B:198:PHE:CD1	2:B:199:VAL:HG23	2.20	0.76
2:D:352:ASP:OD1	5:D:605:SAH:H1'	1.83	0.76
1:C:46:CYS:HB3	1:C:48:HIS:ND1	2.00	0.76
2:D:27:LEU:H	2:D:27:LEU:HD23	1.49	0.76
2:B:295:GLU:HA	2:B:423:LYS:HZ2	1.47	0.76
2:B:156:GLY:HA3	2:B:157:LEU:HD13	1.68	0.76
2:D:260:HIS:CD2	2:D:283:HIS:CE1	2.74	0.76
2:D:331:ASP:HB3	2:D:350:PHE:HB3	1.67	0.76
2:B:181:VAL:HG22	2:B:227:TRP:CZ2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:PHE:HD1	2:B:402:ASP:N	1.84	0.75
2:B:252:ASN:OD1	2:B:255:SER:HB3	1.87	0.75
2:D:282:VAL:HG23	2:D:286:PHE:HD2	1.51	0.75
1:A:76:TYR:CD2	1:A:84:PRO:HD3	2.22	0.74
2:D:334:ASN:ND2	2:D:336:LYS:O	2.20	0.74
2:B:83:VAL:HG21	2:B:286:PHE:HZ	1.52	0.74
5:B:605:SAH:OXT	6:B:606:G3A:H18	1.87	0.74
1:C:92:LEU:HD11	1:C:111:THR:HG21	1.67	0.74
2:D:483:VAL:HG13	2:D:488:ALA:HB2	1.70	0.74
2:D:511:TYR:CE1	2:D:514:PHE:HB2	2.23	0.74
2:B:446:TYR:HB3	2:B:473:CYS:HB2	1.70	0.74
2:B:385:TRP:O	5:B:605:SAH:N	2.19	0.74
2:B:249:PHE:HB3	2:B:256:ASN:ND2	2.02	0.74
2:D:336:LYS:NZ	6:D:606:G3A:H251	2.01	0.74
2:D:336:LYS:HZ3	6:D:606:G3A:H251	1.54	0.73
2:B:21:THR:O	2:B:22:GLN:HG2	1.89	0.73
2:D:253:LEU:HD13	2:D:254:GLN:N	2.04	0.72
2:B:423:LYS:CE	2:B:424:HIS:H	2.02	0.72
1:A:93:LYS:HD3	2:B:128:GLU:O	1.90	0.72
1:C:83:HIS:NE2	1:C:90:CYS:HB2	2.05	0.72
2:D:15:ILE:H	2:D:15:ILE:HD13	1.54	0.72
2:B:48:ASP:OD1	2:B:48:ASP:N	2.17	0.72
2:D:366:LEU:HD21	2:D:373:HIS:CE1	2.25	0.72
2:D:309:CYS:HA	2:D:501:MET:CE	2.19	0.71
1:C:16:PHE:CE2	1:C:26:ALA:HB1	2.25	0.71
2:D:71:ASN:OD1	2:D:71:ASN:N	2.22	0.71
2:D:421:VAL:HG13	2:D:425:ALA:HB2	1.72	0.71
2:B:401:PHE:HD2	6:B:606:G3A:H322	1.34	0.71
2:B:423:LYS:NZ	2:B:424:HIS:H	1.88	0.71
2:B:19:HIS:CG	2:B:20:PRO:HD2	2.26	0.71
2:B:310:ARG:CA	6:B:606:G3A:H12	2.19	0.71
2:B:135:ARG:CG	2:B:135:ARG:HH11	2.03	0.71
2:B:337:ALA:HB2	2:B:362:LYS:HD3	1.72	0.70
2:B:447:TYR:CD2	2:B:519:LEU:HD13	2.21	0.70
2:D:50:THR:HA	2:D:128:GLU:HG2	1.73	0.70
2:B:135:ARG:HG2	2:B:135:ARG:HH11	1.53	0.70
2:D:82:HIS:HD2	2:D:180:ARG:HD2	1.53	0.70
1:A:74:CYS:HB3	1:A:77:CYS:HB2	1.73	0.70
2:D:215:THR:HG21	2:D:227:TRP:NE1	2.07	0.70
1:C:13:VAL:HG13	1:C:30:TYR:CD2	2.27	0.70
2:D:27:LEU:HD23	2:D:27:LEU:N	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:257:HIS:CD2	2:D:276:MET:HG3	2.28	0.69
1:C:120:CYS:HB2	1:C:121:GLY:C	2.12	0.69
2:D:118:VAL:HG23	2:D:156:GLY:HA2	1.74	0.69
2:D:88:GLY:HA2	2:D:184:VAL:HG23	1.72	0.69
2:D:11:CYS:O	2:D:100:ALA:HB1	1.92	0.69
2:D:356:CYS:O	2:D:360:ALA:HB2	1.93	0.69
2:B:171:SER:HA	2:B:227:TRP:CZ3	2.27	0.69
2:D:150:ILE:N	2:D:151:PRO:HD2	2.07	0.69
2:D:224:TYR:HE2	2:D:237:TYR:CE1	2.11	0.69
2:D:88:GLY:O	2:D:111:PHE:HA	1.93	0.69
2:B:163:ARG:NE	2:B:235:TYR:HE1	1.91	0.68
2:B:309:CYS:SG	2:B:501:MET:HE1	2.33	0.68
2:D:317:VAL:HG13	2:D:341:VAL:CG2	2.21	0.68
2:B:450:SER:HB3	2:B:451:PRO:HD2	1.75	0.68
1:C:68:PHE:CD2	1:C:99:ILE:HD13	2.29	0.68
2:D:76:ARG:HD3	2:D:247:TRP:CZ2	2.29	0.68
2:D:428:THR:HG21	6:D:606:G3A:N32	2.07	0.68
2:B:392:TYR:CZ	2:B:398:VAL:HG21	2.29	0.68
2:D:180:ARG:C	2:D:227:TRP:HH2	1.97	0.68
2:D:392:TYR:CZ	2:D:398:VAL:HG21	2.29	0.68
2:D:75:THR:HG23	2:D:78:GLU:HB2	1.73	0.68
2:B:423:LYS:HE2	2:B:424:HIS:H	1.58	0.68
1:A:44:MET:HE1	2:B:20:PRO:HB2	1.75	0.67
2:B:447:TYR:CD2	2:B:474:ILE:HG12	2.30	0.67
1:C:48:HIS:HB3	1:C:61:ALA:HB3	1.77	0.67
1:C:91:ASP:OD1	1:C:91:ASP:N	2.27	0.67
2:D:95:HIS:HB2	2:D:139:LYS:HE2	1.75	0.67
2:D:261:CYS:HA	2:D:415:ASP:HB3	1.77	0.67
2:B:76:ARG:O	2:B:80:ILE:HG12	1.94	0.67
2:D:186:TRP:HE3	2:D:244:VAL:HG23	1.60	0.67
2:D:466:VAL:N	2:D:467:PRO:HD2	2.09	0.67
5:D:605:SAH:C	6:D:606:G3A:C18	2.70	0.67
1:A:38:ILE:HD12	1:A:108:VAL:HG11	1.77	0.66
1:C:42:VAL:HG12	2:D:26:HIS:HA	1.77	0.66
2:D:66:VAL:HG22	2:D:69:TYR:HD2	1.61	0.66
2:B:159:TRP:HB3	2:B:163:ARG:HH12	1.60	0.66
2:B:286:PHE:CD2	2:B:419:LEU:HD13	2.30	0.66
1:A:44:MET:CE	1:A:96:TYR:HE2	2.09	0.66
2:B:228:ASN:HB2	2:B:229:HIS:CE1	2.31	0.66
2:B:475:THR:O	2:B:523:PHE:CE2	2.48	0.66
2:D:379:ASP:N	2:D:379:ASP:OD1	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:CE1	2:B:196:LYS:HA	2.30	0.66
2:B:16:THR:OG1	2:B:16:THR:O	2.14	0.66
2:B:29:VAL:CG2	2:B:34:LYS:HE3	2.25	0.65
2:D:66:VAL:HG22	2:D:69:TYR:CD2	2.31	0.65
2:B:428:THR:HG21	6:B:606:G3A:H321	1.62	0.65
2:D:75:THR:HG23	2:D:78:GLU:CB	2.26	0.65
2:B:257:HIS:CE1	2:B:279:CYS:CB	2.80	0.65
2:B:312:VAL:O	2:B:316:VAL:HG12	1.96	0.65
5:D:605:SAH:OXT	6:D:606:G3A:H18	1.97	0.65
2:D:185:LEU:N	2:D:185:LEU:HD22	2.12	0.65
2:B:132:GLU:O	2:B:134:THR:HG22	1.97	0.64
2:D:19:HIS:CG	2:D:47:LYS:HB3	2.31	0.64
2:D:184:VAL:HG12	2:D:242:ILE:CG2	2.26	0.64
1:A:15:SER:HB3	2:B:62:MET:HE3	1.78	0.64
2:B:368:TYR:CE1	2:B:373:HIS:HB2	2.33	0.64
2:D:317:VAL:HG13	2:D:341:VAL:HG23	1.79	0.64
2:B:487:HIS:H	2:B:487:HIS:CD2	2.13	0.64
2:B:336:LYS:HB2	2:B:338:ILE:HG12	1.78	0.64
2:B:86:TRP:HA	2:B:182:VAL:HG22	1.78	0.64
2:D:10:ASP:OD2	2:D:53:ARG:HD3	1.98	0.64
1:A:76:TYR:CE2	1:A:84:PRO:HD3	2.33	0.64
2:D:205:ARG:HD3	2:D:224:TYR:CE2	2.33	0.64
2:B:476:ARG:NH1	2:B:486:HIS:ND1	2.45	0.64
2:B:313:GLN:O	2:B:317:VAL:HG12	1.98	0.64
1:C:47:THR:OG1	1:C:48:HIS:O	2.13	0.64
2:B:473:CYS:HB3	2:B:491:TYR:CE2	2.33	0.64
1:C:76:TYR:HB2	1:C:83:HIS:ND1	2.13	0.63
1:A:44:MET:CE	2:B:20:PRO:HB2	2.28	0.63
1:C:54:ALA:HB1	1:C:55:ILE:HG23	1.79	0.63
2:B:217:PHE:CD2	2:B:224:TYR:HE1	2.17	0.63
2:D:19:HIS:CD2	2:D:47:LYS:HB3	2.33	0.63
2:B:487:HIS:N	2:B:487:HIS:CD2	2.65	0.63
2:D:363:ILE:N	2:D:363:ILE:HD12	2.13	0.63
1:A:53:GLN:O	1:A:98:GLN:HG3	1.99	0.63
1:C:92:LEU:HD13	1:C:97:VAL:HG21	1.80	0.63
2:D:352:ASP:OD1	2:D:353:ALA:N	2.32	0.63
2:D:84:ARG:CZ	2:D:299:ILE:HD11	2.29	0.63
2:D:317:VAL:HG11	2:D:340:CYS:SG	2.38	0.62
2:D:381:VAL:HG23	2:D:395:ASN:O	1.99	0.62
2:D:173:THR:HG22	2:D:174:LEU:HD13	1.82	0.62
2:D:215:THR:HG21	2:D:227:TRP:CZ2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ILE:HG23	2:B:286:PHE:CE1	2.35	0.62
1:A:71:ALA:HB2	1:A:93:LYS:HG3	1.81	0.62
1:C:92:LEU:HD11	1:C:111:THR:CG2	2.30	0.62
2:D:116:ASN:CG	2:D:271:SER:HG	2.03	0.62
2:D:25:THR:HG22	2:D:28:SER:HB2	1.82	0.62
2:B:411:LEU:HD12	2:B:419:LEU:HD23	1.81	0.62
2:B:136:VAL:HG12	2:B:137:ASN:O	1.99	0.62
2:B:159:TRP:HB3	2:B:163:ARG:NH1	2.15	0.62
1:C:68:PHE:HD2	1:C:99:ILE:HD13	1.63	0.62
1:C:48:HIS:HB3	1:C:61:ALA:O	2.00	0.61
2:D:485:ARG:HG3	2:D:486:HIS:N	2.15	0.61
2:B:107:LEU:HD23	2:B:149:LEU:HD23	1.81	0.61
2:B:423:LYS:HZ3	2:B:424:HIS:N	1.98	0.61
2:B:208:CYS:O	2:B:209:LEU:HG	2.00	0.61
2:B:181:VAL:CG2	2:B:227:TRP:CZ2	2.76	0.61
2:B:31:ILE:HD13	2:B:31:ILE:N	2.15	0.61
1:C:85:ASN:ND2	1:C:86:PRO:HD2	2.15	0.61
2:B:331:ASP:OD2	2:B:334:ASN:ND2	2.33	0.61
2:B:434:SER:O	2:B:437:THR:HG22	2.00	0.61
2:D:72:MET:HB3	2:D:241:MET:HE3	1.83	0.61
1:A:53:GLN:HG2	1:A:122:MET:HE2	1.83	0.61
1:C:41:CYS:HA	1:C:72:SER:HB2	1.83	0.61
2:D:483:VAL:HG22	2:D:484:CYS:H	1.66	0.61
2:D:485:ARG:HG3	2:D:486:HIS:H	1.66	0.61
2:B:188:HIS:ND1	2:B:243:ASP:OD2	2.32	0.61
2:B:315:MET:HG2	2:B:494:TYR:CZ	2.35	0.61
2:B:401:PHE:CD1	2:B:402:ASP:N	2.67	0.61
2:B:392:TYR:HE2	2:B:436:PHE:HE1	1.48	0.61
2:B:473:CYS:SG	2:B:475:THR:HB	2.41	0.60
2:B:333:GLY:O	5:B:605:SAH:HA	2.01	0.60
1:C:106:ASP:OD2	1:C:109:GLY:HA3	1.99	0.60
1:C:13:VAL:HG22	1:C:30:TYR:HE2	1.61	0.60
2:B:447:TYR:HD1	2:B:448:SER:N	2.00	0.60
2:B:510:ILE:HG23	2:B:511:TYR:O	2.01	0.60
2:D:465:TYR:HB3	2:D:467:PRO:HD2	1.83	0.60
1:A:44:MET:HE2	1:A:96:TYR:HE2	1.66	0.60
2:B:186:TRP:CD1	2:B:253:LEU:HB2	2.36	0.60
2:D:21:THR:O	2:D:22:GLN:HG2	2.00	0.60
2:B:185:LEU:H	2:B:185:LEU:HD22	1.67	0.60
2:D:453:GLU:HB3	2:D:485:ARG:CG	2.31	0.60
2:B:383:LEU:HD12	2:B:397:ILE:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:GLN:HG2	1:C:53:GLN:O	2.00	0.60
2:D:440:LYS:HE3	2:D:512:LYS:HA	1.84	0.60
2:D:327:PRO:HD2	2:D:380:GLY:HA2	1.82	0.60
1:C:54:ALA:HA	1:C:98:GLN:HE21	1.65	0.60
2:D:147:LYS:O	2:D:150:ILE:HG23	2.01	0.60
1:A:8:PRO:HD3	2:B:4:VAL:HA	1.84	0.60
2:B:445:PHE:CE2	2:B:514:PHE:HZ	2.20	0.59
2:D:15:ILE:N	2:D:15:ILE:HD13	2.18	0.59
1:C:120:CYS:HB2	1:C:122:MET:N	2.18	0.59
2:D:181:VAL:HG23	2:D:227:TRP:HZ2	1.66	0.59
2:D:278:ARG:HH22	2:D:412:PRO:HG2	1.68	0.59
2:D:508:LEU:HD22	2:D:508:LEU:H	1.67	0.59
2:D:84:ARG:NE	2:D:299:ILE:HD11	2.18	0.59
2:B:401:PHE:HE2	2:B:420:TYR:CD1	2.20	0.59
2:B:13:LYS:HE3	2:B:101:VAL:HG23	1.85	0.59
2:B:499:ASN:O	2:B:502:ILE:HG22	2.03	0.59
2:D:97:THR:HG23	2:D:98:ARG:N	2.18	0.59
2:B:64:TYR:CD1	2:B:64:TYR:N	2.70	0.59
1:C:53:GLN:HA	1:C:122:MET:HG3	1.85	0.59
2:D:141:PRO:HB2	2:D:146:PHE:CB	2.32	0.59
2:B:423:LYS:HE2	2:B:424:HIS:N	2.18	0.58
1:A:7:VAL:HG23	1:A:8:PRO:HD2	1.84	0.58
2:B:447:TYR:C	2:B:447:TYR:CD1	2.77	0.58
2:D:19:HIS:HD2	2:D:21:THR:OG1	1.86	0.58
1:A:125:GLY:C	1:A:127:GLY:HA2	2.22	0.58
1:A:51:THR:HB	1:A:53:GLN:HG3	1.84	0.58
2:B:279:CYS:SG	2:B:414:CYS:HB3	2.43	0.58
2:D:150:ILE:HG13	2:D:151:PRO:N	2.18	0.58
2:D:185:LEU:H	2:D:185:LEU:HD22	1.66	0.58
2:B:476:ARG:CD	2:B:487:HIS:CD2	2.80	0.58
2:B:209:LEU:HD12	2:B:210:CYS:SG	2.44	0.58
2:D:25:THR:HG23	2:D:28:SER:H	1.68	0.58
2:D:336:LYS:NZ	6:D:606:G3A:H23	2.10	0.58
2:B:32:LYS:HD2	2:B:45:ILE:CD1	2.34	0.58
2:D:282:VAL:HG23	2:D:286:PHE:CD2	2.34	0.58
1:C:119:VAL:HG11	1:C:130:CYS:SG	2.44	0.57
2:B:447:TYR:CD1	2:B:448:SER:N	2.72	0.57
2:D:392:TYR:OH	2:D:400:ARG:NH1	2.37	0.57
2:D:257:HIS:CE1	2:D:261:CYS:HB3	2.38	0.57
2:B:398:VAL:HG13	2:B:509:TRP:HB2	1.85	0.57
2:B:101:VAL:HG12	2:B:102:GLY:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:TRP:CD1	2:B:350:PHE:CE1	2.93	0.57
2:B:401:PHE:HE2	2:B:420:TYR:CE1	2.23	0.57
2:D:94:CYS:HB2	2:D:139:LYS:O	2.03	0.57
2:D:181:VAL:CG2	2:D:227:TRP:HZ2	2.16	0.57
2:D:181:VAL:HG23	2:D:227:TRP:CZ2	2.39	0.57
2:B:15:ILE:HD13	2:B:15:ILE:H	1.69	0.57
2:B:17:GLY:HA3	2:B:18:LEU:HG	1.86	0.57
2:B:445:PHE:C	2:B:445:PHE:CD1	2.78	0.57
2:D:361:TYR:CE2	2:D:362:LYS:HG3	2.40	0.57
2:D:453:GLU:HB3	2:D:485:ARG:HG2	1.87	0.57
2:D:51:TYR:CE1	2:D:128:GLU:HA	2.40	0.57
2:D:141:PRO:HB2	2:D:146:PHE:HB3	1.86	0.57
2:D:352:ASP:OD2	5:D:605:SAH:O3'	2.14	0.57
2:B:113:THR:CG2	2:B:115:VAL:HG13	2.34	0.57
2:B:341:VAL:HG12	2:B:341:VAL:O	2.03	0.57
2:B:447:TYR:HD1	2:B:447:TYR:C	2.08	0.57
2:D:501:MET:HG2	2:D:502:ILE:HD13	1.87	0.57
2:D:51:TYR:O	2:D:127:THR:HG22	2.05	0.57
1:A:42:VAL:HG12	1:A:72:SER:HB3	1.85	0.57
2:B:215:THR:HG22	2:B:216:CYS:SG	2.44	0.57
2:B:310:ARG:HG3	6:B:606:G3A:N13	2.20	0.57
2:B:158:PRO:HB2	2:B:160:ASN:OD1	2.03	0.56
2:B:520:TRP:O	2:B:523:PHE:HB2	2.05	0.56
1:A:126:TYR:N	1:A:127:GLY:CA	2.65	0.56
2:B:185:LEU:N	2:B:185:LEU:HD22	2.20	0.56
2:B:296:TYR:H	2:B:423:LYS:NZ	2.02	0.56
2:D:122:THR:HG1	2:D:159:TRP:HD1	1.51	0.56
2:D:163:ARG:HB3	2:D:234:ASP:O	2.05	0.56
2:B:86:TRP:CD1	2:B:182:VAL:HG21	2.41	0.56
1:C:19:PHE:O	2:D:201:ILE:N	2.32	0.56
2:B:217:PHE:CD2	2:B:224:TYR:CE1	2.93	0.56
2:B:227:TRP:CE3	2:B:227:TRP:HA	2.40	0.56
2:D:134:THR:OG1	2:D:135:ARG:N	2.37	0.56
2:D:181:VAL:N	2:D:227:TRP:HH2	2.04	0.56
2:D:428:THR:HG22	6:D:606:G3A:HN31	1.71	0.56
2:B:472:THR:HG23	2:B:472:THR:O	2.06	0.56
2:D:196:LYS:HG3	2:D:196:LYS:O	2.06	0.56
1:C:53:GLN:HB2	1:C:121:GLY:O	2.05	0.56
2:D:337:ALA:HB2	2:D:359:LYS:HD3	1.87	0.56
2:B:11:CYS:O	2:B:100:ALA:HB1	2.05	0.56
2:B:378:THR:OG1	2:B:379:ASP:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:292:TRP:HH2	5:D:605:SAH:H3'	1.69	0.56
2:B:358:ASP:O	2:B:359:LYS:HB2	2.05	0.56
1:C:44:MET:HA	2:D:39:CYS:O	2.05	0.56
1:C:47:THR:N	1:C:48:HIS:HA	2.20	0.56
2:D:181:VAL:CG2	2:D:227:TRP:CZ2	2.89	0.56
1:A:107:PRO:O	1:A:111:THR:HG23	2.07	0.55
2:B:215:THR:HG21	2:B:227:TRP:CZ3	2.41	0.55
2:B:406:LEU:HD13	2:B:407:SER:H	1.71	0.55
1:C:42:VAL:HG23	1:C:69:GLY:H	1.71	0.55
2:D:254:GLN:NE2	2:D:258:ASP:OD2	2.38	0.55
2:B:217:PHE:HD2	2:B:224:TYR:CE1	2.24	0.55
2:B:401:PHE:HD1	2:B:401:PHE:C	2.09	0.55
1:C:82:ASP:N	1:C:82:ASP:OD1	2.33	0.55
2:D:166:ILE:O	2:D:170:LEU:HB2	2.07	0.55
2:D:199:VAL:HG21	2:D:239:PRO:HG3	1.87	0.55
2:B:271:SER:OG	2:B:272:CYS:N	2.38	0.55
2:B:263:VAL:HG23	2:B:415:ASP:HB2	1.88	0.55
2:D:184:VAL:HG12	2:D:242:ILE:HG22	1.88	0.55
2:B:401:PHE:CD1	2:B:401:PHE:C	2.80	0.55
2:D:366:LEU:HD13	2:D:367:PHE:N	2.21	0.55
1:A:55:ILE:O	1:A:55:ILE:HD13	2.06	0.55
2:D:521:ASN:O	2:D:525:ARG:N	2.39	0.55
2:B:19:HIS:O	2:B:23:ALA:HB2	2.06	0.55
2:B:406:LEU:HD13	2:B:407:SER:N	2.22	0.55
1:A:53:GLN:HG2	1:A:122:MET:CE	2.37	0.55
2:B:445:PHE:O	2:B:445:PHE:HD1	1.90	0.55
2:B:481:GLY:N	2:B:482:ALA:HA	2.22	0.55
2:B:93:GLY:HA2	2:B:107:LEU:H	1.72	0.55
2:B:298:ILE:CG1	2:B:302:GLU:HB3	2.31	0.54
1:C:54:ALA:HB1	1:C:55:ILE:CG2	2.35	0.54
1:C:92:LEU:CD1	1:C:111:THR:HG21	2.34	0.54
2:D:257:HIS:CD2	2:D:276:MET:CG	2.89	0.54
2:D:336:LYS:HZ3	6:D:606:G3A:C23	2.11	0.54
5:D:605:SAH:OXT	6:D:606:G3A:C18	2.55	0.54
2:B:474:ILE:HG13	2:B:474:ILE:O	2.06	0.54
2:D:15:ILE:H	2:D:15:ILE:CD1	2.16	0.54
2:B:467:PRO:HB2	2:B:483:VAL:HG21	1.88	0.54
2:D:473:CYS:HB2	2:D:491:TYR:CD2	2.42	0.54
2:B:136:VAL:HG12	2:B:137:ASN:N	2.21	0.54
2:B:169:MET:SD	2:B:170:LEU:HD23	2.47	0.54
2:B:217:PHE:HD2	2:B:224:TYR:HE1	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:CYS:O	1:C:105:ASN:N	2.40	0.54
1:C:62:ASN:C	1:C:62:ASN:OD1	2.46	0.54
2:B:261:CYS:HA	2:B:415:ASP:HB3	1.88	0.54
2:B:384:PHE:O	2:B:398:VAL:HA	2.07	0.54
2:D:289:ARG:HD3	2:D:289:ARG:H	1.72	0.54
2:D:282:VAL:O	2:D:286:PHE:HB2	2.08	0.53
2:B:299:ILE:O	2:B:299:ILE:HD12	2.07	0.53
2:B:22:GLN:NE2	2:B:47:LYS:HB2	2.22	0.53
2:B:309:CYS:SG	2:B:501:MET:CE	2.96	0.53
2:B:403:THR:HG22	2:B:418:SER:OG	2.09	0.53
2:D:413:GLY:HA3	2:D:427:HIS:HE1	1.73	0.53
2:D:521:ASN:C	2:D:525:ARG:HE	2.12	0.53
2:D:517:TYR:HA	2:D:520:TRP:CD1	2.31	0.53
2:B:474:ILE:C	2:B:474:ILE:HD12	2.28	0.53
2:B:474:ILE:HA	2:B:520:TRP:CH2	2.43	0.53
1:A:62:ASN:HB3	1:A:64:ASP:H	1.74	0.53
2:B:31:ILE:H	2:B:31:ILE:HD13	1.74	0.53
2:B:80:ILE:HG23	2:B:286:PHE:HE1	1.74	0.53
1:C:71:ALA:HB2	1:C:93:LYS:HB2	1.91	0.53
2:B:5:THR:HB	2:B:6:GLY:CA	2.39	0.52
2:D:195:MET:HB3	2:D:199:VAL:CG1	2.39	0.52
2:D:519:LEU:O	2:D:522:THR:OG1	2.22	0.52
1:A:96:TYR:OH	2:B:41:ASP:HB2	2.10	0.52
2:B:168:GLN:HG3	2:B:169:MET:N	2.24	0.52
1:C:42:VAL:HG22	1:C:72:SER:OG	2.09	0.52
2:D:51:TYR:HE1	2:D:128:GLU:HA	1.75	0.52
2:B:215:THR:HG21	2:B:227:TRP:CH2	2.43	0.52
2:D:40:VAL:HG22	2:D:42:ILE:HG13	1.92	0.52
2:B:314:HIS:CE1	2:B:341:VAL:HG22	2.45	0.52
2:B:445:PHE:HE2	2:B:514:PHE:HZ	1.55	0.52
2:B:391:ARG:HD3	2:B:437:THR:CG2	2.39	0.52
2:B:392:TYR:CE2	2:B:436:PHE:HE1	2.27	0.52
2:D:317:VAL:O	2:D:321:LEU:HB2	2.09	0.52
2:D:406:LEU:HD22	2:D:406:LEU:N	2.25	0.52
2:D:522:THR:N	2:D:525:ARG:HE	2.07	0.52
2:D:310:ARG:HG3	6:D:606:G3A:N13	2.24	0.52
2:B:450:SER:HB2	2:B:476:ARG:NE	2.24	0.52
2:B:85:ALA:HB3	2:B:182:VAL:HG13	1.90	0.52
1:C:55:ILE:HD12	1:C:55:ILE:O	2.10	0.52
2:B:98:ARG:HB3	2:B:137:ASN:HD22	1.75	0.52
2:D:483:VAL:HG13	2:D:488:ALA:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASN:ND2	2:B:25:THR:HG1	2.05	0.52
2:B:261:CYS:HB2	2:B:414:CYS:HB2	1.91	0.52
2:D:465:TYR:C	2:D:467:PRO:HD2	2.30	0.52
2:D:97:THR:HG23	2:D:98:ARG:H	1.73	0.52
2:B:205:ARG:HG3	2:B:224:TYR:CE2	2.44	0.51
2:D:186:TRP:CE3	2:D:244:VAL:HG23	2.43	0.51
2:D:271:SER:O	2:D:274:ALA:N	2.43	0.51
2:D:466:VAL:N	2:D:467:PRO:CD	2.74	0.51
2:D:498:TYR:O	2:D:502:ILE:HG12	2.09	0.51
1:A:44:MET:HE2	1:A:96:TYR:CE2	2.43	0.51
2:B:336:LYS:HB2	2:B:338:ILE:CG1	2.40	0.51
2:B:7:LEU:O	2:B:8:PHE:HB2	2.09	0.51
2:D:124:TYR:CE1	2:D:133:PHE:HD1	2.28	0.51
2:D:186:TRP:CD1	2:D:253:LEU:HB3	2.46	0.51
2:D:26:HIS:O	2:D:29:VAL:HG23	2.10	0.51
2:B:205:ARG:HH11	2:B:224:TYR:HE2	1.59	0.51
2:D:200:LYS:O	2:D:237:TYR:O	2.27	0.51
1:C:98:GLN:C	1:C:99:ILE:HD12	2.31	0.51
2:D:18:LEU:HD13	2:D:23:ALA:HA	1.93	0.51
2:D:278:ARG:O	2:D:282:VAL:HG12	2.09	0.51
2:B:318:LYS:O	2:B:322:LEU:HD13	2.11	0.51
2:D:385:TRP:CZ3	2:D:399:CYS:HB2	2.45	0.51
2:B:84:ARG:CA	2:B:86:TRP:H	2.24	0.51
2:B:236:VAL:HG12	2:B:239:PRO:HD3	1.91	0.51
2:B:237:TYR:C	2:B:237:TYR:CD1	2.84	0.51
2:D:150:ILE:N	2:D:151:PRO:CD	2.73	0.51
2:D:361:TYR:CD2	2:D:362:LYS:HG3	2.46	0.51
2:B:174:LEU:HD23	2:B:180:ARG:O	2.11	0.50
2:B:69:TYR:HE1	2:B:203:PRO:HD3	1.75	0.50
2:D:522:THR:N	2:D:525:ARG:HH21	2.09	0.50
1:A:44:MET:HB2	1:A:67:SER:HB3	1.93	0.50
2:B:396:ALA:H	2:B:511:TYR:HB3	1.76	0.50
2:D:403:THR:HB	2:D:418:SER:HB2	1.93	0.50
2:B:182:VAL:HA	2:B:240:PHE:O	2.12	0.50
2:B:286:PHE:HD2	2:B:419:LEU:CD1	2.19	0.50
2:B:119:ALA:HA	2:B:157:LEU:H	1.77	0.50
2:B:294:VAL:HG23	2:B:294:VAL:O	2.11	0.50
2:B:477:CYS:O	2:B:482:ALA:HB3	2.10	0.50
2:B:5:THR:HB	2:B:6:GLY:C	2.30	0.50
1:C:19:PHE:CE1	2:D:196:LYS:HA	2.46	0.50
2:B:120:VAL:O	2:B:122:THR:CG2	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:ALA:O	2:B:269:VAL:N	2.44	0.50
1:C:16:PHE:HE2	1:C:26:ALA:HB1	1.73	0.50
2:D:260:HIS:NE2	2:D:283:HIS:HE1	2.08	0.50
5:D:605:SAH:OXT	6:D:606:G3A:H22	2.11	0.50
2:D:82:HIS:CD2	2:D:180:ARG:CD	2.85	0.50
2:B:475:THR:O	2:B:523:PHE:HE2	1.93	0.50
2:B:88:GLY:O	2:B:111:PHE:HA	2.12	0.50
1:C:62:ASN:OD1	1:C:64:ASP:N	2.43	0.50
2:D:149:LEU:HA	2:D:152:LEU:HD13	1.94	0.50
2:D:368:TYR:OH	2:D:393:PRO:HG3	2.11	0.50
2:D:384:PHE:HB2	2:D:398:VAL:HG23	1.94	0.50
2:B:83:VAL:HG11	2:B:286:PHE:HE2	1.77	0.50
2:D:521:ASN:O	2:D:525:ARG:HB2	2.12	0.50
2:B:163:ARG:NH2	2:B:235:TYR:OH	2.40	0.49
2:B:286:PHE:CD2	2:B:419:LEU:CD1	2.95	0.49
2:D:151:PRO:HG2	2:D:152:LEU:HD12	1.94	0.49
2:D:508:LEU:N	2:D:508:LEU:HD22	2.27	0.49
2:B:186:TRP:CG	2:B:253:LEU:HB2	2.47	0.49
2:B:18:LEU:HD21	2:B:53:ARG:NE	2.28	0.49
2:B:88:GLY:C	2:B:274:ALA:HB1	2.33	0.49
2:D:335:PRO:HG3	5:D:605:SAH:O3'	2.12	0.49
1:A:73:CYS:O	1:A:111:THR:HG21	2.11	0.49
2:B:14:ILE:HG22	2:B:15:ILE:O	2.12	0.49
1:A:21:VAL:CG1	2:B:200:LYS:HG2	2.43	0.49
1:C:120:CYS:HB2	1:C:121:GLY:CA	2.43	0.49
2:D:113:THR:HB	2:D:115:VAL:HG12	1.93	0.49
2:B:164:ILE:HD11	2:B:232:GLY:C	2.33	0.49
2:B:491:TYR:C	2:B:491:TYR:CD1	2.86	0.49
2:D:292:TRP:HH2	5:D:605:SAH:C3'	2.26	0.49
2:B:15:ILE:N	2:B:15:ILE:HD13	2.27	0.49
2:B:218:SER:HB2	2:B:233:PHE:CD1	2.47	0.49
2:B:5:THR:HG21	2:B:7:LEU:HB2	1.94	0.49
2:D:201:ILE:HG12	2:D:202:GLY:H	1.78	0.49
2:B:185:LEU:HD22	2:B:242:ILE:O	2.12	0.49
2:B:278:ARG:O	2:B:281:ALA:HB3	2.12	0.49
2:D:111:PHE:O	2:D:113:THR:O	2.29	0.49
1:A:117:CYS:SG	1:A:119:VAL:HB	2.53	0.49
1:A:99:ILE:HG21	1:A:104:ALA:HA	1.94	0.49
1:A:20:ALA:HA	2:B:201:ILE:HG22	1.94	0.49
2:B:521:ASN:N	2:B:521:ASN:OD1	2.46	0.49
1:C:58:THR:OG1	1:C:59:PRO:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:18:LEU:HD21	2:D:53:ARG:NE	2.28	0.49
1:A:123:TRP:HA	1:A:123:TRP:CE3	2.47	0.48
2:B:147:LYS:C	2:B:147:LYS:HD2	2.34	0.48
2:B:442:LEU:HD23	2:B:510:ILE:HB	1.94	0.48
1:C:42:VAL:O	1:C:42:VAL:HG23	2.13	0.48
2:D:313:GLN:HB2	2:D:385:TRP:CZ2	2.48	0.48
2:D:312:VAL:O	2:D:316:VAL:HG22	2.13	0.48
2:B:192:LEU:O	2:B:192:LEU:HD23	2.14	0.48
1:C:79:CYS:HB2	1:C:81:ILE:HD13	1.95	0.48
2:D:257:HIS:O	2:D:260:HIS:N	2.40	0.48
2:D:468:LEU:CD2	2:D:483:VAL:HG11	2.28	0.48
2:B:249:PHE:HB3	2:B:256:ASN:HD21	1.75	0.48
2:B:300:GLY:O	2:B:301:ASP:OD1	2.30	0.48
2:B:31:ILE:CD1	2:B:31:ILE:H	2.27	0.48
6:B:606:G3A:N16	6:B:606:G3A:H42	2.29	0.48
1:C:57:VAL:HG23	1:C:95:LYS:HE3	1.94	0.48
2:D:287:VAL:HG22	2:D:427:HIS:CD2	2.49	0.48
2:B:444:PHE:CE2	2:B:495:LEU:HD12	2.48	0.48
2:B:8:PHE:HA	2:B:55:ILE:HG22	1.95	0.48
2:B:401:PHE:CE2	2:B:420:TYR:CD1	3.01	0.48
1:C:55:ILE:CG2	1:C:97:VAL:HA	2.38	0.48
2:D:260:HIS:NE2	2:D:283:HIS:CE1	2.81	0.48
2:D:27:LEU:CD2	2:D:27:LEU:N	2.74	0.48
2:D:309:CYS:SG	2:D:501:MET:CE	3.02	0.48
2:D:317:VAL:HG13	2:D:341:VAL:HG21	1.95	0.48
2:D:384:PHE:HE2	2:D:393:PRO:HD2	1.78	0.48
1:A:13:VAL:HG22	1:A:30:TYR:CZ	2.49	0.48
1:A:21:VAL:HG13	2:B:200:LYS:HG2	1.95	0.48
2:B:295:GLU:HA	2:B:423:LYS:CE	2.43	0.48
2:D:7:LEU:HD23	2:D:59:GLY:O	2.13	0.48
1:C:8:PRO:HG3	2:D:5:THR:CG2	2.42	0.48
2:B:423:LYS:CE	2:B:424:HIS:N	2.73	0.48
2:D:91:VAL:HG23	2:D:191:GLU:HG3	1.96	0.48
2:D:62:MET:HB2	2:D:64:TYR:CD1	2.49	0.48
2:B:428:THR:HG21	6:B:606:G3A:N32	2.29	0.48
2:B:62:MET:HB2	2:B:64:TYR:HE1	1.79	0.48
1:C:16:PHE:CZ	2:D:66:VAL:HG11	2.49	0.48
2:B:11:CYS:SG	2:B:103:THR:HB	2.54	0.47
1:C:25:LYS:HE2	1:C:29:ASP:OD2	2.15	0.47
2:D:370:TYR:HE2	2:D:391:ARG:NH2	2.00	0.47
2:D:264:HIS:CD2	2:D:264:HIS:O	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:VAL:O	2:B:171:SER:HB2	2.14	0.47
2:B:218:SER:HB2	2:B:233:PHE:CG	2.50	0.47
2:B:415:ASP:OD1	2:B:415:ASP:O	2.33	0.47
2:B:352:ASP:OD1	5:B:605:SAH:H1'	2.14	0.47
1:A:87:LYS:HA	1:A:88:GLY:HA2	1.64	0.47
1:C:10:ASN:ND2	1:C:38:ILE:HG23	2.30	0.47
2:D:336:LYS:HZ3	6:D:606:G3A:C25	2.25	0.47
2:D:18:LEU:HD21	2:D:53:ARG:HE	1.79	0.47
1:A:37:PRO:HB3	1:A:106:ASP:OD1	2.14	0.47
2:D:180:ARG:C	2:D:227:TRP:CH2	2.82	0.47
2:D:19:HIS:HB2	2:D:47:LYS:HA	1.97	0.47
2:B:286:PHE:CD1	2:B:286:PHE:N	2.78	0.47
2:B:308:ALA:CB	2:B:497:ALA:HB1	2.45	0.47
2:B:120:VAL:O	2:B:122:THR:HG22	2.14	0.47
2:B:426:PHE:CE2	6:B:606:G3A:H452	2.49	0.47
2:B:452:CYS:SG	2:B:487:HIS:CD2	2.98	0.47
2:B:7:LEU:HD23	2:B:58:MET:O	2.15	0.47
6:B:606:G3A:C38	6:B:606:G3A:H452	2.45	0.47
5:B:605:SAH:O	6:B:606:G3A:H22	2.15	0.47
1:C:15:SER:HB2	2:D:62:MET:HE1	1.97	0.47
2:D:317:VAL:CG1	2:D:341:VAL:HG23	2.44	0.47
2:D:398:VAL:CG1	2:D:509:TRP:HB2	2.45	0.47
2:D:400:ARG:HG2	2:D:400:ARG:HH11	1.79	0.47
2:B:327:PRO:O	2:B:346:VAL:HG23	2.15	0.46
2:D:384:PHE:CD2	2:D:392:TYR:CD1	3.03	0.46
2:D:519:LEU:HD13	2:D:519:LEU:HA	1.80	0.46
2:D:58:MET:HA	2:D:193:THR:OG1	2.15	0.46
1:C:117:CYS:HB2	1:C:124:LYS:HD3	1.97	0.46
2:B:49:MET:HE3	2:B:49:MET:H	1.75	0.46
1:C:87:LYS:HD2	1:C:87:LYS:HA	1.47	0.46
1:A:47:THR:O	1:A:48:HIS:HB2	2.16	0.46
2:D:186:TRP:HH2	2:D:249:PHE:CD2	2.33	0.46
2:D:334:ASN:O	2:D:334:ASN:ND2	2.48	0.46
2:B:175:LYS:HA	2:B:227:TRP:HB3	1.98	0.46
1:C:7:VAL:HG22	1:C:8:PRO:HD2	1.97	0.46
2:D:122:THR:OG1	2:D:159:TRP:CD1	2.68	0.46
1:C:5:THR:HG23	1:C:5:THR:O	2.15	0.46
2:D:283:HIS:CD2	2:D:287:VAL:HB	2.51	0.46
2:B:296:TYR:HE2	2:B:425:ALA:H	1.64	0.46
2:D:95:HIS:O	2:D:139:LYS:N	2.43	0.46
2:B:481:GLY:N	2:B:482:ALA:CA	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ALA:HA	1:C:55:ILE:HA	1.61	0.46
1:C:56:THR:CG2	1:C:60:GLU:HG3	2.38	0.46
2:D:289:ARG:HB2	2:D:354:GLN:HG3	1.97	0.46
2:D:314:HIS:CG	2:D:314:HIS:O	2.69	0.46
2:B:166:ILE:HG22	2:B:167:VAL:N	2.30	0.46
2:B:479:LEU:HD22	2:B:479:LEU:O	2.16	0.46
1:C:70:GLY:N	1:C:95:LYS:O	2.48	0.46
2:D:82:HIS:HD2	2:D:180:ARG:CD	2.23	0.46
1:A:3:ASN:O	2:B:10:ASP:N	2.44	0.45
2:B:29:VAL:HG21	2:B:39:CYS:SG	2.56	0.45
2:B:310:ARG:HH22	6:B:606:G3A:PA	2.39	0.45
2:D:76:ARG:HD3	2:D:247:TRP:CE2	2.51	0.45
2:B:315:MET:HG2	2:B:494:TYR:OH	2.17	0.45
2:B:352:ASP:OD2	2:B:354:GLN:N	2.41	0.45
2:B:441:GLN:HG3	2:B:509:TRP:CH2	2.51	0.45
2:D:215:THR:N	2:D:225:ALA:O	2.50	0.45
2:D:298:ILE:HA	2:D:302:GLU:OE1	2.15	0.45
2:B:101:VAL:HG12	2:B:102:GLY:H	1.81	0.45
2:B:136:VAL:CG1	2:B:137:ASN:N	2.80	0.45
2:B:215:THR:HG21	2:B:227:TRP:CE3	2.51	0.45
2:B:17:GLY:HA2	2:B:53:ARG:NH2	2.32	0.45
2:D:331:ASP:HA	2:D:383:LEU:HD23	1.98	0.45
2:D:337:ALA:CB	2:D:359:LYS:HD3	2.47	0.45
2:D:400:ARG:HG2	2:D:400:ARG:NH1	2.31	0.45
1:A:21:VAL:HG13	2:B:200:LYS:HB3	1.98	0.45
1:A:57:VAL:HG13	1:A:58:THR:HG23	1.97	0.45
2:B:296:TYR:H	2:B:423:LYS:HZ1	1.64	0.45
6:B:606:G3A:H18	6:B:606:G3A:H23	1.98	0.45
2:D:264:HIS:HD2	2:D:264:HIS:O	1.99	0.45
2:D:421:VAL:HA	2:D:425:ALA:HA	1.98	0.45
2:B:299:ILE:HA	2:B:300:GLY:HA2	1.77	0.45
2:D:122:THR:OG1	2:D:159:TRP:HD1	2.00	0.45
2:D:192:LEU:HD23	2:D:192:LEU:O	2.16	0.45
1:C:19:PHE:C	2:D:201:ILE:HG22	2.37	0.45
2:D:50:THR:HA	2:D:128:GLU:HG3	1.96	0.45
1:A:43:LYS:HE3	1:A:66:GLU:OE1	2.16	0.45
2:B:339:LYS:HE3	2:B:348:TRP:CB	2.47	0.45
2:D:200:LYS:HD2	2:D:235:TYR:CE2	2.52	0.45
2:D:289:ARG:CD	2:D:289:ARG:H	2.29	0.45
2:D:441:GLN:HB2	2:D:509:TRP:CZ3	2.52	0.45
2:B:253:LEU:HD23	2:B:254:GLN:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:GLN:HE22	2:B:47:LYS:HB2	1.82	0.45
2:B:83:VAL:HG21	2:B:286:PHE:CE2	2.51	0.45
2:D:392:TYR:CE1	2:D:398:VAL:HG21	2.52	0.45
2:D:450:SER:O	2:D:487:HIS:NE2	2.47	0.45
1:A:65:GLN:HE21	1:A:98:GLN:CB	2.30	0.45
2:B:30:ASP:OD2	2:B:32:LYS:HG3	2.17	0.45
1:A:96:TYR:CZ	2:B:41:ASP:HB2	2.52	0.45
1:C:10:ASN:HD21	1:C:38:ILE:HG23	1.81	0.45
1:C:16:PHE:CD1	2:D:64:TYR:CG	3.05	0.45
5:B:605:SAH:OXT	6:B:606:G3A:C18	2.59	0.45
1:C:15:SER:HB3	2:D:60:PHE:HD1	1.81	0.45
2:D:249:PHE:HZ	2:D:284:GLU:HG3	1.82	0.45
1:A:22:ASP:OD1	1:A:25:LYS:CB	2.65	0.44
2:D:162:VAL:O	2:D:166:ILE:HG13	2.17	0.44
1:A:42:VAL:HG12	1:A:72:SER:CB	2.47	0.44
1:A:79:CYS:HB2	1:A:81:ILE:HD13	1.99	0.44
2:B:69:TYR:CE1	2:B:203:PRO:HD3	2.51	0.44
2:B:476:ARG:HH11	2:B:487:HIS:CD2	2.34	0.44
2:D:163:ARG:HD3	2:D:198:PHE:HA	1.99	0.44
2:B:198:PHE:CE1	2:B:199:VAL:HG23	2.53	0.44
2:B:229:HIS:N	2:B:229:HIS:ND1	2.64	0.44
2:B:307:SER:OG	2:B:308:ALA:N	2.51	0.44
1:C:123:TRP:HA	1:C:123:TRP:CE3	2.53	0.44
2:D:122:THR:HG22	2:D:135:ARG:HA	1.99	0.44
2:D:129:ASN:OD1	2:D:129:ASN:N	2.50	0.44
2:D:194:SER:O	2:D:197:TYR:HB2	2.17	0.44
2:B:146:PHE:O	2:B:149:LEU:HB2	2.17	0.44
2:B:204:GLU:OE2	2:B:204:GLU:HA	2.18	0.44
2:B:17:GLY:CA	2:B:53:ARG:NH2	2.81	0.44
1:C:43:LYS:HE2	1:C:66:GLU:HG2	1.99	0.44
2:D:17:GLY:HA2	2:D:18:LEU:HA	1.65	0.44
2:D:219:THR:HG23	2:D:234:ASP:OD2	2.18	0.44
6:D:606:G3A:H22	6:D:606:G3A:H18	1.80	0.44
1:A:33:SER:OG	2:B:66:VAL:HA	2.17	0.44
2:B:329:LEU:HD22	2:B:348:TRP:CE2	2.53	0.44
2:D:278:ARG:O	2:D:281:ALA:HB3	2.17	0.44
2:D:341:VAL:HG12	2:D:341:VAL:O	2.17	0.44
2:B:256:ASN:O	2:B:259:GLN:HB2	2.17	0.44
2:B:305:VAL:O	2:B:309:CYS:HB2	2.17	0.44
2:B:510:ILE:HG13	2:B:511:TYR:CD1	2.53	0.44
2:B:80:ILE:HG12	2:B:80:ILE:H	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:THR:HG23	2:D:78:GLU:HB3	2.00	0.44
2:B:9:LYS:HE3	2:B:102:GLY:O	2.18	0.43
2:D:522:THR:HA	2:D:525:ARG:HE	1.82	0.43
2:B:86:TRP:CD1	2:B:182:VAL:CG2	3.01	0.43
2:B:414:CYS:HA	2:B:415:ASP:HA	1.66	0.43
2:D:115:VAL:HG11	2:D:169:MET:SD	2.58	0.43
2:D:57:MET:HB3	2:D:193:THR:HG23	1.99	0.43
2:B:170:LEU:HB3	2:B:227:TRP:CH2	2.52	0.43
2:B:255:SER:OG	2:B:256:ASN:N	2.51	0.43
5:B:605:SAH:C	6:B:606:G3A:C18	2.96	0.43
1:A:16:PHE:CE1	2:B:64:TYR:CE2	3.06	0.43
2:D:169:MET:CE	2:D:170:LEU:HD13	2.46	0.43
2:B:168:GLN:CG	2:B:169:MET:N	2.81	0.43
2:B:88:GLY:HA3	2:B:274:ALA:O	2.19	0.43
2:D:385:TRP:CE3	2:D:399:CYS:HB2	2.54	0.43
1:C:16:PHE:HD1	2:D:64:TYR:CG	2.36	0.43
1:A:45:LEU:HD12	1:A:46:CYS:N	2.34	0.43
2:B:32:LYS:HD2	2:B:45:ILE:HD12	2.00	0.43
2:B:76:ARG:HD3	2:B:247:TRP:CE2	2.53	0.43
1:C:120:CYS:N	1:C:121:GLY:HA2	2.33	0.43
2:D:98:ARG:HG3	2:D:99:ASP:N	2.34	0.43
1:A:94:GLY:O	2:B:47:LYS:NZ	2.51	0.43
2:B:423:LYS:CE	2:B:423:LYS:HA	2.36	0.43
2:B:18:LEU:HD21	2:B:53:ARG:HE	1.82	0.43
1:C:10:ASN:HB3	1:C:14:LEU:HD11	2.00	0.43
2:D:385:TRP:HB3	5:D:605:SAH:N	2.34	0.43
1:A:76:TYR:HD2	1:A:82:ASP:O	2.01	0.43
1:C:58:THR:O	1:C:60:GLU:HG2	2.18	0.43
2:D:148:HIS:ND1	2:D:148:HIS:C	2.71	0.43
2:D:361:TYR:CE2	2:D:362:LYS:HE3	2.54	0.43
2:D:385:TRP:HB3	5:D:605:SAH:HN2	1.82	0.43
2:B:401:PHE:CB	6:B:606:G3A:N32	2.82	0.43
2:B:261:CYS:CA	2:B:415:ASP:HB3	2.49	0.43
2:B:445:PHE:O	2:B:445:PHE:CD1	2.70	0.43
2:B:473:CYS:HB3	2:B:491:TYR:CD2	2.53	0.43
2:D:143:GLY:HA2	2:D:147:LYS:CG	2.49	0.43
2:D:296:TYR:CD1	2:D:296:TYR:N	2.86	0.43
2:D:332:ILE:HG21	2:D:384:PHE:HE1	1.83	0.43
1:A:30:TYR:CE1	1:A:35:GLY:HA3	2.54	0.43
2:B:80:ILE:HG23	2:B:286:PHE:CZ	2.54	0.43
2:B:438:ASN:O	2:B:512:LYS:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:381:VAL:HG22	2:D:382:CYS:N	2.33	0.43
2:D:477:CYS:HB2	2:D:484:CYS:CB	2.47	0.43
1:A:106:ASP:OD2	1:A:109:GLY:HA3	2.18	0.43
2:B:310:ARG:NH2	6:B:606:G3A:O1	2.51	0.43
2:B:361:TYR:CE2	2:B:362:LYS:HG3	2.54	0.43
2:D:336:LYS:HD3	6:D:606:G3A:O23	2.19	0.43
2:B:295:GLU:CA	2:B:423:LYS:NZ	2.73	0.42
1:C:68:PHE:HB2	1:C:73:CYS:SG	2.59	0.42
1:A:44:MET:HE1	2:B:20:PRO:CB	2.47	0.42
2:B:172:ASP:C	2:B:172:ASP:OD1	2.58	0.42
2:B:475:THR:OG1	2:B:476:ARG:N	2.51	0.42
1:C:15:SER:HB2	2:D:62:MET:CE	2.49	0.42
2:D:257:HIS:CG	2:D:276:MET:HG2	2.54	0.42
2:B:352:ASP:OD1	5:B:605:SAH:O3'	2.35	0.42
2:D:259:GLN:OE1	2:D:260:HIS:CD2	2.72	0.42
2:D:465:TYR:CB	2:D:467:PRO:HD2	2.50	0.42
2:D:473:CYS:HB2	2:D:491:TYR:CE2	2.54	0.42
2:B:480:GLY:C	2:B:482:ALA:HB2	2.40	0.42
1:A:15:SER:OG	2:B:60:PHE:HD1	2.02	0.42
2:D:25:THR:CG2	2:D:28:SER:HB2	2.48	0.42
2:D:329:LEU:HD23	2:D:381:VAL:HG13	2.01	0.42
2:D:329:LEU:HD21	2:D:383:LEU:HD22	2.02	0.42
2:B:395:ASN:CG	2:B:395:ASN:O	2.57	0.42
1:C:40:ASN:ND2	2:D:25:THR:HG1	2.17	0.42
2:D:109:LEU:O	2:D:116:ASN:HA	2.20	0.42
2:D:259:GLN:C	2:D:259:GLN:OE1	2.58	0.42
2:D:331:ASP:CB	2:D:350:PHE:HB3	2.43	0.42
2:D:42:ILE:HG22	2:D:43:PRO:O	2.20	0.42
2:D:510:ILE:HG13	2:D:511:TYR:N	2.34	0.42
2:D:60:PHE:HB3	2:D:62:MET:CE	2.50	0.42
2:B:346:VAL:HG22	2:B:347:GLU:O	2.20	0.42
2:D:52:ARG:HA	2:D:126:ASP:O	2.19	0.42
2:B:192:LEU:O	2:B:195:MET:HB2	2.20	0.42
2:B:423:LYS:O	2:B:424:HIS:HB2	2.20	0.42
2:D:302:GLU:HB3	2:D:422:ASN:OD1	2.19	0.42
2:B:204:GLU:OE2	2:B:213:ARG:NH1	2.52	0.42
2:B:5:THR:HB	2:B:6:GLY:HA2	2.01	0.42
2:D:244:VAL:HG12	2:D:247:TRP:CZ3	2.55	0.42
2:B:2:GLU:HG3	2:B:3:ASN:N	2.35	0.41
2:B:445:PHE:C	2:B:445:PHE:HD1	2.21	0.41
2:D:309:CYS:CA	2:D:501:MET:HE3	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:292:TRP:CH2	5:D:605:SAH:H3'	2.52	0.41
1:A:93:LYS:NZ	2:B:127:THR:O	2.37	0.41
2:B:159:TRP:O	2:B:163:ARG:HD2	2.19	0.41
2:B:215:THR:HG21	2:B:227:TRP:CZ2	2.55	0.41
2:B:26:HIS:O	2:B:29:VAL:HG22	2.21	0.41
2:D:113:THR:HB	2:D:115:VAL:CG1	2.50	0.41
2:D:301:ASP:OD1	2:D:301:ASP:O	2.37	0.41
2:D:392:TYR:O	2:D:438:ASN:OD1	2.38	0.41
5:B:605:SAH:C	6:B:606:G3A:H18	2.48	0.41
2:B:63:ASN:OD1	2:B:63:ASN:N	2.53	0.41
2:D:485:ARG:HE	2:D:485:ARG:HA	1.85	0.41
1:A:5:THR:HG23	1:A:6:GLU:HG2	2.03	0.41
1:A:76:TYR:CD1	1:A:76:TYR:N	2.88	0.41
2:B:73:PHE:CZ	2:B:241:MET:HG3	2.56	0.41
2:B:337:ALA:HA	2:B:350:PHE:CE2	2.55	0.41
1:A:80:HIS:CE1	2:B:55:ILE:HG21	2.55	0.41
2:D:420:TYR:CE2	2:D:422:ASN:HB2	2.56	0.41
2:D:485:ARG:HE	2:D:485:ARG:C	2.23	0.41
1:A:62:ASN:HB2	1:A:65:GLN:H	1.86	0.41
2:B:209:LEU:O	2:B:210:CYS:SG	2.79	0.41
2:B:237:TYR:O	2:B:237:TYR:CD1	2.73	0.41
2:B:62:MET:H	2:B:62:MET:HG2	1.77	0.41
2:D:149:LEU:O	2:D:152:LEU:HB2	2.20	0.41
2:D:257:HIS:NE2	2:D:261:CYS:HB3	2.35	0.41
2:D:296:TYR:HA	2:D:297:PRO:HD3	1.82	0.41
2:D:384:PHE:CD2	2:D:392:TYR:HD1	2.39	0.41
2:D:485:ARG:CG	2:D:486:HIS:N	2.77	0.41
2:D:56:SER:OG	2:D:58:MET:HG3	2.20	0.41
2:B:271:SER:O	2:B:274:ALA:N	2.52	0.41
2:B:468:LEU:H	2:B:468:LEU:HD23	1.85	0.41
2:B:483:VAL:HG23	2:B:483:VAL:O	2.20	0.41
2:B:484:CYS:O	2:B:486:HIS:N	2.54	0.41
2:D:144:ASP:OD2	2:D:145:GLN:NE2	2.54	0.41
2:D:326:PHE:HA	2:D:327:PRO:HD3	1.79	0.41
2:B:340:CYS:HG	2:B:348:TRP:HH2	1.65	0.41
2:B:261:CYS:CB	2:B:415:ASP:HB3	2.51	0.41
2:B:473:CYS:O	2:B:475:THR:HG22	2.20	0.41
1:C:31:LEU:HD23	1:C:35:GLY:O	2.21	0.41
2:D:186:TRP:CE2	2:D:253:LEU:HB3	2.55	0.41
2:D:423:LYS:O	2:D:424:HIS:C	2.59	0.41
2:D:428:THR:HA	2:D:429:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:HD12	1:A:46:CYS:H	1.86	0.41
2:B:308:ALA:HB1	2:B:497:ALA:O	2.20	0.41
2:B:447:TYR:HA	2:B:474:ILE:HG13	2.03	0.41
2:B:513:GLN:H	2:B:513:GLN:HG2	1.51	0.41
2:D:107:LEU:O	2:D:118:VAL:HA	2.21	0.41
2:D:260:HIS:CG	2:D:283:HIS:CE1	3.08	0.41
1:A:25:LYS:HZ2	1:A:29:ASP:CG	2.23	0.41
2:B:198:PHE:HD1	2:B:199:VAL:HG23	1.78	0.41
2:D:403:THR:HG22	2:D:428:THR:OG1	2.21	0.41
2:D:87:ILE:HD12	2:D:170:LEU:CD1	2.51	0.41
2:B:296:TYR:N	2:B:423:LYS:HZ1	2.19	0.40
2:B:512:LYS:HB3	2:B:512:LYS:HE3	1.67	0.40
1:C:40:ASN:HD22	2:D:25:THR:HG1	1.69	0.40
2:D:30:ASP:OD2	2:D:32:LYS:HD2	2.21	0.40
2:D:351:TYR:HA	2:D:363:ILE:HG23	2.03	0.40
1:A:71:ALA:CB	1:A:93:LYS:HG3	2.48	0.40
2:B:298:ILE:HD12	2:B:299:ILE:N	2.36	0.40
2:B:337:ALA:CB	2:B:362:LYS:HD3	2.48	0.40
2:B:446:TYR:CE1	2:B:448:SER:HB2	2.56	0.40
2:D:108:GLN:HG2	2:D:270:ALA:HB2	2.03	0.40
2:D:185:LEU:N	2:D:185:LEU:CD2	2.81	0.40
2:B:337:ALA:O	2:B:350:PHE:CZ	2.75	0.40
2:B:476:ARG:HH12	2:B:486:HIS:CE1	2.35	0.40
2:B:308:ALA:HB1	2:B:497:ALA:HB1	2.03	0.40
2:D:260:HIS:CG	2:D:283:HIS:ND1	2.89	0.40
2:B:159:TRP:CE2	2:B:197:TYR:CD2	3.10	0.40
1:A:44:MET:HE3	1:A:96:TYR:HE2	1.86	0.40
2:B:217:PHE:CE2	2:B:224:TYR:HE1	2.40	0.40
2:B:334:ASN:O	2:B:363:ILE:HD13	2.22	0.40
2:B:33:PHE:N	2:B:33:PHE:CD1	2.89	0.40
2:B:398:VAL:CG1	2:B:509:TRP:HB2	2.51	0.40
2:D:424:HIS:N	2:D:424:HIS:ND1	2.70	0.40
2:D:316:VAL:HG12	2:D:442:LEU:HD11	2.02	0.40
2:D:522:THR:H	2:D:525:ARG:HH21	1.69	0.40
2:D:428:THR:CG2	6:D:606:G3A:HN31	2.34	0.40

There are no symmetry-related clashes.

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	131/144 (91%)	126 (96%)	5 (4%)	0	100 100
1	C	131/144 (91%)	127 (97%)	4 (3%)	0	100 100
2	B	510/527 (97%)	490 (96%)	17 (3%)	3 (1%)	25 57
2	D	510/527 (97%)	484 (95%)	26 (5%)	0	100 100
All	All	1282/1342 (96%)	1227 (96%)	52 (4%)	3 (0%)	47 76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	337	ALA
2	B	338	ILE
2	B	389	VAL

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	107/117 (92%)	90 (84%)	17 (16%)	2 11
1	C	107/117 (92%)	82 (77%)	25 (23%)	1 3
2	B	451/463 (97%)	371 (82%)	80 (18%)	2 8
2	D	451/463 (97%)	364 (81%)	87 (19%)	1 6
All	All	1116/1160 (96%)	907 (81%)	209 (19%)	1 7

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	7	VAL
1	A	11	SER
1	A	21	VAL
1	A	42	VAL
1	A	47	THR
1	A	48	HIS
1	A	51	THR
1	A	55	ILE
1	A	63	MET
1	A	67	SER
1	A	81	ILE
1	A	82	ASP
1	A	103	CYS
1	A	108	VAL
1	A	118	THR
1	A	123	TRP
2	B	5	THR
2	B	15	ILE
2	B	27	LEU
2	B	31	ILE
2	B	40	VAL
2	B	48	ASP
2	B	49	MET
2	B	60	PHE
2	B	62	MET
2	B	72	MET
2	B	84	ARG
2	B	97	THR
2	B	109	LEU
2	B	115	VAL
2	B	122	THR
2	B	129	ASN
2	B	134	THR
2	B	135	ARG
2	B	147	LYS
2	B	163	ARG
2	B	164	ILE
2	B	170	LEU
2	B	171	SER
2	B	182	VAL
2	B	185	LEU
2	B	200	LYS

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Mol	Chain	Res	Type
2	B	201	ILE
2	B	212	LYS
2	B	213	ARG
2	B	219	THR
2	B	226	CYS
2	B	227	TRP
2	B	229	HIS
2	B	230	SER
2	B	231	VAL
2	B	246	GLN
2	B	262	GLN
2	B	273	ASP
2	B	279	CYS
2	B	284	GLU
2	B	289	ARG
2	B	290	VAL
2	B	292	TRP
2	B	301	ASP
2	B	302	GLU
2	B	303	LEU
2	B	316	VAL
2	B	336	LYS
2	B	343	GLN
2	B	372	THR
2	B	388	ASN
2	B	389	VAL
2	B	391	ARG
2	B	400	ARG
2	B	401	PHE
2	B	403	THR
2	B	406	LEU
2	B	410	ASN
2	B	422	ASN
2	B	423	LYS
2	B	428	THR
2	B	434	SER
2	B	437	THR
2	B	445	PHE
2	B	447	TYR
2	B	452	CYS
2	B	469	LYS
2	B	474	ILE

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Mol	Chain	Res	Type
2	B	475	THR
2	B	477	CYS
2	B	479	LEU
2	B	487	HIS
2	B	495	LEU
2	B	501	MET
2	B	510	ILE
2	B	512	LYS
2	B	513	GLN
2	B	521	ASN
2	B	524	THR
2	B	525	ARG
1	C	5	THR
1	C	7	VAL
1	C	21	VAL
1	C	25	LYS
1	C	36	GLN
1	C	39	THR
1	C	41	CYS
1	C	47	THR
1	C	49	THR
1	C	53	GLN
1	C	57	VAL
1	C	60	GLU
1	C	62	ASN
1	C	67	SER
1	C	74	CYS
1	C	81	ILE
1	C	82	ASP
1	C	87	LYS
1	C	91	ASP
1	C	93	LYS
1	C	102	THR
1	C	108	VAL
1	C	113	ARG
1	C	116	VAL
1	C	124	LYS
2	D	15	ILE
2	D	18	LEU
2	D	27	LEU
2	D	31	ILE
2	D	40	VAL

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Mol	Chain	Res	Type
2	D	48	ASP
2	D	50	THR
2	D	57	MET
2	D	63	ASN
2	D	66	VAL
2	D	71	ASN
2	D	72	MET
2	D	74	ILE
2	D	75	THR
2	D	76	ARG
2	D	99	ASP
2	D	109	LEU
2	D	113	THR
2	D	115	VAL
2	D	120	VAL
2	D	127	THR
2	D	129	ASN
2	D	145	GLN
2	D	148	HIS
2	D	150	ILE
2	D	153	MET
2	D	155	LYS
2	D	165	LYS
2	D	170	LEU
2	D	174	LEU
2	D	185	LEU
2	D	196	LYS
2	D	199	VAL
2	D	201	ILE
2	D	209	LEU
2	D	212	LYS
2	D	216	CYS
2	D	222	ASP
2	D	241	MET
2	D	244	VAL
2	D	253	LEU
2	D	255	SER
2	D	262	GLN
2	D	271	SER
2	D	272	CYS
2	D	273	ASP
2	D	278	ARG

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Mol	Chain	Res	Type
2	D	280	LEU
2	D	285	CYS
2	D	289	ARG
2	D	303	LEU
2	D	307	SER
2	D	316	VAL
2	D	321	LEU
2	D	329	LEU
2	D	345	GLU
2	D	350	PHE
2	D	351	TYR
2	D	356	CYS
2	D	365	GLU
2	D	376	LYS
2	D	378	THR
2	D	379	ASP
2	D	387	CYS
2	D	400	ARG
2	D	406	LEU
2	D	409	LEU
2	D	423	LYS
2	D	424	HIS
2	D	428	THR
2	D	431	PHE
2	D	439	LEU
2	D	465	TYR
2	D	468	LEU
2	D	472	THR
2	D	474	ILE
2	D	475	THR
2	D	479	LEU
2	D	484	CYS
2	D	486	HIS
2	D	492	ARG
2	D	495	LEU
2	D	501	MET
2	D	508	LEU
2	D	513	GLN
2	D	516	THR
2	D	519	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
2	B	22	GLN
2	B	137	ASN
2	B	229	HIS
2	B	256	ASN
2	B	257	HIS
2	B	395	ASN
2	B	487	HIS
1	C	40	ASN
1	C	83	HIS
2	D	19	HIS
2	D	229	HIS
2	D	257	HIS
2	D	260	HIS
2	D	283	HIS
2	D	373	HIS
2	D	427	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\|>2$
6	G3A	D	606	-	44,55,55	2.33	11 (25%)	49,86,86	1.90	13 (26%)
5	SAH	B	605	-	21,28,28	1.32	2 (9%)	20,40,40	1.82	3 (15%)
6	G3A	B	606	-	44,55,55	2.32	12 (27%)	49,86,86	1.92	14 (28%)
5	SAH	D	605	-	21,28,28	1.36	2 (9%)	20,40,40	1.50	1 (5%)

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
6	G3A	D	606	-	-	15/24/64/64	0/6/6/6
5	SAH	B	605	-	-	3/7/31/31	0/3/3/3
6	G3A	B	606	-	-	10/24/64/64	0/6/6/6
5	SAH	D	605	-	-	5/7/31/31	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	606	G3A	C32-N32	7.35	1.48	1.33
6	D	606	G3A	O36-C36	6.82	1.41	1.24
6	B	606	G3A	O36-C36	6.68	1.41	1.24
6	B	606	G3A	C32-N32	6.66	1.47	1.33
6	B	606	G3A	C22-C21	-5.23	1.45	1.53
6	B	606	G3A	C42-C41	-4.88	1.46	1.53
6	D	606	G3A	C42-C41	-4.87	1.46	1.53
6	D	606	G3A	C22-C21	-4.69	1.46	1.53
5	D	605	SAH	C2-N3	4.67	1.39	1.32
5	B	605	SAH	C2-N3	4.53	1.39	1.32
6	B	606	G3A	C16-N16	4.13	1.49	1.34
6	D	606	G3A	C16-N16	4.08	1.49	1.34
6	D	606	G3A	C22-C23	-3.44	1.43	1.53
6	D	606	G3A	C43-C44	-3.37	1.44	1.53
6	B	606	G3A	C22-C23	-3.37	1.44	1.53
6	B	606	G3A	C43-C44	-3.18	1.44	1.53
6	D	606	G3A	C43-C42	-2.79	1.45	1.53
6	B	606	G3A	C43-C42	-2.78	1.45	1.53
6	D	606	G3A	O23-C23	-2.76	1.36	1.43
6	B	606	G3A	O23-C23	-2.74	1.36	1.43
5	D	605	SAH	C2-N1	2.64	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	606	G3A	PG-O1G	2.34	1.59	1.50
5	B	605	SAH	C2-N1	2.23	1.38	1.33
6	D	606	G3A	C23-C24	-2.22	1.47	1.53
6	B	606	G3A	O42-C42	-2.21	1.37	1.43
6	D	606	G3A	O42-C42	-2.17	1.37	1.43
6	B	606	G3A	C23-C24	-2.01	1.47	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	605	SAH	N3-C2-N1	-5.79	119.62	128.68
5	D	605	SAH	N3-C2-N1	-5.44	120.17	128.68
6	B	606	G3A	N33-C32-N31	-4.65	121.02	127.22
6	D	606	G3A	N33-C32-N31	-4.41	121.34	127.22
6	D	606	G3A	C23-C22-C21	4.28	107.42	100.98
6	B	606	G3A	C41-N39-C34	-4.27	119.14	126.64
6	D	606	G3A	N13-C12-N11	-4.14	122.21	128.68
6	B	606	G3A	O25-C25-C24	4.02	122.81	108.99
6	D	606	G3A	O25-C25-C24	3.92	122.50	108.99
6	D	606	G3A	C32-N33-C34	3.92	119.83	115.36
6	B	606	G3A	C36-N31-C32	3.88	122.10	115.93
6	B	606	G3A	C36-C35-C34	-3.86	117.11	120.80
6	D	606	G3A	C35-C36-N31	-3.78	118.25	123.43
6	B	606	G3A	C32-N33-C34	3.63	119.51	115.36
6	D	606	G3A	C36-N31-C32	3.50	121.48	115.93
6	B	606	G3A	C35-C36-N31	-3.36	118.83	123.43
6	B	606	G3A	N13-C12-N11	-3.29	123.53	128.68
6	D	606	G3A	C34-C35-N37	-3.13	106.13	109.40
6	B	606	G3A	C43-C42-C41	3.08	105.62	100.98
6	B	606	G3A	O45-C45-C44	2.75	118.44	108.99
6	D	606	G3A	O45-C45-C44	2.71	118.32	108.99
6	B	606	G3A	C34-C35-N37	-2.57	106.72	109.40
6	B	606	G3A	C42-C43-C44	2.53	107.56	102.64
6	D	606	G3A	C43-C42-C41	2.43	104.64	100.98
6	B	606	G3A	PG-O3A-PB	-2.35	124.75	132.83
6	D	606	G3A	C41-N39-C34	-2.31	122.58	126.64
6	D	606	G3A	PB-O1-PA	-2.27	125.04	132.83
6	B	606	G3A	C14-C15-N17	-2.21	107.10	109.40
6	D	606	G3A	C22-C23-C24	2.17	106.86	102.64
5	B	605	SAH	C5'-SD-CG	-2.04	96.14	102.27
5	B	605	SAH	C1'-N9-C4	-2.02	123.09	126.64

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	606	G3A	C45-O45-PA-O1A
6	D	606	G3A	C45-O45-PA-O2A
6	D	606	G3A	PB-O1-PA-O45
6	D	606	G3A	C25-O25-PG-O3A
6	D	606	G3A	C25-O25-PG-O1G
6	D	606	G3A	C25-O25-PG-O2G
5	D	605	SAH	O4'-C4'-C5'-SD
5	D	605	SAH	C3'-C4'-C5'-SD
6	B	606	G3A	C45-O45-PA-O1A
6	B	606	G3A	C45-O45-PA-O2A
6	B	606	G3A	C25-O25-PG-O3A
6	B	606	G3A	C25-O25-PG-O1G
6	B	606	G3A	C25-O25-PG-O2G
5	B	605	SAH	O4'-C4'-C5'-SD
5	B	605	SAH	C3'-C4'-C5'-SD
6	D	606	G3A	O44-C44-C45-O45
6	D	606	G3A	C23-C24-C25-O25
6	B	606	G3A	O44-C44-C45-O45
6	B	606	G3A	C23-C24-C25-O25
6	B	606	G3A	O24-C24-C25-O25
5	B	605	SAH	CA-CB-CG-SD
6	B	606	G3A	C43-C44-C45-O45
6	D	606	G3A	O24-C24-C25-O25
6	D	606	G3A	C43-C44-C45-O45
6	D	606	G3A	C24-C25-O25-PG
5	D	605	SAH	CA-CB-CG-SD
6	D	606	G3A	PA-O1-PB-O3B
5	D	605	SAH	CB-CG-SD-C5'
6	D	606	G3A	C45-O45-PA-O1
5	D	605	SAH	N-CA-CB-CG
6	B	606	G3A	C45-O45-PA-O1
6	D	606	G3A	PA-O1-PB-O2B
6	D	606	G3A	PB-O3A-PG-O1G

There are no ring outliers.

4 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	606	G3A	19	0
5	B	605	SAH	9	0

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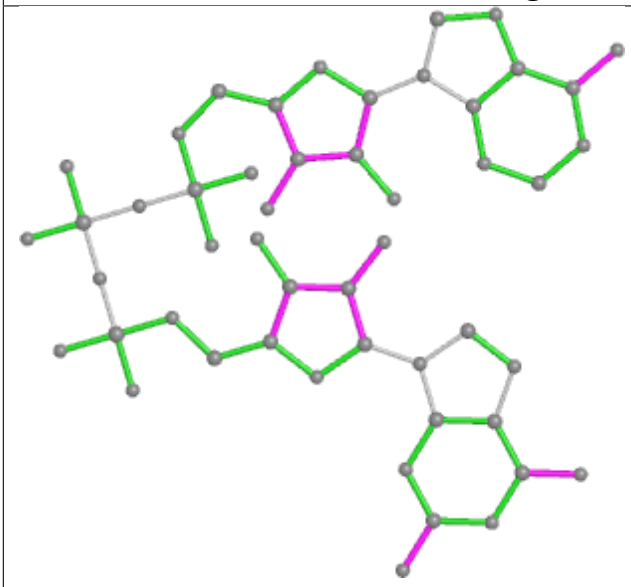
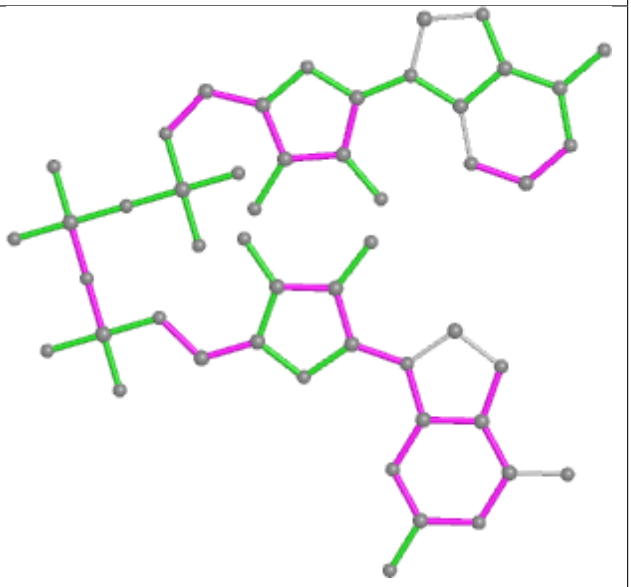
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	606	G3A	19	0
5	D	605	SAH	15	0

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.

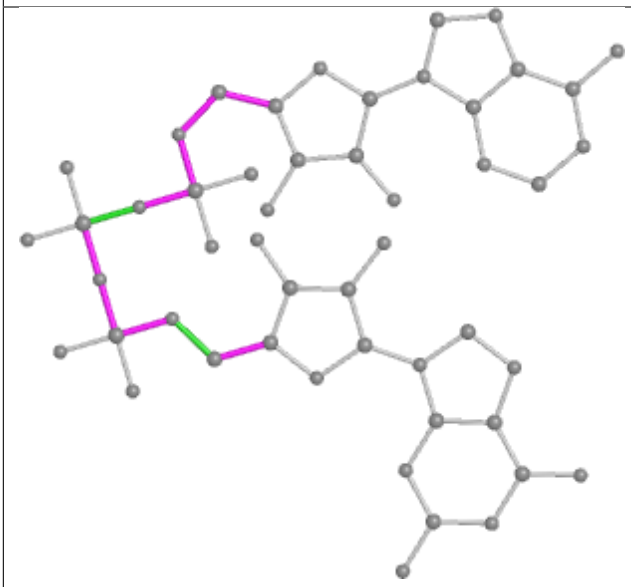
Ligand G3A D 606



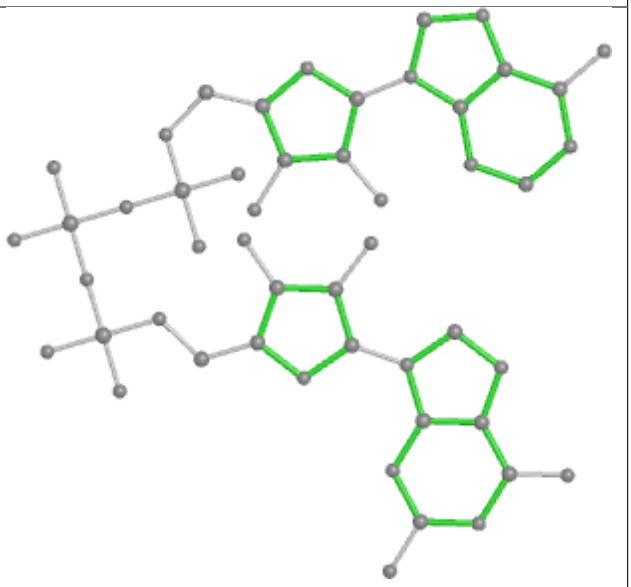
Bond lengths



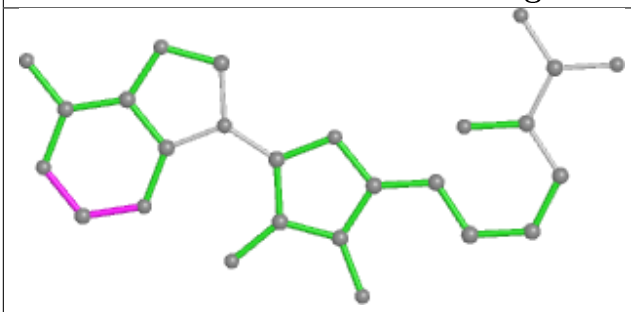
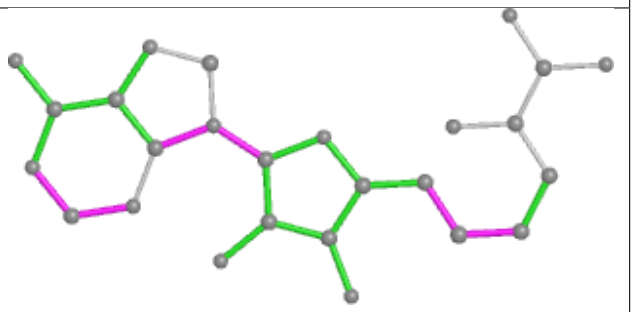
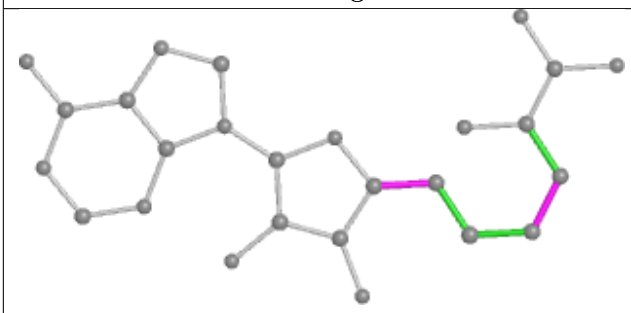
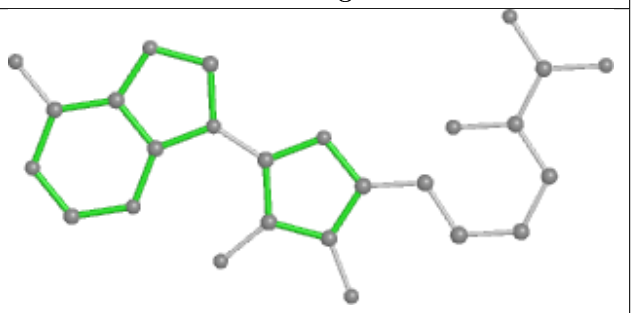
Bond angles



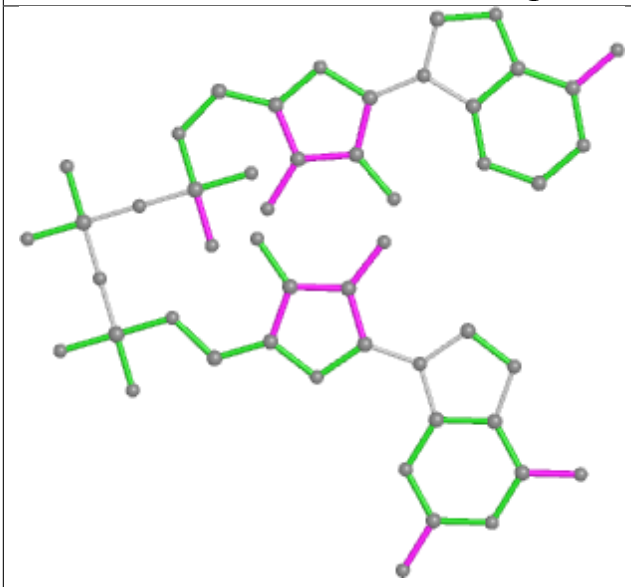
Torsions



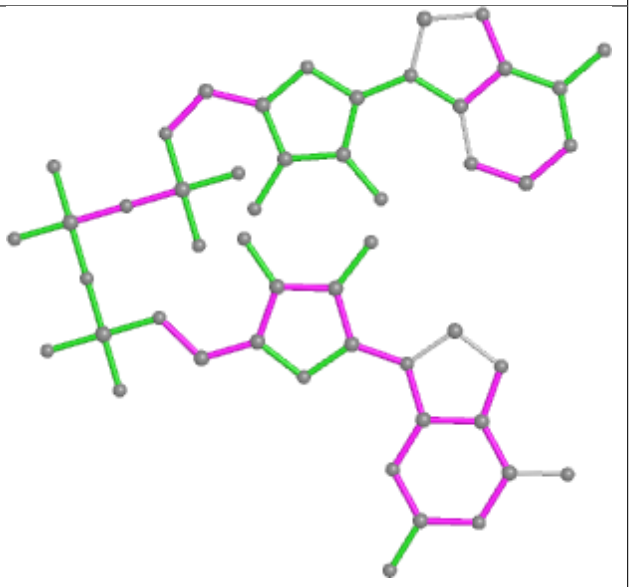
Rings

Ligand SAH B 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

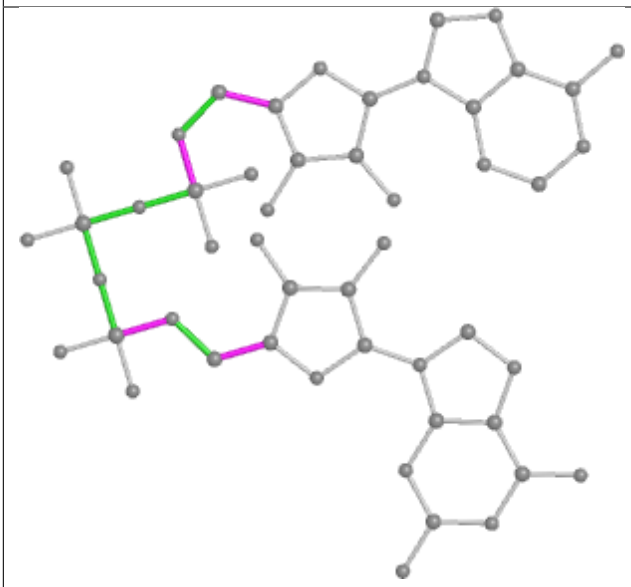
Ligand G3A B 606



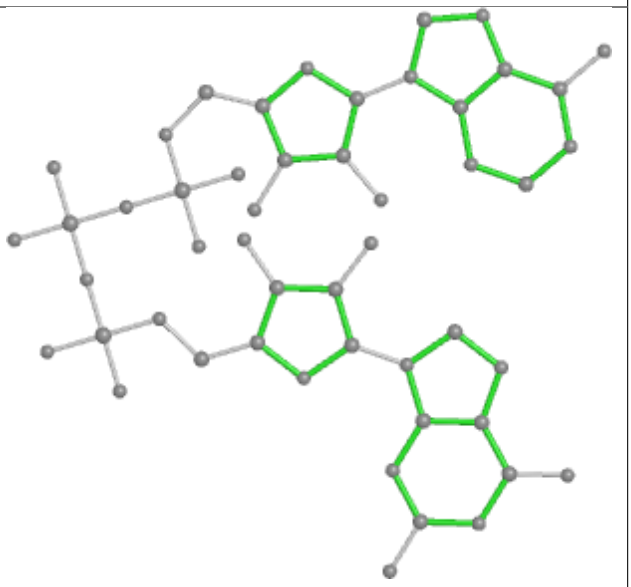
Bond lengths



Bond angles

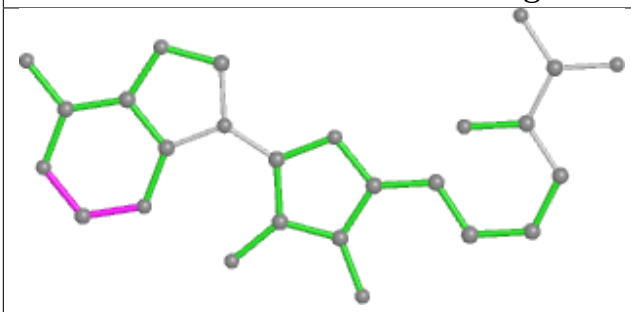


Torsions

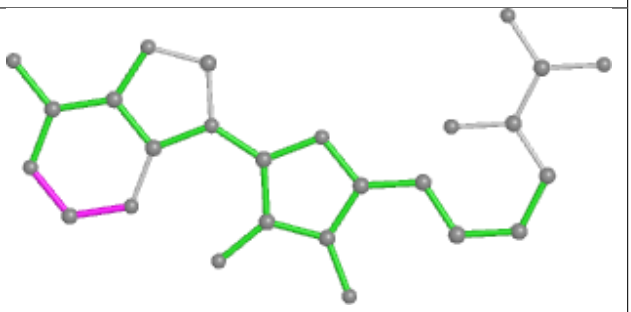


Rings

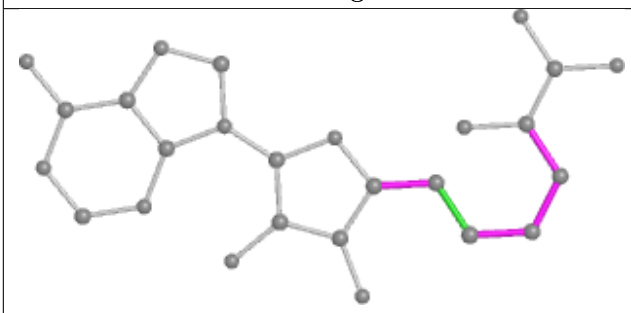
Ligand SAH D 605



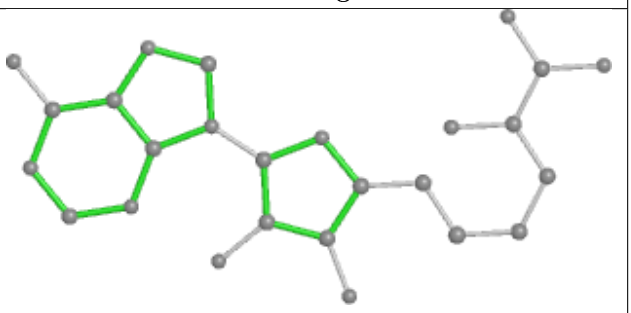
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	133/144 (92%)	0.16	7 (5%)	26	26	94, 134, 179, 206	0
1	C	133/144 (92%)	0.11	2 (1%)	73	72	99, 124, 153, 189	0
2	B	514/527 (97%)	0.03	8 (1%)	72	70	83, 119, 153, 204	0
2	D	514/527 (97%)	0.12	10 (1%)	66	65	88, 119, 165, 180	0
All	All	1294/1342 (96%)	0.09	27 (2%)	63	62	83, 121, 163, 206	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	ASP	3.9
1	A	123	TRP	3.4
1	A	126	TYR	3.1
2	D	368	TYR	3.1
2	B	465	TYR	3.0
2	B	468	LEU	2.8
2	B	519	LEU	2.8
2	B	524	THR	2.7
2	D	147	LYS	2.7
1	A	121	GLY	2.5
2	B	483	VAL	2.5
2	D	436	PHE	2.5
2	D	348	TRP	2.5
2	D	431	PHE	2.5
1	A	116	VAL	2.4
2	B	471	ALA	2.4
2	D	319	SER	2.3
2	D	447	TYR	2.3
1	A	55	ILE	2.3
2	D	142	PRO	2.3
2	D	146	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	359	LYS	2.2
2	B	466	VAL	2.1
1	C	116	VAL	2.1
1	A	82	ASP	2.1
2	B	1	ALA	2.1
1	C	123	TRP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

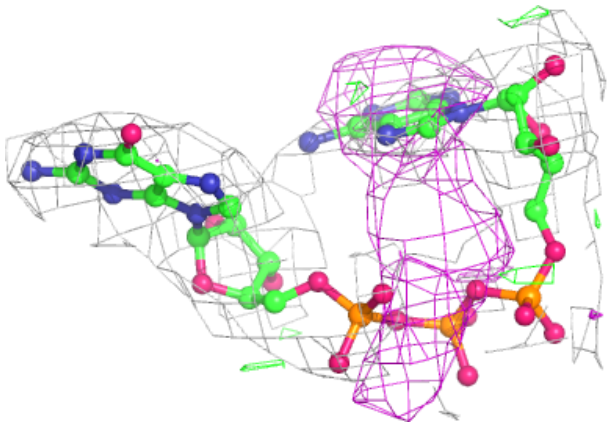
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

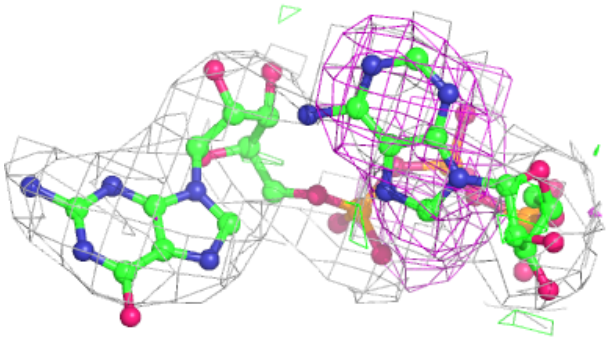
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	G3A	B	606	50/50	0.80	0.25	107,145,181,198	0
6	G3A	D	606	50/50	0.89	0.26	119,138,161,166	0
5	SAH	D	605	26/26	0.90	0.28	118,142,156,161	0
4	MG	B	604	1/1	0.90	0.38	118,118,118,118	0
4	MG	D	604	1/1	0.91	0.11	125,125,125,125	0
3	ZN	A	202	1/1	0.91	0.05	191,191,191,191	0
3	ZN	C	202	1/1	0.93	0.05	148,148,148,148	0
5	SAH	B	605	26/26	0.94	0.23	112,127,149,170	0
3	ZN	B	601	1/1	0.95	0.11	178,178,178,178	0
3	ZN	B	603	1/1	0.97	0.05	140,140,140,140	0
3	ZN	D	602	1/1	0.98	0.09	136,136,136,136	0
3	ZN	B	602	1/1	0.98	0.12	107,107,107,107	0
3	ZN	A	201	1/1	0.98	0.19	126,126,126,126	0
3	ZN	D	603	1/1	0.98	0.08	113,113,113,113	0
3	ZN	D	601	1/1	0.99	0.16	108,108,108,108	0
3	ZN	C	201	1/1	1.00	0.19	113,113,113,113	0

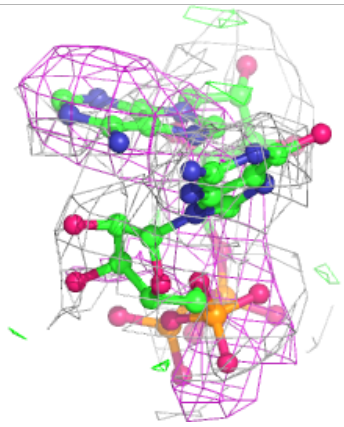
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G3A B 606:

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

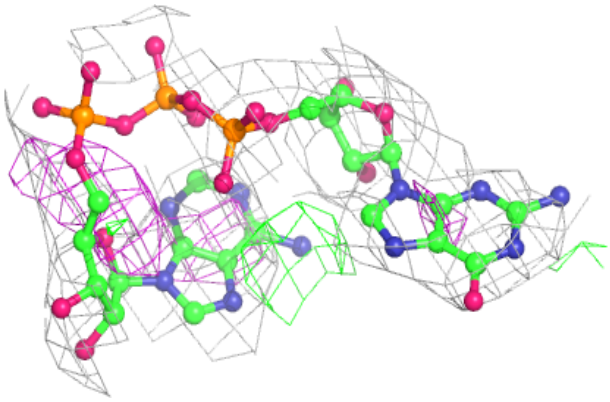


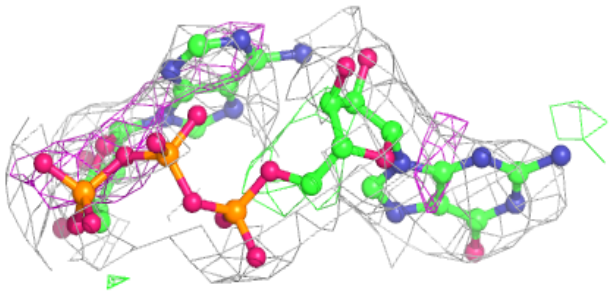


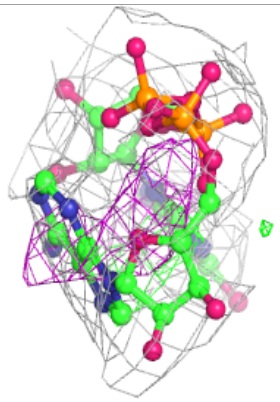


Electron density around G3A D 606:

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

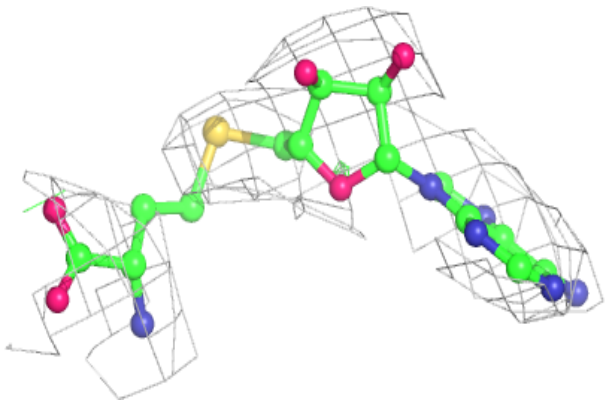


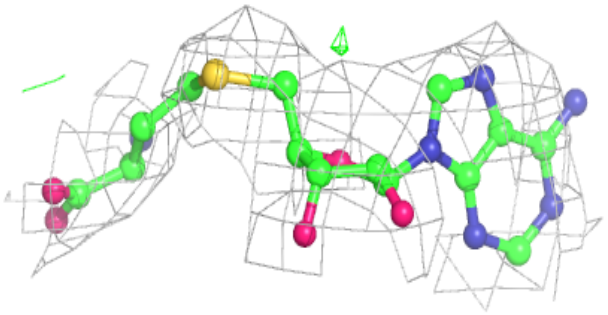


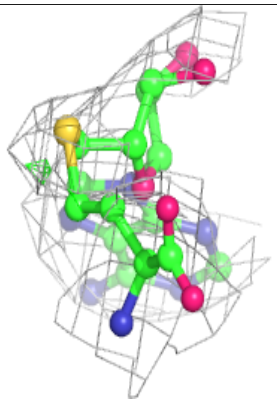


Electron density around SAH D 605:

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

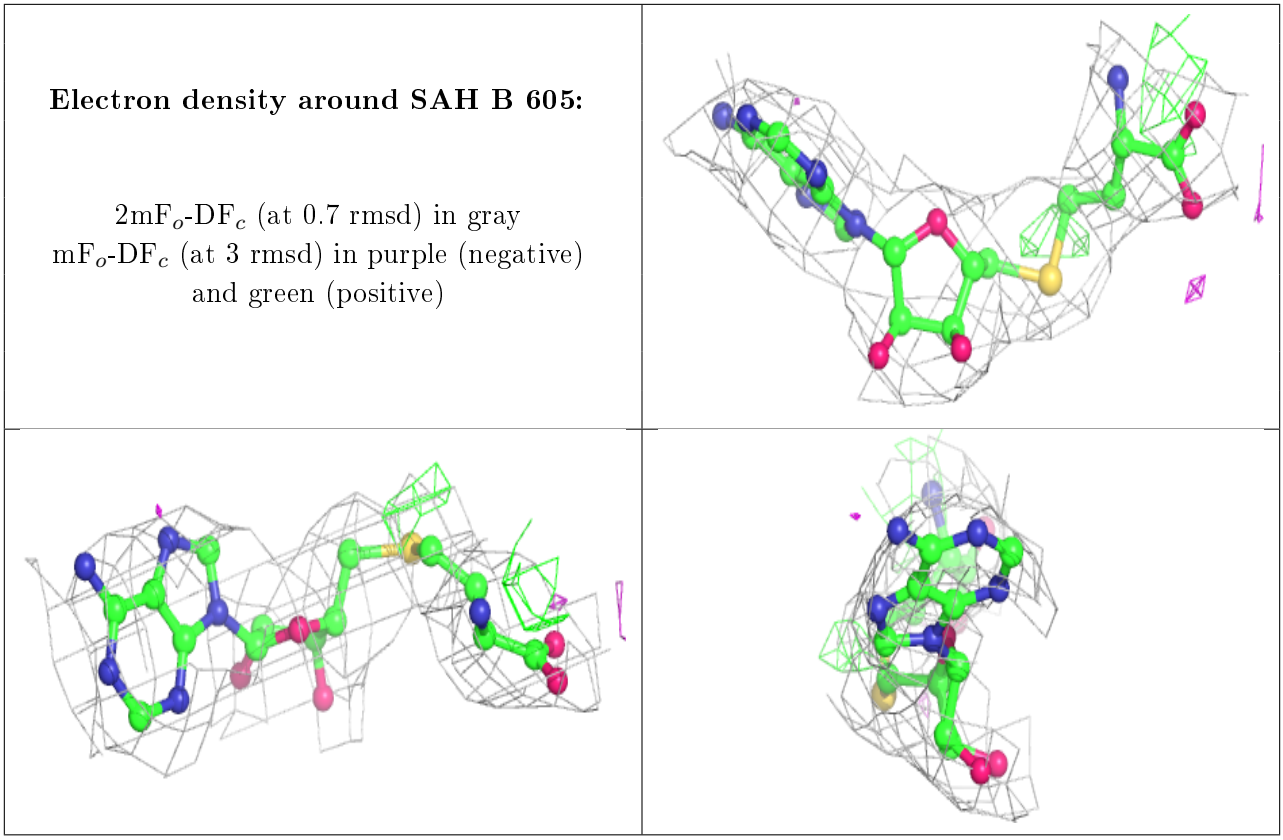






Electron density around SAH B 605:

$2mF_o$-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.