Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2026 – 12:53 pm BST

PDB ID	:	4AUN / pdb_00004aun
Title	:	Crystal structure, recombinant expression and mutagenesis studies of the bi-functional catalase-phenol oxidase from Scytalidium thermophilum
Authors	:	Yuzugullu, Y.; Trinh, C.H.; Smith, M.A.; Pearson, A.R.; Phillips, S.E.V.; Sutay Kocabas, D.; Bakir, U.; Ogel, Z.B.; McPherson, M.J.
Deposited on	:	2012-05-18
Resolution	:	1.92 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

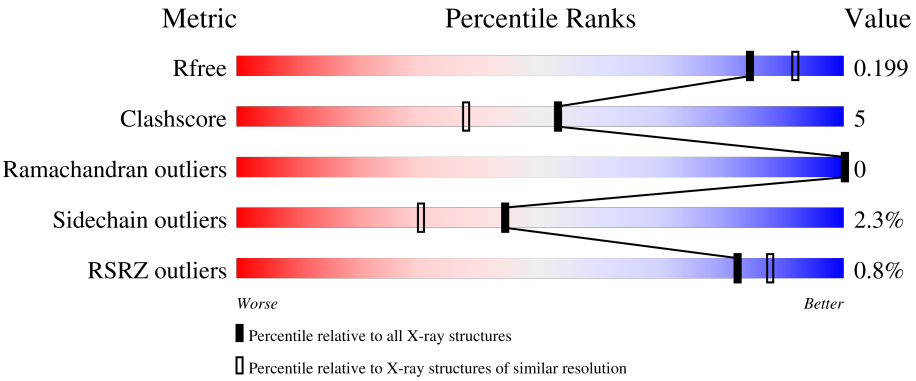
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



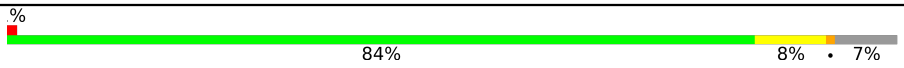
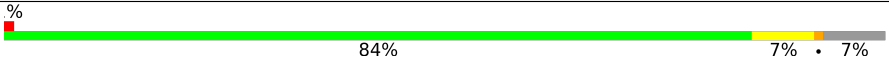
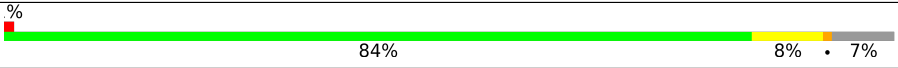
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	719	% 84% 8% • 7%
1	B	719	85% 8% • 6%
1	C	719	85% 8% • 6%
1	D	719	86% 7% • 6%

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Mol	Chain	Length	Quality of chain
1	E	719	
1	F	719	
1	G	719	
1	H	719	

2 Entry composition (i)

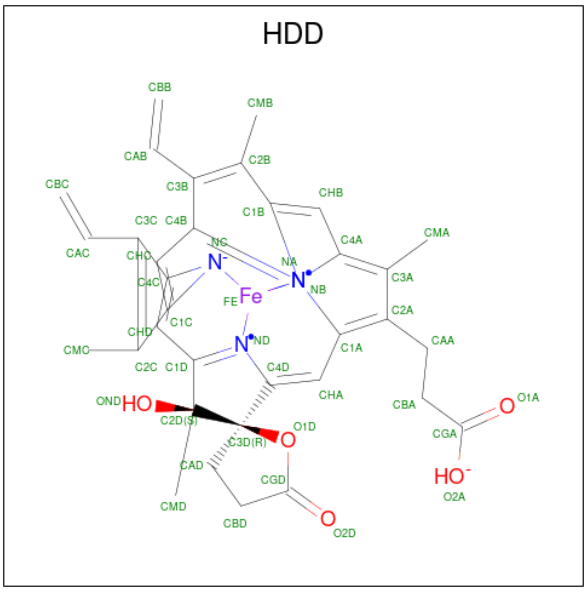
There are 4 unique types of molecules in this entry. The entry contains 46567 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CATALASE-PHENOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	671	Total	C	N	O	S	0	19	0
			5357	3388	933	1025	11			
1	B	673	Total	C	N	O	S	0	19	0
			5364	3395	931	1026	12			
1	C	673	Total	C	N	O	S	0	20	0
			5375	3401	937	1025	12			
1	D	674	Total	C	N	O	S	0	18	0
			5368	3396	937	1023	12			
1	E	668	Total	C	N	O	S	0	19	0
			5324	3371	925	1017	11			
1	F	668	Total	C	N	O	S	0	16	0
			5314	3365	928	1010	11			
1	G	673	Total	C	N	O	S	0	21	0
			5374	3402	935	1025	12			
1	H	670	Total	C	N	O	S	0	16	0
			5325	3371	927	1016	11			

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	C	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	D	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	E	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	F	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	G	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	H	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0
3	H	1	Total Ca 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	521	Total O 521 521	0	0
4	B	420	Total O 420 420	0	0
4	C	470	Total O 470 470	0	0
4	D	468	Total O 468 468	0	0
4	E	341	Total O 341 341	0	0
4	F	381	Total O 381 381	0	0
4	G	454	Total O 454 454	0	0
4	H	350	Total O 350 350	0	0

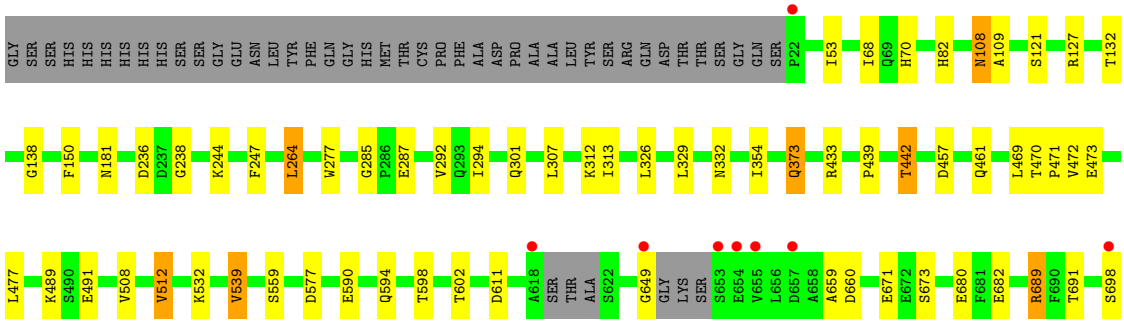
3 Residue-property plots (i)

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

• Molecule 1: CATALASE-PHENOL OXIDASE

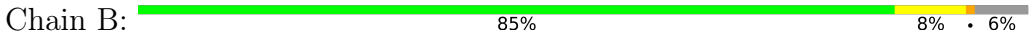
Chain A:

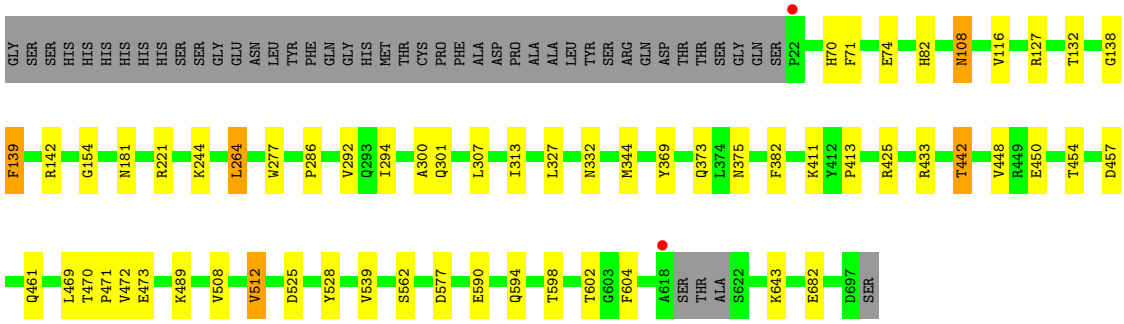




• Molecule 1: CATALASE-PHENOL OXIDASE

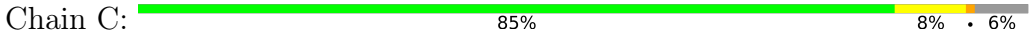
Chain B:

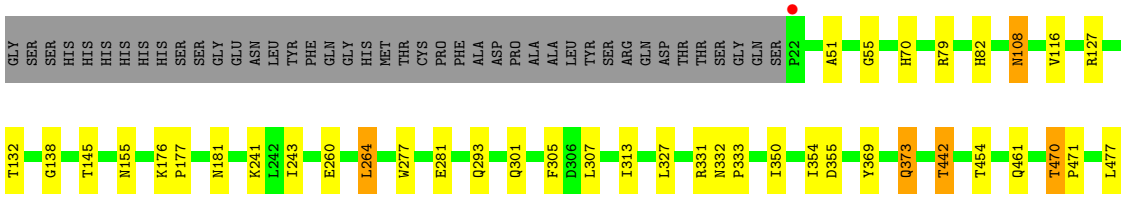




• Molecule 1: CATALASE-PHENOL OXIDASE

Chain C:



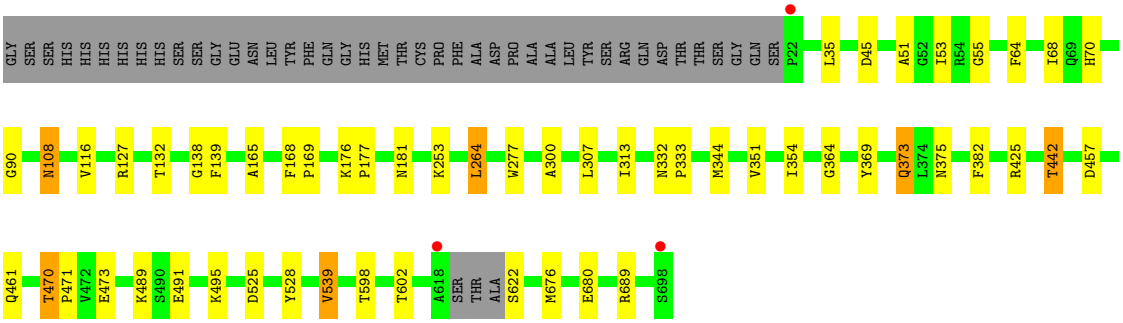




• Molecule 1: CATALASE-PHENOL OXIDASE

Chain D:

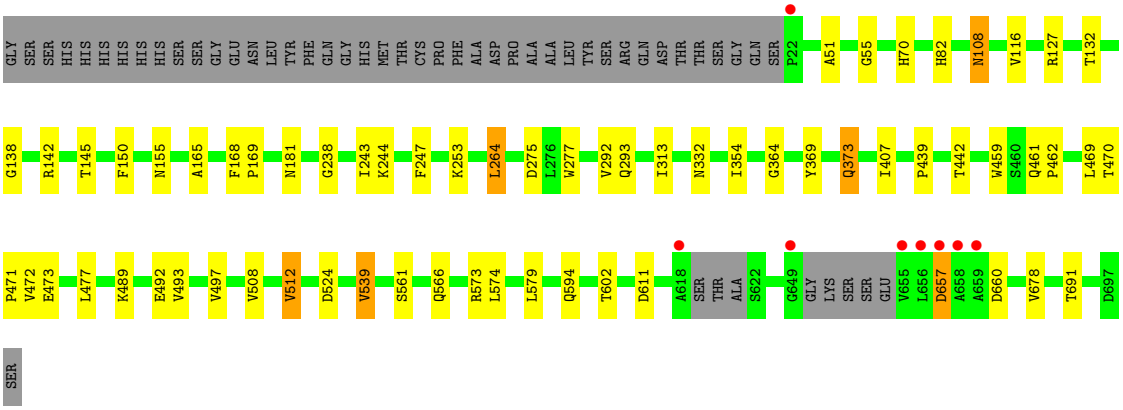




• Molecule 1: CATALASE-PHENOL OXIDASE

Chain E:

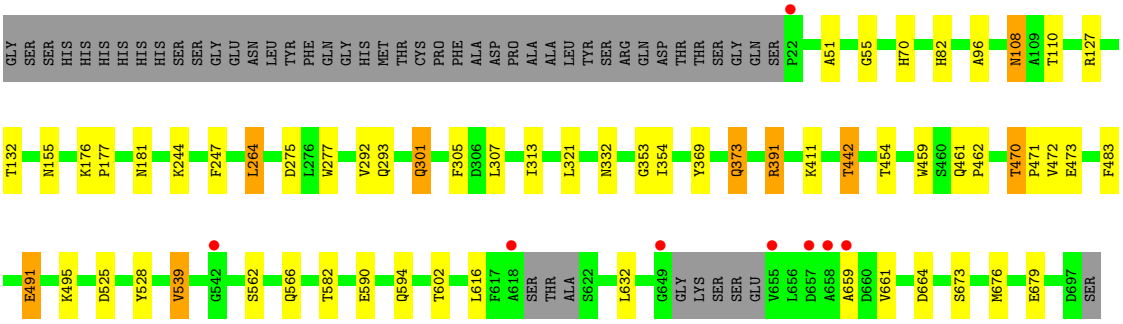




• Molecule 1: CATALASE-PHENOL OXIDASE

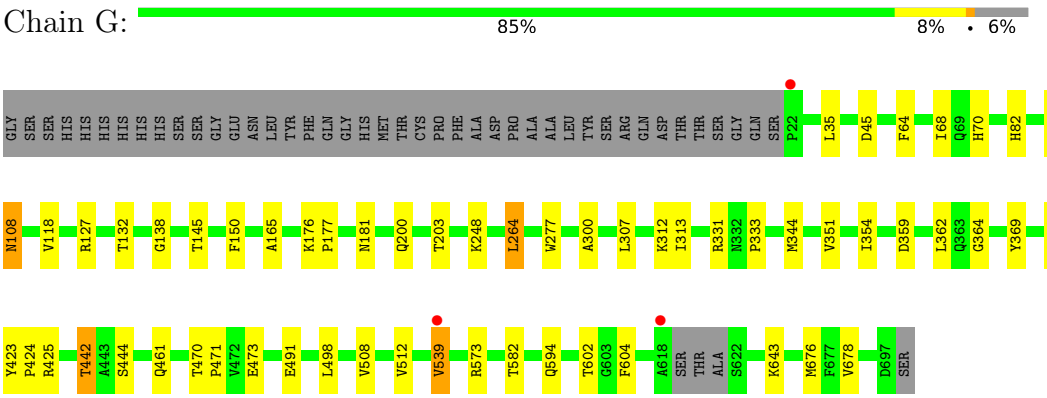
Chain F:





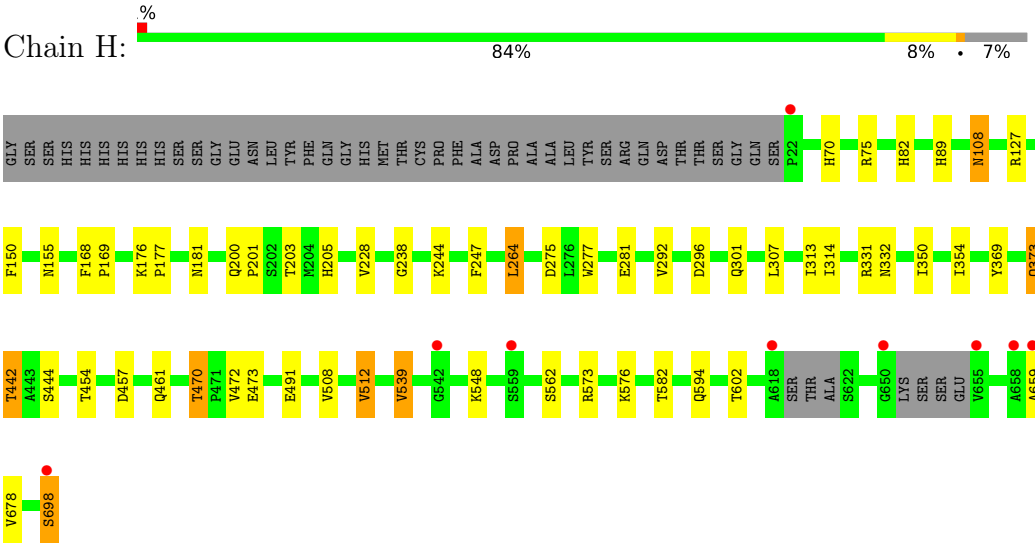
• Molecule 1: CATALASE-PHENOL OXIDASE

Chain G:



• Molecule 1: CATALASE-PHENOL OXIDASE

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	253.37Å 243.29Å 97.06Å 90.00° 104.16° 90.00°	Depositor
Resolution (Å)	69.94 – 1.92 69.94 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.5 (69.94-1.92) 99.6 (69.94-1.92)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.164 , 0.201 0.163 , 0.199	Depositor DCC
R_{free} test set	21640 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	14.7	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 35.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	46567	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2225e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: HDD, CA

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	0/5536	0.66	0/7520
1	B	0.59	0/5544	0.67	0/7533
1	C	0.59	0/5555	0.67	0/7547
1	D	0.60	0/5551	0.67	0/7539
1	E	0.60	0/5509	0.65	0/7487
1	F	0.60	0/5490	0.67	0/7460
1	G	0.60	0/5563	0.68	1/7558 (0.0%)
1	H	0.59	1/5498 (0.0%)	0.66	0/7470
All	All	0.60	1/44246 (0.0%)	0.67	1/60114 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	698	SER	C-OXT	5.21	1.33	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	400	ASP	CB-CA-C	-5.11	109.19	116.34

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	5357	0	5161	56	0
1	B	5364	0	5173	59	0
1	C	5375	0	5189	54	0
1	D	5368	0	5188	49	0
1	E	5324	0	5134	54	0
1	F	5314	0	5130	50	0
1	G	5374	0	5195	53	0
1	H	5325	0	5133	52	0
2	A	44	0	31	2	0
2	B	44	0	31	3	0
2	C	44	0	31	4	0
2	D	44	0	31	2	0
2	E	44	0	31	3	0
2	F	44	0	31	4	0
2	G	44	0	31	2	0
2	H	44	0	31	3	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	521	0	0	10	0
4	B	420	0	0	8	0
4	C	470	0	0	15	0
4	D	468	0	0	11	0
4	E	341	0	0	3	0
4	F	381	0	0	8	0
4	G	454	0	0	7	0
4	H	350	0	0	6	0
All	All	46567	0	41551	420	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 5.

All (420) 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:B:470[A]:THR:HG21	4:B:2340:HOH:O	1.31	1.25
1:A:470[A]:THR:HG21	4:A:2427:HOH:O	1.35	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:2186:HOH:O	1:E:127[A]:ARG:NH2	1.71	1.17
1:D:253:LYS:HG2	4:D:2201:HOH:O	1.47	1.14
1:D:470[A]:THR:HG21	4:D:2362:HOH:O	1.48	1.12
1:C:470[A]:THR:HG21	4:C:2368:HOH:O	1.50	1.11
1:G:470[A]:THR:HG22	1:G:471:PRO:HD2	1.14	1.11
1:G:89:HIS:HB2	1:G:331[B]:ARG:HG2	1.34	1.09
1:C:589[B]:ARG:HH11	1:C:589[B]:ARG:HG3	0.91	1.07
1:F:470[A]:THR:HG21	4:F:2312:HOH:O	1.55	1.05
4:C:2187:HOH:O	1:E:127[A]:ARG:O	1.77	1.01
1:C:589[B]:ARG:HG3	1:C:589[B]:ARG:NH1	1.67	0.99
1:G:470[A]:THR:CG2	1:G:471:PRO:HD2	1.94	0.98
1:E:253:LYS:HG2	4:E:2137:HOH:O	1.64	0.95
1:B:470[A]:THR:HG23	1:B:471:PRO:HD2	1.49	0.94
1:G:470[A]:THR:HG22	1:G:471:PRO:CD	1.97	0.94
1:C:604:PHE:O	1:C:643:LYS:HE2	1.68	0.93
1:D:313:ILE:H	1:D:461:GLN:HE22	1.13	0.92
1:G:313:ILE:H	1:G:461:GLN:HE22	1.18	0.92
1:C:589[B]:ARG:HH11	1:C:589[B]:ARG:CG	1.81	0.91
1:E:313:ILE:H	1:E:461:GLN:HE22	1.17	0.91
1:D:495:LYS:HE2	4:D:2380:HOH:O	1.70	0.91
1:A:470[A]:THR:HG23	1:A:471:PRO:HD2	1.50	0.91
1:G:470[A]:THR:HG21	4:G:2343:HOH:O	1.72	0.90
1:C:127[B]:ARG:O	4:C:2080:HOH:O	1.89	0.89
1:G:423:TYR:CE1	1:G:425:ARG:HD2	2.09	0.87
1:B:313:ILE:H	1:B:461:GLN:HE22	1.20	0.87
1:H:313:ILE:H	1:H:461:GLN:HE22	1.19	0.87
1:G:248:LYS:HD2	4:G:2188:HOH:O	1.76	0.86
1:B:604:PHE:O	1:B:643:LYS:HE2	1.75	0.86
1:F:313:ILE:H	1:F:461:GLN:HE22	1.18	0.86
1:H:508:VAL:O	1:H:512[A]:VAL:HG13	1.76	0.86
1:H:264:LEU:HG	1:H:602:THR:HB	1.58	0.85
1:E:470[A]:THR:HG22	1:E:471:PRO:HD2	1.58	0.85
1:E:264:LEU:HG	1:E:602:THR:HB	1.58	0.85
1:C:442:THR:HG22	4:C:2349:HOH:O	1.78	0.84
1:G:604:PHE:O	1:G:643:LYS:HE2	1.78	0.84
1:A:313:ILE:H	1:A:461:GLN:HE22	1.22	0.84
1:D:264:LEU:HG	1:D:602:THR:HB	1.59	0.84
1:F:470[A]:THR:HG23	1:F:471:PRO:HD2	1.59	0.83
1:D:127[A]:ARG:NH1	4:D:2125:HOH:O	2.11	0.82
1:E:150:PHE:CZ	1:E:354[A]:ILE:HD13	2.15	0.82
1:G:264:LEU:HG	1:G:602:THR:HB	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ILE:H	1:C:461:GLN:HE22	1.27	0.80
1:F:264:LEU:HG	1:F:602:THR:HB	1.65	0.79
1:A:470[A]:THR:CG2	1:A:471:PRO:HD2	2.13	0.78
1:A:611:ASP:HB2	1:A:649:GLY:HA3	1.66	0.77
1:A:264:LEU:HG	1:A:602:THR:HB	1.68	0.76
1:B:264:LEU:HG	1:B:602:THR:HB	1.67	0.75
1:D:689[B]:ARG:CZ	4:D:2443:HOH:O	2.34	0.75
1:B:448:VAL:HB	1:B:450:GLU:HG3	1.67	0.75
1:H:108:ASN:C	1:H:108:ASN:HD22	1.96	0.74
1:C:264:LEU:HG	1:C:602:THR:HB	1.68	0.73
1:G:108:ASN:C	1:G:108:ASN:HD22	1.95	0.73
1:B:590[B]:GLU:CD	1:B:590[B]:GLU:H	1.96	0.73
1:A:108:ASN:C	1:A:108:ASN:HD22	1.94	0.73
1:E:470[A]:THR:CG2	1:E:471:PRO:HD2	2.18	0.73
2:F:900:HDD:HMC1	2:F:900:HDD:HBC1	1.70	0.73
1:H:373:GLN:HE21	1:H:373:GLN:HA	1.53	0.72
1:A:689[A]:ARG:NE	4:A:2504:HOH:O	2.22	0.71
1:C:604:PHE:O	1:C:643:LYS:CE	2.38	0.71
1:D:473:GLU:CD	1:D:539:VAL:HG13	2.14	0.71
1:D:470[A]:THR:HG23	1:D:471:PRO:HD2	1.72	0.71
1:E:489:LYS:HE2	4:E:2122:HOH:O	1.91	0.71
1:D:489:LYS:HD2	4:D:2186:HOH:O	1.90	0.70
1:G:248:LYS:CD	4:G:2188:HOH:O	2.35	0.70
1:F:108:ASN:C	1:F:108:ASN:HD22	1.99	0.69
1:D:689[B]:ARG:NE	4:D:2443:HOH:O	2.25	0.69
1:G:423:TYR:HE1	1:G:425:ARG:HD2	1.59	0.68
1:B:108:ASN:C	1:B:108:ASN:HD22	2.00	0.68
1:A:373:GLN:HA	1:A:373:GLN:HE21	1.57	0.67
4:C:2186:HOH:O	1:E:127[A]:ARG:CZ	2.28	0.67
1:F:277:TRP:CZ3	1:F:332:ASN:HB3	2.29	0.67
1:H:473:GLU:CD	1:H:539:VAL:HG13	2.20	0.67
1:B:470[A]:THR:HG23	1:B:471:PRO:CD	2.22	0.67
1:H:573:ARG:HG2	1:H:678:VAL:HG21	1.76	0.66
1:G:181:ASN:HB3	1:H:277:TRP:CE3	2.29	0.66
1:H:470[A]:THR:HG22	1:H:473:GLU:HB2	1.76	0.66
1:A:508:VAL:O	1:A:512:VAL:HG13	1.96	0.66
1:B:508:VAL:O	1:B:512[A]:VAL:HG13	1.96	0.66
1:F:373:GLN:HA	1:F:373:GLN:HE21	1.58	0.66
1:E:470[A]:THR:HG22	1:E:471:PRO:CD	2.26	0.66
1:F:470[A]:THR:HG23	1:F:471:PRO:CD	2.27	0.65
1:B:132:THR:HG21	1:B:264:LEU:HD13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:GLN:HA	1:D:373:GLN:HE21	1.61	0.65
1:C:373:GLN:HE21	1:C:373:GLN:HA	1.60	0.65
1:C:470[A]:THR:HG23	1:C:471:PRO:HD2	1.80	0.64
1:B:489:LYS:HD2	4:B:2149:HOH:O	1.97	0.64
1:C:82:HIS:HE1	4:C:2075:HOH:O	1.80	0.64
1:A:442:THR:HB	4:A:2404:HOH:O	1.97	0.63
1:C:108:ASN:C	1:C:108:ASN:HD22	2.07	0.63
1:G:181:ASN:HB3	1:H:277:TRP:CZ3	2.34	0.63
1:B:373:GLN:HE21	1:B:373:GLN:HA	1.63	0.62
1:F:491[B]:GLU:HG2	1:F:495:LYS:HE3	1.80	0.62
1:G:573:ARG:HG2	1:G:678:VAL:HG21	1.81	0.62
1:C:689[B]:ARG:NE	4:C:2445:HOH:O	2.32	0.62
1:F:82:HIS:HE1	4:F:2052:HOH:O	1.81	0.62
1:G:442:THR:HB	4:G:2325:HOH:O	1.99	0.62
1:A:698:SER:N	4:A:2518:HOH:O	2.33	0.61
1:A:470[A]:THR:CG2	1:A:471:PRO:CD	2.78	0.61
1:F:132:THR:HG21	1:F:264:LEU:HD13	1.82	0.61
1:H:470[A]:THR:HG22	1:H:473:GLU:H	1.66	0.61
1:F:582:THR:HG21	1:F:594:GLN:HE21	1.65	0.61
1:F:473:GLU:CD	1:F:539:VAL:HG13	2.26	0.60
1:E:108:ASN:HD22	1:E:108:ASN:C	2.08	0.60
1:A:108:ASN:C	1:A:108:ASN:ND2	2.60	0.60
1:D:277:TRP:CZ3	1:D:333:PRO:HD2	2.36	0.60
1:G:470[A]:THR:CG2	1:G:471:PRO:CD	2.71	0.60
1:A:132:THR:HG21	1:A:264:LEU:HD13	1.82	0.60
1:B:442:THR:HG23	4:B:2323:HOH:O	2.00	0.60
1:E:508:VAL:O	1:E:512:VAL:HG13	2.02	0.60
1:C:132:THR:HG21	1:C:264:LEU:HD13	1.83	0.60
1:A:82:HIS:HE1	4:A:2086:HOH:O	1.84	0.60
1:G:127[B]:ARG:NH1	4:G:2112:HOH:O	2.34	0.60
1:D:132:THR:HG21	1:D:264:LEU:HD13	1.84	0.59
1:H:132:THR:HG21	1:H:264:LEU:HD13	1.84	0.59
1:G:313:ILE:N	1:G:461:GLN:HE22	1.95	0.59
1:G:373:GLN:HE21	1:G:373:GLN:HA	1.67	0.59
1:E:373:GLN:HA	1:E:373:GLN:HE21	1.66	0.59
1:D:108:ASN:C	1:D:108:ASN:HD22	2.08	0.59
1:H:307:LEU:HD21	1:H:314:ILE:HD11	1.85	0.59
1:C:301:GLN:HE22	1:C:454:THR:HG21	1.68	0.59
1:F:442:THR:CG2	4:F:2297:HOH:O	2.51	0.59
1:B:108:ASN:C	1:B:108:ASN:ND2	2.61	0.58
1:F:442:THR:HG22	4:F:2297:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470[A]:THR:HG23	1:D:471:PRO:CD	2.34	0.58
1:C:277:TRP:CE3	1:E:181:ASN:HB3	2.38	0.58
1:E:573:ARG:HG2	1:E:678:VAL:HG21	1.86	0.58
1:A:181:ASN:HB3	1:B:277:TRP:CE3	2.40	0.57
1:H:108:ASN:C	1:H:108:ASN:ND2	2.63	0.57
1:A:470[A]:THR:HG23	1:A:471:PRO:CD	2.28	0.57
1:A:313:ILE:N	1:A:461:GLN:HE22	2.00	0.57
1:G:132:THR:HG21	1:G:264:LEU:HD13	1.86	0.56
1:D:470[A]:THR:CG2	4:D:2362:HOH:O	2.26	0.56
1:E:150:PHE:CE1	1:E:354[A]:ILE:HD13	2.40	0.56
1:E:473:GLU:CD	1:E:539:VAL:HG13	2.30	0.56
1:D:277:TRP:CE3	1:F:181:ASN:HB3	2.41	0.56
1:C:689[B]:ARG:CZ	4:C:2445:HOH:O	2.54	0.56
1:G:277:TRP:CZ3	1:G:333:PRO:HD2	2.41	0.56
1:B:294[B]:ILE:HG23	1:B:294[B]:ILE:O	2.06	0.55
1:C:350:ILE:HD11	1:C:354[A]:ILE:HG22	1.89	0.55
1:C:641:TRP:O	1:C:689[B]:ARG:NE	2.34	0.55
1:B:442:THR:HG22	4:B:2321:HOH:O	2.05	0.55
1:A:472:VAL:HG11	1:A:691:THR:HB	1.89	0.55
1:F:470[A]:THR:HG23	4:F:2313:HOH:O	2.07	0.55
1:G:277:TRP:CE3	1:H:181:ASN:HB3	2.42	0.54
1:A:82:HIS:HD2	1:A:121:SER:OG	1.90	0.54
1:B:300:ALA:HA	1:B:307:LEU:HD12	1.88	0.54
1:F:673:SER:HB3	1:F:676:MET:HE3	1.90	0.54
1:C:508:VAL:O	1:C:512[A]:VAL:HG13	2.07	0.54
1:E:155:ASN:CG	2:E:900:HDD:HMB2	2.33	0.54
1:F:470[A]:THR:CG2	4:F:2313:HOH:O	2.55	0.53
1:H:350:ILE:HD11	1:H:354[A]:ILE:HG22	1.89	0.53
1:G:108:ASN:C	1:G:108:ASN:ND2	2.60	0.53
1:A:671:GLU:OE2	1:A:680[B]:GLU:OE2	2.27	0.53
1:E:657:ASP:OD1	1:E:657:ASP:N	2.39	0.53
1:F:391[B]:ARG:NH1	4:F:2109:HOH:O	2.41	0.53
1:C:277:TRP:CZ3	1:E:181:ASN:HB3	2.44	0.53
1:E:132:THR:HG21	1:E:264:LEU:HD13	1.91	0.52
1:A:470[A]:THR:HG22	1:A:471:PRO:N	2.25	0.52
1:B:82:HIS:HE1	4:B:2058:HOH:O	1.92	0.52
1:G:351:VAL:HG23	1:G:354[A]:ILE:HD12	1.90	0.52
1:H:442:THR:HG22	4:H:2262:HOH:O	2.09	0.52
1:C:176:LYS:HB3	1:C:177:PRO:CD	2.40	0.52
1:E:277:TRP:CZ3	1:E:332:ASN:HB3	2.45	0.52
1:D:181:ASN:HB3	1:F:277:TRP:CE3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:373:GLN:HE21	1:H:373:GLN:CA	2.21	0.52
1:B:301:GLN:HE22	1:B:454:THR:HG21	1.76	0.51
1:D:277:TRP:HZ3	1:D:333:PRO:HD2	1.74	0.51
1:E:108:ASN:C	1:E:108:ASN:ND2	2.68	0.51
1:E:470[A]:THR:CG2	1:E:471:PRO:CD	2.85	0.51
1:C:277:TRP:CZ3	1:C:332:ASN:HB3	2.46	0.51
1:G:582:THR:HG21	1:G:594:GLN:HE21	1.74	0.51
1:E:469:LEU:HB3	1:E:473:GLU:HB3	1.93	0.51
1:H:373:GLN:HA	1:H:373:GLN:NE2	2.24	0.51
1:C:108:ASN:C	1:C:108:ASN:ND2	2.69	0.51
1:G:277:TRP:HZ3	1:G:333:PRO:HD2	1.76	0.51
1:A:469:LEU:HB3	1:A:473:GLU:HB3	1.93	0.51
1:A:181:ASN:HB3	1:B:277:TRP:CZ3	2.46	0.51
1:H:470[A]:THR:HG21	4:H:2279:HOH:O	2.10	0.51
1:H:82:HIS:HE1	4:H:2030:HOH:O	1.93	0.51
1:E:369:TYR:O	1:E:373:GLN:HG2	2.10	0.51
1:F:525:ASP:HA	1:F:528:TYR:CD2	2.46	0.51
1:B:71:PHE:HA	1:B:74:GLU:HG3	1.93	0.50
1:B:469:LEU:HB3	1:B:473:GLU:HB3	1.94	0.50
1:C:573:ARG:HG2	1:C:678:VAL:HG21	1.91	0.50
1:F:369:TYR:O	1:F:373:GLN:HG2	2.11	0.50
1:G:508:VAL:O	1:G:512[A]:VAL:HG13	2.11	0.50
1:H:150:PHE:CZ	1:H:354[A]:ILE:HD13	2.47	0.50
1:D:369:TYR:O	1:D:373:GLN:HG2	2.11	0.50
1:B:116:VAL:HG21	1:B:327:LEU:HD11	1.93	0.50
1:C:676[A]:MET:HE1	1:C:679:GLU:OE2	2.12	0.49
1:D:313:ILE:N	1:D:461:GLN:HE22	1.95	0.49
1:F:176:LYS:HB3	1:F:177:PRO:CD	2.42	0.49
1:B:470[B]:THR:OG1	1:B:539:VAL:HG21	2.11	0.49
1:H:168:PHE:HB3	1:H:169:PRO:HD3	1.94	0.49
1:F:108:ASN:C	1:F:108:ASN:ND2	2.64	0.49
1:D:138:GLY:HA3	2:D:900:HDD:HMA2	1.94	0.49
1:B:470[A]:THR:CG2	1:B:471:PRO:CD	2.91	0.49
1:D:108:ASN:C	1:D:108:ASN:ND2	2.71	0.49
1:H:150:PHE:CE1	1:H:354[A]:ILE:HD13	2.47	0.49
1:H:442:THR:CG2	4:H:2262:HOH:O	2.60	0.49
1:A:150:PHE:CZ	1:A:354[A]:ILE:HD13	2.48	0.49
1:B:525:ASP:HA	1:B:528:TYR:CD2	2.48	0.48
1:A:373:GLN:HE21	1:A:373:GLN:CA	2.24	0.48
1:D:168:PHE:HB3	1:D:169:PRO:HD3	1.95	0.48
1:D:442:THR:HB	4:D:2337:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689[A]:ARG:CZ	4:A:2504:HOH:O	2.57	0.48
1:B:470[A]:THR:HG22	1:B:472:VAL:H	1.78	0.48
1:A:594:GLN:HG3	1:A:598:THR:OG1	2.14	0.48
1:E:524:ASP:C	1:E:524:ASP:OD1	2.56	0.48
1:F:301:GLN:HE22	1:F:454:THR:HG21	1.78	0.48
1:A:277:TRP:CE3	1:B:181:ASN:HB3	2.49	0.48
1:B:473:GLU:CD	1:B:539:VAL:HG22	2.39	0.48
1:E:459:TRP:C	1:E:462:PRO:HD2	2.39	0.48
1:D:525:ASP:HA	1:D:528:TYR:CD2	2.48	0.48
1:H:301:GLN:NE2	4:H:2193:HOH:O	2.27	0.48
1:D:277:TRP:CZ3	1:D:332:ASN:HB3	2.49	0.47
1:E:313:ILE:N	1:E:461:GLN:HE22	1.97	0.47
1:F:470[A]:THR:CG2	1:F:472:VAL:HG12	2.44	0.47
1:F:562:SER:O	1:F:566:GLN:HG3	2.14	0.47
1:F:632:LEU:HD11	1:F:659:ALA:HA	1.96	0.47
1:G:369:TYR:O	1:G:373:GLN:HG2	2.14	0.47
1:G:277:TRP:CZ3	1:H:181:ASN:HB3	2.49	0.47
1:E:472:VAL:HG21	1:E:691:THR:HB	1.96	0.47
1:C:470[A]:THR:HG23	1:C:471:PRO:CD	2.43	0.47
1:E:493:VAL:O	1:E:497:VAL:HG23	2.14	0.47
1:G:473:GLU:CD	1:G:539:VAL:HG13	2.40	0.47
1:H:470[A]:THR:CG2	1:H:472:VAL:HG12	2.43	0.47
1:F:176:LYS:HB3	1:F:177:PRO:HD2	1.96	0.47
1:F:305:PHE:HE2	1:F:307:LEU:HD23	1.79	0.47
1:G:351:VAL:CG2	1:G:354[A]:ILE:HD12	2.44	0.47
1:B:116:VAL:HA	1:B:142:ARG:O	2.14	0.47
1:C:79:ARG:HB3	2:C:900:HDD:HBD1	1.97	0.47
1:C:127[A]:ARG:NH2	4:C:2126:HOH:O	2.47	0.47
1:H:155:ASN:CG	2:H:900:HDD:HMB2	2.40	0.46
1:C:313:ILE:N	1:C:461:GLN:HE22	2.04	0.46
1:B:643:LYS:HE3	4:B:2389:HOH:O	2.15	0.46
1:D:676[A]:MET:HE2	1:D:680:GLU:HG3	1.96	0.46
1:A:294[B]:ILE:HG23	1:A:294[B]:ILE:O	2.14	0.46
1:C:525:ASP:HA	1:C:528:TYR:CD2	2.51	0.46
1:H:277:TRP:CZ3	1:H:332:ASN:HB3	2.50	0.46
1:A:127[B]:ARG:NH1	4:A:2132:HOH:O	2.47	0.46
1:C:305:PHE:CE2	1:C:307:LEU:HD23	2.50	0.46
1:F:305:PHE:CE2	1:F:307:LEU:HD23	2.50	0.46
1:H:281[A]:GLU:HG2	1:H:332:ASN:ND2	2.31	0.46
1:H:296:ASP:HB3	4:H:2189:HOH:O	2.14	0.46
1:B:470[B]:THR:HG21	1:B:539:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:PHE:CZ	1:G:68:ILE:HG13	2.51	0.46
1:E:168:PHE:HB3	1:E:169:PRO:HD3	1.96	0.46
1:E:247:PHE:N	1:E:247:PHE:HD1	2.14	0.46
1:G:82:HIS:HE1	4:G:2058:HOH:O	1.99	0.46
1:G:359:ASP:HB3	1:G:362:LEU:HB3	1.97	0.46
1:A:489:LYS:HD2	4:A:2202:HOH:O	2.16	0.46
2:D:900:HDD:HMB1	2:D:900:HDD:HBB1	1.98	0.46
1:F:659:ALA:HB1	1:F:661:VAL:HG23	1.98	0.46
1:D:676[B]:MET:HE2	1:D:676[B]:MET:HB2	1.75	0.46
1:H:582:THR:CG2	1:H:594:GLN:HG2	2.46	0.46
1:B:577:ASP:OD2	1:B:682:GLU:OE2	2.33	0.45
1:F:353:GLY:C	1:F:354[A]:ILE:HD12	2.41	0.45
1:H:238:GLY:O	1:H:439:PRO:HD2	2.16	0.45
1:D:165:ALA:CB	1:D:364:GLY:HA3	2.46	0.45
1:D:470[A]:THR:CG2	1:D:471:PRO:N	2.80	0.45
1:G:373:GLN:HA	1:G:373:GLN:NE2	2.32	0.45
1:D:35:LEU:HD21	1:D:45:ASP:HB3	1.99	0.45
2:H:900:HDD:HMD3	2:H:900:HDD:HAD2	1.59	0.45
1:A:82:HIS:CD2	1:A:121:SER:OG	2.70	0.45
1:A:236:ASP:CG	1:A:433[B]:ARG:HH22	2.24	0.45
1:B:470[A]:THR:CG2	1:B:471:PRO:N	2.79	0.45
1:B:470[A]:THR:CG2	1:B:471:PRO:HD2	2.34	0.45
1:A:473:GLU:CD	1:A:539:VAL:HG13	2.42	0.45
1:H:176:LYS:HB3	1:H:177:PRO:HD2	1.97	0.45
1:C:260:GLU:OE2	1:C:643:LYS:NZ	2.50	0.45
1:D:64:PHE:CZ	1:D:68:ILE:HG13	2.51	0.45
1:D:373:GLN:HE21	1:D:373:GLN:CA	2.25	0.45
1:A:477:LEU:C	1:A:477:LEU:HD23	2.42	0.45
1:B:375:ASN:ND2	4:B:2052:HOH:O	2.50	0.45
1:H:89:HIS:HB2	1:H:331:ARG:HB3	1.98	0.45
1:A:312:LYS:HA	1:A:461:GLN:NE2	2.31	0.45
1:B:470[A]:THR:HB	1:B:539:VAL:CG2	2.47	0.45
1:C:369:TYR:O	1:C:373:GLN:HG2	2.17	0.45
1:E:247:PHE:N	1:E:247:PHE:CD1	2.84	0.45
1:E:477:LEU:C	1:E:477:LEU:HD23	2.42	0.45
1:F:293:GLN:HG3	1:F:321:LEU:HD23	1.99	0.45
1:A:277:TRP:CZ3	1:B:181:ASN:HB3	2.52	0.44
1:A:277:TRP:CH2	1:A:332:ASN:HB3	2.52	0.44
1:B:470[B]:THR:CG2	1:B:539:VAL:HG23	2.47	0.44
1:C:181:ASN:HB3	1:E:277:TRP:CZ3	2.53	0.44
4:C:2123:HOH:O	1:E:127[A]:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ASN:HB3	1:E:277:TRP:CE3	2.53	0.44
1:C:116:VAL:HG21	1:C:327:LEU:HD11	2.00	0.44
1:F:664:ASP:OD2	4:F:2370:HOH:O	2.21	0.44
4:G:2108:HOH:O	1:H:127[A]:ARG:NH1	2.49	0.44
1:A:238:GLY:O	1:A:439:PRO:HD2	2.18	0.44
1:C:155:ASN:CG	2:C:900:HDD:HMB2	2.43	0.44
1:F:313:ILE:N	1:F:461:GLN:HE22	2.00	0.44
1:B:138:GLY:HA3	2:B:900:HDD:HMA2	2.00	0.44
1:B:313:ILE:N	1:B:461:GLN:HE22	2.02	0.44
1:C:277:TRP:CZ3	1:C:333:PRO:HD2	2.53	0.44
1:C:508:VAL:O	1:C:512[A]:VAL:CG1	2.66	0.44
1:E:165:ALA:CB	1:E:364:GLY:HA3	2.48	0.44
1:A:470[A]:THR:CG2	1:A:471:PRO:N	2.81	0.44
1:D:300:ALA:HA	1:D:307:LEU:HD12	2.00	0.44
1:E:116:VAL:HA	1:E:142:ARG:O	2.18	0.44
1:G:176:LYS:HB3	1:G:177:PRO:CD	2.48	0.44
1:H:176:LYS:HB3	1:H:177:PRO:CD	2.49	0.43
1:H:369:TYR:O	1:H:373:GLN:HG2	2.18	0.43
1:G:176:LYS:HE3	1:H:75:ARG:HH21	1.83	0.43
2:G:900:HDD:HMD3	2:G:900:HDD:HAD2	1.53	0.43
1:C:138:GLY:HA3	2:C:900:HDD:HMA2	2.01	0.43
4:D:2124:HOH:O	1:F:127[B]:ARG:NH1	2.52	0.43
1:G:344:MET:HG2	1:G:373:GLN:NE2	2.33	0.43
1:A:470[A]:THR:HG22	4:A:2428:HOH:O	2.17	0.43
1:C:373:GLN:HE21	1:C:373:GLN:CA	2.26	0.43
2:C:900:HDD:HAD2	2:C:900:HDD:HMD3	1.54	0.43
1:C:51:ALA:O	1:C:55:GLY:HA3	2.18	0.43
1:D:51:ALA:O	1:D:55:GLY:HA3	2.19	0.43
1:C:176:LYS:HB3	1:C:177:PRO:HD2	1.99	0.43
1:G:300:ALA:HA	1:G:307:LEU:HD12	2.00	0.43
1:B:373:GLN:HE21	1:B:373:GLN:CA	2.28	0.43
1:C:470[A]:THR:CG2	1:C:471:PRO:N	2.81	0.43
1:G:423:TYR:HA	1:G:424:PRO:C	2.44	0.43
1:A:108:ASN:HD22	1:A:109:ALA:N	2.16	0.43
1:B:277:TRP:CZ3	1:B:332:ASN:HB3	2.54	0.43
2:B:900:HDD:HMD3	2:B:900:HDD:HAD2	1.58	0.43
1:C:442:THR:CG2	4:C:2349:HOH:O	2.50	0.43
2:F:900:HDD:HBC1	2:F:900:HDD:CMC	2.42	0.43
1:G:138:GLY:HA3	2:G:900:HDD:HMA2	2.01	0.43
1:G:498:LEU:HD21	1:G:512[A]:VAL:HG23	2.01	0.43
1:A:373:GLN:HA	1:A:373:GLN:NE2	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:ASP:OD1	1:D:457:ASP:C	2.62	0.42
1:G:35:LEU:HD21	1:G:45:ASP:HB3	2.01	0.42
1:E:82:HIS:HE1	4:E:2039:HOH:O	2.02	0.42
1:E:566:GLN:NE2	1:E:611[B]:ASP:OD1	2.40	0.42
1:E:573:ARG:CG	1:E:678:VAL:HG21	2.47	0.42
1:G:165:ALA:CB	1:G:364:GLY:HA3	2.49	0.42
1:B:369:TYR:O	1:B:373:GLN:HG2	2.19	0.42
1:D:375:ASN:ND2	4:D:2069:HOH:O	2.53	0.42
1:G:200:GLN:O	1:G:203:THR:HG23	2.19	0.42
1:E:138:GLY:HA3	2:E:900:HDD:HMA2	2.01	0.42
1:H:301:GLN:HE22	1:H:454:THR:HG21	1.84	0.42
1:B:594:GLN:HG3	1:B:598:THR:OG1	2.18	0.42
1:F:96:ALA:HA	1:F:110:THR:OG1	2.19	0.42
1:G:248:LYS:HB3	1:G:248:LYS:HE3	1.85	0.42
1:A:457:ASP:OD1	1:A:457:ASP:C	2.63	0.42
1:A:577:ASP:OD2	1:A:682:GLU:OE2	2.37	0.42
1:B:221:ARG:HG2	1:B:286:PRO:HG3	2.01	0.42
1:G:573:ARG:CG	1:G:678:VAL:HG21	2.49	0.42
1:G:87:GLY:HA2	1:G:118:VAL:O	2.20	0.42
1:H:228:VAL:HG11	2:H:900:HDD:HBB2	2.02	0.42
1:E:155:ASN:ND2	2:E:900:HDD:HMB2	2.35	0.42
1:F:470[A]:THR:HG22	1:F:472:VAL:HG12	2.02	0.42
1:A:277:TRP:CZ3	1:A:332:ASN:HB3	2.55	0.42
2:A:900:HDD:HMD2	2:A:900:HDD:HAD2	1.57	0.42
1:F:51:ALA:O	1:F:55:GLY:HA3	2.20	0.42
1:F:459:TRP:C	1:F:462:PRO:HD2	2.44	0.42
1:A:307:LEU:HD23	1:A:307:LEU:HA	1.88	0.42
4:A:2127:HOH:O	1:B:127[A]:ARG:NH1	2.53	0.42
1:E:277:TRP:CH2	1:E:332:ASN:HB3	2.54	0.42
1:E:492[B]:GLU:HG2	1:E:493:VAL:N	2.35	0.42
1:F:155:ASN:CG	2:F:900:HDD:HMB2	2.45	0.42
1:F:470[A]:THR:CG2	1:F:471:PRO:N	2.81	0.42
1:H:373:GLN:CA	1:H:373:GLN:NE2	2.81	0.42
1:B:139:PHE:C	1:B:139:PHE:CD1	2.98	0.41
1:F:673:SER:CB	1:F:676:MET:HE3	2.50	0.41
1:A:244:LYS:O	1:A:292:VAL:HA	2.20	0.41
4:C:2068:HOH:O	1:E:127[B]:ARG:NH2	2.42	0.41
1:D:373:GLN:HA	1:D:373:GLN:NE2	2.30	0.41
1:C:243:ILE:HA	1:C:293:GLN:O	2.21	0.41
1:C:477:LEU:C	1:C:477:LEU:HD23	2.44	0.41
1:A:138:GLY:HA3	2:A:900:HDD:HMA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:LYS:C	1:B:413:PRO:HD3	2.46	0.41
1:B:433[B]:ARG:NH2	4:B:2171:HOH:O	2.52	0.41
2:F:900:HDD:HMD3	2:F:900:HDD:HAD2	1.62	0.41
1:B:139:PHE:C	1:B:139:PHE:HD1	2.28	0.41
1:C:373:GLN:HA	1:C:373:GLN:NE2	2.31	0.41
1:D:176:LYS:HB3	1:D:177:PRO:CD	2.51	0.41
1:E:244:LYS:O	1:E:292:VAL:HA	2.20	0.41
1:E:574:LEU:HD22	1:E:579:LEU:HD13	2.02	0.41
1:G:150:PHE:CZ	1:G:354[A]:ILE:HD13	2.56	0.41
1:E:51:ALA:O	1:E:55:GLY:HA3	2.20	0.41
1:H:200:GLN:O	1:H:203:THR:HG23	2.21	0.41
1:B:373:GLN:HA	1:B:373:GLN:NE2	2.31	0.41
1:E:238:GLY:O	1:E:439:PRO:HD2	2.20	0.41
1:F:244:LYS:O	1:F:292:VAL:HA	2.21	0.41
1:H:244:LYS:O	1:H:292:VAL:HA	2.21	0.41
1:A:285:GLY:HA3	1:A:329:LEU:O	2.21	0.41
1:B:244:LYS:O	1:B:292:VAL:HA	2.21	0.41
1:D:470[A]:THR:HG23	1:D:471:PRO:N	2.35	0.41
1:E:243:ILE:HA	1:E:293:GLN:O	2.21	0.41
1:G:89:HIS:HB2	1:G:331[B]:ARG:CG	2.26	0.41
1:G:312:LYS:HA	1:G:461:GLN:NE2	2.36	0.41
1:H:247:PHE:HD1	1:H:247:PHE:N	2.19	0.41
1:H:247:PHE:N	1:H:247:PHE:CD1	2.89	0.41
1:B:344:MET:SD	1:B:382:PHE:HB2	2.61	0.41
1:H:438:ALA:HA	1:H:439:PRO:HD3	1.88	0.41
1:A:287:GLU:HB3	1:A:326:LEU:HD11	2.03	0.40
1:C:355:ASP:HB2	4:C:2288:HOH:O	2.20	0.40
1:C:331:ARG:HD3	4:C:2272:HOH:O	2.20	0.40
1:H:201:PRO:C	1:H:203:THR:N	2.78	0.40
1:H:205:HIS:CE1	1:H:461:GLN:HE21	2.39	0.40
1:A:68:ILE:HD13	1:A:68:ILE:HA	1.96	0.40
1:A:247:PHE:N	1:A:247:PHE:CD1	2.89	0.40
1:B:594:GLN:HE21	1:B:594:GLN:HB2	1.64	0.40
1:A:659:ALA:O	1:A:660:ASP:HB2	2.21	0.40
1:D:90:GLY:C	1:D:116:VAL:HG22	2.47	0.40
1:D:344:MET:HG2	1:D:373:GLN:NE2	2.37	0.40
1:D:344:MET:SD	1:D:382:PHE:HB2	2.62	0.40
1:D:351:VAL:HG23	1:D:354[A]:ILE:HD12	2.04	0.40
1:D:598:THR:HG22	1:F:483:PHE:CD2	2.56	0.40
1:H:659:ALA:O	1:H:660:ASP:HB2	2.20	0.40
1:B:154:GLY:O	2:B:900:HDD:HMA1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ASP:C	1:B:457:ASP:OD1	2.65	0.40
1:D:139:PHE:C	1:D:139:PHE:CD1	3.00	0.40
1:D:373:GLN:CA	1:D:373:GLN:NE2	2.84	0.40
1:F:247:PHE:N	1:F:247:PHE:HD1	2.20	0.40
1:H:457:ASP:OD1	1:H:457:ASP:C	2.64	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	684/719 (95%)	663 (97%)	21 (3%)	0	100	100
1	B	688/719 (96%)	665 (97%)	23 (3%)	0	100	100
1	C	689/719 (96%)	668 (97%)	21 (3%)	0	100	100
1	D	688/719 (96%)	672 (98%)	16 (2%)	0	100	100
1	E	681/719 (95%)	660 (97%)	21 (3%)	0	100	100
1	F	678/719 (94%)	660 (97%)	18 (3%)	0	100	100
1	G	690/719 (96%)	672 (97%)	18 (3%)	0	100	100
1	H	680/719 (95%)	661 (97%)	19 (3%)	0	100	100
All	All	5478/5752 (95%)	5321 (97%)	157 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	575/596 (96%)	556 (97%)	19 (3%)	33	17
1	B	576/596 (97%)	567 (98%)	9 (2%)	55	44
1	C	577/596 (97%)	560 (97%)	17 (3%)	37	21
1	D	576/596 (97%)	563 (98%)	13 (2%)	44	30
1	E	572/596 (96%)	558 (98%)	14 (2%)	43	28
1	F	569/596 (96%)	552 (97%)	17 (3%)	36	20
1	G	578/596 (97%)	567 (98%)	11 (2%)	50	37
1	H	570/596 (96%)	550 (96%)	20 (4%)	32	16
All	All	4593/4768 (96%)	4473 (97%)	120 (3%)	44	24

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ILE
1	A	70	HIS
1	A	108	ASN
1	A	264	LEU
1	A	301	GLN
1	A	373	GLN
1	A	442	THR
1	A	491[A]	GLU
1	A	491[B]	GLU
1	A	512	VAL
1	A	532	LYS
1	A	539	VAL
1	A	559[A]	SER
1	A	559[B]	SER
1	A	590[A]	GLU
1	A	590[B]	GLU
1	A	673	SER
1	A	689[A]	ARG
1	A	689[B]	ARG
1	B	70	HIS
1	B	108	ASN
1	B	139	PHE
1	B	264	LEU
1	B	425	ARG

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Mol	Chain	Res	Type
1	B	442	THR
1	B	512[A]	VAL
1	B	512[B]	VAL
1	B	562	SER
1	C	70	HIS
1	C	108	ASN
1	C	145	THR
1	C	241	LYS
1	C	264	LEU
1	C	373	GLN
1	C	442	THR
1	C	470[A]	THR
1	C	470[B]	THR
1	C	491[A]	GLU
1	C	491[B]	GLU
1	C	512[A]	VAL
1	C	512[B]	VAL
1	C	539	VAL
1	C	590	GLU
1	C	594	GLN
1	C	622	SER
1	D	53	ILE
1	D	70	HIS
1	D	108	ASN
1	D	264	LEU
1	D	373	GLN
1	D	425	ARG
1	D	442	THR
1	D	470[A]	THR
1	D	470[B]	THR
1	D	491[A]	GLU
1	D	491[B]	GLU
1	D	539	VAL
1	D	622	SER
1	E	70	HIS
1	E	108	ASN
1	E	145	THR
1	E	264	LEU
1	E	275	ASP
1	E	373	GLN
1	E	407	ILE
1	E	442	THR

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Mol	Chain	Res	Type
1	E	512	VAL
1	E	539	VAL
1	E	561	SER
1	E	594	GLN
1	E	657	ASP
1	E	660	ASP
1	F	70	HIS
1	F	108	ASN
1	F	264	LEU
1	F	275	ASP
1	F	301	GLN
1	F	373	GLN
1	F	391[A]	ARG
1	F	391[B]	ARG
1	F	411	LYS
1	F	442	THR
1	F	470[A]	THR
1	F	470[B]	THR
1	F	491[A]	GLU
1	F	491[B]	GLU
1	F	539	VAL
1	F	616	LEU
1	F	679	GLU
1	G	70	HIS
1	G	108	ASN
1	G	145	THR
1	G	264	LEU
1	G	442	THR
1	G	444	SER
1	G	491[A]	GLU
1	G	491[B]	GLU
1	G	539	VAL
1	G	676[A]	MET
1	G	676[B]	MET
1	H	70	HIS
1	H	108	ASN
1	H	145	THR
1	H	264	LEU
1	H	275	ASP
1	H	373	GLN
1	H	442	THR
1	H	444	SER

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Mol	Chain	Res	Type
1	H	470[A]	THR
1	H	470[B]	THR
1	H	491[A]	GLU
1	H	491[B]	GLU
1	H	512[A]	VAL
1	H	512[B]	VAL
1	H	539	VAL
1	H	548	LYS
1	H	562	SER
1	H	576	LYS
1	H	676	MET
1	H	698	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	108	ASN
1	A	113	GLN
1	A	373	GLN
1	A	461	GLN
1	A	594	GLN
1	B	82	HIS
1	B	108	ASN
1	B	167	GLN
1	B	301	GLN
1	B	346	GLN
1	B	373	GLN
1	B	461	GLN
1	B	594	GLN
1	C	82	HIS
1	C	108	ASN
1	C	301	GLN
1	C	373	GLN
1	C	375	ASN
1	C	395	HIS
1	C	461	GLN
1	D	82	HIS
1	D	108	ASN
1	D	301	GLN
1	D	373	GLN
1	D	375	ASN

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Mol	Chain	Res	Type
1	D	430	ASN
1	D	461	GLN
1	D	594	GLN
1	E	82	HIS
1	E	108	ASN
1	E	246	HIS
1	E	301	GLN
1	E	332	ASN
1	E	373	GLN
1	E	375	ASN
1	E	461	GLN
1	E	594	GLN
1	F	82	HIS
1	F	108	ASN
1	F	113	GLN
1	F	301	GLN
1	F	373	GLN
1	F	461	GLN
1	F	569	GLN
1	F	594	GLN
1	G	82	HIS
1	G	108	ASN
1	G	113	GLN
1	G	301	GLN
1	G	373	GLN
1	G	461	GLN
1	G	569	GLN
1	G	594	GLN
1	H	46	GLN
1	H	82	HIS
1	H	108	ASN
1	H	246	HIS
1	H	301	GLN
1	H	373	GLN
1	H	375	ASN
1	H	377	ASN
1	H	461	GLN
1	H	633	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides 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	$\#\|Z\| > 2$
2	HDD	D	900	4,1	50,52,52	2.57	21 (42%)	56,89,89	2.69	22 (39%)
2	HDD	H	900	4,1	50,52,52	2.56	20 (40%)	56,89,89	2.55	22 (39%)
2	HDD	G	900	4,1	50,52,52	2.55	22 (44%)	56,89,89	2.66	23 (41%)
2	HDD	B	900	4,1	50,52,52	2.55	22 (44%)	56,89,89	2.71	26 (46%)
2	HDD	A	900	4,1	50,52,52	2.56	22 (44%)	56,89,89	2.54	22 (39%)
2	HDD	E	900	4,1	50,52,52	2.56	22 (44%)	56,89,89	2.64	23 (41%)
2	HDD	F	900	4,1	50,52,52	2.51	21 (42%)	56,89,89	2.54	23 (41%)
2	HDD	C	900	4,1	50,52,52	2.54	21 (42%)	56,89,89	2.73	25 (44%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HDD	D	900	4,1	-	5/9/89/89	0/1/9/9
2	HDD	H	900	4,1	-	4/9/89/89	0/1/9/9
2	HDD	G	900	4,1	-	4/9/89/89	0/1/9/9
2	HDD	B	900	4,1	-	4/9/89/89	0/1/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HDD	A	900	4,1	-	5/9/89/89	0/1/9/9
2	HDD	E	900	4,1	-	4/9/89/89	0/1/9/9
2	HDD	F	900	4,1	-	3/9/89/89	0/1/9/9
2	HDD	C	900	4,1	-	4/9/89/89	0/1/9/9

All (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	HDD	O1D-CGD	5.78	1.45	1.35
2	H	900	HDD	O1D-CGD	5.64	1.44	1.35
2	C	900	HDD	O1D-CGD	5.63	1.44	1.35
2	D	900	HDD	O1D-CGD	5.52	1.44	1.35
2	B	900	HDD	O1D-CGD	5.50	1.44	1.35
2	E	900	HDD	O1D-CGD	5.36	1.44	1.35
2	A	900	HDD	FE-NB	5.33	2.11	1.94
2	G	900	HDD	FE-NB	5.32	2.11	1.94
2	G	900	HDD	O1D-CGD	5.27	1.44	1.35
2	F	900	HDD	O1D-CGD	5.26	1.44	1.35
2	E	900	HDD	FE-NB	5.23	2.11	1.94
2	D	900	HDD	FE-NB	5.17	2.10	1.94
2	C	900	HDD	FE-NB	5.16	2.10	1.94
2	F	900	HDD	FE-NB	5.12	2.10	1.94
2	B	900	HDD	C3B-C2B	5.07	1.47	1.37
2	H	900	HDD	FE-NB	5.06	2.10	1.94
2	D	900	HDD	C3B-C2B	5.06	1.47	1.37
2	D	900	HDD	C3C-C2C	5.06	1.47	1.37
2	B	900	HDD	FE-NB	5.05	2.10	1.94
2	E	900	HDD	C3B-C2B	4.99	1.47	1.37
2	H	900	HDD	C3B-C2B	4.97	1.47	1.37
2	A	900	HDD	C3B-C2B	4.96	1.47	1.37
2	E	900	HDD	C3C-C2C	4.91	1.47	1.37
2	H	900	HDD	CHD-C4C	4.82	1.47	1.38
2	A	900	HDD	C3C-C2C	4.82	1.47	1.37
2	G	900	HDD	CHC-C1C	4.78	1.47	1.38
2	G	900	HDD	C3B-C2B	4.76	1.46	1.37
2	B	900	HDD	C3C-C2C	4.76	1.46	1.37
2	H	900	HDD	C3C-C2C	4.76	1.46	1.37
2	F	900	HDD	C3B-C2B	4.76	1.46	1.37
2	G	900	HDD	C3C-C2C	4.75	1.46	1.37
2	C	900	HDD	C3B-C2B	4.72	1.46	1.37
2	F	900	HDD	C3C-C2C	4.68	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	HDD	CHC-C1C	4.63	1.47	1.38
2	G	900	HDD	FE-NC	4.63	2.10	1.95
2	H	900	HDD	FE-NC	4.63	2.10	1.95
2	E	900	HDD	FE-NC	4.62	2.10	1.95
2	C	900	HDD	C3C-C2C	4.60	1.46	1.37
2	B	900	HDD	FE-NC	4.57	2.10	1.95
2	B	900	HDD	CHD-C4C	4.56	1.47	1.38
2	B	900	HDD	CHC-C1C	4.55	1.47	1.38
2	E	900	HDD	CHD-C4C	4.52	1.47	1.38
2	F	900	HDD	CHC-C1C	4.51	1.47	1.38
2	C	900	HDD	CHD-C4C	4.50	1.47	1.38
2	H	900	HDD	CHB-C1B	4.48	1.47	1.38
2	H	900	HDD	CHC-C1C	4.48	1.47	1.38
2	A	900	HDD	CHC-C1C	4.47	1.47	1.38
2	D	900	HDD	FE-NA	4.46	2.10	1.95
2	F	900	HDD	CHD-C4C	4.45	1.47	1.38
2	D	900	HDD	CHD-C4C	4.44	1.47	1.38
2	E	900	HDD	CHB-C1B	4.43	1.47	1.38
2	C	900	HDD	FE-NC	4.43	2.10	1.95
2	A	900	HDD	CHD-C4C	4.41	1.47	1.38
2	D	900	HDD	FE-NC	4.40	2.10	1.95
2	F	900	HDD	FE-NC	4.39	2.10	1.95
2	E	900	HDD	CHC-C1C	4.38	1.46	1.38
2	D	900	HDD	CHB-C1B	4.38	1.47	1.38
2	F	900	HDD	CHB-C1B	4.36	1.47	1.38
2	D	900	HDD	CHC-C1C	4.34	1.46	1.38
2	A	900	HDD	CHB-C1B	4.32	1.47	1.38
2	B	900	HDD	FE-NA	4.32	2.09	1.95
2	H	900	HDD	FE-NA	4.32	2.09	1.95
2	G	900	HDD	CHB-C1B	4.31	1.47	1.38
2	G	900	HDD	CHD-C4C	4.31	1.46	1.38
2	A	900	HDD	FE-NC	4.30	2.09	1.95
2	A	900	HDD	FE-NA	4.28	2.09	1.95
2	F	900	HDD	FE-NA	4.24	2.09	1.95
2	C	900	HDD	FE-NA	4.23	2.09	1.95
2	B	900	HDD	CHB-C1B	4.19	1.47	1.38
2	G	900	HDD	FE-NA	4.07	2.08	1.95
2	C	900	HDD	CHB-C1B	4.06	1.46	1.38
2	E	900	HDD	FE-NA	4.05	2.08	1.95
2	E	900	HDD	CHA-C1A	3.96	1.48	1.39
2	A	900	HDD	CHA-C1A	3.89	1.48	1.39
2	D	900	HDD	CHB-C4A	3.84	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	900	HDD	CHA-C1A	3.84	1.48	1.39
2	B	900	HDD	CHC-C4B	3.80	1.47	1.39
2	F	900	HDD	CHA-C1A	3.79	1.47	1.39
2	D	900	HDD	CHA-C1A	3.75	1.47	1.39
2	B	900	HDD	CHA-C1A	3.75	1.47	1.39
2	C	900	HDD	CHB-C4A	3.67	1.47	1.39
2	C	900	HDD	CHA-C1A	3.65	1.47	1.39
2	G	900	HDD	CHC-C4B	3.61	1.47	1.39
2	F	900	HDD	CHC-C4B	3.60	1.47	1.39
2	C	900	HDD	CHC-C4B	3.59	1.47	1.39
2	H	900	HDD	CHC-C4B	3.59	1.47	1.39
2	H	900	HDD	CHA-C1A	3.53	1.47	1.39
2	A	900	HDD	CHC-C4B	3.51	1.47	1.39
2	B	900	HDD	CHB-C4A	3.50	1.47	1.39
2	F	900	HDD	CHB-C4A	3.50	1.47	1.39
2	H	900	HDD	CHB-C4A	3.49	1.47	1.39
2	G	900	HDD	CHB-C4A	3.49	1.47	1.39
2	E	900	HDD	CHC-C4B	3.46	1.47	1.39
2	E	900	HDD	CHB-C4A	3.46	1.47	1.39
2	A	900	HDD	CHB-C4A	3.45	1.47	1.39
2	D	900	HDD	CHC-C4B	3.42	1.47	1.39
2	D	900	HDD	C2A-C3A	3.31	1.47	1.38
2	C	900	HDD	C2A-C3A	3.23	1.47	1.38
2	H	900	HDD	C2A-C3A	3.21	1.47	1.38
2	F	900	HDD	C2A-C3A	3.19	1.47	1.38
2	G	900	HDD	C2A-C3A	3.16	1.47	1.38
2	B	900	HDD	C2A-C3A	3.13	1.47	1.38
2	A	900	HDD	C2A-C3A	3.05	1.47	1.38
2	E	900	HDD	C2A-C3A	3.03	1.46	1.38
2	G	900	HDD	C1B-NB	-2.84	1.35	1.40
2	C	900	HDD	C1A-NA	-2.81	1.34	1.39
2	E	900	HDD	CHD-C1D	-2.78	1.33	1.41
2	A	900	HDD	CHD-C1D	-2.77	1.33	1.41
2	F	900	HDD	C1A-NA	-2.76	1.34	1.39
2	H	900	HDD	C1A-NA	-2.73	1.34	1.39
2	H	900	HDD	C1B-NB	-2.72	1.35	1.40
2	D	900	HDD	C1A-NA	-2.71	1.34	1.39
2	D	900	HDD	CHD-C1D	-2.70	1.33	1.41
2	B	900	HDD	C1A-NA	-2.70	1.34	1.39
2	D	900	HDD	C4C-NC	-2.68	1.34	1.39
2	C	900	HDD	C1B-NB	-2.64	1.35	1.40
2	C	900	HDD	C4C-NC	-2.64	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	900	HDD	C1B-C2B	2.64	1.49	1.44
2	F	900	HDD	CHD-C1D	-2.63	1.33	1.41
2	G	900	HDD	CHD-C1D	-2.62	1.33	1.41
2	C	900	HDD	CHD-C1D	-2.61	1.33	1.41
2	G	900	HDD	C1A-NA	-2.61	1.34	1.39
2	E	900	HDD	C1B-NB	-2.60	1.35	1.40
2	B	900	HDD	CHD-C1D	-2.59	1.33	1.41
2	E	900	HDD	C1A-NA	-2.54	1.34	1.39
2	E	900	HDD	C4C-NC	-2.54	1.34	1.39
2	G	900	HDD	C4C-NC	-2.50	1.34	1.39
2	A	900	HDD	C1B-NB	-2.49	1.36	1.40
2	D	900	HDD	C1B-NB	-2.48	1.36	1.40
2	H	900	HDD	CHD-C1D	-2.47	1.34	1.41
2	H	900	HDD	C1B-C2B	2.47	1.49	1.44
2	B	900	HDD	C1B-NB	-2.46	1.36	1.40
2	F	900	HDD	C1B-NB	-2.45	1.36	1.40
2	A	900	HDD	C1B-C2B	2.41	1.49	1.44
2	G	900	HDD	C1B-C2B	2.41	1.49	1.44
2	D	900	HDD	C1B-C2B	2.40	1.49	1.44
2	A	900	HDD	C4A-NA	-2.40	1.35	1.39
2	A	900	HDD	C1A-NA	-2.39	1.35	1.39
2	A	900	HDD	C4C-NC	-2.38	1.35	1.39
2	B	900	HDD	C1B-C2B	2.36	1.49	1.44
2	C	900	HDD	C1B-C2B	2.36	1.49	1.44
2	C	900	HDD	C4A-NA	-2.35	1.35	1.39
2	E	900	HDD	C4A-NA	-2.35	1.35	1.39
2	F	900	HDD	C4A-NA	-2.35	1.35	1.39
2	B	900	HDD	C4C-NC	-2.33	1.35	1.39
2	D	900	HDD	C1A-C2A	2.33	1.49	1.44
2	F	900	HDD	C1B-C2B	2.32	1.49	1.44
2	B	900	HDD	C1A-C2A	2.31	1.49	1.44
2	H	900	HDD	C4C-NC	-2.31	1.35	1.39
2	F	900	HDD	C4C-NC	-2.29	1.35	1.39
2	D	900	HDD	C4A-C3A	2.29	1.48	1.43
2	H	900	HDD	C1A-C2A	2.28	1.49	1.44
2	B	900	HDD	C4A-C3A	2.27	1.48	1.43
2	G	900	HDD	C4A-NA	-2.23	1.35	1.39
2	B	900	HDD	C4A-NA	-2.23	1.35	1.39
2	G	900	HDD	C1A-C2A	2.22	1.49	1.44
2	A	900	HDD	C1C-NC	-2.21	1.35	1.39
2	A	900	HDD	C4A-C3A	2.17	1.48	1.43
2	E	900	HDD	C1C-C2C	2.16	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	HDD	C1C-NC	-2.14	1.35	1.39
2	F	900	HDD	C1A-C2A	2.14	1.48	1.44
2	E	900	HDD	C4A-C3A	2.13	1.48	1.43
2	E	900	HDD	C1A-C2A	2.13	1.48	1.44
2	A	900	HDD	C1A-C2A	2.12	1.48	1.44
2	D	900	HDD	C4A-NA	-2.10	1.35	1.39
2	G	900	HDD	C1C-C2C	2.09	1.49	1.45
2	G	900	HDD	C4A-C3A	2.08	1.48	1.43
2	B	900	HDD	C1C-C2C	2.08	1.49	1.45
2	H	900	HDD	C4A-C3A	2.05	1.48	1.43
2	C	900	HDD	C1C-C2C	2.00	1.49	1.45
2	F	900	HDD	C4A-C3A	2.00	1.48	1.43

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	900	HDD	C3B-C2B-C1B	-9.49	99.44	106.49
2	C	900	HDD	C3B-C2B-C1B	-8.90	99.88	106.49
2	B	900	HDD	C3B-C2B-C1B	-8.72	100.02	106.49
2	E	900	HDD	C3B-C2B-C1B	-8.62	100.09	106.49
2	F	900	HDD	C3B-C2B-C1B	-8.45	100.21	106.49
2	G	900	HDD	C3B-C2B-C1B	-8.29	100.33	106.49
2	A	900	HDD	C3B-C2B-C1B	-8.17	100.43	106.49
2	E	900	HDD	C3C-C2C-C1C	-7.92	99.51	107.08
2	H	900	HDD	C3B-C2B-C1B	-7.74	100.75	106.49
2	H	900	HDD	C3C-C2C-C1C	-7.68	99.74	107.08
2	D	900	HDD	C3C-C2C-C1C	-7.61	99.81	107.08
2	G	900	HDD	C3C-C2C-C1C	-7.34	100.06	107.08
2	C	900	HDD	C3C-C2C-C1C	-7.23	100.17	107.08
2	F	900	HDD	C3C-C2C-C1C	-7.21	100.19	107.08
2	A	900	HDD	C3C-C2C-C1C	-7.20	100.20	107.08
2	B	900	HDD	C3C-C2C-C1C	-7.13	100.27	107.08
2	G	900	HDD	CHD-C4C-NC	-5.56	118.42	124.44
2	G	900	HDD	C2B-C1B-NB	5.55	116.41	109.84
2	A	900	HDD	C2B-C1B-NB	5.40	116.24	109.84
2	C	900	HDD	C2B-C1B-NB	5.23	116.04	109.84
2	F	900	HDD	C2B-C1B-NB	5.19	115.99	109.84
2	C	900	HDD	CHD-C4C-NC	-4.70	119.36	124.44
2	B	900	HDD	C2B-C1B-NB	4.67	115.38	109.84
2	E	900	HDD	C2B-C1B-NB	4.66	115.36	109.84
2	B	900	HDD	CHD-C4C-NC	-4.49	119.58	124.44
2	C	900	HDD	C4A-C3A-C2A	-4.48	101.59	106.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	900	HDD	CHC-C1C-NC	-4.47	119.60	124.44
2	E	900	HDD	C2D-C1D-CHD	-4.34	116.46	123.33
2	H	900	HDD	C2B-C1B-NB	4.34	114.98	109.84
2	B	900	HDD	C4A-C3A-C2A	-4.31	101.79	106.83
2	F	900	HDD	C4A-C3A-C2A	-4.28	101.82	106.83
2	A	900	HDD	C4C-C3C-C2C	-4.23	103.28	106.75
2	D	900	HDD	C2B-C1B-NB	4.23	114.85	109.84
2	B	900	HDD	C4C-NC-C1C	-4.19	101.25	105.35
2	H	900	HDD	C4A-C3A-C2A	-4.16	101.96	106.83
2	B	900	HDD	CHC-C1C-NC	-4.10	120.00	124.44
2	H	900	HDD	CHD-C4C-NC	-4.08	120.02	124.44
2	D	900	HDD	C4A-C3A-C2A	-4.04	102.10	106.83
2	G	900	HDD	C4A-C3A-C2A	-4.03	102.12	106.83
2	E	900	HDD	C4A-C3A-C2A	-4.02	102.13	106.83
2	A	900	HDD	C4A-C3A-C2A	-3.80	102.39	106.83
2	B	900	HDD	CAA-CBA-CGA	-3.79	105.45	113.60
2	A	900	HDD	CHC-C1C-NC	-3.79	120.34	124.44
2	D	900	HDD	O1D-CGD-O2D	3.75	124.14	120.80
2	D	900	HDD	CHC-C1C-NC	-3.75	120.39	124.44
2	B	900	HDD	CHA-C1A-NA	-3.69	117.05	123.85
2	D	900	HDD	C4B-C3B-C2B	-3.68	104.19	107.11
2	H	900	HDD	CHA-C1A-NA	-3.67	117.08	123.85
2	C	900	HDD	CAA-CBA-CGA	-3.65	105.75	113.60
2	G	900	HDD	CAA-CBA-CGA	-3.64	105.76	113.60
2	B	900	HDD	C4C-C3C-C2C	-3.64	103.76	106.75
2	D	900	HDD	CHA-C1A-NA	-3.64	117.16	123.85
2	A	900	HDD	O1D-CGD-O2D	3.62	124.03	120.80
2	E	900	HDD	CAA-CBA-CGA	-3.61	105.83	113.60
2	C	900	HDD	C2D-C1D-CHD	-3.60	117.64	123.33
2	G	900	HDD	CHA-C1A-NA	-3.57	117.27	123.85
2	D	900	HDD	CHD-C4C-NC	-3.57	120.58	124.44
2	A	900	HDD	CHA-C1A-NA	-3.54	117.34	123.85
2	H	900	HDD	CHC-C1C-NC	-3.54	120.61	124.44
2	H	900	HDD	O1D-CGD-O2D	3.50	123.92	120.80
2	C	900	HDD	CHA-C1A-NA	-3.49	117.42	123.85
2	H	900	HDD	C3A-C4A-NA	3.42	115.28	110.08
2	F	900	HDD	CAA-CBA-CGA	-3.39	106.32	113.60
2	D	900	HDD	C2C-C1C-NC	3.36	115.88	109.69
2	G	900	HDD	C4C-C3C-C2C	-3.35	104.00	106.75
2	C	900	HDD	CMC-C2C-C1C	3.35	130.61	124.71
2	G	900	HDD	C4C-NC-C1C	-3.33	102.09	105.35
2	F	900	HDD	CHA-C1A-NA	-3.32	117.73	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	900	HDD	CAA-CBA-CGA	-3.31	106.48	113.60
2	E	900	HDD	CHA-C1A-NA	-3.31	117.76	123.85
2	B	900	HDD	C3A-C4A-NA	3.26	115.05	110.08
2	D	900	HDD	C2D-C1D-CHD	-3.26	118.17	123.33
2	H	900	HDD	C2A-C1A-NA	3.24	113.77	110.15
2	B	900	HDD	C2D-C1D-CHD	-3.22	118.24	123.33
2	C	900	HDD	C3A-C4A-NA	3.22	114.98	110.08
2	B	900	HDD	CMC-C2C-C1C	3.19	130.34	124.71
2	H	900	HDD	CMC-C2C-C1C	3.19	130.34	124.71
2	G	900	HDD	CMC-C2C-C1C	3.18	130.32	124.71
2	G	900	HDD	C3A-C4A-NA	3.17	114.91	110.08
2	F	900	HDD	C2C-C1C-NC	3.16	115.53	109.69
2	F	900	HDD	CHD-C4C-NC	-3.16	121.03	124.44
2	C	900	HDD	CMB-C2B-C1B	3.16	129.84	125.04
2	E	900	HDD	C3A-C4A-NA	3.15	114.88	110.08
2	A	900	HDD	C2D-C1D-CHD	-3.15	118.34	123.33
2	A	900	HDD	C3A-C4A-NA	3.13	114.84	110.08
2	D	900	HDD	C2A-C1A-NA	3.13	113.64	110.15
2	D	900	HDD	C3A-C4A-NA	3.12	114.84	110.08
2	A	900	HDD	C2A-C1A-NA	3.12	113.64	110.15
2	F	900	HDD	C2D-C1D-CHD	-3.12	118.40	123.33
2	F	900	HDD	C3A-C4A-NA	3.11	114.82	110.08
2	H	900	HDD	C4C-NC-C1C	-3.10	102.31	105.35
2	E	900	HDD	CHB-C1B-NB	-3.09	120.56	124.37
2	E	900	HDD	C2C-C1C-NC	3.09	115.39	109.69
2	A	900	HDD	CAA-CBA-CGA	-3.08	106.98	113.60
2	E	900	HDD	CMC-C2C-C1C	3.07	130.13	124.71
2	H	900	HDD	C2C-C1C-NC	3.04	115.30	109.69
2	C	900	HDD	C4C-C3C-C2C	-3.02	104.27	106.75
2	E	900	HDD	C4C-NC-C1C	-3.01	102.40	105.35
2	C	900	HDD	C4C-NC-C1C	-3.01	102.40	105.35
2	G	900	HDD	C2C-C1C-NC	3.00	115.23	109.69
2	E	900	HDD	C4C-C3C-C2C	-3.00	104.29	106.75
2	G	900	HDD	C2D-C1D-CHD	-3.00	118.59	123.33
2	D	900	HDD	C1A-C2A-C3A	-2.97	102.22	106.89
2	C	900	HDD	C4A-NA-C1A	-2.97	102.44	105.35
2	B	900	HDD	C2A-C1A-NA	2.96	113.46	110.15
2	F	900	HDD	C4C-NC-C1C	-2.96	102.45	105.35
2	F	900	HDD	CMB-C2B-C1B	2.96	129.54	125.04
2	E	900	HDD	O1D-CGD-O2D	2.96	123.44	120.80
2	F	900	HDD	C2A-C1A-NA	2.94	113.44	110.15
2	C	900	HDD	C2C-C1C-NC	2.93	115.10	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	900	HDD	CHD-C4C-NC	-2.91	121.29	124.44
2	A	900	HDD	C1A-C2A-C3A	-2.86	102.39	106.89
2	G	900	HDD	C2A-C1A-NA	2.86	113.35	110.15
2	H	900	HDD	CMB-C2B-C1B	2.85	129.38	125.04
2	H	900	HDD	CAA-CBA-CGA	-2.85	107.47	113.60
2	B	900	HDD	O1D-CGD-O2D	2.83	123.32	120.80
2	F	900	HDD	CHC-C1C-NC	-2.83	121.38	124.44
2	C	900	HDD	C1A-C2A-C3A	-2.80	102.49	106.89
2	C	900	HDD	O1D-CGD-O2D	2.79	123.29	120.80
2	F	900	HDD	CMC-C2C-C1C	2.79	129.64	124.71
2	B	900	HDD	CHD-C4C-C3C	-2.78	120.50	125.26
2	H	900	HDD	C2D-C1D-CHD	-2.77	118.94	123.33
2	E	900	HDD	C2A-C1A-NA	2.76	113.23	110.15
2	A	900	HDD	CHD-C4C-NC	-2.76	121.45	124.44
2	D	900	HDD	CHC-C4B-NB	-2.76	121.42	124.42
2	F	900	HDD	O1D-CGD-O2D	2.75	123.25	120.80
2	G	900	HDD	CHD-C4C-C3C	-2.74	120.58	125.26
2	H	900	HDD	CHB-C1B-NB	-2.74	121.00	124.37
2	A	900	HDD	C2C-C1C-NC	2.73	114.72	109.69
2	B	900	HDD	C2C-C1C-NC	2.71	114.68	109.69
2	G	900	HDD	CMB-C2B-C1B	2.68	129.11	125.04
2	G	900	HDD	C1A-C2A-C3A	-2.67	102.70	106.89
2	C	900	HDD	CHC-C4B-NB	-2.66	121.52	124.42
2	C	900	HDD	C2A-C1A-NA	2.66	113.12	110.15
2	D	900	HDD	CMC-C2C-C1C	2.65	129.39	124.71
2	D	900	HDD	CHB-C1B-NB	-2.65	121.11	124.37
2	F	900	HDD	C1A-C2A-C3A	-2.61	102.78	106.89
2	C	900	HDD	CHC-C4B-C3B	-2.61	119.52	125.13
2	D	900	HDD	C4C-NC-C1C	-2.60	102.80	105.35
2	B	900	HDD	C1A-C2A-C3A	-2.60	102.80	106.89
2	C	900	HDD	CHD-C4C-C3C	-2.59	120.83	125.26
2	E	900	HDD	C1A-C2A-C3A	-2.57	102.84	106.89
2	C	900	HDD	CHC-C1C-NC	-2.55	121.68	124.44
2	A	900	HDD	CAA-C2A-C1A	2.54	129.89	124.89
2	D	900	HDD	CMB-C2B-C1B	2.54	128.90	125.04
2	F	900	HDD	C4A-NA-C1A	-2.52	102.88	105.35
2	E	900	HDD	CMB-C2B-C1B	2.51	128.85	125.04
2	B	900	HDD	CHB-C1B-NB	-2.50	121.29	124.37
2	H	900	HDD	C1A-C2A-C3A	-2.50	102.96	106.89
2	H	900	HDD	CMA-C3A-C4A	2.48	129.15	125.37
2	G	900	HDD	O1D-CGD-O2D	2.43	122.97	120.80
2	A	900	HDD	CMA-C3A-C4A	2.41	129.04	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	900	HDD	C4B-C3B-C2B	-2.39	105.22	107.11
2	G	900	HDD	C4B-C3B-C2B	-2.39	105.22	107.11
2	G	900	HDD	CAA-C2A-C1A	2.39	129.59	124.89
2	B	900	HDD	C4A-NA-C1A	-2.38	103.01	105.35
2	C	900	HDD	CMA-C3A-C2A	2.38	130.76	125.61
2	B	900	HDD	CAA-C2A-C1A	2.38	129.57	124.89
2	B	900	HDD	CHC-C1C-C2C	-2.38	120.50	125.48
2	C	900	HDD	CHB-C4A-C3A	-2.36	120.57	127.24
2	E	900	HDD	C4B-C3B-C2B	-2.36	105.24	107.11
2	A	900	HDD	CMB-C2B-C1B	2.36	128.63	125.04
2	G	900	HDD	CHC-C1C-NC	-2.32	121.92	124.44
2	B	900	HDD	CHB-C1B-C2B	-2.32	120.28	126.73
2	G	900	HDD	CHB-C1B-NB	-2.32	121.51	124.37
2	A	900	HDD	C4A-NA-C1A	-2.29	103.10	105.35
2	B	900	HDD	CMA-C3A-C4A	2.29	128.85	125.37
2	C	900	HDD	C4B-C3B-C2B	-2.27	105.31	107.11
2	B	900	HDD	C4B-C3B-C2B	-2.27	105.31	107.11
2	F	900	HDD	CMA-C3A-C4A	2.24	128.77	125.37
2	F	900	HDD	CAA-C2A-C1A	2.17	129.16	124.89
2	F	900	HDD	CHB-C4A-C3A	-2.16	121.14	127.24
2	G	900	HDD	CHB-C4A-C3A	-2.13	121.21	127.24
2	E	900	HDD	CMA-C3A-C4A	2.12	128.60	125.37
2	E	900	HDD	CAA-C2A-C1A	2.11	129.04	124.89
2	F	900	HDD	C4C-C3C-C2C	-2.10	105.02	106.75
2	A	900	HDD	C4B-C3B-C2B	-2.09	105.45	107.11
2	H	900	HDD	CHC-C1C-C2C	-2.09	121.10	125.48
2	E	900	HDD	CHB-C1B-C2B	-2.08	120.96	126.73
2	F	900	HDD	CHC-C1C-C2C	-2.07	121.14	125.48
2	D	900	HDD	CMA-C3A-C4A	2.06	128.51	125.37
2	B	900	HDD	CHB-C4A-C3A	-2.06	121.42	127.24
2	H	900	HDD	CHB-C1B-C2B	-2.06	121.02	126.73
2	D	900	HDD	C4C-C3C-C2C	-2.04	105.07	106.75
2	A	900	HDD	CHB-C1B-C2B	-2.02	121.12	126.73
2	A	900	HDD	CMC-C2C-C1C	2.00	128.24	124.71

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	900	HDD	C2B-C3B-CAB-CBB
2	G	900	HDD	C2B-C3B-CAB-CBB
2	G	900	HDD	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	H	900	HDD	C4C-C3C-CAC-CBC
2	A	900	HDD	C2B-C3B-CAB-CBB
2	A	900	HDD	C2C-C3C-CAC-CBC
2	C	900	HDD	C2B-C3B-CAB-CBB
2	D	900	HDD	C2C-C3C-CAC-CBC
2	E	900	HDD	C2C-C3C-CAC-CBC
2	F	900	HDD	C2B-C3B-CAB-CBB
2	H	900	HDD	C2C-C3C-CAC-CBC
2	A	900	HDD	C4B-C3B-CAB-CBB
2	B	900	HDD	C4C-C3C-CAC-CBC
2	C	900	HDD	C4C-C3C-CAC-CBC
2	A	900	HDD	CAA-CBA-CGA-O2A
2	B	900	HDD	CAA-CBA-CGA-O2A
2	A	900	HDD	CAA-CBA-CGA-O1A
2	E	900	HDD	CAA-CBA-CGA-O1A
2	C	900	HDD	CAA-CBA-CGA-O1A
2	E	900	HDD	CAA-CBA-CGA-O2A
2	F	900	HDD	CAA-CBA-CGA-O1A
2	H	900	HDD	CAA-CBA-CGA-O1A
2	G	900	HDD	CAA-CBA-CGA-O1A
2	D	900	HDD	CAA-CBA-CGA-O2A
2	G	900	HDD	CAA-CBA-CGA-O2A
2	C	900	HDD	CAA-CBA-CGA-O2A
2	D	900	HDD	CAA-CBA-CGA-O1A
2	F	900	HDD	CAA-CBA-CGA-O2A
2	H	900	HDD	CAA-CBA-CGA-O2A
2	B	900	HDD	CAA-CBA-CGA-O1A
2	D	900	HDD	C4B-C3B-CAB-CBB
2	D	900	HDD	C4C-C3C-CAC-CBC
2	E	900	HDD	C4B-C3B-CAB-CBB

There are no ring outliers.

8 monomers are involved in 23 short contacts:

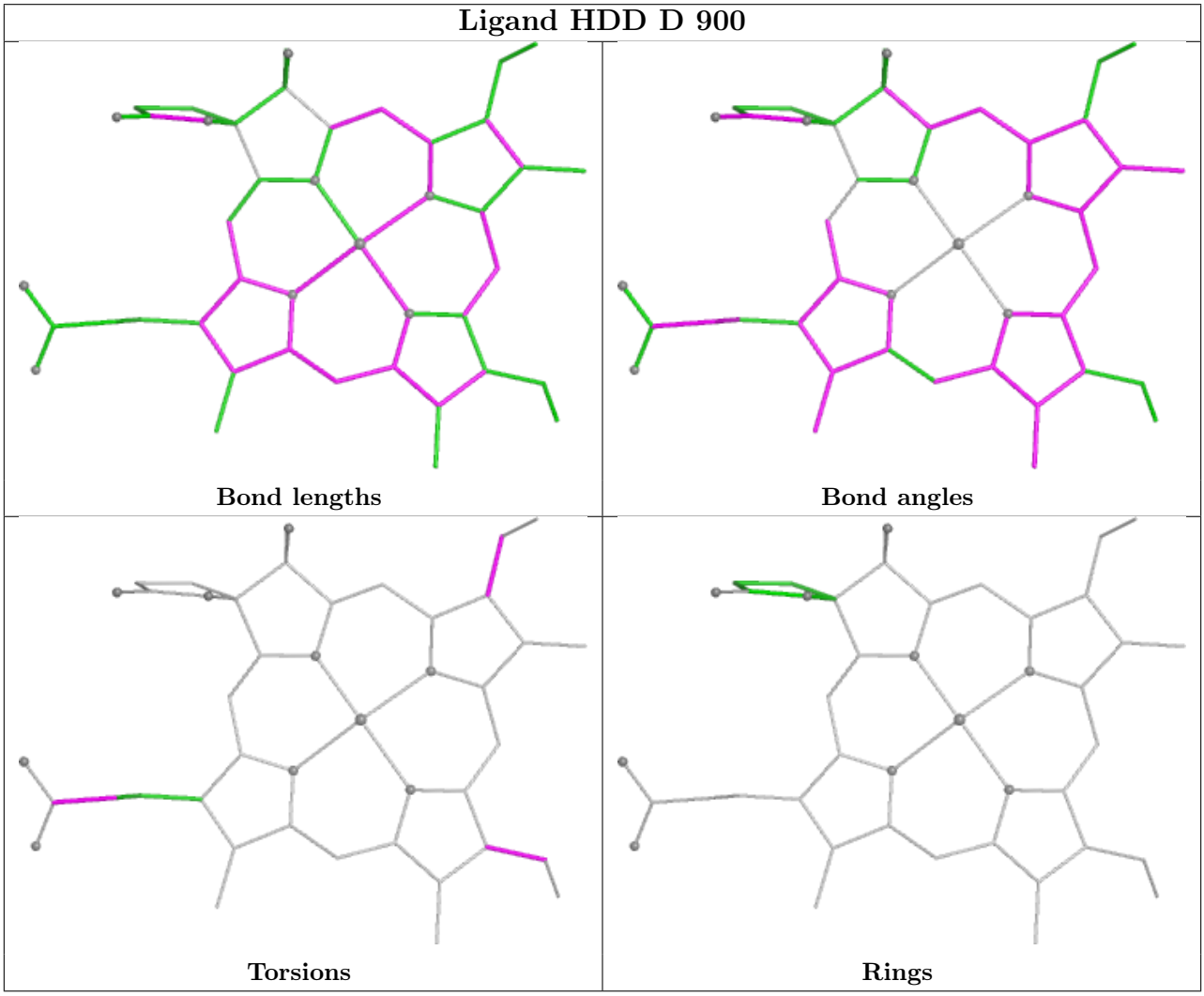
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	900	HDD	2	0
2	H	900	HDD	3	0
2	G	900	HDD	2	0
2	B	900	HDD	3	0
2	A	900	HDD	2	0
2	E	900	HDD	3	0
2	F	900	HDD	4	0

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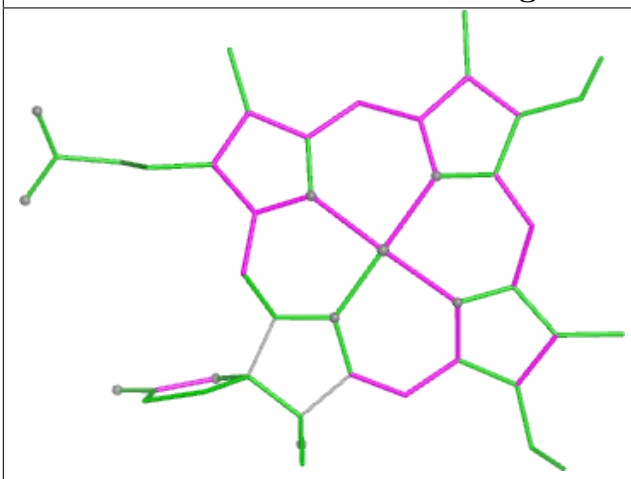
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	900	HDD	4	0

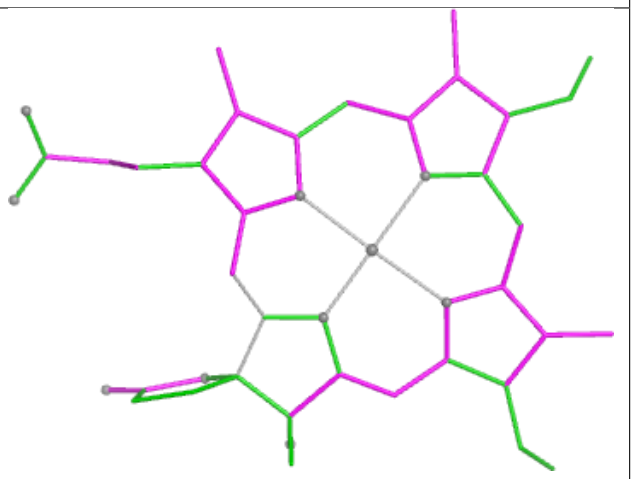
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



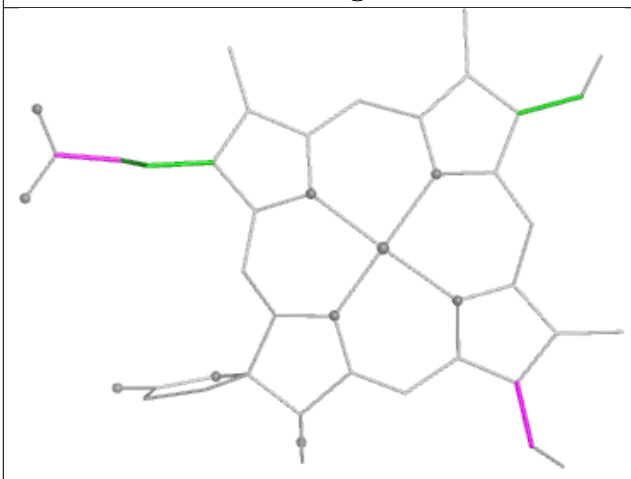
Ligand HDD H 900



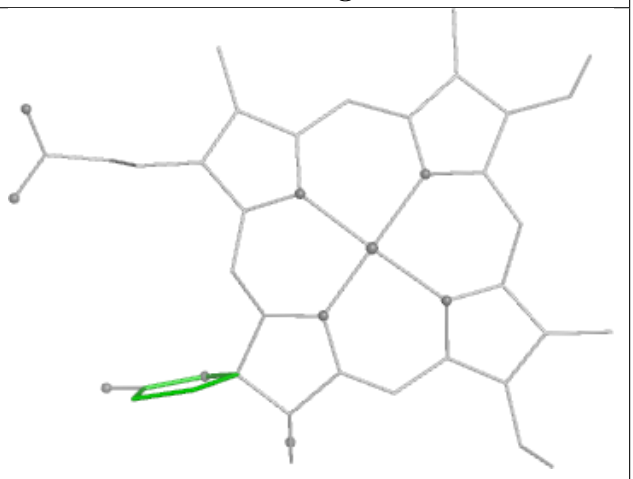
Bond lengths



Bond angles

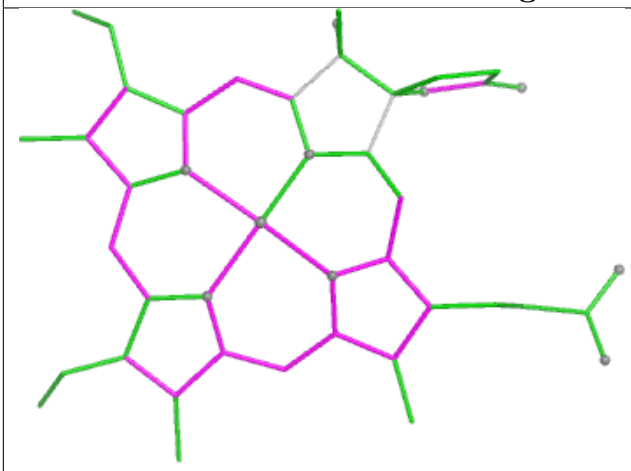


Torsions

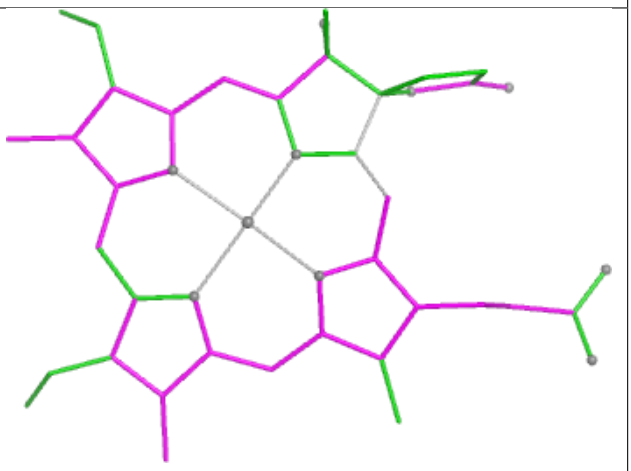


Rings

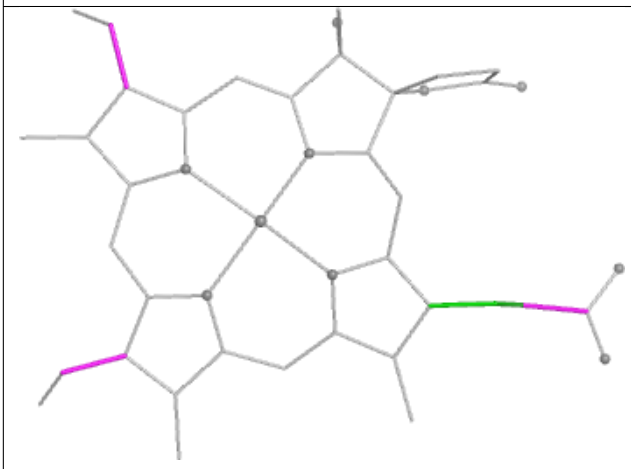
Ligand HDD G 900



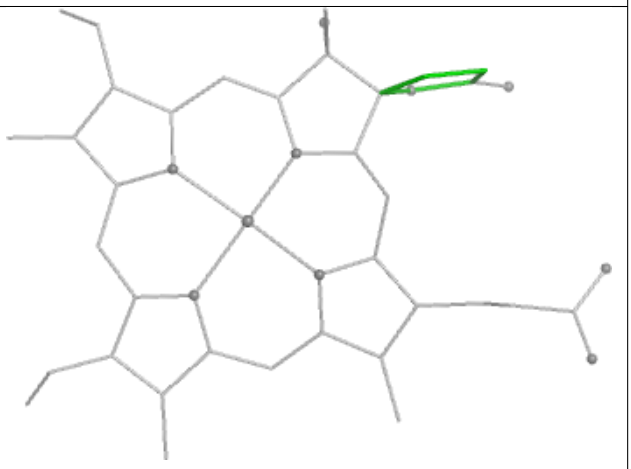
Bond lengths



Bond angles

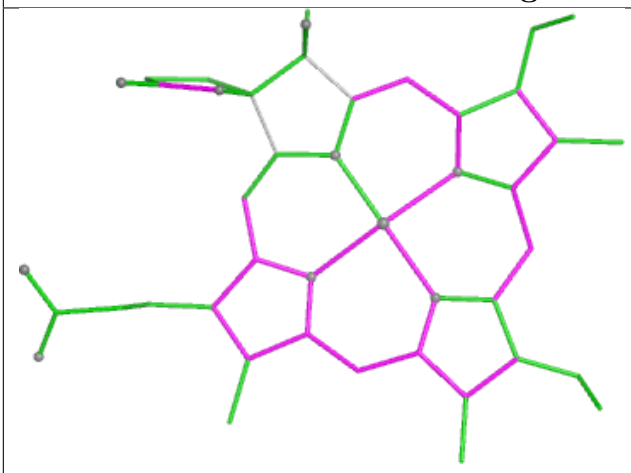


Torsions

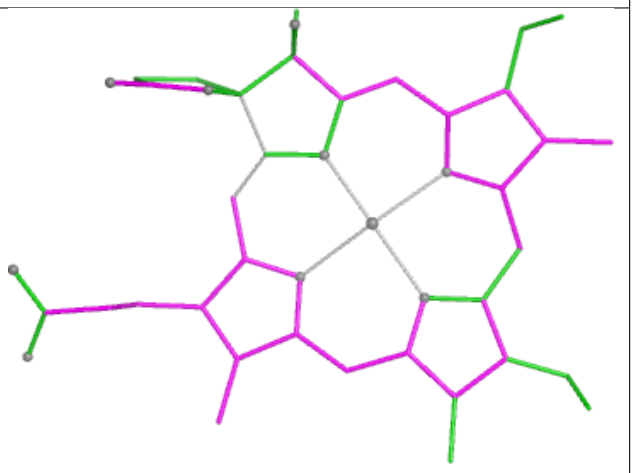


Rings

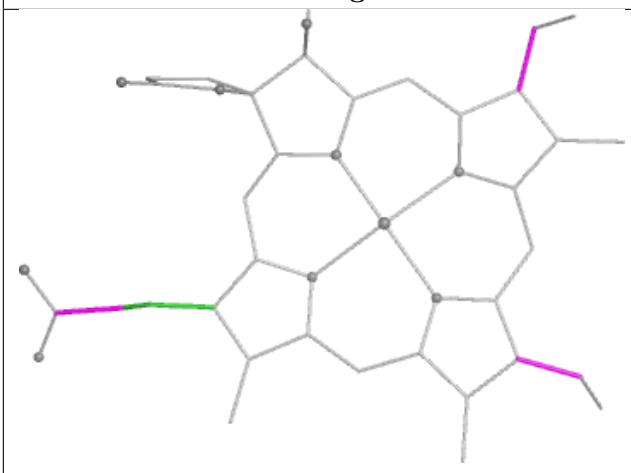
Ligand HDD B 900



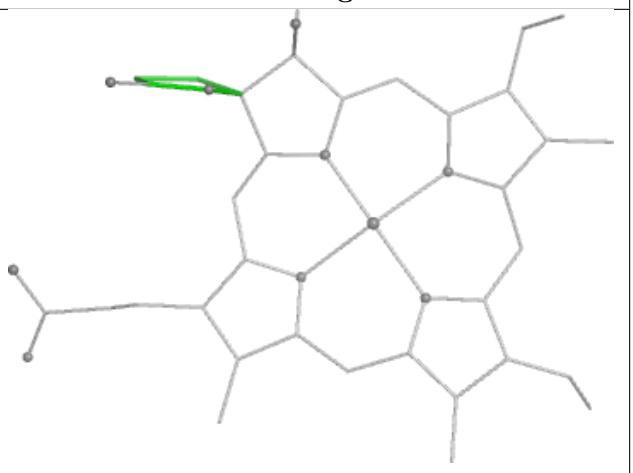
Bond lengths



Bond angles

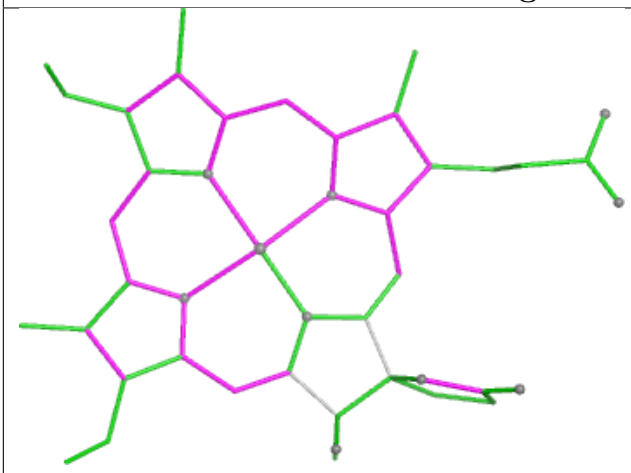


Torsions

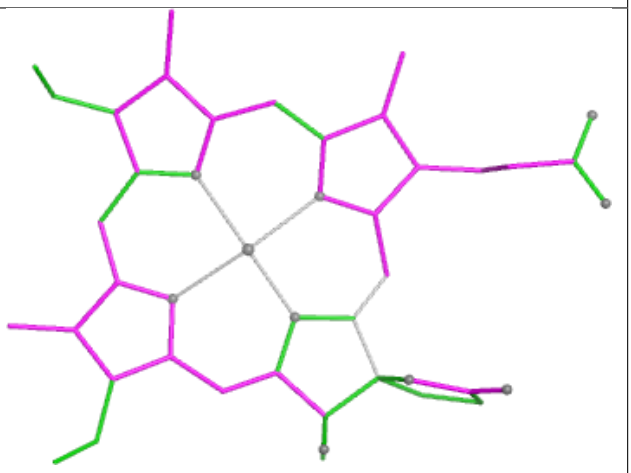


Rings

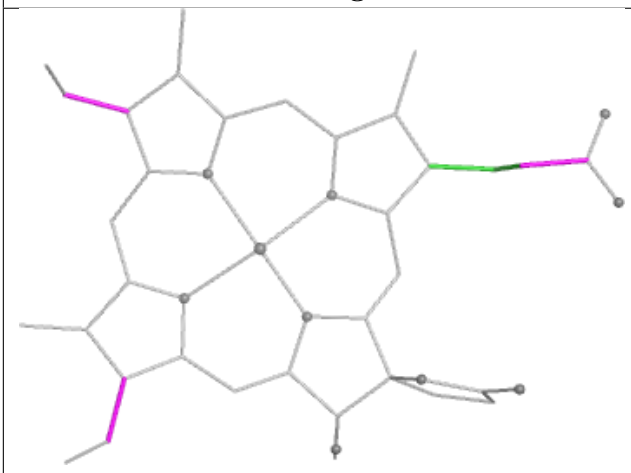
Ligand HDD A 900



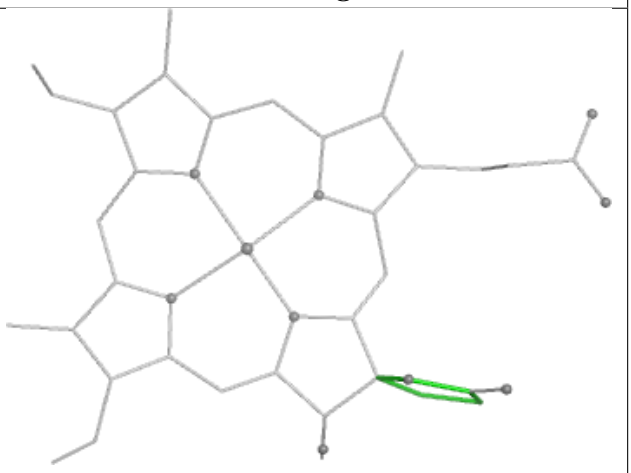
Bond lengths



Bond angles

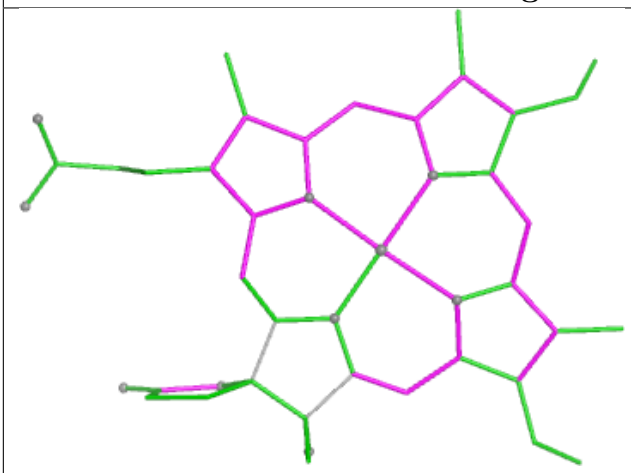


Torsions

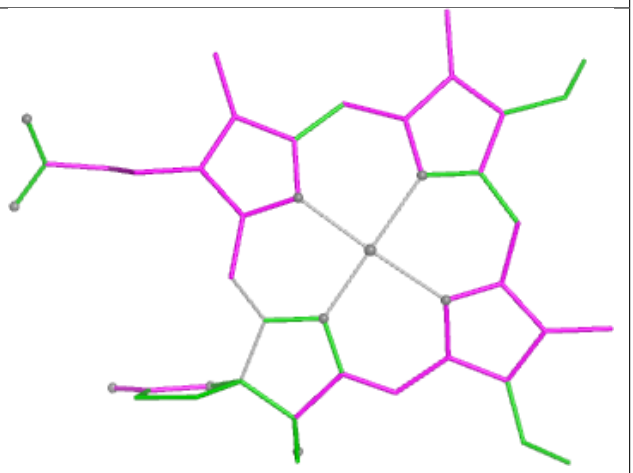


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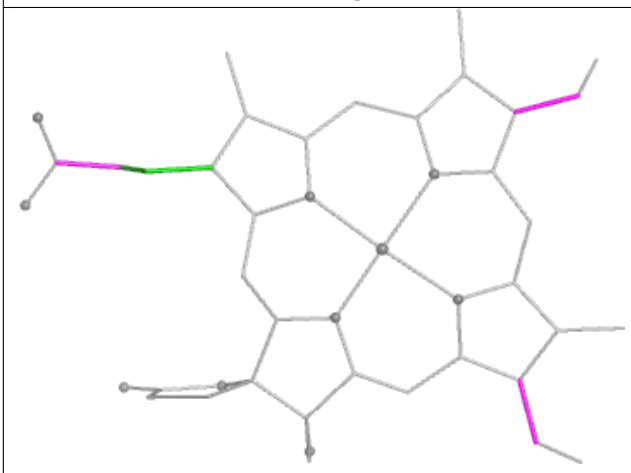
Ligand HDD E 900



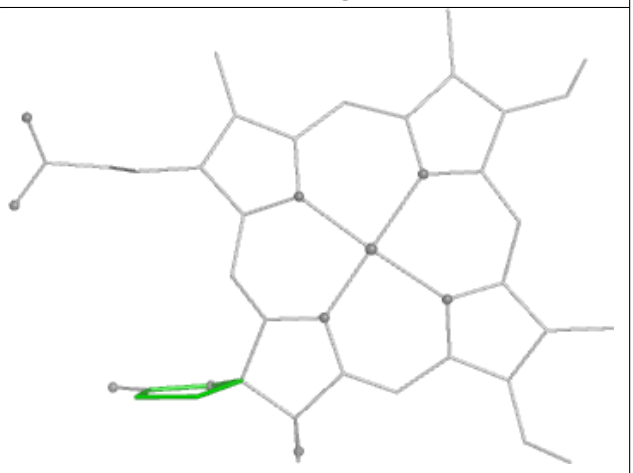
Bond lengths



Bond angles

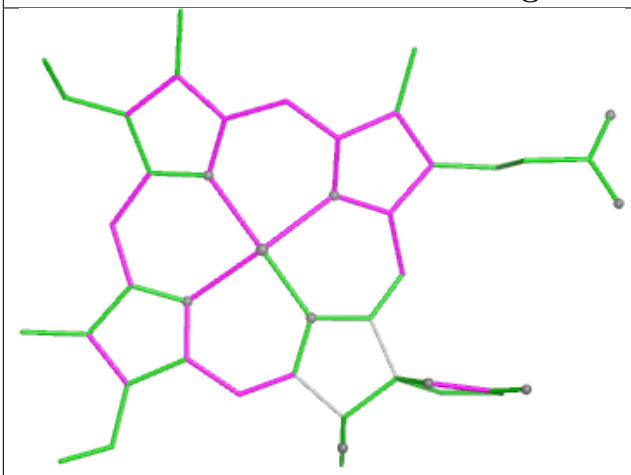


Torsions

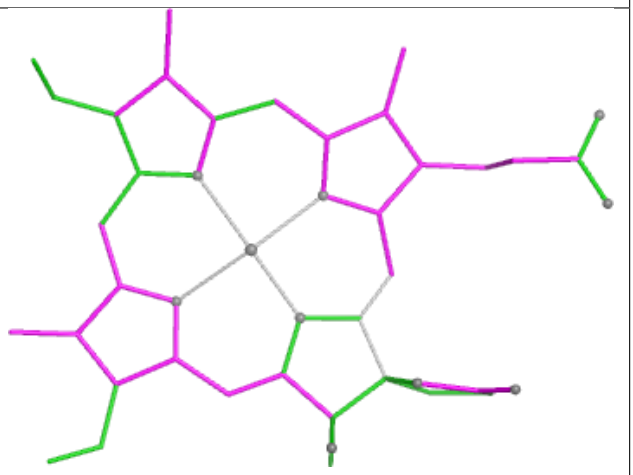


Rings

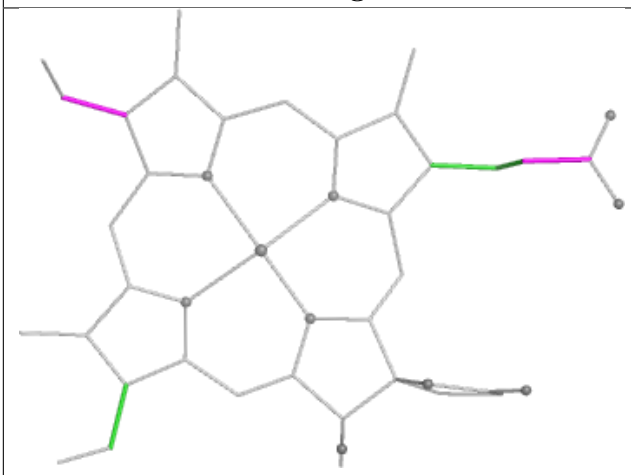
Ligand HDD F 900



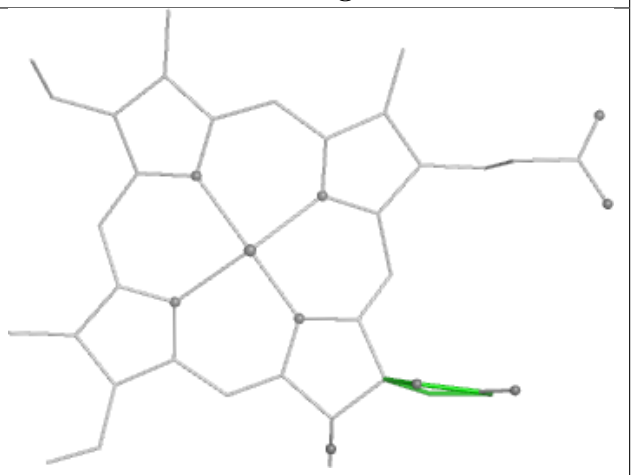
Bond lengths



Bond angles

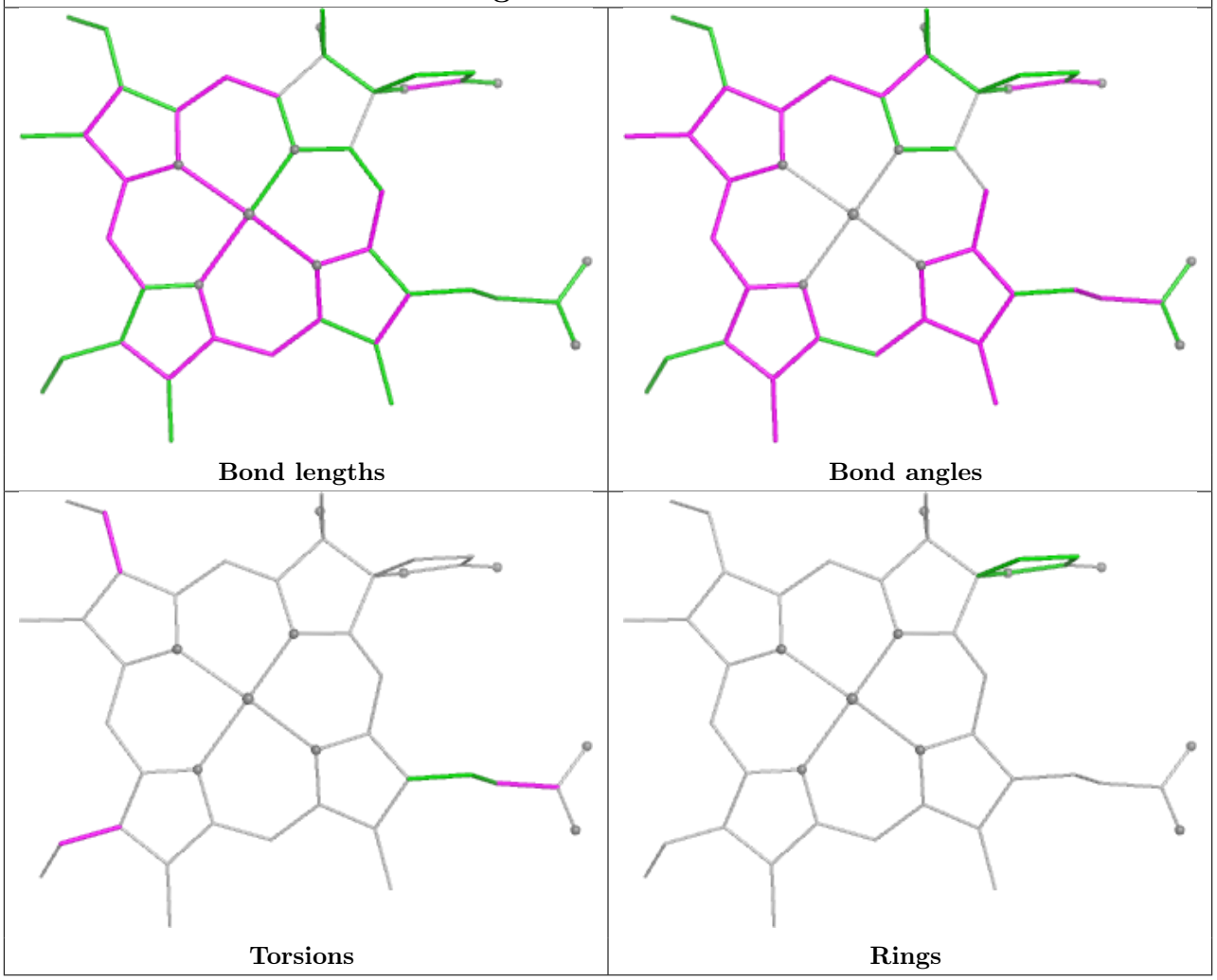


Torsions



Rings

Ligand HDD C 900



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	671/719 (93%)	-0.44	8 (1%)	76	82	5, 14, 30, 49	19 (2%)
1	B	673/719 (93%)	-0.50	2 (0%)	90	93	5, 14, 26, 38	19 (2%)
1	C	673/719 (93%)	-0.51	3 (0%)	88	92	5, 13, 26, 37	20 (2%)
1	D	674/719 (93%)	-0.57	3 (0%)	88	92	4, 12, 24, 48	18 (2%)
1	E	668/719 (92%)	-0.37	8 (1%)	76	82	5, 15, 31, 60	19 (2%)
1	F	668/719 (92%)	-0.40	8 (1%)	76	82	4, 13, 30, 56	16 (2%)
1	G	673/719 (93%)	-0.52	3 (0%)	88	92	5, 13, 25, 40	21 (3%)
1	H	670/719 (93%)	-0.39	10 (1%)	72	79	5, 14, 32, 50	16 (2%)
All	All	5370/5752 (93%)	-0.46	45 (0%)	82	88	4, 13, 28, 60	148 (2%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	655	VAL	7.2
1	F	655	VAL	6.4
1	F	22	PRO	6.4
1	H	22	PRO	5.0
1	H	618	ALA	4.4
1	F	618	ALA	4.1
1	A	698	SER	4.1
1	H	650	GLY	4.0
1	F	658	ALA	4.0
1	A	653	SER	3.6
1	A	22	PRO	3.4
1	D	22	PRO	3.4
1	H	698	SER	3.3
1	G	618	ALA	3.3
1	A	618	ALA	3.2
1	B	618	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	22	PRO	3.2
1	A	649	GLY	3.1
1	E	649	GLY	3.1
1	E	22	PRO	3.1
1	D	698	SER	3.0
1	E	657	ASP	3.0
1	E	618	ALA	3.0
1	A	655	VAL	2.9
1	C	618	ALA	2.8
1	E	658	ALA	2.7
1	F	649	GLY	2.7
1	H	559[A]	SER	2.6
1	E	659	ALA	2.6
1	H	655	VAL	2.6
1	E	656	LEU	2.4
1	H	676	MET	2.4
1	F	659	ALA	2.4
1	B	22	PRO	2.4
1	G	539	VAL	2.4
1	A	654	GLU	2.4
1	H	542	GLY	2.4
1	H	658	ALA	2.3
1	H	659	ALA	2.3
1	C	22	PRO	2.3
1	A	657	ASP	2.2
1	F	657	ASP	2.2
1	F	542	GLY	2.1
1	D	618	ALA	2.0
1	C	539	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

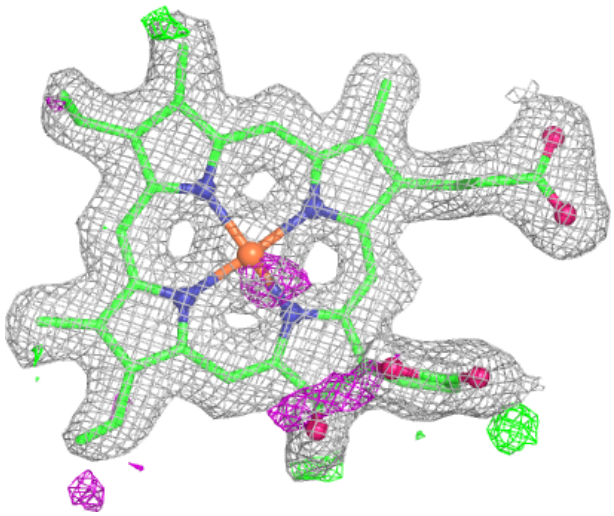
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

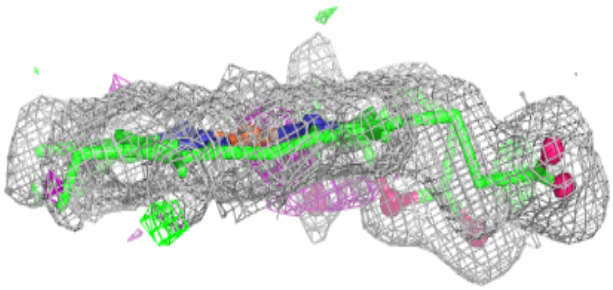
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HDD	A	900	44/44	0.96	0.08	8,13,22,24	0
2	HDD	B	900	44/44	0.96	0.08	10,14,19,22	0
2	HDD	C	900	44/44	0.96	0.08	8,14,18,21	0
2	HDD	D	900	44/44	0.96	0.08	7,11,18,23	0
2	HDD	E	900	44/44	0.96	0.08	9,14,22,28	0
2	HDD	F	900	44/44	0.96	0.07	7,12,17,22	0
2	HDD	G	900	44/44	0.96	0.08	7,13,19,23	0
2	HDD	H	900	44/44	0.96	0.08	9,13,22,24	0
3	CA	A	1700	1/1	0.98	0.03	19,19,19,19	1
3	CA	D	1700	1/1	0.98	0.04	9,9,9,9	1
3	CA	E	1700	1/1	0.98	0.04	8,8,8,8	1
3	CA	B	1700	1/1	0.99	0.01	10,10,10,10	1
3	CA	C	1700	1/1	0.99	0.02	10,10,10,10	1
3	CA	G	1700	1/1	0.99	0.02	12,12,12,12	1
3	CA	F	1700	1/1	1.00	0.01	8,8,8,8	1
3	CA	A	1701	1/1	1.00	0.01	8,8,8,8	1
3	CA	H	1700	1/1	1.00	0.01	7,7,7,7	1

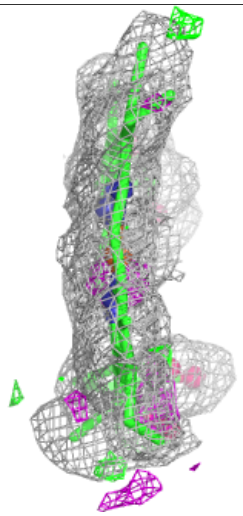
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HDD A 900:

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

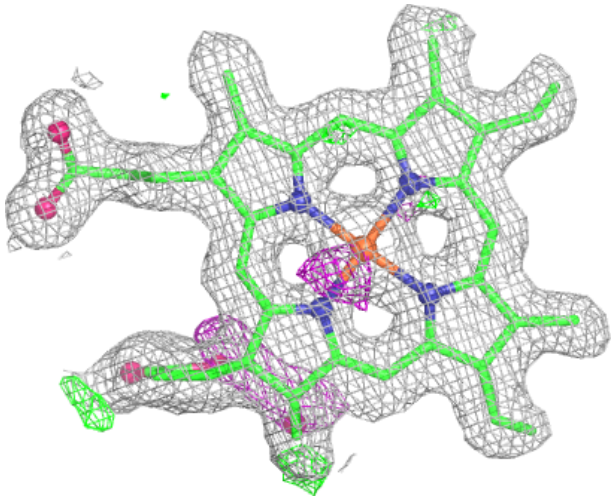


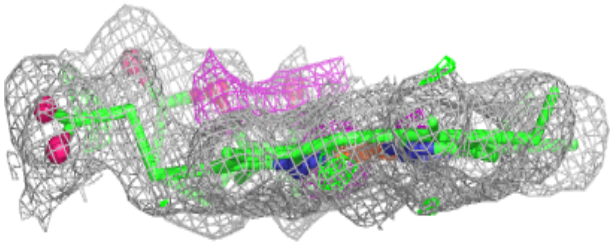


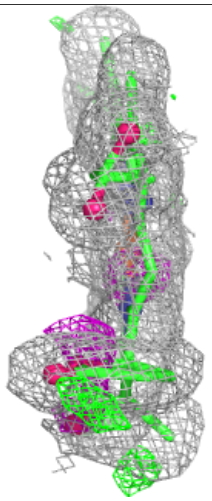


Electron density around HDD B 900:

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

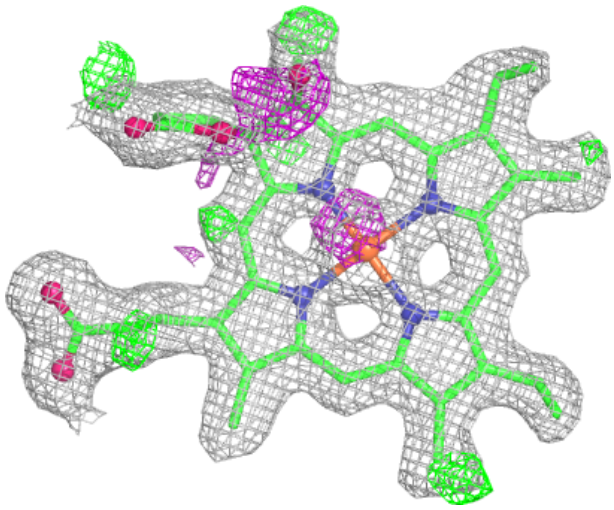


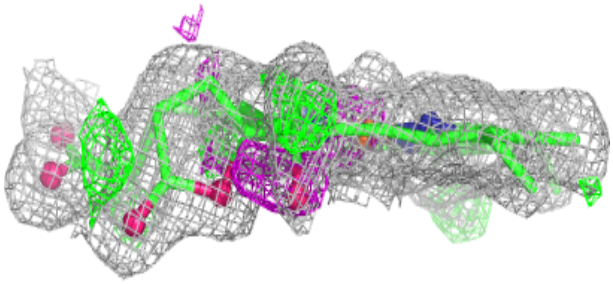


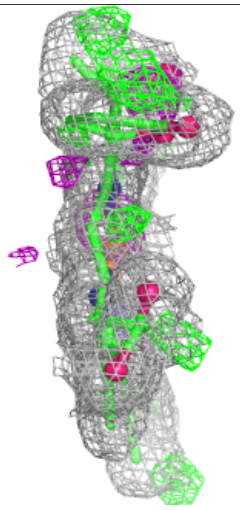


Electron density around HDD C 900:

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

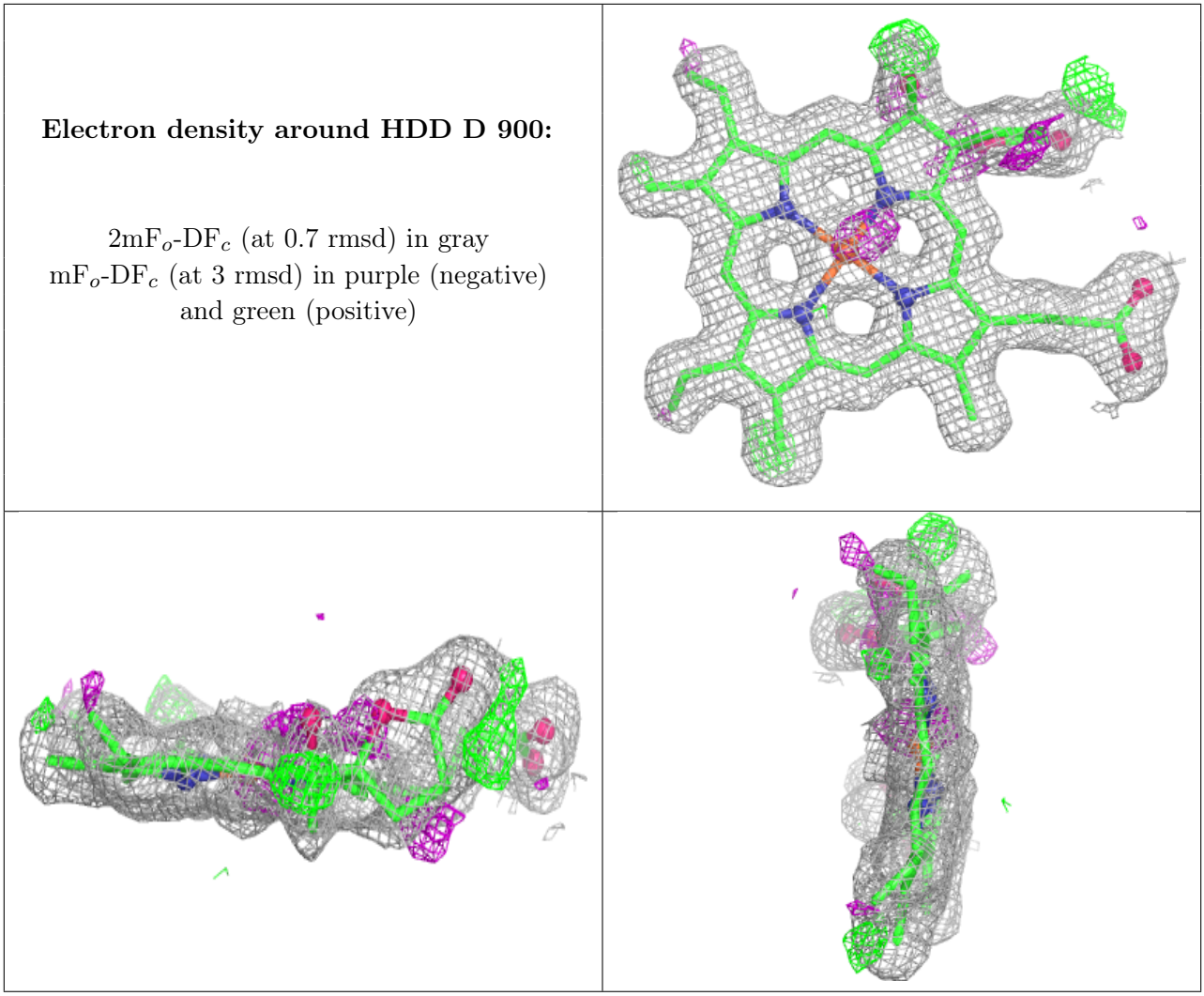






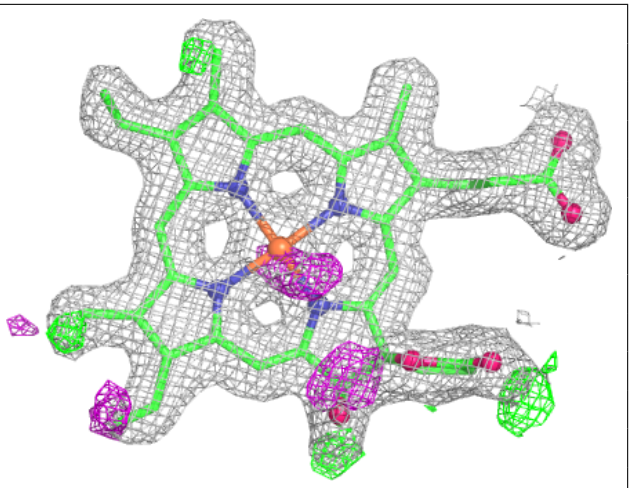
Electron density around HDD D 900:

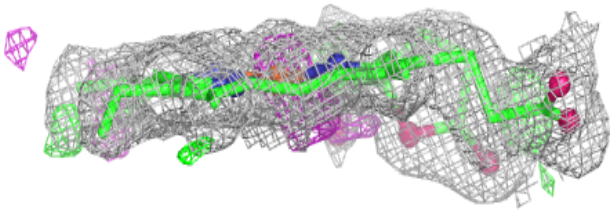
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

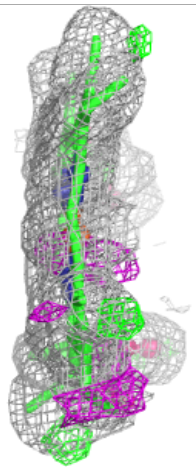


Electron density around HDD E 900:

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

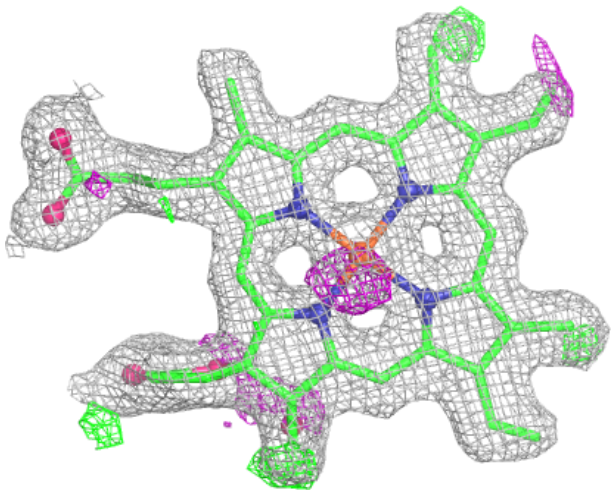


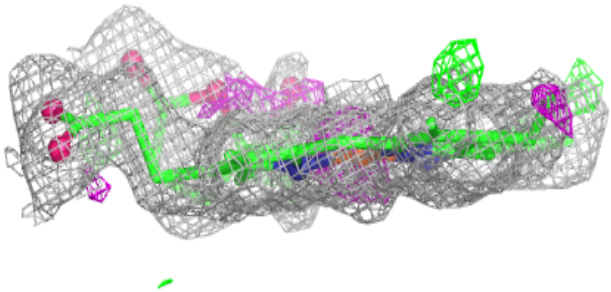


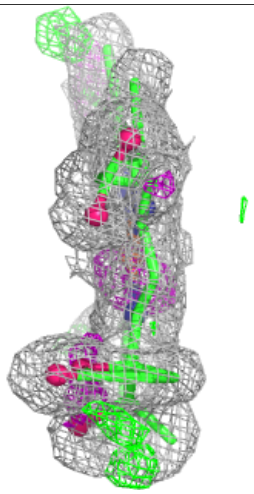


Electron density around HDD F 900:

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

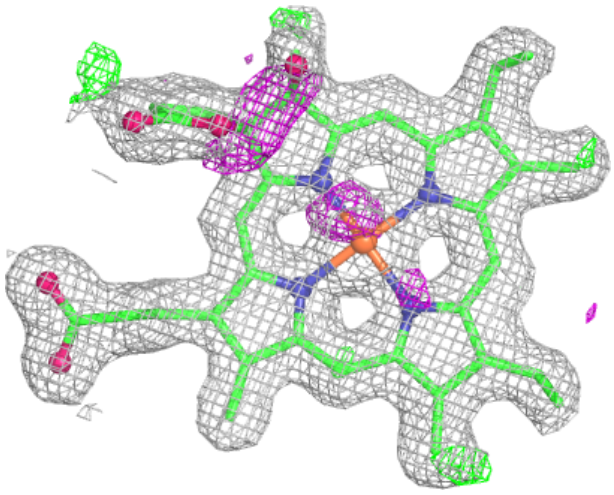


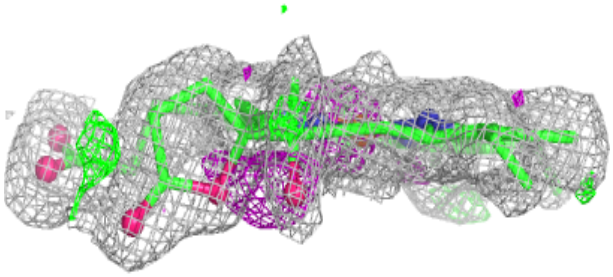


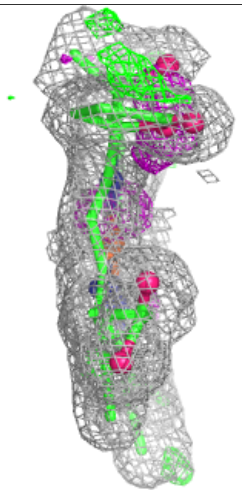


Electron density around HDD G 900:

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

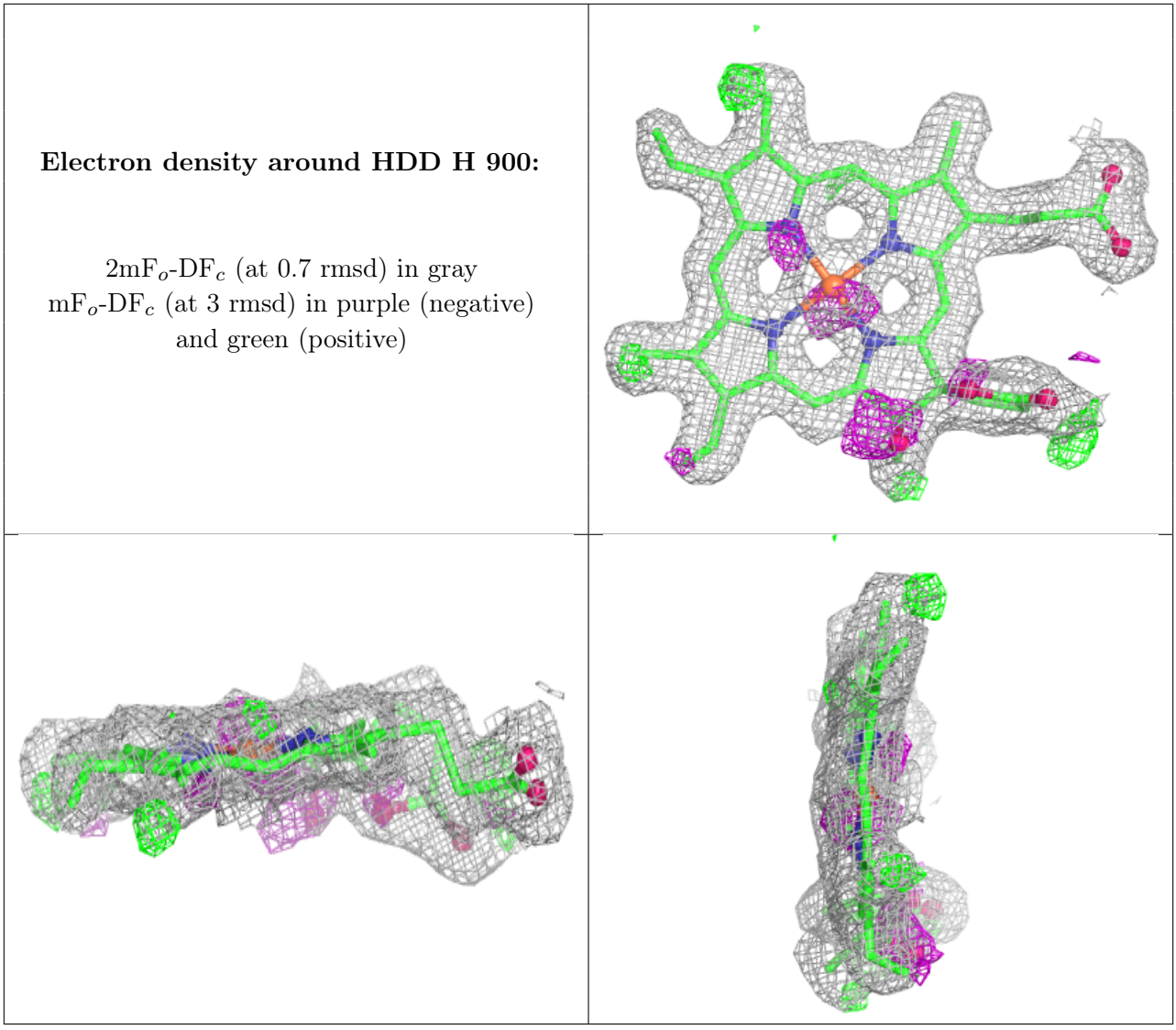






Electron density around HDD H 900:

$2mF_o$-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.