Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 12:02 AM EDT

PDB ID	:	1SO2
Title	:	CATALYTIC DOMAIN OF HUMAN PHOSPHODIESTERASE 3B In COMPLEX WITH A DIHYDROPYRIDAZINE INHIBITOR
Authors	:	Scapin, G.; Patel, S.B.; Chung, C.; Varnerin, J.P.; Edmondson, S.D.; Mastracchio, A.; Parmee, E.R.; Becker, J.W.; Singh, S.B.; Van Der Ploeg, L.H.; Tota, M.R.
Deposited on	:	2004-03-12
Resolution	:	2.40 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 (i) 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 (1)) were used in the production of this report:

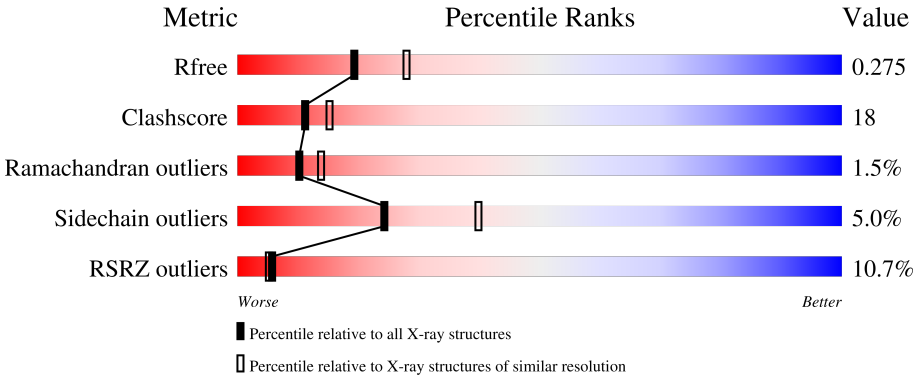
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	420	9% 61% 23% • 14%
1	B	420	8% 60% 24% • 14%
1	C	420	9% 63% 24% • 11%
1	D	420	12% 50% 33% 5% 13%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12292 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.

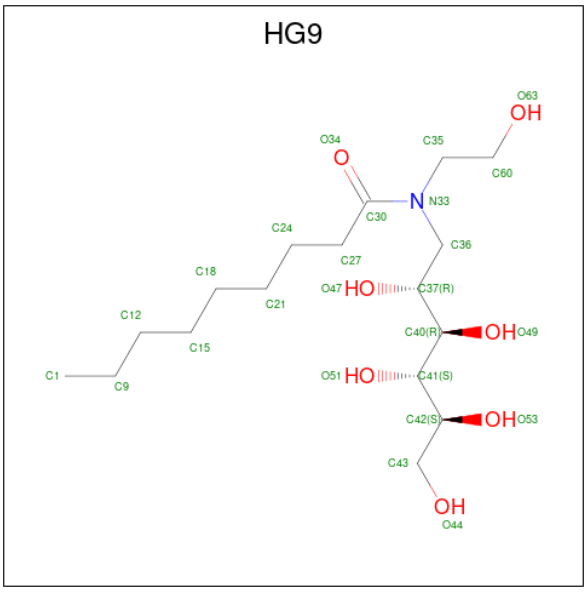
- Molecule 1 is a protein called cGMP-inhibited 3',5'-cyclic phosphodiesterase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2916	1868	501	533	14			
1	B	363	Total	C	N	O	S	0	0	0
			2909	1863	500	532	14			
1	C	372	Total	C	N	O	S	0	0	0
			2964	1897	508	545	14			
1	D	365	Total	C	N	O	S	0	0	0
			2916	1867	500	535	14			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

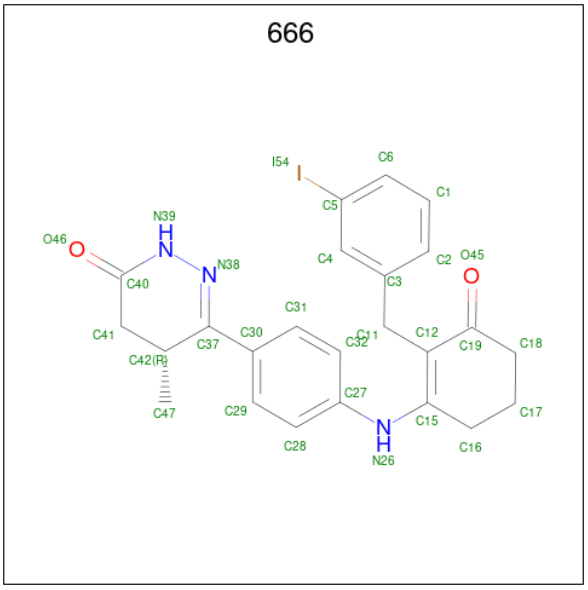
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mg	0	0
			3	3		
2	B	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 1-DEOXY-1-[(2-HYDROXYETHYL)(NONANOYL)AMINO]HEXITOL (three-letter code: HG9) (formula: $C_{17}H_{35}NO_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	16	1	7		
3	A	1	Total	C	N	O	0	0
			24	16	1	7		
3	B	1	Total	C	N	O	0	0
			24	16	1	7		
3	B	1	Total	C	N	O	0	0
			24	16	1	7		

- Molecule 4 is 6-(4-{[2-(3-IODOBENZYL)-3-OXOCYCLOHEX-1-EN-1-YL]AMINO}PHENYL)-5-METHYL-4,5-DIHYDROPYRIDAZIN-3(2H)-ONE (three-letter code: 666) (formula: $C_{24}H_{24}IN_3O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	I	N	O	0	0
			30	24	1	3	2		
4	B	1	Total	C	I	N	O	0	0
			30	24	1	3	2		
4	C	1	Total	C	I	N	O	0	0
			30	24	1	3	2		
4	D	1	Total	C	I	N	O	0	0
			30	24	1	3	2		

- Molecule 5 is water.

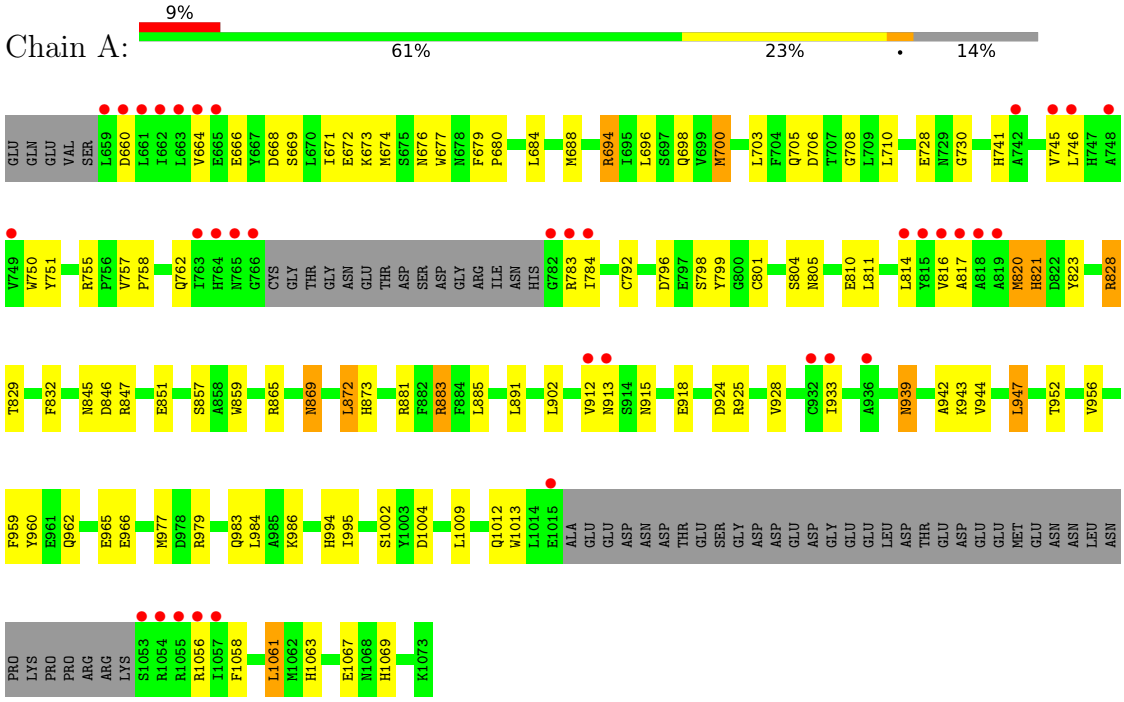
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		
5	B	115	Total	O	0	0
			115	115		
5	C	70	Total	O	0	0
			70	70		
5	D	58	Total	O	0	0
			58	58		

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.

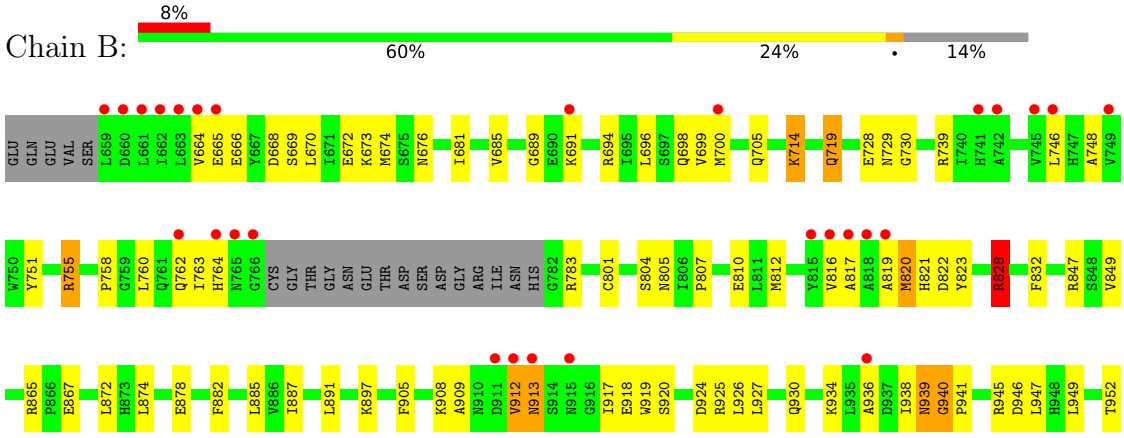
• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

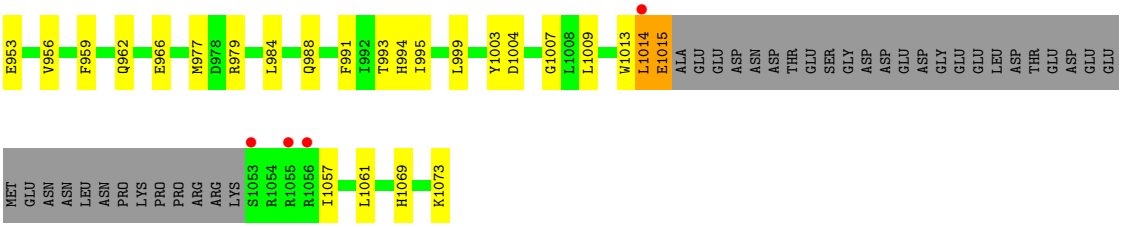
Chain A:



• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

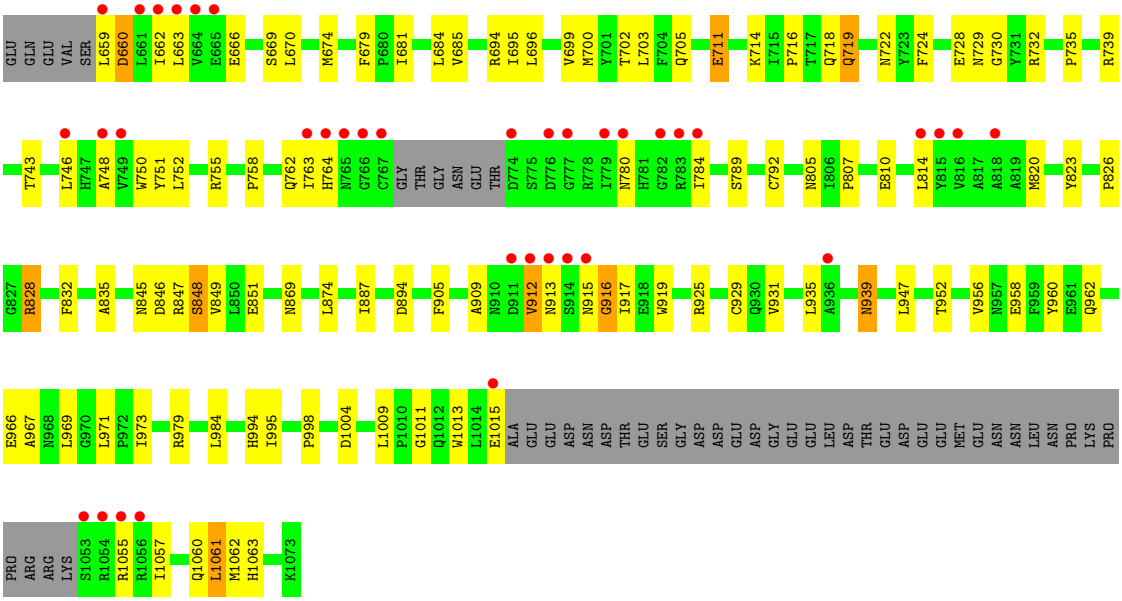
Chain B:





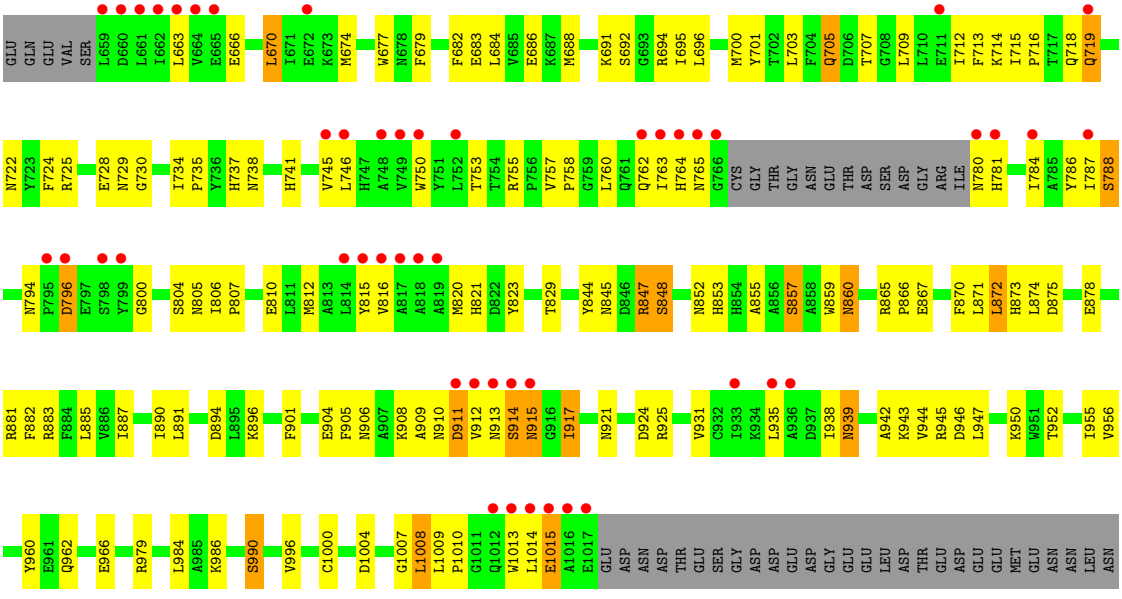
• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

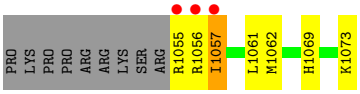
Chain C:



• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

Chain D:




PRO
LYS
PRO
PRO
ARG
ARG
LYS
SER
ARG
R1055
R1056
I1057
L1061
M1062
H1069
K1073

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	147.48Å 121.77Å 126.67Å 90.00° 100.74° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.40) 99.8 (29.82-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.10 (at 2.39Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.232 , 0.277 0.228 , 0.275	Depositor DCC
R_{free} test set	4345 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.881	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12292	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: MG, 666, HG9

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	0.59	0/2992	0.67	1/4063 (0.0%)
1	B	0.58	0/2985	0.70	1/4054 (0.0%)
1	C	0.55	0/3040	0.66	0/4129
1	D	0.58	0/2992	0.64	0/4065
All	All	0.57	0/12009	0.67	2/16311 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	828	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	821	HIS	N-CA-C	5.22	125.09	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2916	0	2803	83	0
1	B	2909	0	2788	107	0
1	C	2964	0	2834	87	0
1	D	2916	0	2788	148	0
2	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	48	0	60	2	0
3	B	48	0	60	2	0
4	A	30	0	24	2	0
4	B	30	0	24	2	0
4	C	30	0	24	1	0
4	D	30	0	24	3	0
5	A	119	0	0	2	0
5	B	115	0	0	6	0
5	C	70	0	0	3	0
5	D	58	0	0	4	0
All	All	12292	0	11429	419	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 18.

All (419) 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:A:700:MET:HE3	1:A:746:LEU:HD21	1.38	1.00
1:C:828:ARG:HG2	1:C:832:PHE:CD2	1.96	0.99
1:C:967:ALA:HB2	1:C:973:ILE:HD11	1.45	0.96
1:B:828:ARG:HG2	1:B:832:PHE:CD2	2.04	0.93
1:B:719:GLN:H	1:B:719:GLN:HE21	0.99	0.92
1:A:1061:LEU:HD23	1:A:1061:LEU:H	1.38	0.89
1:B:719:GLN:HE21	1:B:719:GLN:N	1.70	0.89
1:B:1014:LEU:HD12	1:B:1014:LEU:H	1.39	0.87
1:B:1009:LEU:HD22	1:B:1061:LEU:HD21	1.58	0.86
1:C:670:LEU:HD22	1:C:702:THR:HG21	1.58	0.86
1:C:994:HIS:O	1:C:995:ILE:HD13	1.76	0.85
1:D:679:PHE:HZ	1:D:684:LEU:HD22	1.41	0.84
1:A:828:ARG:HG2	1:A:832:PHE:CD2	2.15	0.81
1:B:939:ASN:C	1:B:939:ASN:HD22	1.83	0.81
1:A:939:ASN:C	1:A:939:ASN:HD22	1.85	0.80
1:B:700:MET:HE3	1:B:746:LEU:HD13	1.65	0.78
1:B:719:GLN:H	1:B:719:GLN:NE2	1.80	0.77
1:B:1015:GLU:OE1	1:B:1015:GLU:HA	1.85	0.75
1:D:872:LEU:HD13	1:D:873:HIS:CD2	2.22	0.75
1:A:847:ARG:CZ	1:B:891:LEU:HD13	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:716:PRO:HB2	1:D:719:GLN:HE22	1.53	0.73
1:C:730:GLY:HA3	1:C:823:TYR:CE1	2.23	0.73
1:C:751:TYR:CE2	1:C:755:ARG:HG3	2.24	0.73
1:B:905:PHE:HA	1:B:927:LEU:HD21	1.69	0.73
1:A:730:GLY:HA3	1:A:823:TYR:CE1	2.23	0.73
1:D:816:VAL:O	1:D:820:MET:HG2	1.89	0.73
1:B:1009:LEU:CD2	1:B:1061:LEU:HD21	2.20	0.72
1:D:956:VAL:HG11	1:D:984:LEU:HD13	1.69	0.72
1:B:909:ALA:HB2	1:B:917:ILE:HD11	1.70	0.72
1:D:921:ASN:HB3	1:D:924:ASP:HB2	1.72	0.72
1:A:979:ARG:HH11	3:A:453:HG9:H602	1.53	0.71
1:B:991:PHE:HA	1:B:995:ILE:HD13	1.72	0.71
1:C:828:ARG:HG2	1:C:832:PHE:CG	2.26	0.71
1:D:881:ARG:HH11	1:D:881:ARG:HG3	1.56	0.71
1:B:764:HIS:HB2	1:B:804:SER:O	1.90	0.71
1:B:995:ILE:HD12	1:B:995:ILE:N	2.07	0.70
1:D:716:PRO:HB2	1:D:719:GLN:NE2	2.06	0.70
1:A:762:GLN:NE2	1:A:801:CYS:H	1.90	0.70
4:C:463:666:H162	4:C:463:666:H28	1.72	0.69
1:D:688:MET:HE2	1:D:692:SER:HA	1.74	0.69
1:B:1014:LEU:HD12	1:B:1014:LEU:N	2.06	0.69
1:B:1069:HIS:NE2	1:B:1073:LYS:HD2	2.08	0.69
1:D:709:LEU:HD23	1:D:787:ILE:HD11	1.75	0.69
1:D:762:GLN:OE1	1:D:804:SER:HB2	1.93	0.69
1:D:784:ILE:HD12	1:D:807:PRO:HB3	1.74	0.68
1:B:1069:HIS:CD2	1:B:1073:LYS:HD2	2.29	0.67
1:D:935:LEU:HD11	1:D:1000:CYS:SG	2.34	0.67
1:D:865:ARG:HH11	1:D:865:ARG:HG2	1.59	0.67
1:A:883:ARG:HG2	1:A:883:ARG:HH11	1.59	0.67
1:C:912:VAL:HG23	1:C:913:ASN:N	2.10	0.67
1:D:718:GLN:HE21	1:D:722:ASN:HD21	1.41	0.67
1:D:700:MET:HE2	1:D:746:LEU:HD21	1.77	0.67
1:D:906:ASN:O	1:D:911:ASP:HB2	1.95	0.67
1:A:700:MET:HE3	1:A:746:LEU:CD2	2.20	0.66
1:D:1013:TRP:HA	1:D:1057:ILE:HG22	1.75	0.66
1:B:700:MET:HE3	1:B:746:LEU:CD1	2.25	0.66
1:A:939:ASN:C	1:A:939:ASN:ND2	2.46	0.66
1:C:763:ILE:HG13	1:C:764:HIS:N	2.10	0.66
1:D:1004:ASP:HB2	1:D:1009:LEU:HD12	1.77	0.66
1:D:725:ARG:O	1:D:729:ASN:ND2	2.29	0.66
1:D:763:ILE:C	1:D:765:ASN:H	2.00	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:960:TYR:HB3	1:C:979:ARG:NH2	2.11	0.65
1:C:962:GLN:O	1:C:966:GLU:HG3	1.96	0.65
1:A:816:VAL:O	1:A:820:MET:HG3	1.97	0.64
1:C:696:LEU:HB3	1:C:728:GLU:HG2	1.79	0.64
1:A:1063:HIS:O	1:A:1067:GLU:HG3	1.98	0.64
1:D:804:SER:C	1:D:805:ASN:HD22	2.00	0.64
1:D:912:VAL:C	1:D:914:SER:H	1.99	0.64
1:C:732:ARG:NH1	1:C:826:PRO:HA	2.12	0.63
1:A:1012:GLN:HE21	1:A:1058:PHE:HD2	1.45	0.63
1:D:853:HIS:O	1:D:857:SER:HB2	1.98	0.63
1:A:696:LEU:HB3	1:A:728:GLU:HG2	1.80	0.63
1:B:739:ARG:HG3	5:B:348:HOH:O	1.98	0.63
1:B:751:TYR:CZ	1:B:755:ARG:HG3	2.34	0.63
1:B:939:ASN:C	1:B:939:ASN:ND2	2.52	0.63
1:B:810:GLU:OE1	1:B:925:ARG:HD2	1.99	0.63
1:D:730:GLY:HA3	1:D:823:TYR:CE1	2.34	0.63
1:C:912:VAL:HG23	1:C:913:ASN:OD1	1.99	0.63
1:A:700:MET:HE1	1:A:746:LEU:HD11	1.81	0.63
1:A:959:PHE:HB3	1:A:977:MET:HG2	1.80	0.62
1:B:979:ARG:HH11	3:B:451:HG9:H602	1.64	0.62
1:C:994:HIS:C	1:C:995:ILE:HD13	2.19	0.62
1:D:763:ILE:H	1:D:805:ASN:HD21	1.46	0.62
1:C:700:MET:HE2	1:C:746:LEU:HD21	1.82	0.62
1:C:751:TYR:CZ	1:C:755:ARG:HG3	2.34	0.62
4:B:462:666:H162	4:B:462:666:H28	1.82	0.62
1:D:881:ARG:O	1:D:885:LEU:HD13	2.00	0.62
1:C:758:PRO:HD3	1:C:1011:GLY:H	1.64	0.61
1:D:1008:LEU:HD23	1:D:1008:LEU:N	2.14	0.61
1:C:719:GLN:HA	1:C:722:ASN:HD22	1.66	0.61
1:C:784:ILE:HG21	1:C:807:PRO:HB3	1.82	0.60
1:D:718:GLN:NE2	1:D:722:ASN:HD21	1.99	0.60
1:B:681:ILE:O	1:B:685:VAL:HG23	2.02	0.60
1:C:1013:TRP:CZ3	1:C:1055:ARG:HB3	2.37	0.60
1:D:865:ARG:HG2	1:D:865:ARG:NH1	2.17	0.60
1:C:703:LEU:HD22	1:C:750:TRP:CE2	2.37	0.60
1:D:829:THR:HG22	4:D:464:666:H182	1.84	0.59
1:C:814:LEU:HD13	1:C:929:CYS:HB3	1.84	0.59
1:B:1069:HIS:HE2	1:B:1073:LYS:HD2	1.67	0.59
1:A:664:VAL:HG12	1:A:668:ASP:OD2	2.01	0.59
1:A:694:ARG:O	1:A:698:GLN:HG2	2.01	0.59
1:B:828:ARG:HG2	1:B:832:PHE:CG	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:ASN:HB3	1:B:887:ILE:HD13	1.84	0.59
1:D:707:THR:HB	1:D:787:ILE:HG21	1.85	0.59
1:B:664:VAL:HG12	1:B:668:ASP:OD2	2.03	0.58
1:C:752:LEU:HD11	1:C:935:LEU:HD22	1.84	0.58
1:D:914:SER:O	1:D:915:ASN:HB2	2.03	0.58
1:B:1014:LEU:O	1:B:1015:GLU:HG2	2.02	0.58
1:B:730:GLY:HA3	1:B:823:TYR:CE1	2.39	0.58
1:B:939:ASN:HD22	1:B:940:GLY:N	2.02	0.58
1:B:917:ILE:HG23	1:B:924:ASP:HB3	1.85	0.58
1:D:716:PRO:CG	1:D:719:GLN:NE2	2.67	0.58
1:B:930:GLN:O	1:B:934:LYS:HG3	2.03	0.58
1:A:757:VAL:HG13	1:A:1009:LEU:O	2.04	0.58
1:D:719:GLN:NE2	1:D:719:GLN:H	2.01	0.58
1:B:700:MET:HE2	1:B:700:MET:HA	1.86	0.57
1:B:698:GLN:NE2	5:B:374:HOH:O	2.37	0.57
1:D:905:PHE:CD1	1:D:931:VAL:HG21	2.39	0.57
1:D:763:ILE:H	1:D:805:ASN:ND2	2.02	0.57
1:A:730:GLY:HA3	1:A:823:TYR:HE1	1.69	0.57
1:B:1003:TYR:HD2	1:B:1009:LEU:HG	1.70	0.57
1:C:700:MET:HE2	1:C:746:LEU:CD2	2.33	0.57
1:D:810:GLU:OE1	1:D:925:ARG:HD2	2.05	0.57
1:A:883:ARG:HG2	1:A:883:ARG:NH1	2.19	0.56
1:A:995:ILE:N	1:A:995:ILE:HD12	2.20	0.56
1:C:660:ASP:O	1:C:663:LEU:HB2	2.05	0.56
1:D:696:LEU:HB3	1:D:728:GLU:HG2	1.87	0.56
1:D:741:HIS:O	1:D:745:VAL:HG23	2.05	0.56
1:A:684:LEU:O	1:A:688:MET:HG3	2.05	0.56
1:D:812:MET:O	1:D:816:VAL:HG23	2.05	0.56
1:D:701:TYR:CZ	1:D:705:GLN:HG3	2.41	0.56
1:C:724:PHE:O	1:C:728:GLU:HG3	2.06	0.56
1:A:804:SER:C	1:A:805:ASN:HD22	2.09	0.56
1:B:874:LEU:HD22	1:B:878:GLU:HB3	1.87	0.55
1:A:881:ARG:HG3	1:A:881:ARG:HH11	1.71	0.55
1:A:783:ARG:HG2	1:A:784:ILE:N	2.21	0.55
1:D:763:ILE:O	1:D:765:ASN:N	2.39	0.55
1:C:1015:GLU:O	1:C:1055:ARG:HD3	2.07	0.55
1:A:979:ARG:NH1	3:A:453:HG9:H602	2.22	0.55
1:D:962:GLN:O	1:D:966:GLU:HG3	2.07	0.55
1:A:912:VAL:O	1:A:913:ASN:HB2	2.07	0.55
1:D:896:LYS:HD3	5:D:373:HOH:O	2.07	0.55
1:C:912:VAL:HG23	1:C:913:ASN:H	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:712:ILE:HD12	1:D:787:ILE:CD1	2.37	0.54
1:A:751:TYR:CZ	1:A:755:ARG:HG3	2.42	0.54
1:C:1061:LEU:C	1:C:1061:LEU:HD12	2.28	0.54
1:D:734:ILE:HB	1:D:735:PRO:HD2	1.88	0.54
1:D:912:VAL:O	1:D:914:SER:N	2.40	0.54
1:A:962:GLN:O	1:A:966:GLU:HG3	2.08	0.54
1:D:716:PRO:CB	1:D:719:GLN:NE2	2.71	0.54
1:A:828:ARG:HG2	1:A:832:PHE:CG	2.42	0.54
4:A:461:666:H162	4:A:461:666:H28	1.89	0.54
1:B:816:VAL:O	1:B:820:MET:HG3	2.08	0.54
1:A:708:GLY:HA2	5:A:128:HOH:O	2.07	0.54
1:D:724:PHE:O	1:D:728:GLU:HG3	2.07	0.54
1:D:787:ILE:HG22	1:D:788:SER:N	2.21	0.54
1:D:914:SER:O	1:D:915:ASN:CB	2.56	0.54
1:D:714:LYS:HA	1:D:714:LYS:HE2	1.89	0.54
1:A:783:ARG:HG2	1:A:784:ILE:H	1.72	0.53
1:D:716:PRO:HG2	1:D:719:GLN:HE21	1.74	0.53
1:C:1004:ASP:HB2	1:C:1009:LEU:HD12	1.89	0.53
1:B:956:VAL:HG11	1:B:984:LEU:HD13	1.88	0.53
1:D:674:MET:CE	1:D:703:LEU:HD21	2.38	0.53
1:D:1061:LEU:HD12	1:D:1062:MET:N	2.23	0.53
1:A:952:THR:O	1:A:956:VAL:HG13	2.08	0.53
1:B:918:GLU:O	1:B:920:SER:N	2.42	0.53
1:B:1009:LEU:HD22	1:B:1061:LEU:CD2	2.36	0.53
1:C:847:ARG:CZ	1:D:891:LEU:HD13	2.38	0.53
1:D:1069:HIS:NE2	1:D:1073:LYS:HD3	2.23	0.53
1:A:762:GLN:HE22	1:A:801:CYS:H	1.55	0.53
1:D:682:PHE:CE1	1:D:950:LYS:HG2	2.44	0.53
1:A:700:MET:HA	1:A:700:MET:CE	2.39	0.53
1:D:938:ILE:HD12	1:D:996:VAL:HG22	1.91	0.53
1:B:729:ASN:HA	1:B:739:ARG:NH2	2.23	0.53
1:C:905:PHE:CD1	1:C:931:VAL:HG21	2.43	0.53
1:B:1004:ASP:O	1:B:1007:GLY:N	2.40	0.52
1:C:935:LEU:C	1:C:935:LEU:HD23	2.30	0.52
1:D:944:VAL:HG12	1:D:947:LEU:HD12	1.92	0.52
1:B:905:PHE:HA	1:B:927:LEU:CD2	2.38	0.52
1:A:1004:ASP:HB2	1:A:1009:LEU:HD12	1.92	0.52
1:C:663:LEU:HD12	1:C:666:GLU:HB2	1.91	0.52
1:D:694:ARG:HA	1:D:728:GLU:OE1	2.08	0.52
1:A:817:ALA:O	1:A:821:HIS:HB3	2.10	0.52
1:B:926:LEU:O	1:B:930:GLN:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:719:GLN:H	1:C:719:GLN:NE2	2.08	0.52
1:B:979:ARG:NH1	3:B:451:HG9:H602	2.25	0.51
1:C:735:PRO:HG2	1:C:958:GLU:HB2	1.91	0.51
1:A:829:THR:HG22	4:A:461:666:H182	1.92	0.51
1:D:1061:LEU:HD12	1:D:1061:LEU:C	2.31	0.51
1:A:751:TYR:CE2	1:A:755:ARG:HG3	2.46	0.51
1:A:865:ARG:NH2	1:C:874:LEU:O	2.44	0.51
1:C:716:PRO:HB2	1:C:719:GLN:NE2	2.26	0.51
1:C:784:ILE:CG2	1:C:807:PRO:HB3	2.40	0.51
1:B:696:LEU:HB3	1:B:728:GLU:HG2	1.93	0.50
1:D:986:LYS:O	1:D:990:SER:HB2	2.11	0.50
1:D:663:LEU:O	1:D:666:GLU:HB2	2.11	0.50
1:B:700:MET:HE2	1:B:746:LEU:HD21	1.94	0.50
1:B:751:TYR:CE2	1:B:755:ARG:HG3	2.47	0.50
1:A:912:VAL:O	1:A:913:ASN:CB	2.60	0.50
1:C:659:LEU:N	1:C:694:ARG:HH22	2.09	0.50
1:C:679:PHE:HZ	1:C:684:LEU:HD22	1.76	0.50
1:D:784:ILE:HG13	1:D:786:TYR:CE1	2.46	0.50
1:A:669:SER:O	1:A:673:LYS:HG3	2.12	0.50
1:B:817:ALA:O	1:B:821:HIS:HB3	2.11	0.50
1:D:707:THR:HB	1:D:787:ILE:CG2	2.42	0.50
1:D:914:SER:O	1:D:915:ASN:ND2	2.43	0.50
1:D:677:TRP:NE1	1:D:1061:LEU:HB3	2.27	0.50
1:D:700:MET:CE	1:D:746:LEU:CD2	2.90	0.50
1:D:763:ILE:C	1:D:765:ASN:N	2.65	0.49
1:D:1069:HIS:HE2	1:D:1073:LYS:HD3	1.76	0.49
1:A:881:ARG:O	1:A:885:LEU:HG	2.11	0.49
1:A:942:ALA:HB1	1:A:1061:LEU:HB2	1.93	0.49
1:B:666:GLU:O	1:B:669:SER:HB3	2.12	0.49
1:D:844:TYR:CE2	1:D:852:ASN:HB3	2.47	0.49
1:A:705:GLN:OE1	1:A:710:LEU:HD12	2.12	0.49
1:D:866:PRO:HG2	1:D:867:GLU:OE1	2.13	0.49
1:C:969:LEU:HB2	1:C:971:LEU:HD12	1.95	0.49
1:D:787:ILE:CG2	1:D:788:SER:N	2.76	0.49
1:A:810:GLU:OE1	1:A:925:ARG:HD2	2.13	0.49
1:D:753:THR:HG1	1:D:815:TYR:HH	1.56	0.49
1:B:962:GLN:O	1:B:966:GLU:HG3	2.13	0.49
1:C:966:GLU:O	1:C:971:LEU:HB2	2.13	0.49
1:C:679:PHE:O	1:C:681:ILE:N	2.44	0.48
1:C:956:VAL:HG11	1:C:984:LEU:HD13	1.95	0.48
1:D:913:ASN:O	1:D:915:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:ARG:HA	1:B:728:GLU:OE1	2.13	0.48
1:B:897:LYS:NZ	5:B:363:HOH:O	2.46	0.48
1:B:849:VAL:HG23	5:B:100:HOH:O	2.13	0.48
1:D:815:TYR:N	1:D:815:TYR:CD2	2.80	0.48
1:D:912:VAL:C	1:D:914:SER:N	2.67	0.48
1:D:955:ILE:HG23	1:D:956:VAL:N	2.27	0.48
1:A:872:LEU:HD13	1:A:873:HIS:N	2.29	0.48
1:D:816:VAL:HG21	1:D:882:PHE:HZ	1.78	0.48
1:D:894:ASP:OD1	1:D:896:LYS:HB3	2.14	0.48
1:D:901:PHE:O	1:D:904:GLU:HB2	2.14	0.48
1:C:912:VAL:CG2	1:C:913:ASN:N	2.75	0.48
1:D:679:PHE:HZ	1:D:684:LEU:CD2	2.20	0.48
1:A:891:LEU:HD13	1:B:847:ARG:CZ	2.44	0.47
1:B:669:SER:O	1:B:672:GLU:HB3	2.14	0.47
1:D:855:ALA:HB2	1:D:890:ILE:HG21	1.95	0.47
1:D:881:ARG:HH11	1:D:881:ARG:CG	2.24	0.47
1:A:700:MET:CE	1:A:746:LEU:HD11	2.44	0.47
1:C:919:TRP:O	1:C:925:ARG:HD3	2.14	0.47
1:B:700:MET:CE	1:B:746:LEU:CD1	2.91	0.47
1:D:712:ILE:CD1	1:D:787:ILE:HD13	2.45	0.47
1:C:711:GLU:OE1	1:C:714:LYS:NZ	2.42	0.47
1:D:917:ILE:HD12	1:D:924:ASP:HB3	1.96	0.47
1:D:1004:ASP:CB	1:D:1009:LEU:HD12	2.44	0.47
1:A:924:ASP:O	1:A:928:VAL:HG23	2.14	0.47
1:B:865:ARG:HD3	1:B:867:GLU:OE2	2.15	0.47
1:C:846:ASP:OD2	1:D:883:ARG:NH1	2.45	0.47
1:D:1009:LEU:HD23	1:D:1010:PRO:HD2	1.97	0.47
1:B:945:ARG:O	1:B:949:LEU:HG	2.15	0.47
1:D:1014:LEU:O	1:D:1015:GLU:O	2.32	0.47
1:A:805:ASN:HD22	1:A:805:ASN:N	2.11	0.47
1:B:912:VAL:HG12	1:B:913:ASN:ND2	2.30	0.47
1:B:993:THR:OG1	1:B:1069:HIS:HE1	1.97	0.47
1:C:718:GLN:HG3	1:C:722:ASN:HD21	1.79	0.47
1:D:760:LEU:HD23	1:D:800:GLY:O	2.15	0.47
1:D:762:GLN:OE1	1:D:804:SER:CB	2.62	0.47
1:B:917:ILE:HG22	1:B:918:GLU:N	2.29	0.46
1:B:938:ILE:HD11	1:B:999:LEU:HD23	1.96	0.46
1:C:1004:ASP:CB	1:C:1009:LEU:HD12	2.45	0.46
1:A:703:LEU:HD22	1:A:750:TRP:CE2	2.50	0.46
1:A:902:LEU:HD11	1:A:1002:SER:OG	2.15	0.46
1:B:994:HIS:HB2	1:B:995:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:LEU:HD11	1:A:933:ILE:HB	1.97	0.46
1:C:912:VAL:CG2	1:C:913:ASN:H	2.29	0.46
1:B:816:VAL:O	1:B:819:ALA:HB3	2.15	0.46
1:D:1007:GLY:C	1:D:1008:LEU:HD23	2.35	0.46
1:A:823:TYR:HE2	1:A:857:SER:HB3	1.80	0.46
1:D:694:ARG:HD2	1:D:725:ARG:HG2	1.97	0.46
1:D:716:PRO:HG2	1:D:719:GLN:NE2	2.31	0.46
1:C:845:ASN:HB3	1:D:887:ILE:HD13	1.98	0.46
1:D:700:MET:CE	1:D:746:LEU:HD21	2.45	0.46
1:B:939:ASN:ND2	1:B:940:GLY:N	2.63	0.46
1:D:960:TYR:HB3	1:D:979:ARG:CZ	2.45	0.46
1:D:1013:TRP:HA	1:D:1057:ILE:CG2	2.44	0.46
1:D:734:ILE:HD11	1:D:737:HIS:HB2	1.98	0.45
1:B:762:GLN:OE1	1:B:762:GLN:HA	2.16	0.45
1:B:918:GLU:C	1:B:920:SER:H	2.20	0.45
1:C:695:ILE:O	1:C:699:VAL:HG23	2.15	0.45
1:D:715:ILE:HG23	1:D:870:PHE:HB2	1.97	0.45
1:D:845:ASN:O	1:D:847:ARG:HG3	2.15	0.45
1:C:703:LEU:HD22	1:C:750:TRP:CD2	2.51	0.45
1:D:670:LEU:HD23	1:D:670:LEU:O	2.16	0.45
1:D:691:LYS:HE2	1:D:691:LYS:HB3	1.83	0.45
1:D:859:TRP:CZ2	1:D:883:ARG:HA	2.51	0.45
1:A:859:TRP:CE2	1:A:883:ARG:HD2	2.51	0.45
1:C:732:ARG:HH11	1:C:826:PRO:HA	1.80	0.45
1:D:794:ASN:OD1	1:D:800:GLY:HA2	2.16	0.45
1:B:783:ARG:HH11	1:B:783:ARG:HG2	1.82	0.45
1:B:1014:LEU:H	1:B:1014:LEU:CD1	2.17	0.45
1:A:851:GLU:HB3	1:A:891:LEU:HD23	1.99	0.45
1:A:944:VAL:HG12	1:A:947:LEU:HD22	1.99	0.45
1:A:960:TYR:HB3	1:A:979:ARG:CZ	2.47	0.45
1:C:729:ASN:HA	1:C:739:ARG:HH22	1.81	0.45
1:C:762:GLN:HA	1:C:805:ASN:HD21	1.82	0.45
1:C:1061:LEU:HD12	1:C:1062:MET:N	2.32	0.45
1:B:700:MET:HE2	1:B:746:LEU:CD2	2.46	0.44
1:C:851:GLU:OE1	1:C:894:ASP:HB2	2.17	0.44
1:D:737:HIS:NE2	5:D:45:HOH:O	2.36	0.44
1:D:847:ARG:O	1:D:848:SER:C	2.54	0.44
1:A:758:PRO:HG3	1:A:799:TYR:CE2	2.51	0.44
1:A:869:ASN:ND2	1:A:872:LEU:HB3	2.33	0.44
1:B:804:SER:C	1:B:805:ASN:HD22	2.20	0.44
1:C:832:PHE:O	1:C:835:ALA:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:909:ALA:HB2	1:B:917:ILE:CD1	2.41	0.44
1:D:738:ASN:HB2	5:D:342:HOH:O	2.18	0.44
1:D:871:LEU:O	1:D:874:LEU:HB2	2.18	0.44
1:D:944:VAL:O	1:D:945:ARG:C	2.56	0.44
1:B:670:LEU:HA	1:B:673:LYS:NZ	2.32	0.44
1:C:847:ARG:O	1:C:848:SER:C	2.55	0.44
1:C:718:GLN:O	1:C:722:ASN:ND2	2.50	0.44
1:C:739:ARG:HG3	5:C:311:HOH:O	2.18	0.44
1:D:674:MET:HE1	1:D:703:LEU:HD21	2.00	0.44
1:A:872:LEU:HD12	1:A:872:LEU:N	2.33	0.43
1:A:891:LEU:HD13	1:B:847:ARG:NH1	2.33	0.43
1:A:881:ARG:HG3	1:A:881:ARG:NH1	2.31	0.43
1:C:846:ASP:CG	1:D:883:ARG:HH12	2.21	0.43
1:C:915:ASN:O	1:C:916:GLY:O	2.37	0.43
1:D:712:ILE:HD12	1:D:787:ILE:HD11	2.00	0.43
1:B:696:LEU:N	1:B:728:GLU:OE2	2.51	0.43
1:C:748:ALA:HB2	5:C:337:HOH:O	2.18	0.43
1:B:670:LEU:O	1:B:674:MET:HG3	2.17	0.43
1:B:674:MET:C	1:B:676:ASN:H	2.21	0.43
1:B:758:PRO:HB2	1:B:1057:ILE:HD13	1.99	0.43
1:C:670:LEU:CD2	1:C:674:MET:SD	3.07	0.43
1:B:694:ARG:O	1:B:698:GLN:HG2	2.19	0.43
1:D:757:VAL:HG13	1:D:1009:LEU:O	2.18	0.43
1:A:796:ASP:OD1	1:A:798:SER:OG	2.12	0.43
1:C:1060:GLN:O	1:C:1063:HIS:HB3	2.18	0.43
1:A:758:PRO:HG3	1:A:799:TYR:HE2	1.84	0.43
1:D:663:LEU:HA	1:D:666:GLU:OE1	2.19	0.43
1:D:1009:LEU:HA	1:D:1010:PRO:HD2	1.91	0.43
1:B:674:MET:CE	1:B:699:VAL:HG13	2.48	0.43
1:B:729:ASN:HA	1:B:739:ARG:HH22	1.82	0.43
1:C:670:LEU:HD23	1:C:674:MET:SD	2.59	0.43
1:D:1055:ARG:CG	1:D:1056:ARG:H	2.32	0.43
1:B:810:GLU:HG2	1:B:885:LEU:HD13	2.01	0.43
1:B:812:MET:HG2	1:B:882:PHE:HE1	1.83	0.43
1:D:952:THR:O	1:D:956:VAL:HG13	2.19	0.43
1:A:994:HIS:HB2	1:A:995:ILE:HD12	2.00	0.42
1:D:700:MET:HE3	1:D:746:LEU:CD2	2.49	0.42
1:B:758:PRO:HB3	1:B:1013:TRP:CE2	2.55	0.42
1:B:908:LYS:HD2	1:B:924:ASP:OD1	2.19	0.42
1:D:750:TRP:CZ2	1:D:755:ARG:NH2	2.85	0.42
1:A:811:LEU:HD23	1:A:811:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:918:GLU:C	1:B:920:SER:N	2.72	0.42
1:C:743:THR:O	1:C:746:LEU:HB3	2.20	0.42
1:C:807:PRO:HG2	1:C:810:GLU:CD	2.40	0.42
1:D:852:ASN:OD1	1:D:891:LEU:HD21	2.18	0.42
1:A:679:PHE:HD1	1:A:680:PRO:HD2	1.84	0.42
1:D:712:ILE:HD12	1:D:787:ILE:HD13	2.00	0.42
1:D:755:ARG:O	1:D:757:VAL:HG23	2.19	0.42
1:D:874:LEU:HG	1:D:878:GLU:OE2	2.19	0.42
1:D:1055:ARG:CG	1:D:1056:ARG:N	2.82	0.42
1:A:669:SER:O	1:A:672:GLU:HB3	2.19	0.42
1:B:941:PRO:HD3	4:B:462:666:C40	2.50	0.42
1:C:755:ARG:NH2	1:C:789:SER:OG	2.52	0.42
1:C:763:ILE:CG1	1:C:764:HIS:N	2.80	0.42
1:D:1062:MET:HA	1:D:1062:MET:HE2	2.01	0.42
1:A:983:GLN:OE1	1:A:986:LYS:HD3	2.20	0.42
1:B:714:LYS:HE3	1:B:714:LYS:HA	2.02	0.42
1:D:990:SER:HB3	4:D:464:666:I54	2.90	0.42
4:D:464:666:H181	5:D:320:HOH:O	2.20	0.42
1:B:865:ARG:HG3	1:B:865:ARG:HH11	1.84	0.42
1:A:758:PRO:HB3	1:A:1013:TRP:CE2	2.55	0.41
1:D:806:ILE:HA	1:D:807:PRO:HD2	1.93	0.41
1:A:956:VAL:HG11	1:A:984:LEU:HD13	2.01	0.41
1:B:691:LYS:HE3	1:B:694:ARG:HH21	1.85	0.41
1:B:812:MET:HG2	1:B:882:PHE:CE1	2.55	0.41
1:C:681:ILE:O	1:C:685:VAL:HG23	2.20	0.41
1:D:935:LEU:HD12	1:D:935:LEU:HA	1.92	0.41
1:D:1062:MET:HB2	1:D:1062:MET:HE3	1.92	0.41
1:B:959:PHE:HB3	1:B:977:MET:HG2	2.00	0.41
1:C:700:MET:HE3	1:C:746:LEU:HD13	2.00	0.41
1:D:691:LYS:HE3	1:D:694:ARG:NH2	2.35	0.41
1:D:695:ILE:HG23	1:D:696:LEU:N	2.35	0.41
1:D:939:ASN:HD22	1:D:943:LYS:HG2	1.86	0.41
1:A:847:ARG:HB3	5:A:229:HOH:O	2.20	0.41
1:B:807:PRO:HD2	1:B:925:ARG:HD3	2.02	0.41
1:C:939:ASN:ND2	1:C:939:ASN:C	2.73	0.41
1:D:860:ASN:ND2	1:D:860:ASN:C	2.74	0.41
1:A:671:ILE:HD13	1:A:671:ILE:HA	1.93	0.41
1:A:677:TRP:O	1:A:943:LYS:HE2	2.20	0.41
1:B:760:LEU:HD23	1:B:801:CYS:N	2.35	0.41
1:B:821:HIS:NE2	1:B:822:ASP:OD2	2.53	0.41
1:B:952:THR:HG23	1:B:988:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1007:GLY:HA2	5:B:251:HOH:O	2.21	0.41
1:B:1014:LEU:O	1:B:1015:GLU:CB	2.68	0.41
1:C:952:THR:O	1:C:956:VAL:HG13	2.20	0.41
1:D:700:MET:HE3	1:D:746:LEU:HD22	2.02	0.41
1:D:713:PHE:O	1:D:714:LYS:C	2.58	0.41
1:D:1013:TRP:CZ3	1:D:1055:ARG:HB3	2.56	0.41
1:A:845:ASN:O	1:A:846:ASP:HB2	2.21	0.41
1:C:674:MET:HE3	1:C:699:VAL:HG13	2.03	0.41
1:B:953:GLU:O	1:B:956:VAL:HG22	2.20	0.41
1:A:741:HIS:O	1:A:745:VAL:HG23	2.21	0.41
1:C:887:ILE:HD13	1:D:845:ASN:HB3	2.03	0.41
1:D:872:LEU:HD12	1:D:872:LEU:N	2.35	0.41
1:B:783:ARG:HG2	1:B:783:ARG:NH1	2.36	0.41
1:D:881:ARG:HG3	1:D:881:ARG:NH1	2.32	0.41
1:C:663:LEU:HD13	1:C:666:GLU:OE1	2.20	0.40
1:C:847:ARG:O	1:C:849:VAL:N	2.54	0.40
1:C:909:ALA:HB2	1:C:917:ILE:CD1	2.52	0.40
1:C:998:PRO:HA	5:C:424:HOH:O	2.21	0.40
1:D:683:GLU:O	1:D:686:GLU:HB3	2.20	0.40
1:D:942:ALA:HB1	1:D:1061:LEU:HB2	2.03	0.40
1:A:1061:LEU:HD23	1:A:1061:LEU:N	2.20	0.40
1:B:755:ARG:HD2	5:B:387:HOH:O	2.20	0.40
1:C:1057:ILE:HD12	1:C:1057:ILE:O	2.21	0.40
1:D:904:GLU:O	1:D:905:PHE:C	2.60	0.40
1:B:748:ALA:HB3	1:B:936:ALA:HB1	2.04	0.40
1:C:960:TYR:HB3	1:C:979:ARG:CZ	2.52	0.40
1:D:688:MET:HE2	1:D:691:LYS:O	2.21	0.40
1:A:674:MET:C	1:A:676:ASN:H	2.25	0.40
1:B:897:LYS:HE2	1:B:897:LYS:HB3	1.91	0.40
1:D:780:ASN:N	1:D:780:ASN:HD22	2.20	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	357/420 (85%)	337 (94%)	18 (5%)	2 (1%)	25 36
1	B	357/420 (85%)	325 (91%)	26 (7%)	6 (2%)	9 11
1	C	366/420 (87%)	336 (92%)	25 (7%)	5 (1%)	11 15
1	D	359/420 (86%)	319 (89%)	31 (9%)	9 (2%)	5 6
All	All	1439/1680 (86%)	1317 (92%)	100 (7%)	22 (2%)	10 14

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	912	VAL
1	B	913	ASN
1	C	660	ASP
1	D	914	SER
1	D	1015	GLU
1	A	869	ASN
1	B	919	TRP
1	C	848	SER
1	C	916	GLY
1	D	764	HIS
1	A	660	ASP
1	B	689	GLY
1	D	848	SER
1	D	908	LYS
1	D	909	ALA
1	C	912	VAL
1	D	796	ASP
1	D	915	ASN
1	C	662	ILE
1	B	763	ILE
1	D	758	PRO
1	B	940	GLY

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	310/370 (84%)	293 (94%)	17 (6%)	21	35
1	B	308/370 (83%)	295 (96%)	13 (4%)	30	47
1	C	313/370 (85%)	301 (96%)	12 (4%)	33	51
1	D	308/370 (83%)	288 (94%)	20 (6%)	17	27
All	All	1239/1480 (84%)	1177 (95%)	62 (5%)	24	40

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	666	GLU
1	A	694	ARG
1	A	700	MET
1	A	706	ASP
1	A	792	CYS
1	A	820	MET
1	A	828	ARG
1	A	872	LEU
1	A	883	ARG
1	A	915	ASN
1	A	918	GLU
1	A	939	ASN
1	A	947	LEU
1	A	965	GLU
1	A	1056	ARG
1	A	1061	LEU
1	A	1069	HIS
1	B	665	GLU
1	B	705	GLN
1	B	714	LYS
1	B	719	GLN
1	B	755	ARG
1	B	820	MET
1	B	828	ARG
1	B	872	LEU
1	B	939	ASN
1	B	946	ASP
1	B	947	LEU
1	B	1014	LEU
1	B	1015	GLU
1	C	669	SER

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Mol	Chain	Res	Type
1	C	705	GLN
1	C	711	GLU
1	C	719	GLN
1	C	780	ASN
1	C	792	CYS
1	C	820	MET
1	C	828	ARG
1	C	869	ASN
1	C	939	ASN
1	C	947	LEU
1	C	1061	LEU
1	D	670	LEU
1	D	705	GLN
1	D	719	GLN
1	D	781	HIS
1	D	788	SER
1	D	796	ASP
1	D	821	HIS
1	D	847	ARG
1	D	857	SER
1	D	860	ASN
1	D	872	LEU
1	D	875	ASP
1	D	910	ASN
1	D	911	ASP
1	D	917	ILE
1	D	939	ASN
1	D	946	ASP
1	D	990	SER
1	D	1008	LEU
1	D	1057	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	762	GLN
1	A	764	HIS
1	A	805	ASN
1	A	923	ASN
1	A	939	ASN
1	A	1012	GLN
1	B	698	GLN

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Mol	Chain	Res	Type
1	B	705	GLN
1	B	718	GLN
1	B	719	GLN
1	B	722	ASN
1	B	805	ASN
1	B	869	ASN
1	B	923	ASN
1	B	939	ASN
1	B	994	HIS
1	B	1060	GLN
1	B	1069	HIS
1	C	705	GLN
1	C	718	GLN
1	C	719	GLN
1	C	722	ASN
1	C	805	ASN
1	C	869	ASN
1	C	923	ASN
1	C	939	ASN
1	D	718	GLN
1	D	719	GLN
1	D	729	ASN
1	D	805	ASN
1	D	860	ASN
1	D	876	HIS
1	D	898	HIS
1	D	913	ASN
1	D	923	ASN
1	D	939	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
3	HG9	A	454	-	23,23,24	1.71	6 (26%)	27,28,29	1.48	4 (14%)
4	666	D	464	-	33,33,33	3.88	25 (75%)	43,46,46	2.74	13 (30%)
3	HG9	B	451	-	23,23,24	1.86	5 (21%)	27,28,29	1.15	2 (7%)
3	HG9	A	453	-	23,23,24	1.51	3 (13%)	27,28,29	1.27	3 (11%)
3	HG9	B	452	-	23,23,24	1.47	3 (13%)	27,28,29	1.29	5 (18%)
4	666	B	462	-	33,33,33	3.81	22 (66%)	43,46,46	2.66	9 (20%)
4	666	A	461	-	33,33,33	3.89	25 (75%)	43,46,46	2.66	12 (27%)
4	666	C	463	-	33,33,33	3.83	24 (72%)	43,46,46	2.73	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HG9	A	454	-	-	6/32/32/33	-
4	666	D	464	-	-	1/12/39/39	0/4/4/4
3	HG9	B	451	-	-	4/32/32/33	-
3	HG9	A	453	-	-	4/32/32/33	-
3	HG9	B	452	-	-	5/32/32/33	-
4	666	B	462	-	-	1/12/39/39	0/4/4/4
4	666	A	461	-	-	1/12/39/39	0/4/4/4
4	666	C	463	-	-	1/12/39/39	0/4/4/4

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	464	666	C15-N26	10.29	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	461	666	C15-N26	10.13	1.49	1.35
4	B	462	666	C37-N38	9.81	1.39	1.29
4	B	462	666	C15-N26	9.80	1.49	1.35
4	A	461	666	C37-N38	9.52	1.38	1.29
4	C	463	666	C15-N26	9.43	1.48	1.35
4	D	464	666	C37-N38	8.96	1.38	1.29
4	C	463	666	C37-N38	7.84	1.37	1.29
4	C	463	666	C4-C5	6.87	1.49	1.38
4	D	464	666	C4-C5	6.66	1.49	1.38
4	B	462	666	C17-C18	6.35	1.72	1.52
4	A	461	666	C4-C5	6.20	1.48	1.38
4	D	464	666	C17-C18	6.01	1.71	1.52
4	A	461	666	C17-C18	5.91	1.71	1.52
4	B	462	666	C4-C5	5.86	1.48	1.38
4	C	463	666	C17-C18	5.79	1.70	1.52
4	C	463	666	C19-C12	5.52	1.58	1.46
4	A	461	666	C19-C12	5.42	1.58	1.46
4	B	462	666	C19-C12	5.40	1.58	1.46
4	C	463	666	C4-C3	4.99	1.47	1.39
4	D	464	666	C42-C37	4.79	1.58	1.51
4	A	461	666	C42-C37	4.62	1.58	1.51
3	A	454	HG9	C27-C30	4.59	1.61	1.51
3	B	452	HG9	C27-C30	4.57	1.61	1.51
4	D	464	666	C19-C12	4.49	1.56	1.46
4	D	464	666	C16-C15	4.42	1.57	1.49
4	B	462	666	C2-C3	4.31	1.48	1.38
4	A	461	666	N39-N38	-4.28	1.27	1.38
3	B	451	HG9	C36-C37	4.24	1.58	1.52
4	C	463	666	C42-C37	4.23	1.57	1.51
3	A	453	HG9	C27-C30	4.22	1.60	1.51
4	C	463	666	C11-C3	4.18	1.58	1.51
4	B	462	666	C42-C37	4.15	1.57	1.51
4	D	464	666	C4-C3	4.00	1.46	1.39
3	B	451	HG9	C30-N33	3.96	1.43	1.35
4	A	461	666	C4-C3	3.88	1.45	1.39
4	C	463	666	N39-N38	-3.87	1.28	1.38
3	B	451	HG9	C27-C30	3.85	1.59	1.51
4	A	461	666	C16-C15	3.85	1.56	1.49
4	D	464	666	C32-C27	3.74	1.45	1.39
4	D	464	666	C2-C3	3.71	1.46	1.38
3	A	454	HG9	C36-C37	3.66	1.57	1.52
4	C	463	666	C2-C3	3.66	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	462	666	C16-C15	3.64	1.55	1.49
4	D	464	666	N39-N38	-3.60	1.29	1.38
4	C	463	666	C16-C15	3.59	1.55	1.49
3	A	453	HG9	C36-C37	3.58	1.57	1.52
4	D	464	666	C31-C30	3.57	1.45	1.39
4	A	461	666	C2-C3	3.56	1.46	1.38
4	B	462	666	N39-N38	-3.52	1.29	1.38
4	B	462	666	C4-C3	3.48	1.45	1.39
4	D	464	666	C41-C40	3.37	1.56	1.50
4	A	461	666	C1-C6	3.36	1.46	1.38
4	A	461	666	C18-C19	3.33	1.55	1.50
4	B	462	666	C1-C2	3.31	1.45	1.38
4	C	463	666	C27-N26	-3.27	1.35	1.41
4	A	461	666	C31-C30	3.25	1.44	1.39
4	C	463	666	C31-C30	3.24	1.44	1.39
4	C	463	666	C11-C12	3.22	1.55	1.51
4	C	463	666	C41-C40	3.16	1.56	1.50
4	C	463	666	C32-C27	3.12	1.44	1.39
4	D	464	666	C11-C3	3.09	1.56	1.51
4	B	462	666	C32-C27	3.07	1.44	1.39
4	A	461	666	C32-C31	3.05	1.44	1.38
4	D	464	666	C32-C31	3.05	1.44	1.38
4	C	463	666	C29-C30	3.02	1.44	1.39
4	B	462	666	C41-C40	3.00	1.55	1.50
4	A	461	666	C27-N26	-3.00	1.35	1.41
4	C	463	666	C1-C6	2.99	1.45	1.38
3	B	451	HG9	C37-C40	2.96	1.59	1.53
4	D	464	666	C18-C19	2.92	1.54	1.50
4	A	461	666	C32-C27	2.89	1.44	1.39
4	B	462	666	C18-C19	2.89	1.54	1.50
3	A	454	HG9	C36-N33	2.87	1.53	1.47
4	B	462	666	C1-C6	2.86	1.44	1.38
4	C	463	666	C1-C2	2.83	1.44	1.38
4	B	462	666	C31-C30	2.81	1.44	1.39
3	B	451	HG9	C36-N33	2.78	1.53	1.47
3	B	452	HG9	C30-N33	2.77	1.40	1.35
4	D	464	666	C29-C30	2.74	1.44	1.39
4	B	462	666	C29-C30	2.73	1.44	1.39
4	D	464	666	C17-C16	2.71	1.60	1.52
4	C	463	666	C6-C5	2.56	1.44	1.38
4	A	461	666	C41-C40	2.51	1.54	1.50
3	A	453	HG9	C30-N33	2.50	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	461	666	C6-C5	2.49	1.44	1.38
4	A	461	666	C1-C2	2.41	1.44	1.38
4	A	461	666	C17-C16	2.41	1.59	1.52
4	B	462	666	C11-C3	2.40	1.55	1.51
4	B	462	666	C27-N26	-2.39	1.36	1.41
3	A	454	HG9	C37-C40	2.37	1.57	1.53
4	A	461	666	C29-C30	2.37	1.43	1.39
4	A	461	666	C5-I54	2.36	2.16	2.10
4	D	464	666	C1-C2	2.36	1.43	1.38
4	C	463	666	C28-C27	2.36	1.43	1.39
4	B	462	666	C28-C27	2.35	1.43	1.39
3	B	452	HG9	C36-C37	2.34	1.56	1.52
4	D	464	666	C6-C5	2.33	1.43	1.38
4	B	462	666	C17-C16	2.33	1.59	1.52
4	D	464	666	C1-C6	2.31	1.43	1.38
4	C	463	666	C32-C31	2.30	1.42	1.38
4	C	463	666	C18-C19	2.29	1.53	1.50
4	D	464	666	C27-N26	-2.25	1.37	1.41
4	D	464	666	O45-C19	-2.22	1.18	1.23
3	A	454	HG9	C30-N33	2.19	1.39	1.35
4	A	461	666	O46-C40	-2.19	1.18	1.23
4	D	464	666	C11-C12	2.19	1.54	1.51
4	B	462	666	C32-C31	2.16	1.42	1.38
4	A	461	666	C28-C27	2.15	1.42	1.39
4	C	463	666	C17-C16	2.13	1.58	1.52
4	A	461	666	C11-C12	2.08	1.54	1.51
4	D	464	666	C28-C27	2.05	1.42	1.39
3	A	454	HG9	C41-C40	2.04	1.57	1.53

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	462	666	C11-C12-C19	-9.79	102.99	118.50
4	D	464	666	C11-C12-C19	-9.57	103.33	118.50
4	A	461	666	C11-C12-C19	-8.99	104.26	118.50
4	C	463	666	C11-C12-C19	-8.21	105.49	118.50
4	C	463	666	C19-C12-C15	-8.16	113.59	120.37
4	D	464	666	C37-N38-N39	8.02	125.83	116.97
4	A	461	666	C19-C12-C15	-7.26	114.34	120.37
4	C	463	666	C37-N38-N39	7.19	124.92	116.97
4	B	462	666	C37-N38-N39	7.17	124.89	116.97
4	A	461	666	C37-N38-N39	7.10	124.82	116.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	462	666	C19-C12-C15	-6.57	114.92	120.37
4	D	464	666	C19-C12-C15	-6.21	115.21	120.37
4	C	463	666	C30-C37-N38	5.75	122.10	117.14
4	D	464	666	C42-C37-N38	-5.62	115.71	122.84
4	B	462	666	C42-C37-N38	-5.22	116.22	122.84
4	B	462	666	C30-C37-N38	5.19	121.62	117.14
4	C	463	666	C42-C37-N38	-5.06	116.42	122.84
4	A	461	666	C42-C37-N38	-4.80	116.75	122.84
4	A	461	666	C30-C37-N38	4.53	121.05	117.14
3	A	454	HG9	C35-N33-C36	4.35	121.58	116.41
4	D	464	666	C27-N26-C15	4.19	136.44	127.21
4	B	462	666	C27-N26-C15	3.90	135.81	127.21
4	A	461	666	C27-N26-C15	3.87	135.73	127.21
4	C	463	666	C27-N26-C15	3.86	135.71	127.21
4	D	464	666	C30-C37-N38	3.66	120.30	117.14
3	A	454	HG9	C36-C37-C40	3.33	119.08	109.79
3	A	453	HG9	C60-C35-N33	3.33	121.17	112.55
4	C	463	666	C16-C15-N26	3.06	123.23	117.40
3	A	454	HG9	C60-C35-N33	3.05	120.45	112.55
4	A	461	666	C16-C15-N26	3.04	123.18	117.40
4	C	463	666	C6-C5-C4	-3.03	117.53	121.09
4	D	464	666	C16-C15-N26	2.96	123.04	117.40
3	B	451	HG9	C36-C37-C40	2.96	118.05	109.79
4	B	462	666	C16-C15-N26	2.92	122.96	117.40
3	A	453	HG9	C35-N33-C36	2.86	119.81	116.41
4	D	464	666	C3-C11-C12	-2.82	109.03	114.32
3	B	452	HG9	C35-N33-C36	2.80	119.74	116.41
4	A	461	666	C6-C5-C4	-2.78	117.83	121.09
4	C	463	666	C18-C17-C16	-2.73	103.22	112.02
3	B	452	HG9	O53-C42-C43	-2.65	102.94	109.14
4	D	464	666	C17-C18-C19	2.57	118.14	113.58
4	A	461	666	C18-C17-C16	-2.57	103.74	112.02
4	B	462	666	C18-C17-C16	-2.56	103.78	112.02
4	A	461	666	C17-C18-C19	2.36	117.77	113.58
4	D	464	666	C6-C5-C4	-2.29	118.39	121.09
4	B	462	666	C17-C18-C19	2.24	117.56	113.58
3	B	452	HG9	O44-C43-C42	-2.24	106.19	111.07
4	D	464	666	C18-C17-C16	-2.23	104.83	112.02
3	B	451	HG9	C60-C35-N33	2.20	118.25	112.55
3	A	454	HG9	C35-N33-C30	-2.20	113.26	121.03
3	B	452	HG9	C36-C37-C40	2.07	115.58	109.79
4	D	464	666	C4-C5-I54	2.06	121.99	119.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	461	666	C29-C30-C37	-2.05	118.32	120.75
4	A	461	666	C42-C41-C40	2.04	113.83	111.22
4	D	464	666	C42-C41-C40	2.03	113.82	111.22
3	A	453	HG9	C36-C37-C40	2.02	115.42	109.79
3	B	452	HG9	C60-C35-N33	2.01	117.76	112.55

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	453	HG9	N33-C36-C37-C40
3	A	453	HG9	N33-C36-C37-O47
3	A	454	HG9	N33-C36-C37-O47
3	B	451	HG9	N33-C36-C37-C40
3	B	451	HG9	N33-C36-C37-O47
3	B	452	HG9	C60-C35-N33-C36
3	B	452	HG9	N33-C36-C37-C40
3	B	452	HG9	N33-C36-C37-O47
4	A	461	666	C3-C11-C12-C19
4	B	462	666	C3-C11-C12-C19
4	C	463	666	C3-C11-C12-C19
4	D	464	666	C3-C11-C12-C19
3	B	452	HG9	C60-C35-N33-C30
3	A	453	HG9	C12-C15-C18-C21
3	A	454	HG9	C60-C35-N33-C36
3	B	452	HG9	C12-C15-C18-C21
3	A	454	HG9	O47-C37-C40-C41
3	B	451	HG9	C12-C15-C18-C21
3	A	454	HG9	C60-C35-N33-C30
3	A	454	HG9	O47-C37-C40-O49
3	A	453	HG9	C9-C12-C15-C18
3	B	451	HG9	O47-C37-C40-O49
3	A	454	HG9	C9-C12-C15-C18

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	464	666	3	0
3	B	451	HG9	2	0
3	A	453	HG9	2	0

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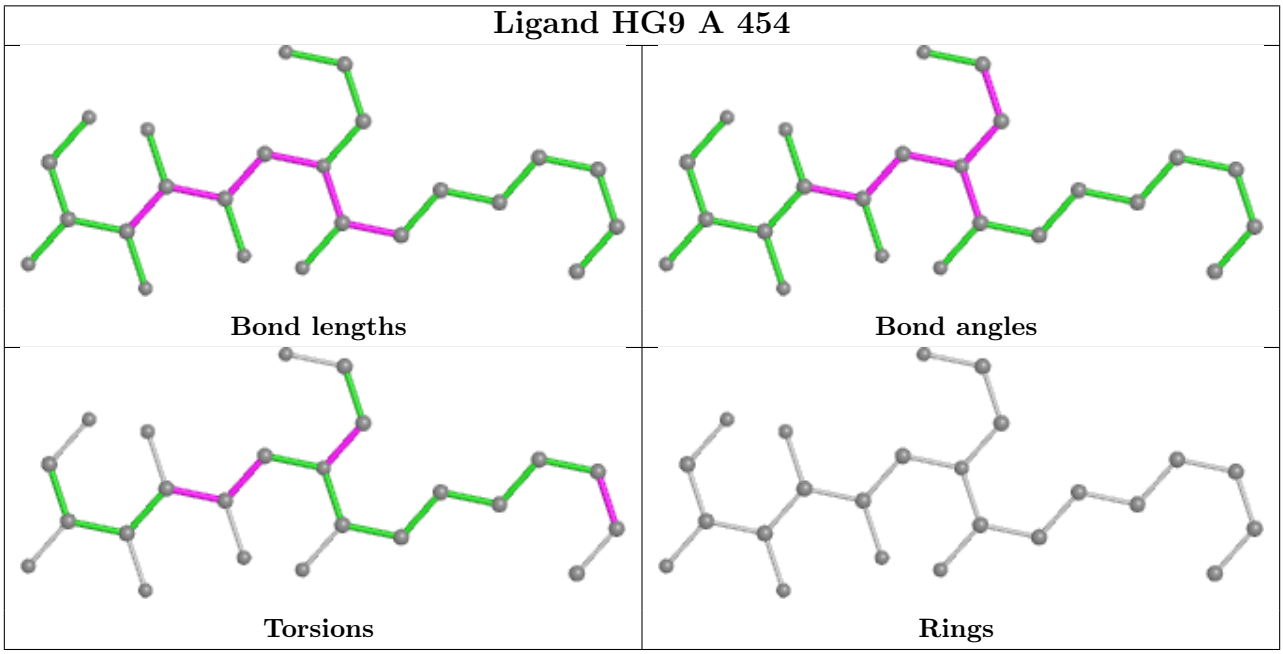
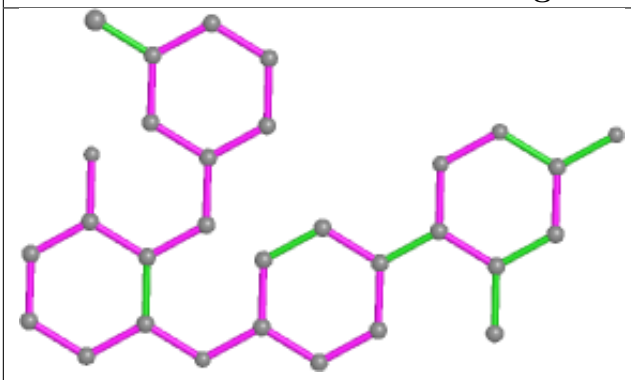
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	462	666	2	0
4	A	461	666	2	0
4	C	463	666	1	0

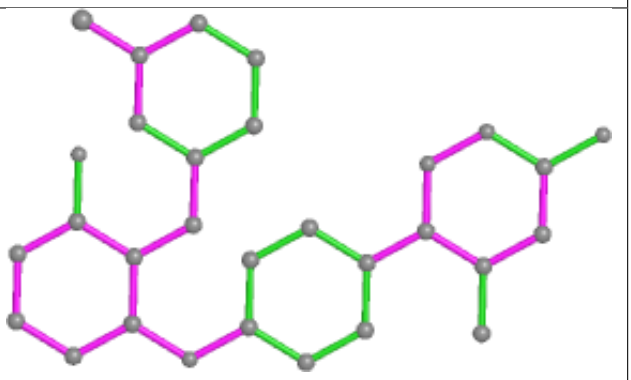
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



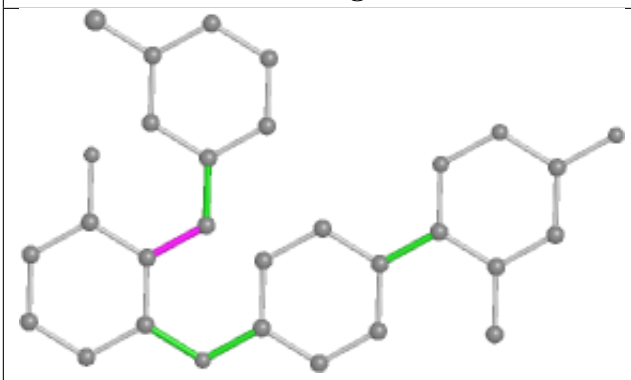
Ligand 666 D 464



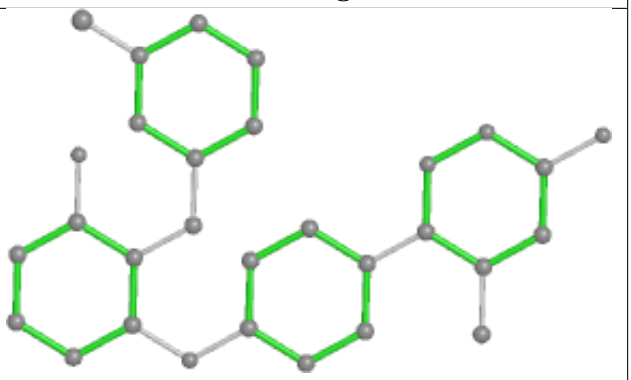
Bond lengths



Bond angles

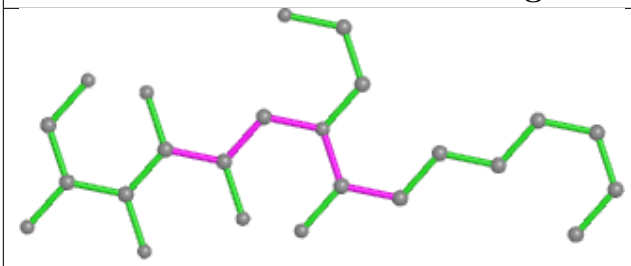


Torsions

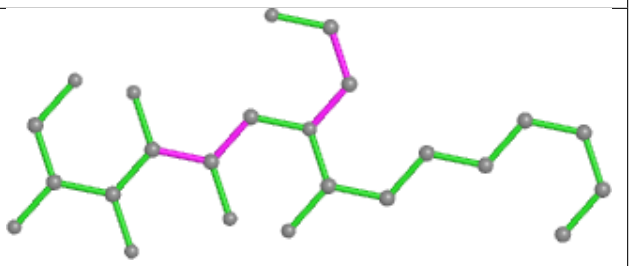


Rings

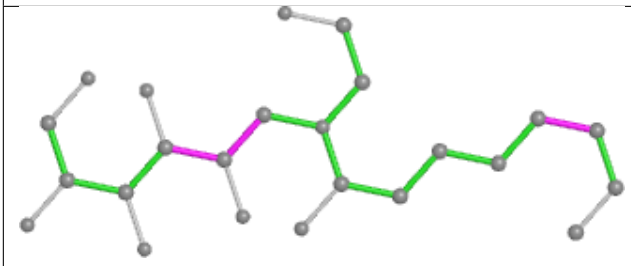
Ligand HG9 B 451



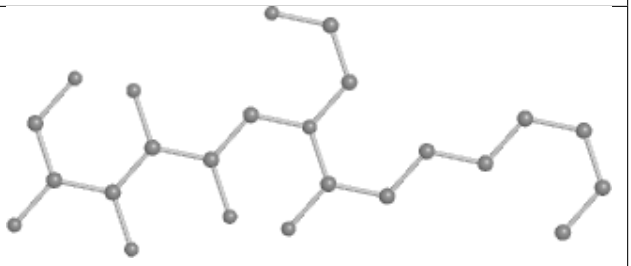
Bond lengths



Bond angles

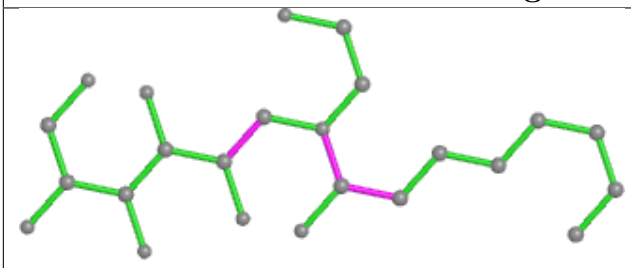


Torsions

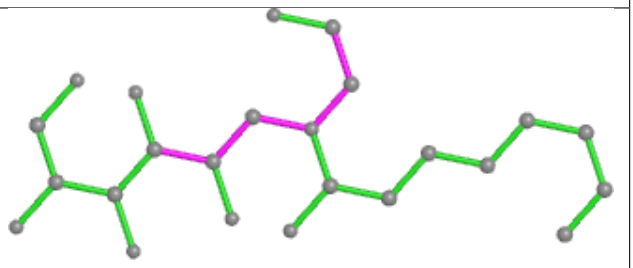


Rings

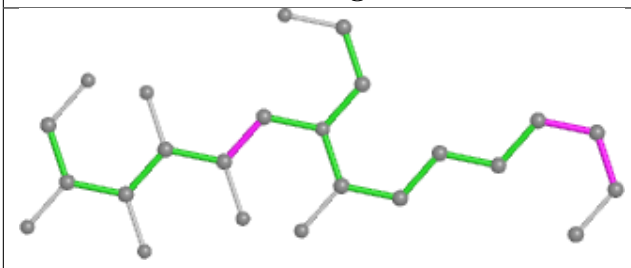
Ligand HG9 A 453



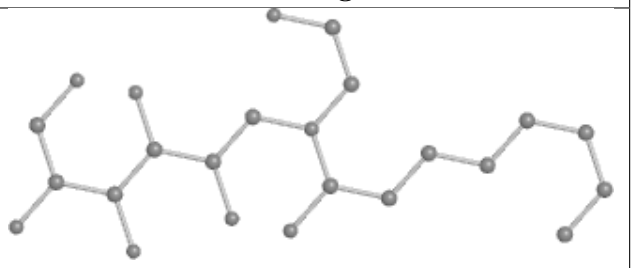
Bond lengths



Bond angles

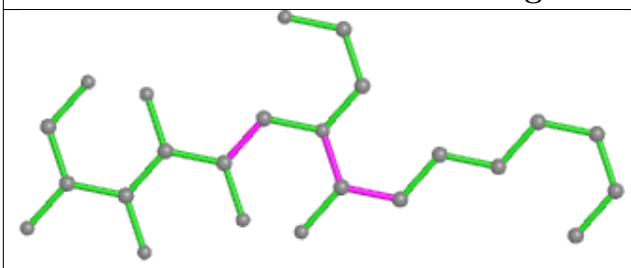


Torsions

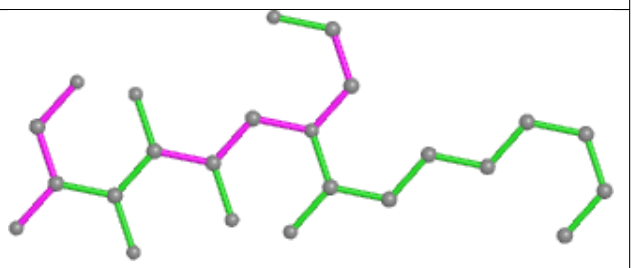


Rings

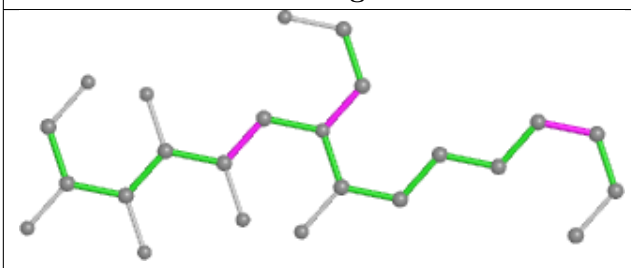
Ligand HG9 B 452



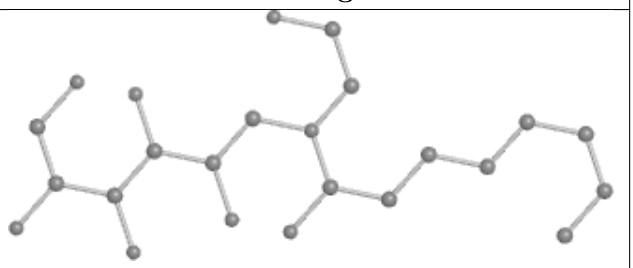
Bond lengths



Bond angles

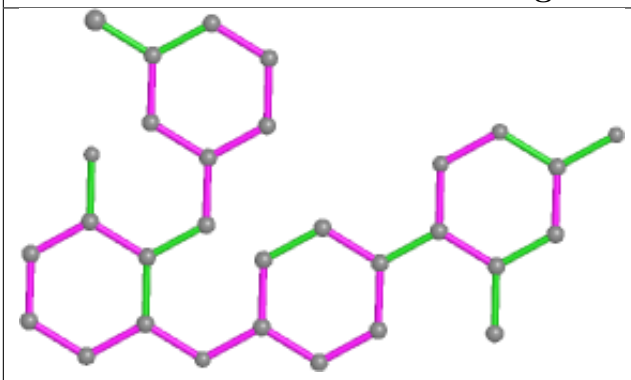


Torsions

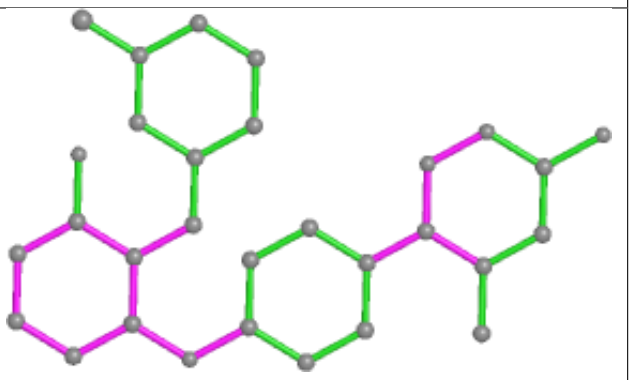


Rings

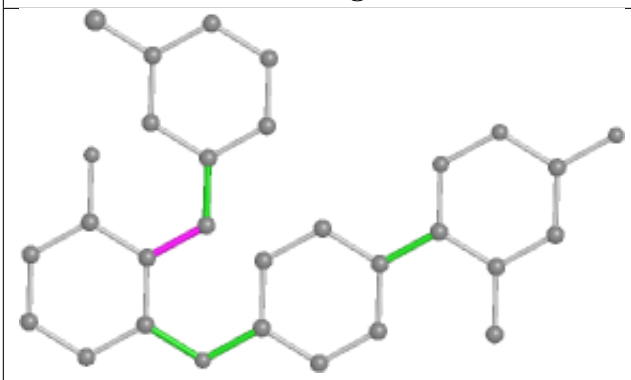
Ligand 666 B 462



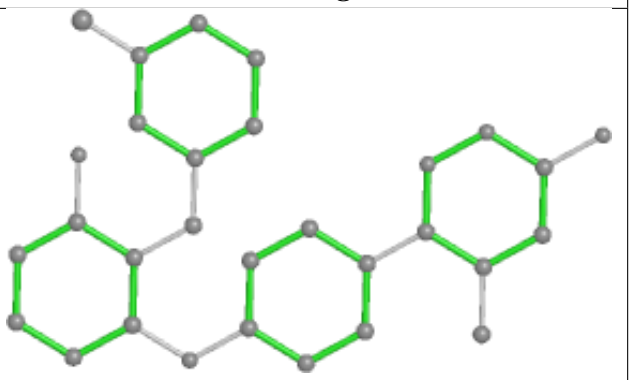
Bond lengths



Bond angles

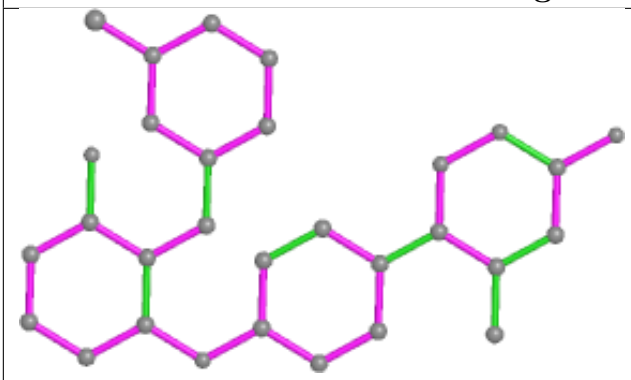


Torsions

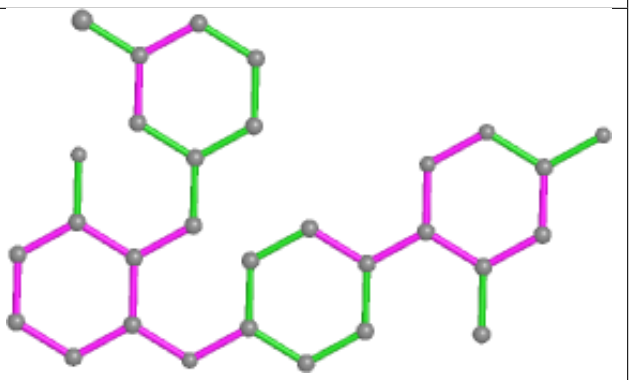


Rings

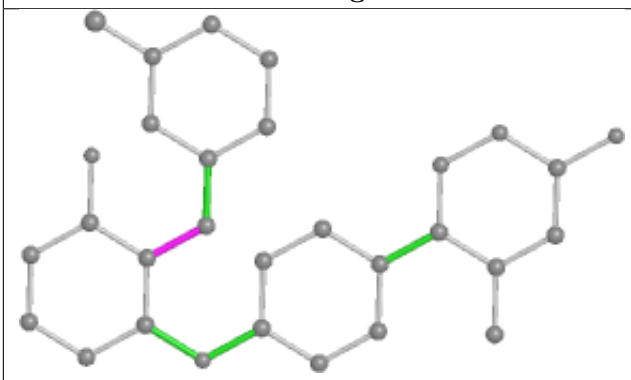
Ligand 666 A 461



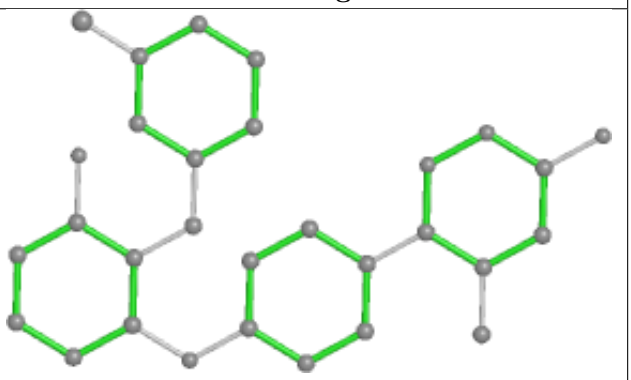
Bond lengths



Bond angles

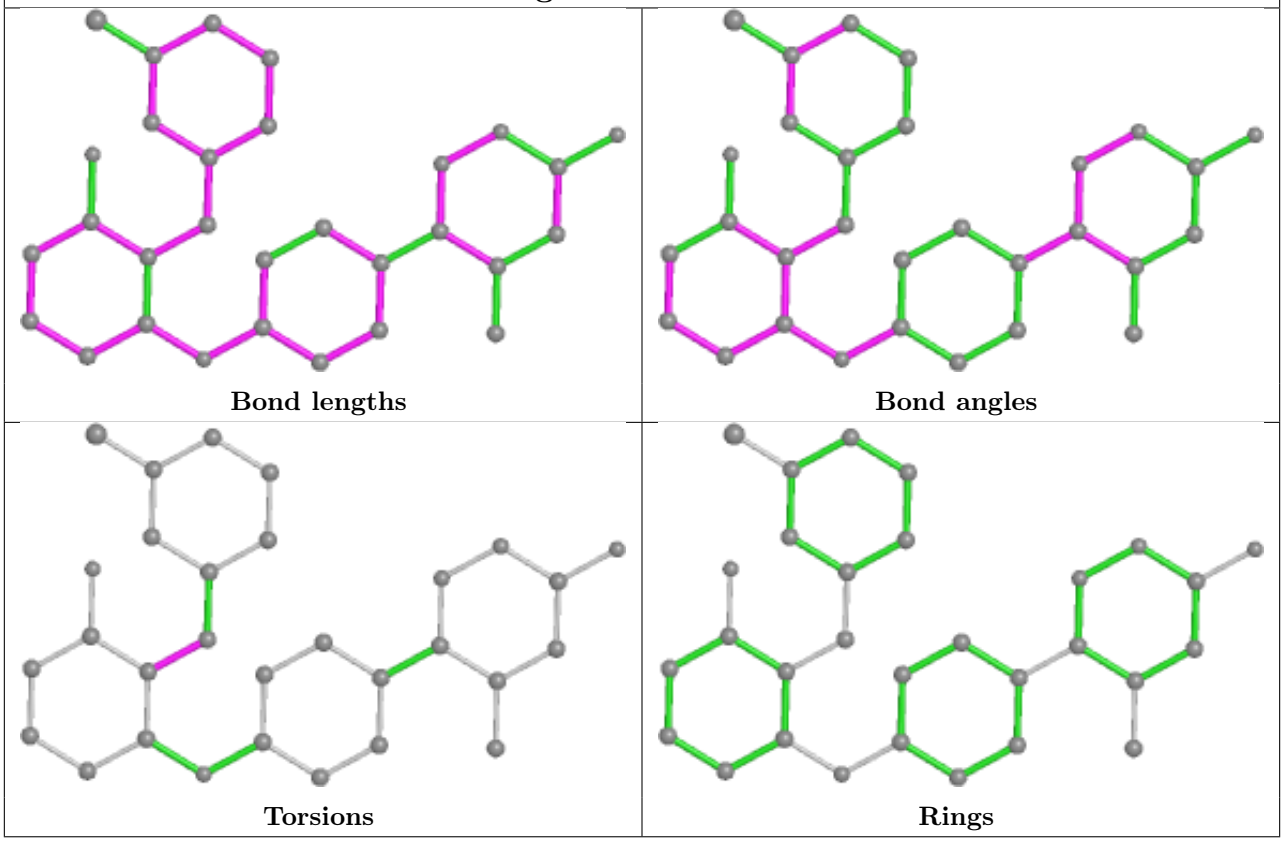


Torsions



Rings

Ligand 666 C 463



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	363/420 (86%)	0.28	36 (9%) 7 6	26, 42, 69, 77	0
1	B	363/420 (86%)	0.29	32 (8%) 10 9	23, 43, 70, 79	0
1	C	372/420 (88%)	0.39	37 (9%) 7 6	34, 49, 72, 78	0
1	D	365/420 (86%)	0.73	52 (14%) 2 2	33, 55, 74, 79	0
All	All	1463/1680 (87%)	0.42	157 (10%) 6 5	23, 48, 72, 79	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1016	ALA	9.5
1	A	662	ILE	8.1
1	C	661	LEU	8.0
1	A	1053	SER	7.4
1	A	659	LEU	7.1
1	B	659	LEU	7.0
1	C	664	VAL	6.9
1	D	662	ILE	6.5
1	B	660	ASP	6.4
1	B	662	ILE	6.3
1	A	661	LEU	6.2
1	A	764	HIS	6.2
1	D	912	VAL	6.2
1	C	662	ILE	5.8
1	B	661	LEU	5.8
1	D	659	LEU	5.8
1	A	765	ASN	5.7
1	A	1055	ARG	5.7
1	A	766	GLY	5.5
1	A	1054	ARG	5.5
1	D	1056	ARG	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	661	LEU	5.2
1	C	765	ASN	4.9
1	C	767	CYS	4.8
1	B	1055	ARG	4.8
1	C	912	VAL	4.8
1	D	795	PRO	4.7
1	C	764	HIS	4.7
1	D	660	ASP	4.6
1	C	665	GLU	4.6
1	D	780	ASN	4.6
1	D	1017	GLU	4.5
1	A	660	ASP	4.4
1	C	766	GLY	4.3
1	D	663	LEU	4.3
1	D	781	HIS	4.3
1	D	784	ILE	4.2
1	D	665	GLU	4.2
1	C	913	ASN	4.1
1	D	749	VAL	4.1
1	B	912	VAL	4.0
1	C	663	LEU	4.0
1	B	663	LEU	3.9
1	D	664	VAL	3.9
1	B	764	HIS	3.9
1	D	764	HIS	3.9
1	C	1053	SER	3.8
1	C	1054	ARG	3.8
1	C	914	SER	3.8
1	A	782	GLY	3.7
1	A	749	VAL	3.7
1	D	748	ALA	3.7
1	D	1055	ARG	3.7
1	D	766	GLY	3.7
1	C	1015	GLU	3.7
1	B	766	GLY	3.6
1	D	815	TYR	3.6
1	C	749	VAL	3.6
1	D	914	SER	3.6
1	B	1053	SER	3.6
1	A	663	LEU	3.5
1	D	1014	LEU	3.5
1	A	783	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	819	ALA	3.5
1	C	779	ILE	3.4
1	B	765	ASN	3.4
1	D	913	ASN	3.3
1	C	746	LEU	3.3
1	A	817	ALA	3.3
1	C	780	ASN	3.3
1	D	936	ALA	3.3
1	A	933	ILE	3.3
1	A	665	GLU	3.2
1	A	1056	ARG	3.2
1	B	816	VAL	3.2
1	D	798	SER	3.2
1	D	1012	GLN	3.2
1	D	745	VAL	3.2
1	D	746	LEU	3.2
1	C	1056	ARG	3.2
1	D	711	GLU	3.1
1	C	659	LEU	3.1
1	C	1055	ARG	3.1
1	D	818	ALA	3.0
1	C	748	ALA	3.0
1	D	816	VAL	3.0
1	B	818	ALA	3.0
1	B	819	ALA	3.0
1	D	1015	GLU	3.0
1	D	765	ASN	3.0
1	B	745	VAL	2.9
1	A	664	VAL	2.9
1	A	818	ALA	2.9
1	A	816	VAL	2.9
1	B	817	ALA	2.9
1	A	748	ALA	2.9
1	A	784	ILE	2.8
1	C	936	ALA	2.8
1	A	932	CYS	2.8
1	A	913	ASN	2.8
1	D	1057	ILE	2.7
1	C	915	ASN	2.7
1	A	745	VAL	2.7
1	B	762	GLN	2.7
1	D	1013	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	911	ASP	2.6
1	D	933	ILE	2.6
1	B	665	GLU	2.6
1	B	913	ASN	2.6
1	D	799	TYR	2.6
1	B	746	LEU	2.6
1	C	776	ASP	2.5
1	D	935	LEU	2.5
1	B	936	ALA	2.5
1	D	817	ALA	2.5
1	A	815	TYR	2.5
1	D	814	LEU	2.5
1	B	691	LYS	2.5
1	D	911	ASP	2.5
1	B	1056	ARG	2.4
1	A	1015	GLU	2.4
1	C	777	GLY	2.4
1	D	915	ASN	2.4
1	A	912	VAL	2.4
1	B	664	VAL	2.4
1	D	750	TRP	2.4
1	A	814	LEU	2.4
1	C	782	GLY	2.3
1	C	763	ILE	2.3
1	D	787	ILE	2.3
1	C	815	TYR	2.3
1	D	762	GLN	2.3
1	A	746	LEU	2.3
1	B	1014	LEU	2.3
1	B	741	HIS	2.3
1	A	742	ALA	2.3
1	C	783	ARG	2.3
1	C	818	ALA	2.3
1	C	774	ASP	2.3
1	D	796	ASP	2.3
1	D	752	LEU	2.3
1	A	936	ALA	2.2
1	B	815	TYR	2.2
1	B	700	MET	2.2
1	B	749	VAL	2.2
1	C	814	LEU	2.2
1	C	911	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	763	ILE	2.1
1	C	784	ILE	2.1
1	B	742	ALA	2.1
1	D	763	ILE	2.1
1	B	915	ASN	2.1
1	D	719	GLN	2.1
1	A	819	ALA	2.1
1	D	672	GLU	2.1
1	A	1057	ILE	2.0
1	C	816	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
3	HG9	B	452	24/25	0.76	0.26	48,54,68,70	0
3	HG9	B	451	24/25	0.78	0.28	37,49,69,70	0
3	HG9	A	453	24/25	0.80	0.27	42,53,65,67	0
3	HG9	A	454	24/25	0.83	0.22	46,61,71,74	0
4	666	C	463	30/30	0.93	0.20	39,53,72,85	0
4	666	A	461	30/30	0.94	0.17	32,43,59,73	0
4	666	B	462	30/30	0.95	0.20	36,43,60,68	0
4	666	D	464	30/30	0.95	0.18	46,50,65,82	0
2	MG	A	472	1/1	0.97	0.19	32,32,32,32	0
2	MG	A	479	1/1	0.97	0.06	39,39,39,39	0
2	MG	B	474	1/1	0.97	0.14	33,33,33,33	0
2	MG	C	476	1/1	0.97	0.18	37,37,37,37	0
2	MG	D	477	1/1	0.99	0.18	34,34,34,34	0

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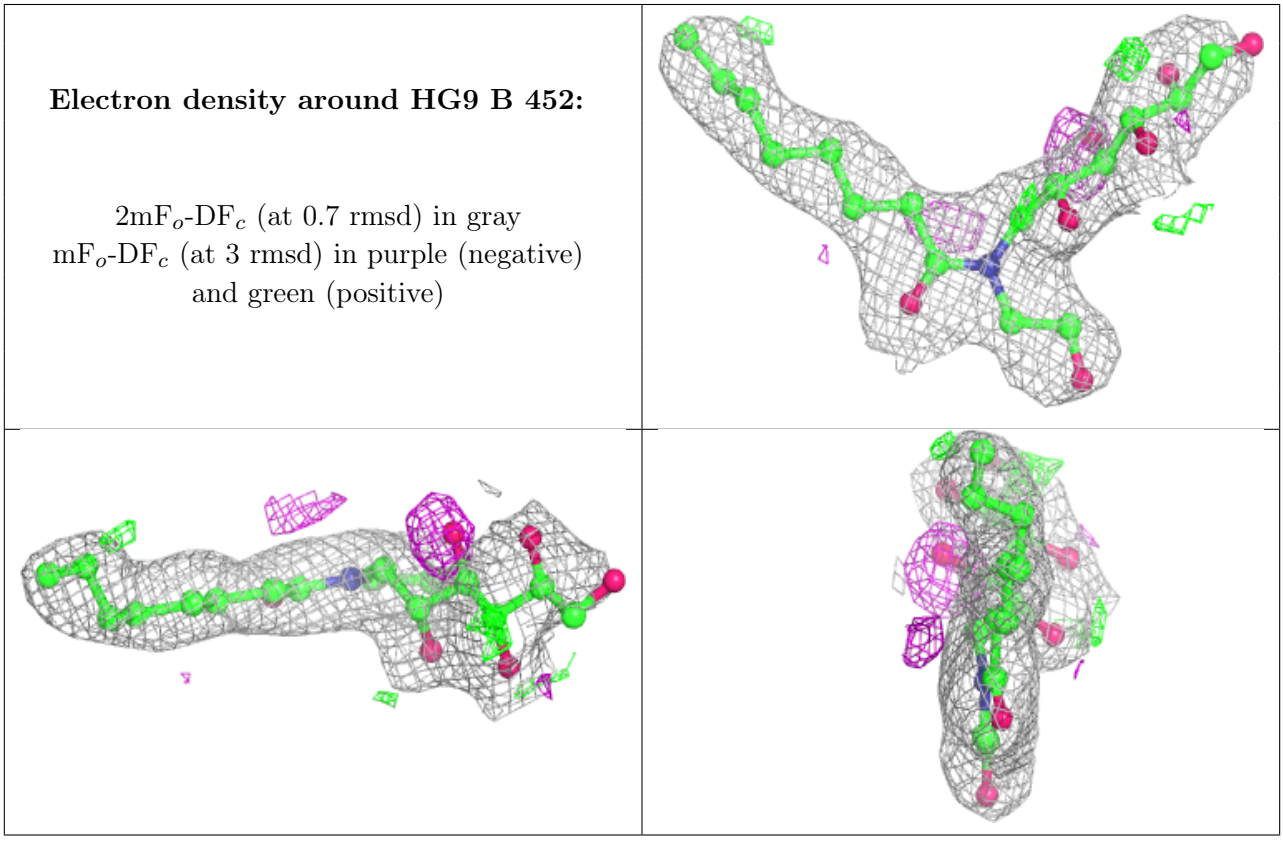
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	D	478	1/1	0.99	0.13	31,31,31,31	0
2	MG	A	471	1/1	0.99	0.27	34,34,34,34	0
2	MG	C	475	1/1	0.99	0.16	28,28,28,28	0
2	MG	B	473	1/1	0.99	0.29	23,23,23,23	0

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.

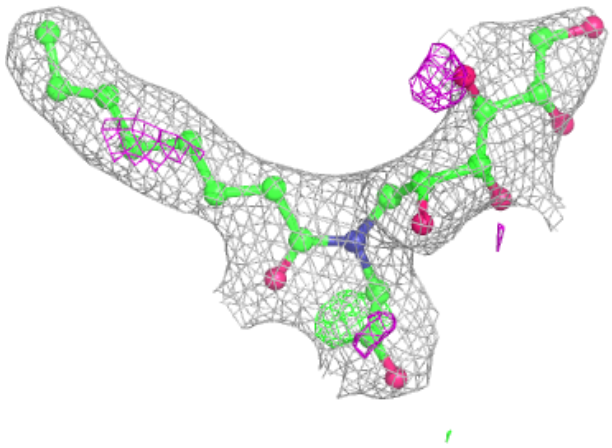
Electron density around HG9 B 452:

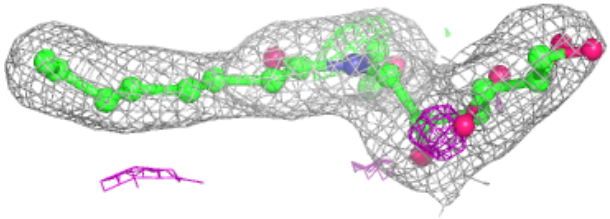
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

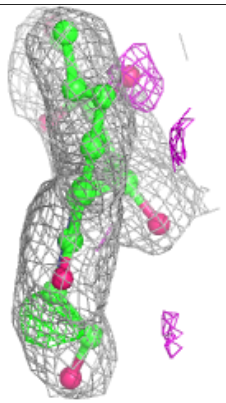


Electron density around HG9 B 451:

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

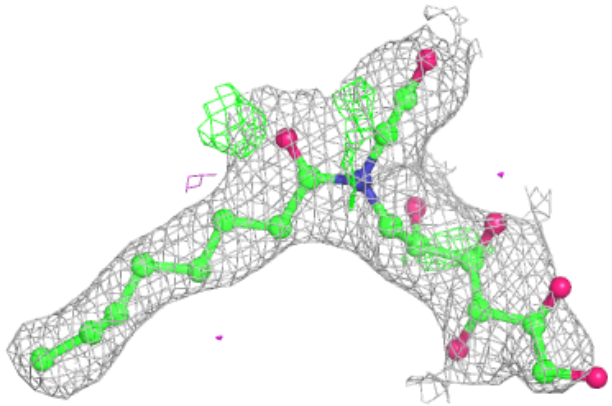


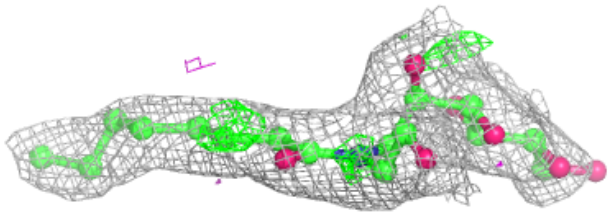


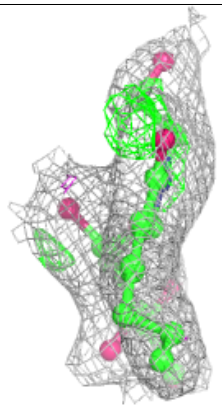


Electron density around HG9 A 453:

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

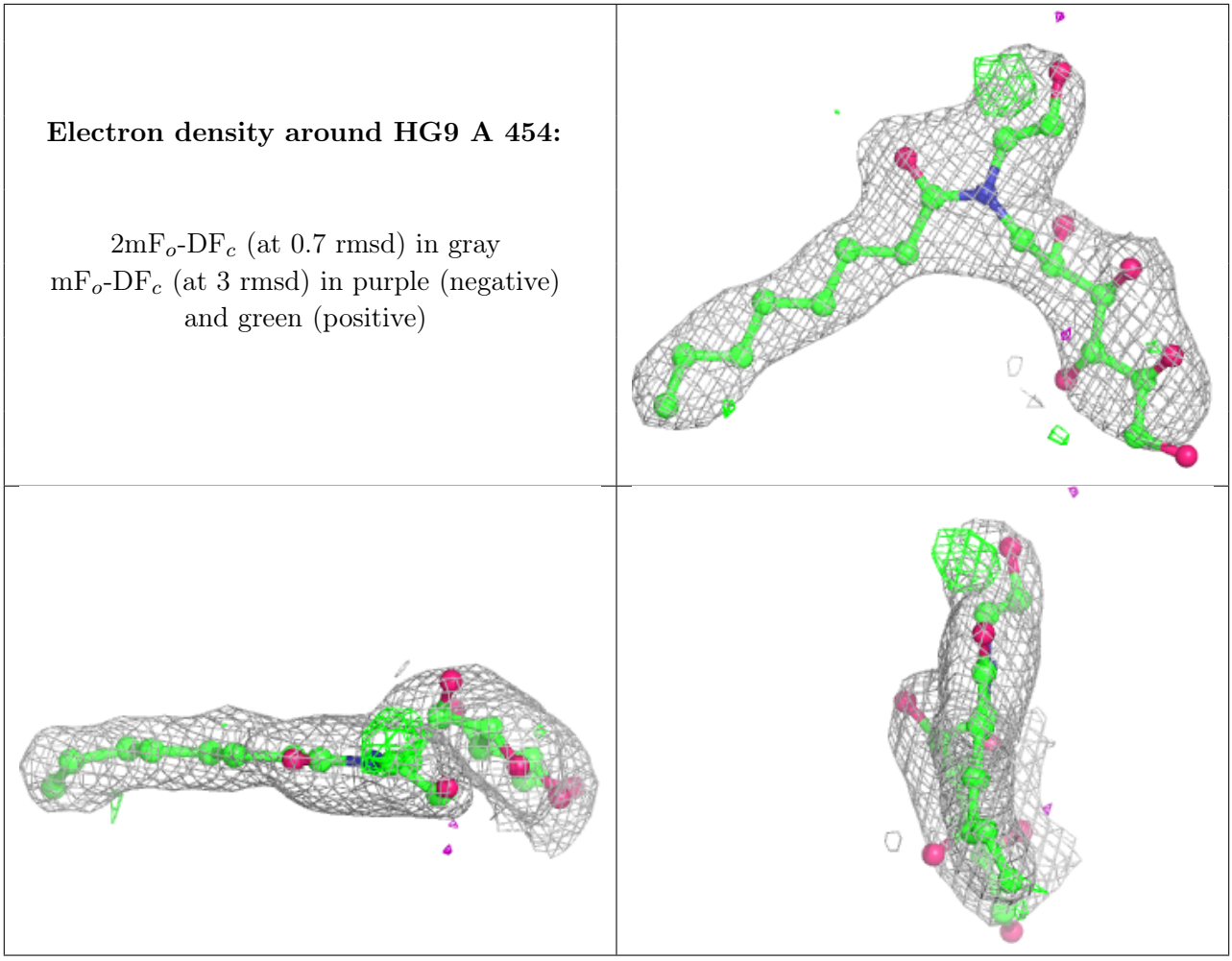






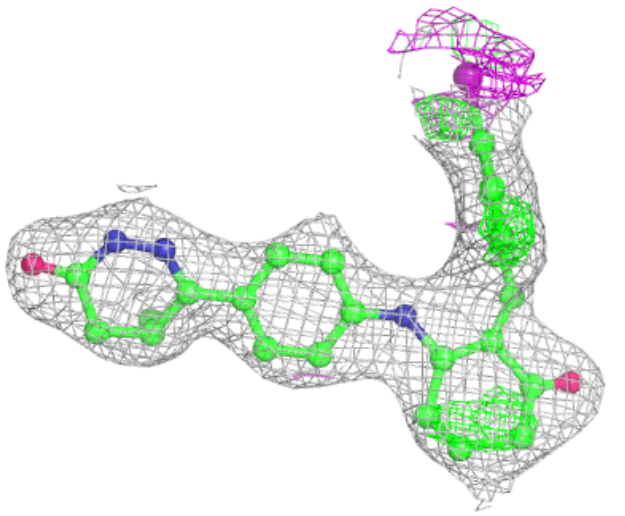
Electron density around HG9 A 454:

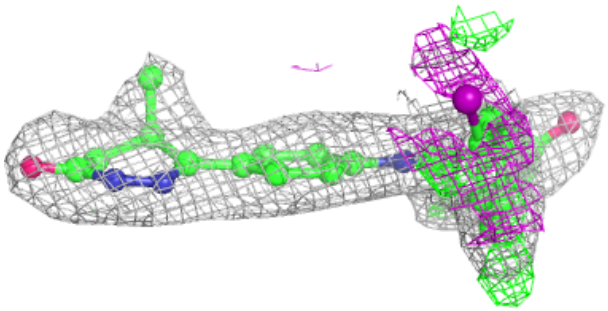
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

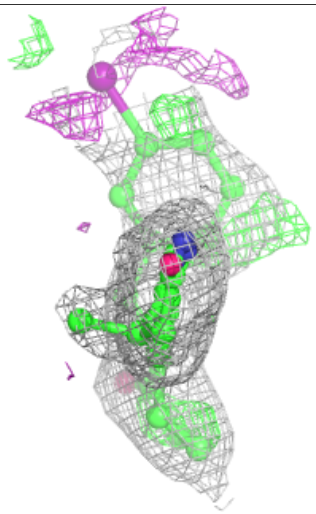


Electron density around 666 C 463:

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

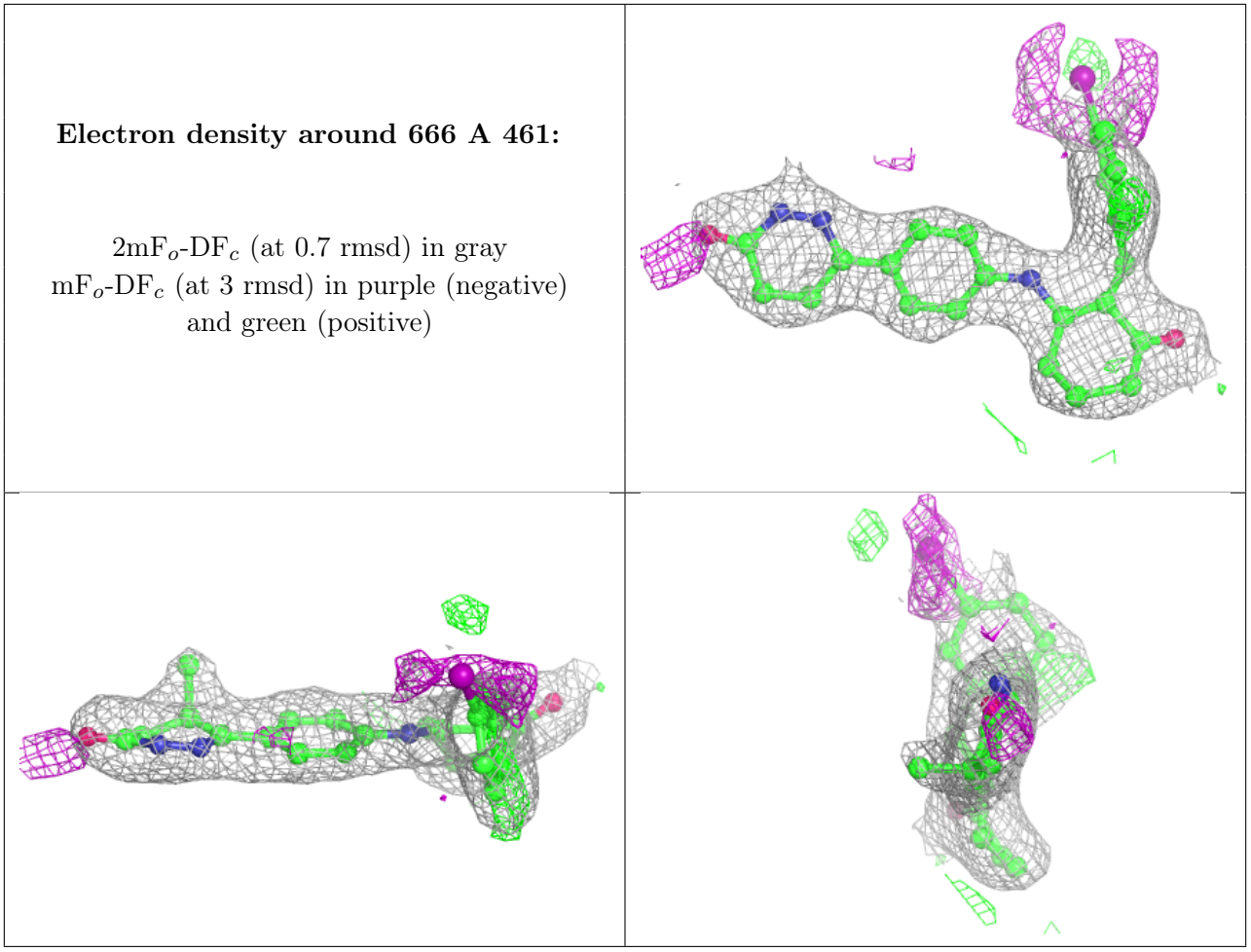






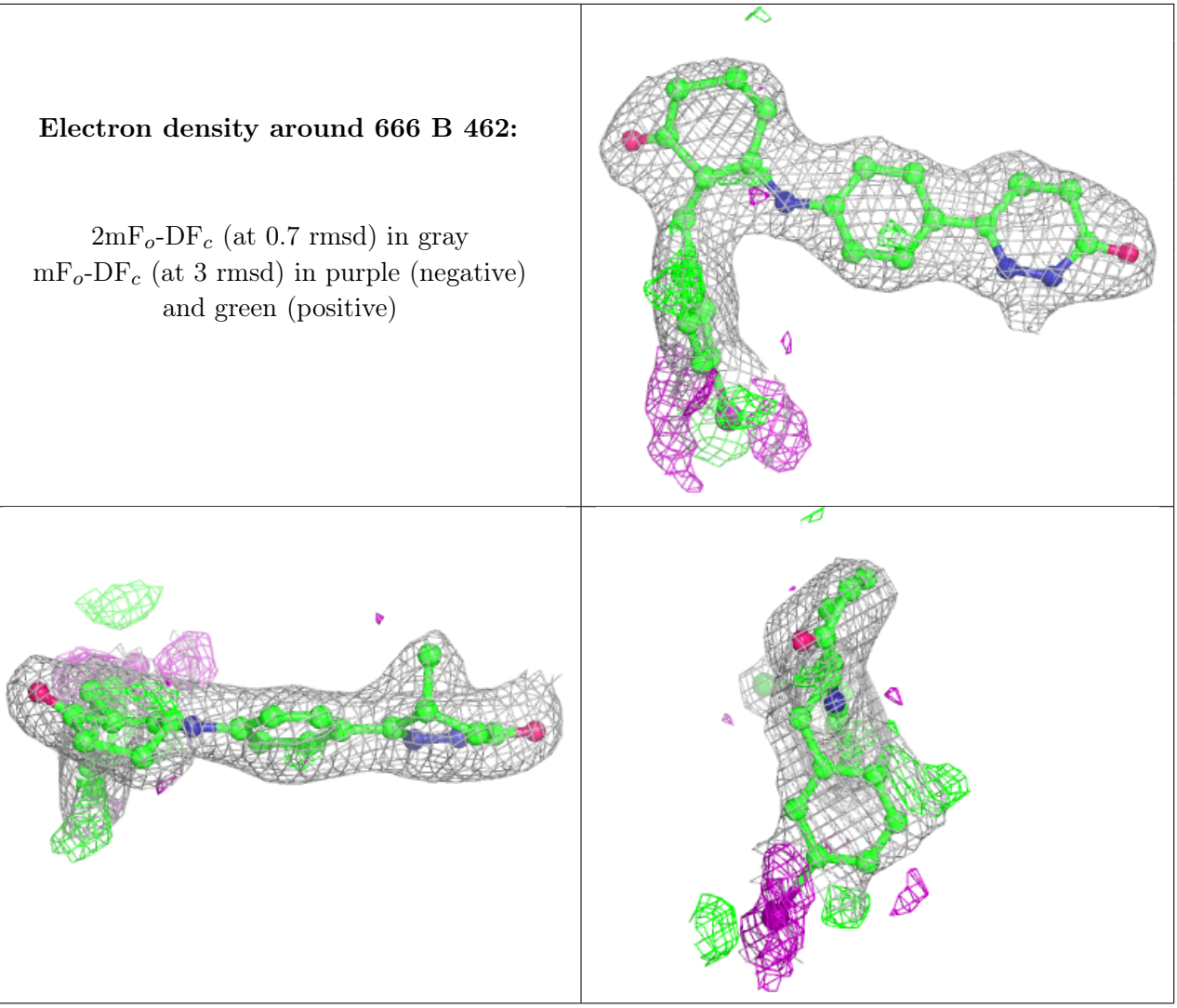
Electron density around 666 A 461:

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



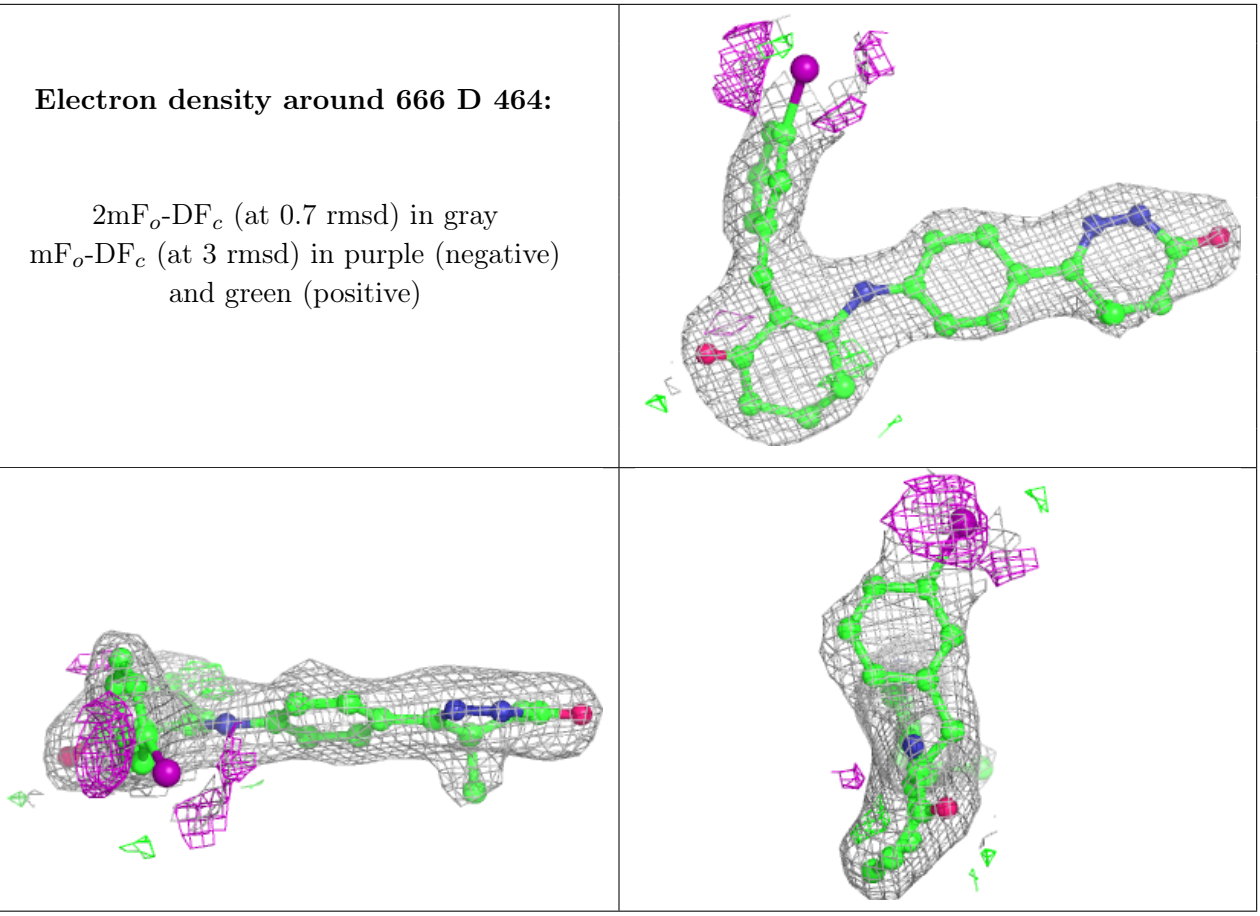
Electron density around 666 B 462:

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



Electron density around 666 D 464:

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



6.5 Other polymers

There are no such residues in this entry.