



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 12:16 AM EDT

PDB ID : 2QD1 / pdb_00002qd1
Title : 2.2 Angstrom Structure of the human ferrochelatase variant E343K with substrate bound
Authors : Medlock, A.E.; Dailey, T.A.; Ross, T.A.; Dailey, H.A.; Lanzilotta, W.N.
Deposited on : 2007-06-20
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (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

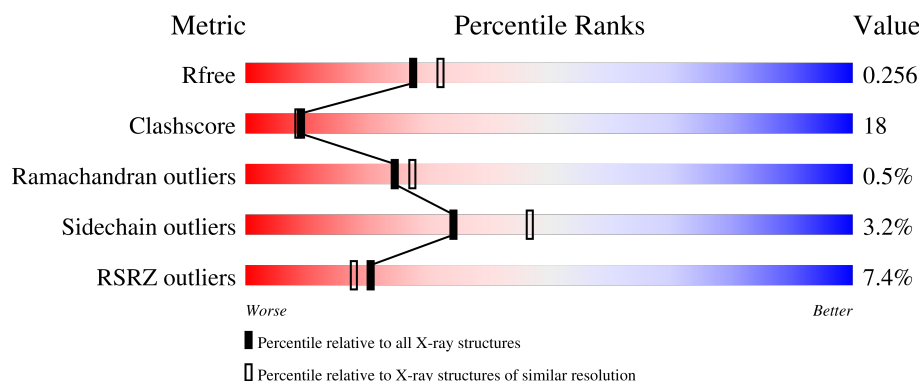
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	359	7% 70% 28% .
1	B	359	6% 66% 32% .
1	C	359	9% 66% 32% .
1	D	359	7% 61% 36% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12677 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.

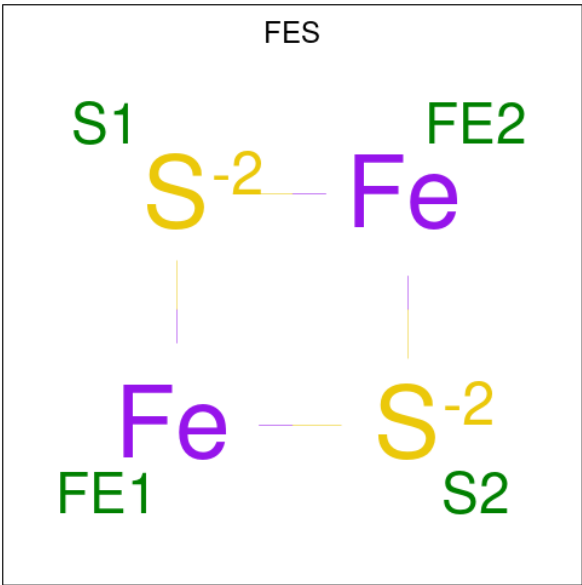
- Molecule 1 is a protein called Ferrochelatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2891	1842	504	527	18			
1	B	359	Total	C	N	O	S	0	4	0
			2927	1865	512	531	19			
1	C	359	Total	C	N	O	S	0	2	0
			2911	1854	510	529	18			
1	D	359	Total	C	N	O	S	0	4	0
			2931	1864	514	535	18			

There are 4 discrepancies between the modelled and reference sequences:

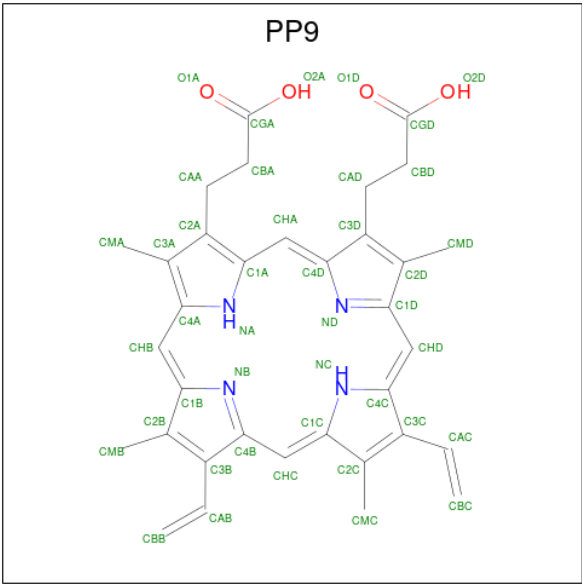
Chain	Residue	Modelled	Actual	Comment	Reference
A	343	LYS	GLU	engineered mutation	UNP P22830
B	343	LYS	GLU	engineered mutation	UNP P22830
C	343	LYS	GLU	engineered mutation	UNP P22830
D	343	LYS	GLU	engineered mutation	UNP P22830

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



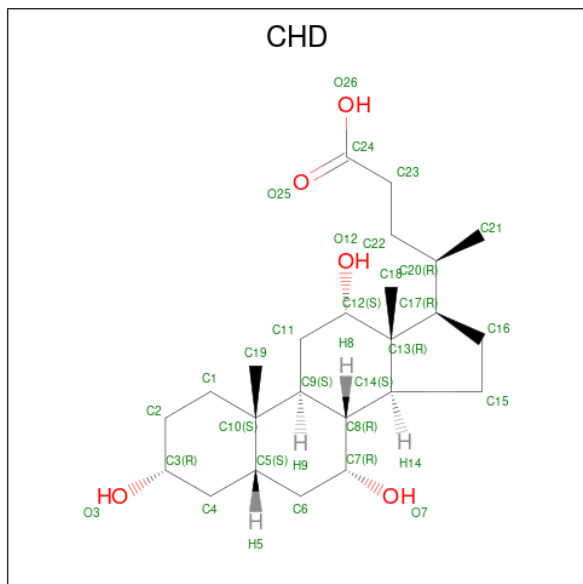
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	C	1	Total	Fe	S	0	0
			4	2	2		
2	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is PROTOPORPHYRIN IX (CCD ID: PP9) (formula: C₃₄H₃₄N₄O₄).



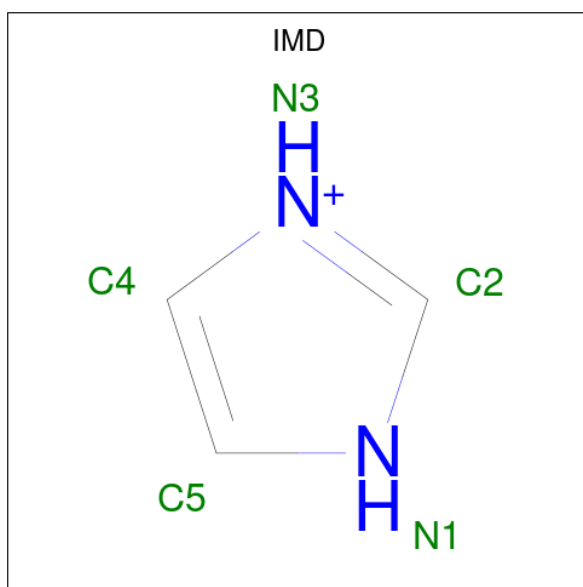
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			42	34	4	4		
3	B	1	Total	C	N	O	0	0
			42	34	4	4		
3	C	1	Total	C	N	O	0	0
			42	34	4	4		
3	D	1	Total	C	N	O	0	0
			42	34	4	4		
3	D	1	Total	C	N	O	0	0
			42	34	4	4		
3	D	1	Total	C	N	O	0	0
			42	34	4	4		

- Molecule 4 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			29	24	5		
4	D	1	Total	C	O	0	0
			29	24	5		

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	N	0	0
			5	3	2		

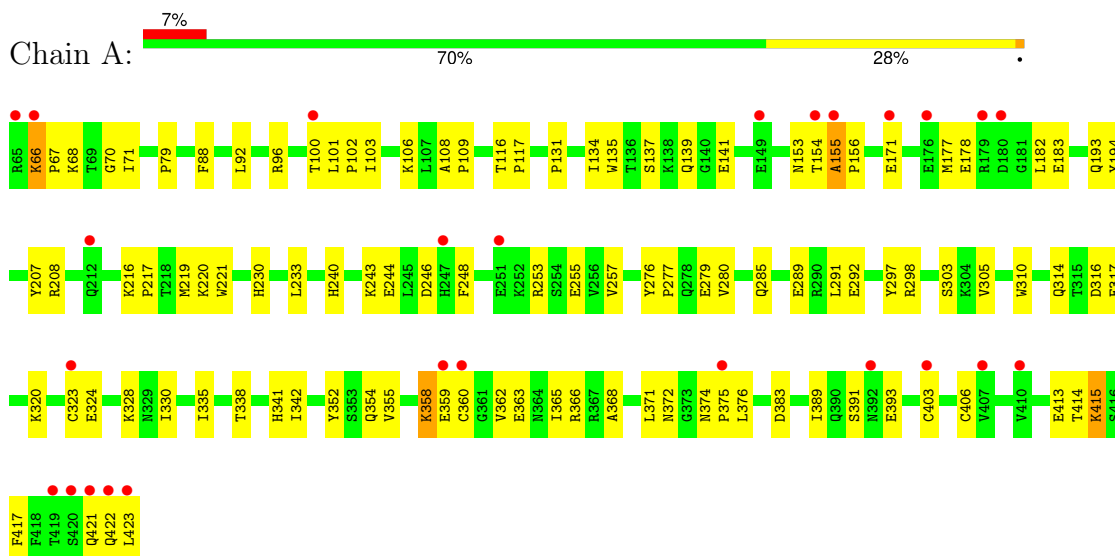
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	188	Total	O	0	0
			188	188		
6	B	175	Total	O	0	0
			175	175		
6	C	167	Total	O	0	0
			167	167		
6	D	156	Total	O	0	0
			156	156		

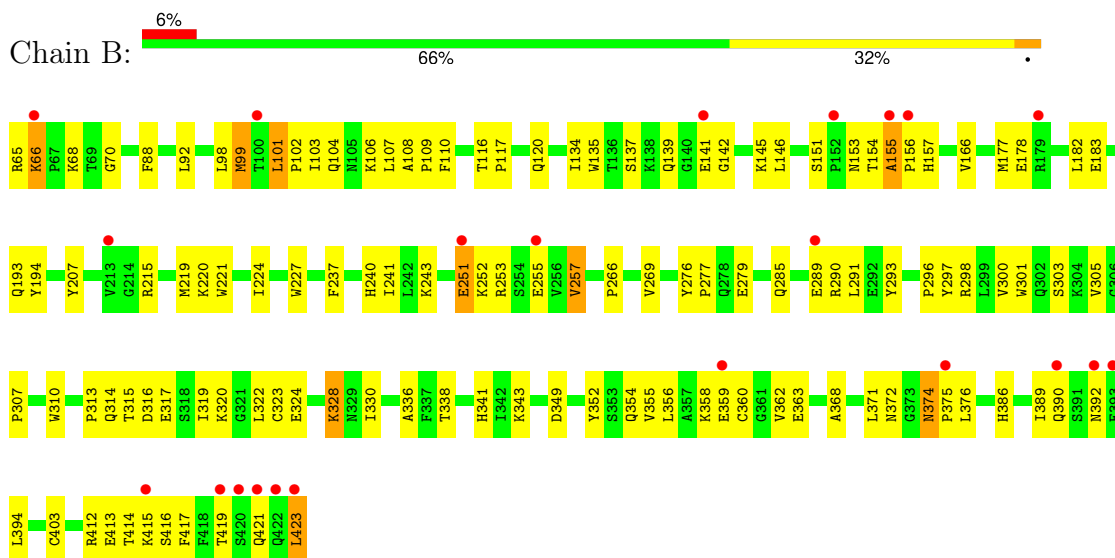
3 Residue-property plots

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: Ferrochelatase

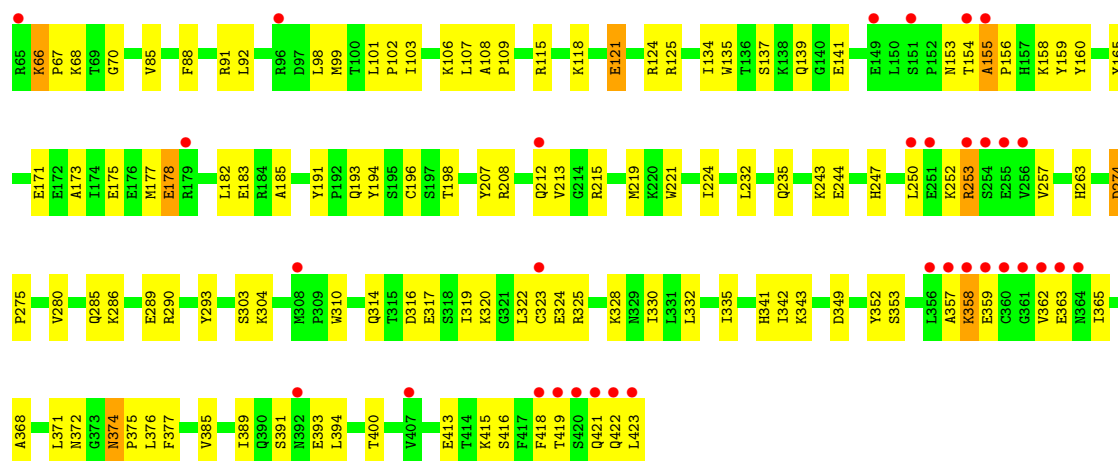


• Molecule 1: Ferrochelatase

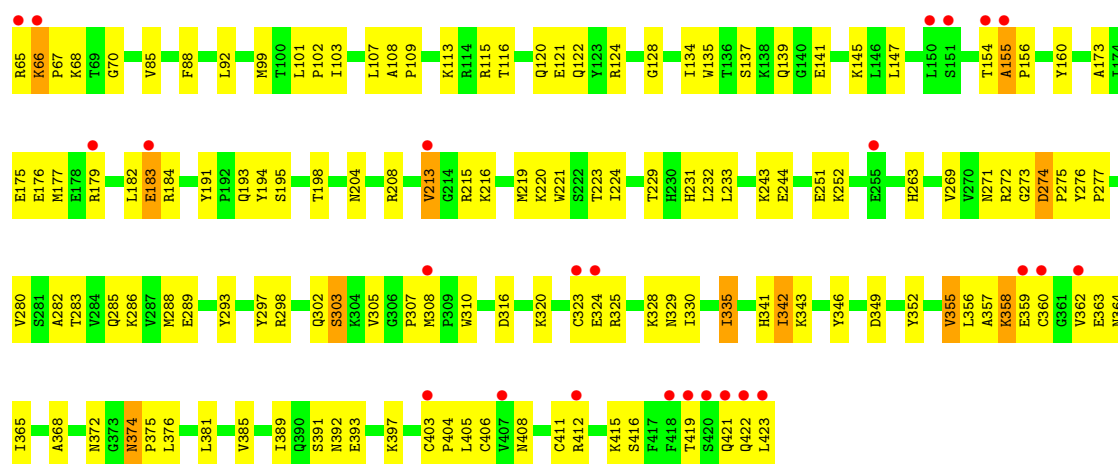


• Molecule 1: Ferrochelatase





• Molecule 1: Ferrochelatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.89Å 88.45Å 93.10Å 102.49° 108.99° 105.55°	Depositor
Resolution (Å)	42.08 – 2.20 42.08 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.4 (42.08-2.20) 95.4 (42.08-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.261 0.216 , 0.256	Depositor DCC
R_{free} test set	5530 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12677	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, PP9, IMD, CHD

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	0.43	0/2961	0.92	4/4010 (0.1%)
1	B	0.42	0/2997	0.90	6/4056 (0.1%)
1	C	0.43	0/2981	0.90	10/4035 (0.2%)
1	D	0.43	0/3001	0.91	11/4062 (0.3%)
All	All	0.43	0/11940	0.91	31/16163 (0.2%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	303	SER	N-CA-C	8.08	123.09	113.23
1	C	303	SER	N-CA-C	8.00	122.48	112.24
1	B	303	SER	N-CA-C	7.57	121.81	112.58
1	A	303	SER	N-CA-C	6.58	121.26	113.23
1	A	233	LEU	N-CA-C	-6.29	104.34	111.14
1	D	233	LEU	N-CA-C	-6.15	104.50	111.14
1	B	194	TYR	N-CA-C	6.12	119.14	109.96
1	A	194	TYR	N-CA-C	5.97	119.25	109.76
1	D	349	ASP	N-CA-C	5.96	117.86	111.36
1	C	224	ILE	N-CA-C	-5.95	96.96	109.34
1	D	335	ILE	N-CA-C	5.90	120.39	111.89
1	D	224	ILE	N-CA-C	-5.84	97.20	109.34
1	C	194	TYR	N-CA-C	5.83	118.70	109.96
1	C	335	ILE	N-CA-C	5.78	120.21	111.89
1	C	85	VAL	N-CA-C	5.70	115.83	110.30
1	C	349	ASP	N-CA-C	5.66	117.52	111.36
1	C	274	ASP	CA-C-N	5.64	125.26	119.56
1	C	274	ASP	C-N-CA	5.64	125.26	119.56
1	B	224	ILE	N-CA-C	-5.57	97.76	109.34
1	A	335	ILE	N-CA-C	5.49	119.80	111.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	194	TYR	N-CA-C	5.42	118.37	109.76
1	C	196	CYS	N-CA-C	-5.38	105.98	112.54
1	D	223	THR	N-CA-C	5.27	117.26	108.99
1	B	253	ARG	N-CA-C	5.26	117.42	111.11
1	D	85	VAL	N-CA-C	5.24	115.38	110.30
1	D	274	ASP	CA-C-N	5.22	124.83	119.56
1	D	274	ASP	C-N-CA	5.22	124.83	119.56
1	C	165	TYR	N-CA-C	5.13	119.08	112.41
1	B	328	LYS	N-CA-C	5.11	118.55	112.72
1	B	368	ALA	N-CA-C	-5.07	103.45	110.35
1	D	183	GLU	N-CA-C	-5.01	107.30	113.41

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	2891	0	2906	94	0
1	B	2927	0	2949	132	0
1	C	2911	0	2930	102	0
1	D	2931	0	2940	116	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	42	0	32	5	0
3	B	42	0	32	9	0
3	C	42	0	32	14	0
3	D	126	0	96	9	0
4	D	58	0	78	2	0
5	D	5	0	5	0	0
6	A	188	0	0	2	0
6	B	175	0	0	3	0
6	C	167	0	0	6	0
6	D	156	0	0	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12677	0	12000	437	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 (437) 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:D:155:ALA:HB1	1:D:156:PRO:HD2	1.35	1.03
1:A:155:ALA:HB1	1:A:156:PRO:HD2	1.36	1.02
1:B:403:CYS:HA	1:D:298:ARG:HH12	1.25	1.01
1:B:392:ASN:HD21	1:B:423:LEU:HD12	1.31	0.93
1:A:221:TRP:N	1:A:421:GLN:HE21	1.67	0.92
1:C:155:ALA:HB1	1:C:156:PRO:CD	1.98	0.92
1:D:422:GLN:HG2	1:D:423:LEU:H	1.33	0.91
1:D:221:TRP:H	1:D:421:GLN:HE21	1.19	0.89
1:B:298:ARG:HH12	1:D:403:CYS:HA	1.36	0.89
1:D:155:ALA:HB1	1:D:156:PRO:CD	2.04	0.87
1:A:221:TRP:H	1:A:421:GLN:NE2	1.73	0.87
1:A:221:TRP:H	1:A:421:GLN:HE21	0.90	0.86
1:B:155:ALA:HB1	1:B:156:PRO:CD	2.05	0.86
1:A:155:ALA:HB1	1:A:156:PRO:CD	2.05	0.86
1:C:68:LYS:HD3	1:C:155:ALA:HB3	1.58	0.85
1:C:213:VAL:HG12	1:C:215:ARG:HG2	1.58	0.84
1:C:155:ALA:HB1	1:C:156:PRO:HD3	1.60	0.84
1:C:328:LYS:HB2	1:C:363:GLU:HG3	1.59	0.82
1:C:358:LYS:HE3	1:C:358:LYS:HA	1.62	0.82
1:C:208:ARG:O	1:C:212:GLN:HG2	1.79	0.81
1:B:285:GLN:O	1:B:289:GLU:HG3	1.79	0.81
1:C:98:LEU:CD1	3:C:705:PP9:HBB1	2.10	0.80
1:A:358:LYS:HA	1:A:358:LYS:HE3	1.62	0.80
1:D:220:LYS:HD2	1:D:423:LEU:HB3	1.62	0.80
1:A:360:CYS:SG	1:A:362:VAL:HG23	2.22	0.79
1:D:323:CYS:SG	1:D:362:VAL:HG22	2.24	0.78
1:A:137:SER:O	1:A:141:GLU:HG3	1.86	0.76
1:C:285:GLN:O	1:C:289:GLU:HG3	1.86	0.75
1:B:314:GLN:HB2	1:B:317:GLU:HG3	1.66	0.75
1:D:355:VAL:O	1:D:359:GLU:HG3	1.86	0.74
1:B:68:LYS:HG3	1:B:183:GLU:OE2	1.89	0.73
1:D:68:LYS:HB3	1:D:155:ALA:HB3	1.71	0.72
1:B:403:CYS:HA	1:D:298:ARG:NH1	2.03	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:LEU:OXT	1:D:423:LEU:HD13	1.90	0.71
1:A:374:ASN:C	1:A:374:ASN:HD22	1.98	0.71
1:B:276:TYR:HB3	1:B:277:PRO:HD3	1.72	0.71
1:C:108:ALA:HB3	1:C:109:PRO:HD3	1.74	0.70
1:D:285:GLN:O	1:D:289:GLU:HG3	1.91	0.70
1:B:320:LYS:O	1:B:324:GLU:HG3	1.92	0.69
1:D:229:THR:HB	1:D:286:LYS:HD3	1.74	0.69
1:B:137:SER:O	1:B:141:GLU:HG3	1.92	0.69
1:A:320:LYS:O	1:A:324:GLU:HG3	1.92	0.69
1:C:98:LEU:HD12	3:C:705:PP9:HBB1	1.74	0.69
1:D:422:GLN:HG2	1:D:423:LEU:N	2.08	0.69
1:D:320:LYS:O	1:D:324:GLU:HG3	1.92	0.69
1:B:251:GLU:OE2	1:B:252:LYS:HG2	1.93	0.68
1:B:135:TRP:O	1:B:139:GLN:HG3	1.93	0.68
1:A:374:ASN:ND2	1:A:376:LEU:H	1.92	0.68
1:D:341:HIS:HB2	3:D:706:PP9:CGD	2.24	0.68
1:D:374:ASN:C	1:D:374:ASN:HD22	2.02	0.68
1:A:285:GLN:O	1:A:289:GLU:HG3	1.94	0.68
1:C:374:ASN:C	1:C:374:ASN:HD22	2.02	0.67
1:A:374:ASN:HD22	1:A:375:PRO:N	1.92	0.67
1:D:416:SER:HA	1:D:419:THR:OG1	1.95	0.67
1:C:323:CYS:SG	1:C:362:VAL:HG12	2.34	0.67
1:B:215:ARG:CB	1:B:215:ARG:HH11	2.08	0.67
1:B:298:ARG:NH1	1:D:403:CYS:HA	2.09	0.67
1:B:68:LYS:HG3	1:B:183:GLU:CD	2.20	0.66
1:B:374:ASN:ND2	1:B:376:LEU:H	1.92	0.66
1:A:155:ALA:CB	1:A:156:PRO:HD2	2.21	0.66
1:C:68:LYS:CD	1:C:155:ALA:HB3	2.24	0.66
1:A:207:TYR:CZ	1:A:413:GLU:HB3	2.31	0.66
1:B:374:ASN:C	1:B:374:ASN:HD22	2.02	0.66
1:D:88:PHE:HE2	3:D:706:PP9:HAA2	1.61	0.66
1:D:108:ALA:HB3	1:D:109:PRO:HD3	1.78	0.66
1:C:341:HIS:HB2	3:C:705:PP9:CGD	2.27	0.65
1:A:423:LEU:OXT	1:A:423:LEU:HD13	1.97	0.65
1:C:320[B]:LYS:O	1:C:324:GLU:HG3	1.97	0.64
1:C:155:ALA:CB	1:C:156:PRO:CD	2.74	0.64
1:A:276:TYR:HB3	1:A:277:PRO:HD3	1.77	0.64
1:C:70:GLY:HA3	1:C:182:LEU:HD13	1.80	0.64
1:A:68:LYS:CB	1:A:155:ALA:HB3	2.28	0.64
1:C:68:LYS:HD3	1:C:155:ALA:CB	2.26	0.64
1:B:154:THR:HG21	1:B:389:ILE:HD13	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LYS:H	1:C:66:LYS:HD3	1.61	0.63
1:D:155:ALA:CB	1:D:156:PRO:HD2	2.22	0.63
1:B:298:ARG:NH1	1:D:404:PRO:HD3	2.14	0.63
1:C:374:ASN:ND2	1:C:376:LEU:H	1.97	0.62
1:B:215:ARG:NH1	1:B:215:ARG:HB2	2.13	0.62
1:D:221:TRP:H	1:D:421:GLN:NE2	1.96	0.62
1:C:98:LEU:O	3:C:705:PP9:HBB2	1.99	0.62
1:B:108:ALA:HB3	1:B:109:PRO:HD3	1.82	0.62
1:A:66:LYS:HE3	1:A:66:LYS:H	1.64	0.62
1:D:276:TYR:HB3	1:D:277:PRO:HD3	1.82	0.62
1:C:115:ARG:HH21	3:C:705:PP9:CGA	2.12	0.61
1:B:155:ALA:HB1	1:B:156:PRO:HD3	1.83	0.61
1:B:374:ASN:HD22	1:B:376:LEU:H	1.46	0.61
1:A:66:LYS:H	1:A:66:LYS:CE	2.12	0.61
1:C:416:SER:HA	1:C:419:THR:OG1	2.00	0.61
1:B:65:ARG:HD3	1:B:65:ARG:N	2.16	0.61
1:C:289:GLU:HG2	1:C:293:TYR:OH	2.00	0.61
1:A:68:LYS:HE3	1:A:183:GLU:OE1	2.00	0.61
1:C:320[A]:LYS:O	1:C:324:GLU:HG3	1.99	0.61
1:C:342:ILE:HG22	3:C:705:PP9:HBD2	1.82	0.61
1:A:341:HIS:HB2	3:A:701:PP9:CGD	2.31	0.61
1:B:155:ALA:HB1	1:B:156:PRO:HD2	1.82	0.61
1:C:137:SER:O	1:C:141:GLU:HG3	2.01	0.61
1:C:235:GLN:HG3	1:C:290:ARG:NH1	2.15	0.61
1:B:221:TRP:O	1:B:421:GLN:HG3	2.02	0.60
1:D:328:LYS:CB	1:D:363:GLU:HG3	2.32	0.60
1:B:240:HIS:HA	1:B:243:LYS:HD3	1.83	0.60
1:B:412:ARG:HG2	1:B:412:ARG:HH11	1.66	0.60
1:C:328:LYS:CB	1:C:363:GLU:HG3	2.31	0.60
1:A:96:ARG:NH1	1:A:100:THR:HG23	2.17	0.59
1:A:135:TRP:O	1:A:139:GLN:HG3	2.01	0.59
1:C:422:GLN:HG2	1:C:423:LEU:HG	1.84	0.59
1:D:374:ASN:ND2	1:D:376:LEU:H	1.99	0.59
1:B:386:HIS:O	1:B:390:GLN:HG3	2.02	0.59
1:C:374:ASN:HD22	1:C:375:PRO:N	2.00	0.59
1:B:99[A]:MET:HB3	3:B:702:PP9:CBB	2.32	0.59
1:C:213:VAL:CG1	1:C:215:ARG:HG2	2.32	0.59
1:D:381:LEU:O	1:D:385:VAL:HG23	2.02	0.59
1:B:98[A]:LEU:HG	3:B:702:PP9:HBB1	1.84	0.59
1:B:153:ASN:C	1:B:155:ALA:H	2.10	0.59
1:B:134:ILE:HG13	6:B:1109:HOH:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:TRP:O	1:D:139:GLN:HG3	2.03	0.58
1:B:215:ARG:CB	1:B:215:ARG:NH1	2.66	0.58
1:D:68:LYS:CB	1:D:155:ALA:HB3	2.33	0.58
1:C:134:ILE:HG13	6:C:1152:HOH:O	2.03	0.58
1:D:66:LYS:HD3	1:D:66:LYS:N	2.18	0.58
1:D:307:PRO:HB3	4:D:802:CHD:H12	1.86	0.58
1:A:240:HIS:HA	1:A:243:LYS:HD3	1.86	0.57
1:D:137:SER:O	1:D:141:GLU:HG3	2.03	0.57
1:D:229:THR:HB	1:D:286:LYS:CD	2.34	0.57
1:D:358:LYS:HE3	1:D:358:LYS:HA	1.84	0.57
1:A:96:ARG:HH12	1:A:100:THR:HG23	1.69	0.57
1:B:154:THR:HG1	1:B:157:HIS:CE1	2.23	0.57
1:A:155:ALA:CB	1:A:156:PRO:CD	2.80	0.57
1:B:215:ARG:HH11	1:B:215:ARG:HB3	1.67	0.57
1:B:305:VAL:HG21	3:B:702:PP9:HMB3	1.85	0.57
1:B:360:CYS:SG	1:B:362:VAL:HG23	2.45	0.57
1:D:116:THR:O	1:D:120:GLN:HG3	2.05	0.57
1:A:193:GLN:HB3	1:A:279:GLU:HB2	1.86	0.57
1:A:391:SER:OG	1:A:393:GLU:HG2	2.05	0.57
1:B:394:LEU:HD22	1:B:421:GLN:HB2	1.87	0.57
1:A:135:TRP:CZ3	1:A:372:ASN:HB3	2.40	0.57
3:D:704:PP9:HHA	3:D:704:PP9:HBA1	1.87	0.57
1:C:115:ARG:NE	3:C:705:PP9:O1A	2.33	0.56
1:B:266:PRO:HG2	1:B:269:VAL:HG23	1.85	0.56
3:D:703:PP9:CHA	3:D:704:PP9:HAA2	2.35	0.56
1:B:415:LYS:HG3	1:B:416:SER:N	2.19	0.56
1:D:155:ALA:CB	1:D:156:PRO:CD	2.81	0.56
1:C:263:HIS:HB2	3:C:705:PP9:HBC1	1.88	0.56
1:A:68:LYS:HB3	1:A:155:ALA:HB3	1.88	0.56
1:A:207:TYR:CE1	1:A:413:GLU:HB3	2.41	0.56
1:A:154:THR:HG21	1:A:389:ILE:HD13	1.89	0.55
1:C:213:VAL:HG11	1:C:215:ARG:CZ	2.37	0.55
1:A:220:LYS:HD3	1:A:220:LYS:C	2.32	0.55
1:B:151:SER:HB2	1:B:386:HIS:HD2	1.72	0.55
1:D:310:TRP:CH2	3:D:706:PP9:HAB	2.41	0.55
1:D:408:ASN:HB3	1:D:411:CYS:SG	2.46	0.55
1:D:374:ASN:HD22	1:D:375:PRO:N	2.05	0.54
1:A:216:LYS:HG3	1:A:217:PRO:HD2	1.89	0.54
1:B:68:LYS:HB3	1:B:155:ALA:HB3	1.89	0.54
1:C:98:LEU:HG	3:C:705:PP9:CBB	2.37	0.54
1:A:305:VAL:CG2	3:A:701:PP9:HMB2	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LYS:CB	1:B:155:ALA:HB3	2.38	0.54
1:B:98[B]:LEU:HG	3:B:702:PP9:HBB1	1.89	0.54
1:C:263:HIS:NE2	1:C:343:LYS:NZ	2.55	0.54
1:A:246:ASP:OD2	1:A:253:ARG:NH1	2.40	0.54
1:C:257:VAL:HG21	1:C:322:LEU:HD13	1.90	0.54
1:A:220:LYS:HD3	1:A:221:TRP:N	2.23	0.54
1:A:285:GLN:NE2	6:A:1146:HOH:O	2.41	0.54
1:B:142:GLY:O	1:B:146:LEU:HG	2.07	0.54
1:B:155:ALA:CB	1:B:156:PRO:CD	2.82	0.53
1:C:135:TRP:O	1:C:139:GLN:HG3	2.08	0.53
1:A:68:LYS:HG3	1:A:183:GLU:OE1	2.08	0.53
1:B:135:TRP:CZ3	1:B:372:ASN:HB3	2.44	0.53
1:C:171:GLU:O	1:C:175:GLU:HG3	2.08	0.53
1:C:285:GLN:HE21	1:C:289:GLU:CD	2.16	0.53
1:C:244:GLU:HA	1:C:247:HIS:HD2	1.72	0.53
1:D:70:GLY:HA3	1:D:182:LEU:HD13	1.89	0.53
1:D:328:LYS:HB2	1:D:363:GLU:HG3	1.91	0.53
1:B:341:HIS:HB2	3:B:702:PP9:CGD	2.39	0.53
1:C:124:ARG:NH1	1:C:125:ARG:HG2	2.24	0.53
1:B:99[B]:MET:HB2	3:B:702:PP9:CBB	2.39	0.53
1:B:102:PRO:C	1:B:103:ILE:HG13	2.34	0.53
1:C:400:THR:HA	1:C:415:LYS:HD2	1.90	0.53
1:C:212:GLN:NE2	6:C:1154:HOH:O	2.42	0.52
1:B:237:PHE:O	1:B:241:ILE:HG13	2.10	0.52
1:C:221:TRP:O	1:C:421:GLN:HG3	2.10	0.52
1:D:272[A]:ARG:HH11	1:D:272[A]:ARG:HG3	1.73	0.52
1:A:314:GLN:HB2	1:A:317:GLU:HG3	1.91	0.52
1:C:316:ASP:HB3	1:C:352:TYR:CE1	2.45	0.52
1:D:283:THR:HG22	1:D:335:ILE:HD11	1.92	0.52
1:C:314:GLN:HB2	1:C:317:GLU:HG3	1.92	0.52
1:C:178:GLU:OE1	1:C:219:MET:HE2	2.09	0.52
1:C:98:LEU:CG	3:C:705:PP9:HBB1	2.40	0.52
1:C:391:SER:OG	1:C:393:GLU:HG2	2.09	0.52
1:D:175:GLU:HG2	1:D:179:ARG:NH1	2.25	0.52
1:C:343:LYS:HD3	6:C:1021:HOH:O	2.09	0.51
1:C:374:ASN:HD22	1:C:376:LEU:H	1.58	0.51
1:C:394:LEU:HD23	1:C:418:PHE:O	2.10	0.51
1:D:135:TRP:CZ3	1:D:372:ASN:HB3	2.45	0.51
1:C:193:GLN:HG2	1:C:280:VAL:HA	1.91	0.51
1:D:92:LEU:HD23	1:D:92:LEU:C	2.35	0.51
1:C:102:PRO:O	1:C:103:ILE:C	2.54	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ARG:HG3	1:C:125:ARG:N	2.24	0.51
1:C:155:ALA:HB1	1:C:156:PRO:HD2	1.89	0.51
1:D:316:ASP:HB3	1:D:352:TYR:CE1	2.45	0.51
1:B:386:HIS:ND1	1:B:390:GLN:NE2	2.59	0.51
1:B:220:LYS:HZ2	1:B:423:LEU:HB3	1.75	0.51
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.93	0.51
1:B:207:TYR:CZ	1:B:413:GLU:HB3	2.46	0.51
1:C:98:LEU:HG	3:C:705:PP9:HBB1	1.93	0.51
1:D:415:LYS:C	1:D:415:LYS:HD3	2.36	0.51
1:B:220:LYS:NZ	1:B:423:LEU:HB3	2.25	0.50
1:B:356:LEU:HA	1:B:359:GLU:HG2	1.93	0.50
1:C:141:GLU:HG2	1:C:159:TYR:HE2	1.76	0.50
1:D:374:ASN:HD22	1:D:376:LEU:H	1.59	0.50
1:D:147:LEU:HD21	1:D:385:VAL:HB	1.93	0.50
1:A:328:LYS:HB3	1:A:363:GLU:HG3	1.92	0.50
1:A:415:LYS:NZ	1:A:415:LYS:HB3	2.26	0.50
1:B:296:PRO:HD3	1:D:397:LYS:HD2	1.93	0.50
1:D:134:ILE:HG13	6:D:1095:HOH:O	2.11	0.50
1:C:244:GLU:HG2	6:C:1027:HOH:O	2.11	0.50
1:B:101:LEU:HB2	1:B:104:GLN:HG3	1.94	0.50
1:D:269:VAL:O	1:D:272[B]:ARG:HG2	2.11	0.50
1:A:106:LYS:O	1:A:109:PRO:HD2	2.12	0.49
1:B:341:HIS:CE1	1:B:343:LYS:HB2	2.48	0.49
1:B:316:ASP:HB3	1:B:352:TYR:CE1	2.48	0.49
1:B:356:LEU:O	1:B:359:GLU:HG3	2.12	0.49
1:A:403:CYS:HB2	1:A:406:CYS:HB2	1.93	0.49
1:B:99[A]:MET:HB3	3:B:702:PP9:HBB2	1.94	0.49
1:B:421:GLN:HE21	1:B:421:GLN:HA	1.78	0.49
1:C:68:LYS:HE3	1:C:183:GLU:OE1	2.12	0.49
1:C:330:ILE:O	1:C:365:ILE:HA	2.12	0.49
1:C:342:ILE:HG22	3:C:705:PP9:CBD	2.42	0.49
1:D:328:LYS:HB3	1:D:363:GLU:HG3	1.95	0.49
1:C:232:LEU:HD22	1:C:376:LEU:HD11	1.95	0.49
1:D:102:PRO:O	1:D:103:ILE:C	2.56	0.49
1:D:302:GLN:HG3	1:D:303:SER:OG	2.13	0.49
1:C:173:ALA:O	1:C:177:MET:HG3	2.12	0.49
1:A:221:TRP:O	1:A:421:GLN:HG3	2.13	0.49
1:B:103:ILE:HD12	1:B:103:ILE:O	2.13	0.48
1:B:412:ARG:O	1:B:415:LYS:HG2	2.12	0.48
1:C:67:PRO:HB2	1:C:182:LEU:CD2	2.43	0.48
1:C:67:PRO:HB2	1:C:182:LEU:HD21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:ASN:HB3	1:D:208:ARG:NH1	2.27	0.48
1:C:341:HIS:CE1	1:C:343:LYS:HB2	2.48	0.48
1:D:183:GLU:OE2	1:D:423:LEU:HD11	2.12	0.48
1:D:328:LYS:HB3	1:D:363:GLU:H	1.77	0.48
1:A:106:LYS:C	1:A:109:PRO:HD2	2.38	0.48
1:B:289:GLU:HG2	1:B:293:TYR:OH	2.13	0.48
1:A:291:LEU:O	1:A:292:GLU:HG2	2.12	0.48
1:B:412:ARG:HG2	1:B:412:ARG:NH1	2.28	0.48
1:C:92:LEU:C	1:C:92:LEU:HD23	2.38	0.48
1:D:288:MET:HG3	1:D:297:TYR:CE2	2.48	0.48
1:A:365:ILE:O	1:A:365:ILE:HG23	2.14	0.48
1:C:88:PHE:HE2	3:C:705:PP9:HAA2	1.79	0.48
1:A:374:ASN:C	1:A:374:ASN:ND2	2.69	0.48
1:B:65:ARG:HB3	1:B:66:LYS:HE3	1.95	0.48
1:C:121:GLU:OE2	1:C:124:ARG:NE	2.47	0.48
1:C:135:TRP:CZ3	1:C:372:ASN:HB3	2.48	0.48
1:A:230:HIS:HE1	1:A:383:ASP:OD2	1.97	0.47
1:D:193:GLN:HG2	1:D:280:VAL:HA	1.97	0.47
1:B:177:MET:HB2	1:B:219:MET:HE1	1.95	0.47
1:D:173:ALA:O	1:D:177:MET:HG3	2.14	0.47
1:D:357:ALA:O	1:D:362:VAL:HG23	2.14	0.47
1:B:313:PRO:HB3	1:D:271:ASN:O	2.14	0.47
1:B:320:LYS:HD3	1:B:356:LEU:HD11	1.96	0.47
1:C:153:ASN:C	1:C:155:ALA:H	2.22	0.47
1:A:255:GLU:O	1:A:255:GLU:HG2	2.13	0.47
1:A:324:GLU:HB3	1:B:324:GLU:OE2	2.14	0.47
1:C:141:GLU:HG2	1:C:159:TYR:CE2	2.49	0.47
1:C:207:TYR:CE1	1:C:413:GLU:HB3	2.49	0.47
1:D:323:CYS:CB	1:D:360:CYS:HG	2.28	0.47
1:B:177:MET:HB3	1:B:182:LEU:HD12	1.97	0.47
1:C:91:ARG:HD2	6:C:1094:HOH:O	2.14	0.47
1:D:154:THR:HG21	1:D:389:ILE:HD13	1.96	0.47
1:A:324:GLU:OE2	1:B:324:GLU:HB3	2.15	0.47
1:D:263:HIS:CD2	1:D:343:LYS:HE3	2.49	0.47
1:A:374:ASN:HD22	1:A:376:LEU:H	1.63	0.46
1:C:357:ALA:HB1	1:C:362:VAL:CG2	2.45	0.46
1:B:99[A]:MET:HG2	3:B:702:PP9:HBB1	1.98	0.46
1:B:356:LEU:HA	1:B:359:GLU:CG	2.46	0.46
1:D:231:HIS:CE1	1:D:232:LEU:HG	2.51	0.46
1:C:252:LYS:O	1:C:253[A]:ARG:C	2.58	0.46
1:D:342:ILE:HD13	1:D:342:ILE:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:LYS:HG3	6:C:1123:HOH:O	2.15	0.46
1:D:412:ARG:HD2	1:D:412:ARG:O	2.15	0.46
1:A:328:LYS:CB	1:A:363:GLU:HG3	2.45	0.46
1:B:257:VAL:CG1	1:B:330:ILE:HG12	2.46	0.46
1:B:343:LYS:NZ	6:B:1135:HOH:O	2.21	0.46
1:C:365:ILE:HG23	1:C:365:ILE:O	2.15	0.46
1:B:102:PRO:O	1:B:103:ILE:C	2.58	0.46
1:D:308:MET:HB2	6:D:1024:HOH:O	2.14	0.46
1:A:338:THR:HA	1:A:371:LEU:HD12	1.97	0.46
1:B:328:LYS:HB3	1:B:363:GLU:HG3	1.97	0.46
1:B:421:GLN:HA	1:B:421:GLN:NE2	2.31	0.46
1:A:414:THR:O	1:A:417:PHE:HB3	2.15	0.46
1:C:422:GLN:HG2	1:C:423:LEU:N	2.31	0.46
1:A:177:MET:CB	1:A:219:MET:HE1	2.46	0.46
1:B:328:LYS:CB	1:B:363:GLU:HG3	2.46	0.46
1:D:68:LYS:HD3	1:D:155:ALA:HB3	1.98	0.46
1:D:183:GLU:OE2	1:D:423:LEU:HD21	2.17	0.46
1:C:385:VAL:O	1:C:389:ILE:HG13	2.15	0.45
1:A:171:GLU:OE1	1:A:171:GLU:N	2.49	0.45
1:A:422:GLN:O	1:A:423:LEU:HB3	2.16	0.45
1:B:338:THR:O	1:B:371:LEU:HB2	2.16	0.45
1:C:319:ILE:HD11	1:C:332:LEU:HD21	1.99	0.45
1:D:141:GLU:O	1:D:145:LYS:HG3	2.15	0.45
1:D:272[A]:ARG:HD3	1:D:406:CYS:HA	1.98	0.45
1:D:289:GLU:HG2	1:D:293:TYR:OH	2.15	0.45
1:A:305:VAL:HG21	3:A:701:PP9:HMB2	1.99	0.45
1:D:195:SER:HB2	1:D:276:TYR:HB2	1.98	0.45
1:A:354:GLN:O	1:A:358:LYS:HB2	2.17	0.45
3:D:703:PP9:HBD2	3:D:703:PP9:HHA	1.99	0.45
1:C:325:ARG:HH11	1:C:325:ARG:HG3	1.81	0.45
1:D:184:ARG:NE	6:D:1114:HOH:O	2.50	0.45
1:B:88:PHE:HD1	1:B:166:VAL:HG13	1.82	0.45
1:B:416:SER:HA	1:B:419:THR:OG1	2.16	0.45
1:D:184:ARG:NE	1:D:220:LYS:HD3	2.32	0.45
1:C:191:TYR:CZ	1:C:198:THR:HB	2.52	0.45
1:C:353:SER:O	1:C:357:ALA:HB3	2.16	0.45
1:D:330:ILE:O	1:D:365:ILE:HA	2.16	0.45
1:A:248:PHE:CE1	1:A:366:ARG:HD3	2.52	0.45
1:D:244:GLU:CG	1:D:368:ALA:HA	2.46	0.45
1:D:422:GLN:CG	1:D:423:LEU:N	2.76	0.45
1:B:116:THR:HB	1:B:117:PRO:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:LEU:O	3:C:705:PP9:CBB	2.64	0.45
1:B:336:ALA:HB1	3:B:702:PP9:HBC2	1.98	0.44
1:C:106:LYS:O	1:C:109:PRO:HD2	2.16	0.44
1:A:92:LEU:HD23	1:A:92:LEU:C	2.42	0.44
1:B:338:THR:HA	1:B:371:LEU:HD12	1.98	0.44
1:A:355:VAL:O	1:A:359:GLU:HG2	2.17	0.44
1:B:315:THR:O	1:B:319:ILE:HG13	2.18	0.44
1:D:323:CYS:SG	1:D:360:CYS:SG	3.12	0.44
1:A:358:LYS:HA	1:A:358:LYS:CE	2.40	0.44
1:D:220:LYS:CD	1:D:423:LEU:HB3	2.41	0.44
1:D:229:THR:CB	1:D:286:LYS:HD3	2.46	0.44
1:B:207:TYR:CE1	1:B:413:GLU:HB3	2.53	0.44
1:B:415:LYS:HD3	6:B:1177:HOH:O	2.17	0.44
1:A:68:LYS:HB2	1:A:155:ALA:HB3	1.98	0.44
1:A:316:ASP:HB3	1:A:352:TYR:CE1	2.53	0.44
1:C:185:ALA:HB2	1:C:219:MET:SD	2.57	0.44
1:B:374:ASN:HD22	1:B:375:PRO:N	2.15	0.44
1:D:272[A]:ARG:HG3	1:D:405:LEU:O	2.18	0.43
1:D:323:CYS:HG	1:D:362:VAL:HG22	1.80	0.43
1:A:70:GLY:HA3	1:A:182:LEU:HD13	2.00	0.43
1:A:208:ARG:NH2	6:A:1027:HOH:O	2.40	0.43
1:A:358:LYS:HE3	1:A:358:LYS:CA	2.39	0.43
1:B:300:VAL:HG12	1:B:313:PRO:HG2	2.00	0.43
1:B:145:LYS:HB2	1:B:145:LYS:HE3	1.76	0.43
1:B:412:ARG:NH2	1:D:325:ARG:O	2.51	0.43
1:D:184:ARG:CD	1:D:220:LYS:HD3	2.49	0.43
1:D:67:PRO:HA	1:D:156:PRO:HG2	2.01	0.43
1:D:124[B]:ARG:HA	1:D:128:GLY:HA2	2.00	0.43
1:B:349:ASP:O	1:B:354:GLN:HG3	2.19	0.43
3:D:703:PP9:HBA2	4:D:801:CHD:H7	2.01	0.43
1:A:131:PRO:O	1:A:134:ILE:HG12	2.19	0.43
1:A:330:ILE:O	1:A:365:ILE:HA	2.19	0.43
1:B:116:THR:O	1:B:120:GLN:HG3	2.18	0.43
1:B:285:GLN:HG2	1:D:282:ALA:HB1	2.00	0.43
1:B:301:TRP:O	1:B:314:GLN:HA	2.19	0.43
1:C:274:ASP:HA	1:C:275:PRO:HD3	1.78	0.43
1:A:305:VAL:HG22	1:A:310:TRP:CZ2	2.54	0.43
1:D:391:SER:OG	1:D:393:GLU:HG2	2.18	0.43
1:A:297:TYR:O	1:A:298:ARG:HD3	2.18	0.43
1:C:252:LYS:O	1:C:253[B]:ARG:C	2.59	0.43
1:A:244:GLU:CG	1:A:368:ALA:HA	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LYS:HE2	1:B:155:ALA:CB	2.48	0.42
1:D:124[A]:ARG:HA	1:D:128:GLY:HA2	2.01	0.42
1:A:220:LYS:C	1:A:220:LYS:CD	2.91	0.42
1:B:99[A]:MET:HE1	1:B:101:LEU:HD22	2.00	0.42
1:B:257:VAL:HG13	1:B:330:ILE:HG12	2.01	0.42
1:C:158:LYS:HD3	1:C:160:TYR:CZ	2.54	0.42
1:B:101:LEU:CB	1:B:104:GLN:HG3	2.49	0.42
1:B:153:ASN:C	1:B:155:ALA:N	2.77	0.42
1:B:255:GLU:O	1:B:255:GLU:HG2	2.18	0.42
1:B:394:LEU:CD2	1:B:421:GLN:HB2	2.48	0.42
1:D:160:TYR:HE2	1:D:176:GLU:HG2	1.84	0.42
1:A:79:PRO:HD3	1:A:88:PHE:CD2	2.55	0.42
1:C:124:ARG:HG3	1:C:124:ARG:HH11	1.83	0.42
1:D:272[A]:ARG:O	1:D:272[A]:ARG:HG2	2.18	0.42
1:B:356:LEU:HD12	1:B:359:GLU:CD	2.45	0.42
1:B:323:CYS:CB	1:B:360:CYS:HG	2.33	0.42
1:D:329:ASN:HD22	1:D:364:ASN:HB2	1.84	0.42
1:A:71:ILE:N	1:A:71:ILE:HD12	2.35	0.42
1:A:116:THR:HB	1:A:117:PRO:HD3	2.01	0.42
1:B:106:LYS:C	1:B:109:PRO:HD2	2.45	0.42
1:D:191:TYR:CZ	1:D:198:THR:HB	2.55	0.42
1:D:352:TYR:HA	1:D:356:LEU:HB3	2.00	0.42
3:D:703:PP9:HHA	3:D:704:PP9:HAA2	2.02	0.42
1:A:342:ILE:HG22	3:A:701:PP9:HBD1	2.02	0.42
1:B:65:ARG:HB3	1:B:66:LYS:CE	2.49	0.42
1:B:193:GLN:HB3	1:B:279:GLU:HB2	2.02	0.42
1:D:65:ARG:HG3	1:D:156:PRO:HG3	2.01	0.42
1:B:68:LYS:HE2	1:B:155:ALA:HB2	2.02	0.42
1:B:354:GLN:O	1:B:358:LYS:HB2	2.19	0.42
1:A:96:ARG:HG3	1:A:96:ARG:HH11	1.85	0.42
1:A:153:ASN:C	1:A:155:ALA:H	2.28	0.42
1:B:305:VAL:HG22	1:B:310:TRP:CZ2	2.54	0.42
1:D:308:MET:HE3	6:D:1087:HOH:O	2.20	0.42
1:B:298:ARG:NH1	1:D:273:GLY:O	2.52	0.41
1:B:374:ASN:ND2	1:B:374:ASN:C	2.74	0.41
1:A:102:PRO:O	1:A:103:ILE:C	2.62	0.41
1:B:376:LEU:HD12	1:B:376:LEU:HA	1.92	0.41
1:C:371:LEU:HD13	1:C:377:PHE:CD2	2.55	0.41
1:D:252:LYS:HE2	1:D:252:LYS:HB3	1.87	0.41
1:A:193:GLN:HG2	1:A:280:VAL:HA	2.02	0.41
1:B:374:ASN:HA	1:B:375:PRO:HD2	1.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:HIS:HB2	3:A:701:PP9:O2D	2.20	0.41
1:C:154:THR:HG21	1:C:389:ILE:HD13	2.01	0.41
1:B:241:ILE:HG21	1:B:291:LEU:HD11	2.01	0.41
1:A:240:HIS:O	1:A:243:LYS:HG2	2.21	0.41
1:B:355:VAL:O	1:B:359:GLU:HG2	2.21	0.41
1:C:257:VAL:O	1:C:257:VAL:HG23	2.20	0.41
1:D:220:LYS:HD2	1:D:423:LEU:HD12	2.02	0.41
1:A:207:TYR:CZ	1:A:413:GLU:CB	3.03	0.41
1:A:220:LYS:NZ	1:A:423:LEU:OXT	2.54	0.41
1:A:323:CYS:CB	1:A:360:CYS:HG	2.33	0.41
1:D:244:GLU:HG3	1:D:368:ALA:HA	2.02	0.41
1:D:272[B]:ARG:HD2	6:D:1052:HOH:O	2.20	0.41
1:A:66:LYS:HA	1:A:67:PRO:HD3	1.93	0.41
1:A:305:VAL:O	1:A:305:VAL:HG23	2.21	0.41
1:D:213:VAL:HG12	1:D:215:ARG:H	1.86	0.41
1:D:342:ILE:HD13	1:D:346:TYR:HB3	2.02	0.41
1:D:412:ARG:HG2	1:D:412:ARG:HH11	1.86	0.41
1:B:107:LEU:O	1:B:110:PHE:HB3	2.21	0.40
1:D:115:ARG:NE	3:D:706:PP9:O1A	2.41	0.40
1:D:122:GLN:HG2	1:D:346:TYR:CE2	2.56	0.40
1:D:219:MET:HE3	1:D:221:TRP:CZ2	2.55	0.40
1:B:151:SER:HB2	1:B:386:HIS:CD2	2.53	0.40
1:C:244:GLU:CG	1:C:368:ALA:HA	2.51	0.40
1:C:304:LYS:HE3	1:C:310:TRP:CD1	2.56	0.40
1:D:243:LYS:HG3	6:D:1139:HOH:O	2.21	0.40
1:B:92:LEU:HD23	1:B:92:LEU:C	2.46	0.40
1:B:106:LYS:O	1:B:109:PRO:HD2	2.21	0.40
1:B:227:TRP:CD1	1:B:227:TRP:N	2.89	0.40
1:B:257:VAL:HG11	1:B:322:LEU:HD13	2.03	0.40
1:B:290:ARG:HG2	1:B:290:ARG:HH11	1.87	0.40
1:B:297:TYR:CD1	1:B:297:TYR:C	2.99	0.40
1:B:414:THR:O	1:B:417:PHE:HB3	2.22	0.40
1:D:274:ASP:HA	1:D:275:PRO:HD3	1.81	0.40
1:B:70:GLY:HA3	1:B:182:LEU:HD13	2.04	0.40
1:C:374:ASN:C	1:C:374:ASN:ND2	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	357/359 (99%)	343 (96%)	13 (4%)	1 (0%)	36	42
1	B	361/359 (101%)	344 (95%)	16 (4%)	1 (0%)	36	42
1	C	359/359 (100%)	336 (94%)	19 (5%)	4 (1%)	11	10
1	D	361/359 (101%)	345 (96%)	14 (4%)	2 (1%)	21	23
All	All	1438/1436 (100%)	1368 (95%)	62 (4%)	8 (1%)	24	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ALA
1	B	155	ALA
1	C	155	ALA
1	C	253[A]	ARG
1	C	253[B]	ARG
1	D	155	ALA
1	C	359	GLU
1	D	355	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/324 (100%)	318 (98%)	6 (2%)	50	66
1	B	328/324 (101%)	318 (97%)	10 (3%)	36	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	326/324 (101%)	314 (96%)	12 (4%)	30	41
1	D	328/324 (101%)	313 (95%)	15 (5%)	24	32
All	All	1306/1296 (101%)	1263 (97%)	43 (3%)	34	45

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LYS
1	A	101	LEU
1	A	178	GLU
1	A	257	VAL
1	A	358	LYS
1	A	415	LYS
1	B	66	LYS
1	B	99[A]	MET
1	B	99[B]	MET
1	B	101	LEU
1	B	178	GLU
1	B	251	GLU
1	B	257	VAL
1	B	307	PRO
1	B	374	ASN
1	B	423	LEU
1	C	66	LYS
1	C	99	MET
1	C	101	LEU
1	C	107	LEU
1	C	118	LYS
1	C	121	GLU
1	C	178	GLU
1	C	243	LYS
1	C	250	LEU
1	C	286	LYS
1	C	358	LYS
1	C	374	ASN
1	D	66	LYS
1	D	99	MET
1	D	101	LEU
1	D	107	LEU
1	D	113	LYS
1	D	121[A]	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	121[B]	GLU
1	D	213	VAL
1	D	216	LYS
1	D	251	GLU
1	D	305	VAL
1	D	342	ILE
1	D	358	LYS
1	D	374	ASN
1	D	392	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	HIS
1	A	285	GLN
1	A	329	ASN
1	A	354	GLN
1	A	364	ASN
1	A	374	ASN
1	A	421	GLN
1	B	120	GLN
1	B	231	HIS
1	B	235	GLN
1	B	285	GLN
1	B	314	GLN
1	B	329	ASN
1	B	354	GLN
1	B	364	ASN
1	B	374	ASN
1	B	390	GLN
1	B	392	ASN
1	B	421	GLN
1	B	422	GLN
1	C	167	HIS
1	C	211	ASN
1	C	212	GLN
1	C	231	HIS
1	C	235	GLN
1	C	247	HIS
1	C	285	GLN
1	C	329	ASN
1	C	364	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	374	ASN
1	C	421	GLN
1	D	212	GLN
1	D	231	HIS
1	D	235	GLN
1	D	329	ASN
1	D	354	GLN
1	D	364	ASN
1	D	374	ASN
1	D	386	HIS
1	D	390	GLN
1	D	421	GLN
1	D	422	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	PP9	A	701	-	36,46,46	2.08	11 (30%)	28,68,68	2.55	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	IMD	D	901	-	5,5,5	0.35	0	5,5,5	0.44	0
3	PP9	C	705	-	36,46,46	2.01	11 (30%)	28,68,68	2.58	10 (35%)
2	FES	B	1002	1	0,4,4	-	-	-	-	-
3	PP9	B	702	-	36,46,46	2.26	13 (36%)	28,68,68	2.42	10 (35%)
3	PP9	D	704	-	36,46,46	2.37	8 (22%)	28,68,68	2.27	8 (28%)
2	FES	D	1004	1	0,4,4	-	-	-	-	-
2	FES	A	1001	1	0,4,4	-	-	-	-	-
3	PP9	D	706	-	36,46,46	2.12	12 (33%)	28,68,68	2.66	10 (35%)
4	CHD	D	801	-	32,32,32	2.17	13 (40%)	51,51,51	1.89	16 (31%)
2	FES	C	1003	1	0,4,4	-	-	-	-	-
4	CHD	D	802	-	32,32,32	2.29	16 (50%)	51,51,51	1.89	16 (31%)
3	PP9	D	703	-	36,46,46	2.20	9 (25%)	28,68,68	2.29	9 (32%)

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	PP9	A	701	-	-	5/12/62/62	0/4/5/5
5	IMD	D	901	-	-	-	0/1/1/1
3	PP9	C	705	-	-	5/12/62/62	0/4/5/5
2	FES	B	1002	1	-	-	0/1/1/1
3	PP9	B	702	-	-	2/12/62/62	0/4/5/5
3	PP9	D	704	-	-	6/12/62/62	0/4/5/5
2	FES	D	1004	1	-	-	0/1/1/1
2	FES	A	1001	1	-	-	0/1/1/1
3	PP9	D	706	-	-	3/12/62/62	0/4/5/5
4	CHD	D	801	-	-	3/9/74/74	0/4/4/4
2	FES	C	1003	1	-	-	0/1/1/1
4	CHD	D	802	-	-	5/9/74/74	0/4/4/4
3	PP9	D	703	-	-	10/12/62/62	0/4/5/5

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	704	PP9	C1A-C2A	6.21	1.46	1.39
3	B	702	PP9	C3C-C4C	5.87	1.47	1.41
3	D	704	PP9	CAB-C3B	5.78	1.54	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	703	PP9	CAB-C3B	5.49	1.54	1.47
3	D	706	PP9	C1A-C2A	5.37	1.45	1.39
3	B	702	PP9	CAB-C3B	5.00	1.53	1.47
3	D	703	PP9	C1A-C2A	4.78	1.44	1.39
4	D	802	CHD	O25-C24	4.74	1.37	1.22
3	D	704	PP9	CBB-CAB	4.63	1.52	1.30
3	D	703	PP9	CBB-CAB	4.62	1.52	1.30
3	B	702	PP9	CBB-CAB	4.61	1.52	1.30
3	A	701	PP9	CBB-CAB	4.55	1.52	1.30
4	D	801	CHD	O25-C24	4.54	1.36	1.22
3	A	701	PP9	C3C-C2C	-4.53	1.34	1.40
3	D	706	PP9	C3C-C2C	-4.52	1.34	1.40
3	D	704	PP9	C1C-C2C	4.52	1.44	1.39
3	D	706	PP9	CBB-CAB	4.51	1.52	1.30
3	C	705	PP9	CBB-CAB	4.50	1.52	1.30
3	B	702	PP9	C1A-C2A	4.45	1.44	1.39
3	D	704	PP9	C3C-C2C	-4.41	1.34	1.40
3	C	705	PP9	C3C-C2C	-4.39	1.34	1.40
3	A	701	PP9	CAB-C3B	4.36	1.52	1.47
3	D	703	PP9	C3C-C2C	-4.35	1.34	1.40
3	D	703	PP9	C4A-C3A	4.29	1.44	1.39
3	A	701	PP9	C1A-C2A	4.21	1.44	1.39
4	D	802	CHD	C11-C9	4.16	1.60	1.53
3	D	704	PP9	C4A-C3A	4.12	1.44	1.39
3	A	701	PP9	C1C-C2C	4.11	1.44	1.39
3	D	706	PP9	CAB-C3B	4.09	1.52	1.47
3	D	703	PP9	C1C-C2C	4.00	1.44	1.39
3	C	705	PP9	C1C-C2C	3.96	1.43	1.39
4	D	801	CHD	C11-C9	3.91	1.60	1.53
3	C	705	PP9	CAB-C3B	3.90	1.52	1.47
3	C	705	PP9	C1A-C2A	3.86	1.43	1.39
4	D	801	CHD	C16-C17	3.85	1.62	1.54
3	D	704	PP9	CBC-CAC	3.76	1.52	1.29
3	A	701	PP9	CBC-CAC	3.74	1.52	1.29
3	D	703	PP9	CBC-CAC	3.69	1.52	1.29
3	D	706	PP9	CBC-CAC	3.67	1.52	1.29
3	B	702	PP9	CBC-CAC	3.67	1.52	1.29
3	C	705	PP9	CBC-CAC	3.66	1.52	1.29
4	D	802	CHD	C16-C17	3.63	1.61	1.54
3	D	704	PP9	C3C-C4C	3.60	1.45	1.41
4	D	802	CHD	C10-C9	3.46	1.62	1.56
3	B	702	PP9	C3C-C2C	-3.26	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	PP9	C1C-C2C	3.21	1.43	1.39
3	D	706	PP9	C3C-C4C	3.16	1.44	1.41
4	D	802	CHD	C6-C5	3.14	1.58	1.53
3	D	706	PP9	C1C-C2C	3.10	1.43	1.39
4	D	801	CHD	C10-C9	3.05	1.61	1.56
4	D	801	CHD	C6-C5	2.98	1.58	1.53
4	D	802	CHD	C8-C14	2.93	1.59	1.53
4	D	801	CHD	C18-C13	2.83	1.58	1.54
3	A	701	PP9	C3C-C4C	2.81	1.44	1.41
4	D	802	CHD	C18-C13	2.77	1.58	1.54
3	B	702	PP9	CBA-CGA	-2.75	1.44	1.50
3	D	703	PP9	C3C-C4C	2.74	1.44	1.41
3	C	705	PP9	C3C-C4C	2.70	1.44	1.41
4	D	801	CHD	C19-C10	2.63	1.58	1.54
3	A	701	PP9	CBA-CGA	-2.57	1.44	1.50
4	D	802	CHD	O26-C24	-2.55	1.22	1.30
4	D	801	CHD	O26-C24	-2.54	1.22	1.30
4	D	801	CHD	C8-C14	2.53	1.58	1.53
4	D	802	CHD	C8-C7	2.51	1.58	1.53
3	A	701	PP9	O2A-CGA	-2.50	1.22	1.30
3	B	702	PP9	O2A-CGA	-2.50	1.22	1.30
4	D	802	CHD	C13-C12	2.49	1.58	1.54
4	D	801	CHD	O12-C12	2.49	1.47	1.43
4	D	802	CHD	C19-C10	2.48	1.58	1.54
3	B	702	PP9	CMB-C2B	2.47	1.54	1.50
4	D	802	CHD	C20-C17	2.47	1.58	1.54
4	D	802	CHD	O12-C12	2.46	1.47	1.43
3	D	706	PP9	O2A-CGA	-2.41	1.22	1.30
3	B	702	PP9	O2D-CGD	-2.37	1.23	1.30
3	C	705	PP9	O2A-CGA	-2.34	1.23	1.30
3	B	702	PP9	CMD-C2D	2.31	1.54	1.50
3	C	705	PP9	CBA-CGA	-2.31	1.45	1.50
4	D	801	CHD	O7-C7	2.29	1.48	1.43
4	D	801	CHD	C8-C7	2.29	1.57	1.53
3	C	705	PP9	CMD-C2D	2.28	1.54	1.50
4	D	801	CHD	C13-C12	2.28	1.58	1.54
3	C	705	PP9	O2D-CGD	-2.27	1.23	1.30
3	D	706	PP9	CMB-C2B	2.27	1.54	1.50
3	D	706	PP9	O2D-CGD	-2.24	1.23	1.30
4	D	802	CHD	O7-C7	2.20	1.47	1.43
3	B	702	PP9	C4A-NA	-2.18	1.34	1.38
4	D	802	CHD	C22-C23	2.16	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	PP9	CMD-C2D	2.12	1.53	1.50
3	A	701	PP9	O2D-CGD	-2.09	1.23	1.30
3	D	703	PP9	O2D-CGD	-2.07	1.24	1.30
4	D	802	CHD	C8-C9	2.06	1.57	1.53
3	D	706	PP9	CMD-C2D	2.05	1.53	1.50
3	D	706	PP9	CBA-CGA	-2.05	1.45	1.50

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	705	PP9	C3C-C4C-NC	6.21	111.51	107.46
3	A	701	PP9	C3C-C4C-NC	6.12	111.46	107.46
3	D	703	PP9	C3C-C4C-NC	6.03	111.39	107.46
3	D	706	PP9	CBA-CAA-C2A	-5.93	102.57	112.54
3	D	704	PP9	C3C-C4C-NC	5.91	111.32	107.46
3	D	706	PP9	C3C-C4C-NC	5.91	111.31	107.46
3	C	705	PP9	CBA-CAA-C2A	-5.76	102.86	112.54
3	D	706	PP9	CAA-CBA-CGA	5.68	129.15	113.83
3	B	702	PP9	CBA-CAA-C2A	-5.63	103.06	112.54
3	B	702	PP9	CAA-CBA-CGA	5.58	128.87	113.83
3	B	702	PP9	C3C-C4C-NC	5.35	110.95	107.46
3	A	701	PP9	CBA-CAA-C2A	-5.35	103.55	112.54
3	D	704	PP9	CBA-CAA-C2A	5.08	121.08	112.54
3	D	703	PP9	CBA-CAA-C2A	4.97	120.89	112.54
3	A	701	PP9	CAA-CBA-CGA	4.78	126.70	113.83
3	C	705	PP9	CAA-CBA-CGA	4.75	126.64	113.83
4	D	801	CHD	O26-C24-C23	4.48	128.14	114.00
4	D	802	CHD	O26-C24-C23	4.28	127.54	114.00
3	A	701	PP9	C4A-NA-C1A	-4.06	102.89	108.82
4	D	801	CHD	C18-C13-C12	-4.02	105.03	109.06
4	D	802	CHD	C18-C13-C12	-3.96	105.09	109.06
4	D	802	CHD	C19-C10-C1	-3.92	102.07	108.31
3	C	705	PP9	C4A-NA-C1A	-3.87	103.18	108.82
3	D	706	PP9	C4A-NA-C1A	-3.86	103.19	108.82
4	D	801	CHD	C19-C10-C1	-3.72	102.38	108.31
3	C	705	PP9	C4C-NC-C1C	-3.70	103.42	108.82
3	D	706	PP9	CBB-CAB-C3B	-3.66	118.66	125.93
3	D	703	PP9	C4A-NA-C1A	-3.64	103.51	108.82
3	D	703	PP9	C4C-NC-C1C	-3.62	103.54	108.82
3	A	701	PP9	C4C-NC-C1C	-3.61	103.55	108.82
3	A	701	PP9	CBB-CAB-C3B	-3.59	118.80	125.93
3	C	705	PP9	CBB-CAB-C3B	-3.56	118.86	125.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	706	PP9	C4C-NC-C1C	-3.55	103.65	108.82
3	D	706	PP9	C3A-C4A-NA	3.54	111.99	109.43
3	B	702	PP9	C2C-C1C-NC	3.53	111.98	109.43
3	B	702	PP9	C4C-NC-C1C	-3.42	103.83	108.82
4	D	802	CHD	C17-C13-C12	3.42	120.75	117.67
3	D	704	PP9	C4C-NC-C1C	-3.39	103.88	108.82
3	D	704	PP9	C4A-NA-C1A	-3.38	103.90	108.82
4	D	802	CHD	O12-C12-C13	-3.35	105.36	111.02
4	D	801	CHD	O12-C12-C13	-3.30	105.45	111.02
3	C	705	PP9	CBD-CAD-C3D	3.21	121.31	112.54
4	D	801	CHD	C17-C13-C14	3.20	103.32	100.11
3	D	703	PP9	C2A-C1A-NA	3.15	111.70	109.43
3	A	701	PP9	CBD-CAD-C3D	3.14	121.14	112.54
3	A	701	PP9	C3A-C4A-NA	3.10	111.67	109.43
3	B	702	PP9	CBD-CAD-C3D	3.05	120.89	112.54
3	D	706	PP9	CBD-CAD-C3D	3.03	120.83	112.54
4	D	802	CHD	O25-C24-C23	-3.02	113.52	123.09
4	D	801	CHD	O25-C24-C23	-3.00	113.57	123.09
4	D	802	CHD	C17-C13-C14	2.99	103.11	100.11
4	D	801	CHD	C17-C13-C12	2.95	120.32	117.67
3	D	706	PP9	C2C-C1C-NC	2.89	111.52	109.43
3	C	705	PP9	C3A-C4A-NA	2.89	111.52	109.43
3	B	702	PP9	CBB-CAB-C3B	-2.82	120.34	125.93
4	D	801	CHD	C6-C5-C10	-2.81	109.67	112.66
4	D	802	CHD	C16-C17-C13	-2.72	100.90	103.54
4	D	802	CHD	C6-C5-C10	-2.71	109.77	112.66
4	D	802	CHD	C11-C12-C13	2.65	113.96	111.26
3	D	703	PP9	CBB-CAB-C3B	-2.65	120.67	125.93
4	D	801	CHD	C11-C12-C13	2.58	113.89	111.26
4	D	802	CHD	C6-C5-C4	2.54	114.12	111.23
4	D	802	CHD	C1-C10-C5	2.54	111.39	107.75
3	A	701	PP9	CAA-C2A-C3A	-2.50	120.06	127.25
3	D	706	PP9	CAA-C2A-C3A	-2.50	120.07	127.25
4	D	801	CHD	C1-C10-C5	2.50	111.33	107.75
3	D	704	PP9	CBB-CAB-C3B	-2.48	121.01	125.93
4	D	801	CHD	C11-C9-C10	-2.46	111.20	113.70
3	B	702	PP9	CAA-C2A-C3A	-2.46	120.18	127.25
3	D	703	PP9	CAD-CBD-CGD	2.42	120.08	113.67
4	D	802	CHD	C11-C9-C10	-2.38	111.28	113.70
4	D	801	CHD	C16-C17-C13	-2.37	101.25	103.54
3	D	704	PP9	CAD-CBD-CGD	2.36	119.93	113.67
3	C	705	PP9	CAA-C2A-C3A	-2.32	120.57	127.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	802	CHD	C9-C8-C7	-2.32	108.94	111.86
4	D	801	CHD	C6-C5-C4	2.31	113.87	111.23
3	D	704	PP9	C2A-C1A-NA	2.31	111.10	109.43
4	D	801	CHD	C9-C8-C7	-2.27	109.00	111.86
3	D	704	PP9	C3A-C4A-NA	2.25	111.06	109.43
4	D	801	CHD	C19-C10-C9	2.23	114.17	111.18
4	D	802	CHD	C19-C10-C9	2.23	114.17	111.18
4	D	801	CHD	C9-C11-C12	-2.17	111.46	114.29
3	B	702	PP9	C2A-C1A-NA	-2.12	107.90	109.43
4	D	802	CHD	C9-C11-C12	-2.11	111.53	114.29
3	C	705	PP9	C2C-C1C-NC	2.10	110.95	109.43
3	D	703	PP9	C2C-C1C-NC	2.09	110.94	109.43
3	B	702	PP9	CAD-C3D-C2D	-2.04	124.05	127.87
3	D	703	PP9	CBD-CAD-C3D	2.01	118.04	112.54

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	705	PP9	C2B-C3B-CAB-CBB
3	C	705	PP9	C4B-C3B-CAB-CBB
3	D	703	PP9	C1A-C2A-CAA-CBA
3	D	703	PP9	C3A-C2A-CAA-CBA
3	D	704	PP9	C1A-C2A-CAA-CBA
3	D	704	PP9	C3A-C2A-CAA-CBA
3	D	706	PP9	C2B-C3B-CAB-CBB
3	D	706	PP9	C4B-C3B-CAB-CBB
4	D	802	CHD	C21-C20-C22-C23
3	A	701	PP9	C2A-CAA-CBA-CGA
3	B	702	PP9	C2A-CAA-CBA-CGA
4	D	801	CHD	C20-C22-C23-C24
3	A	701	PP9	C2D-C3D-CAD-CBD
3	C	705	PP9	C2A-CAA-CBA-CGA
3	B	702	PP9	C4D-C3D-CAD-CBD
3	D	703	PP9	C4D-C3D-CAD-CBD
4	D	801	CHD	C21-C20-C22-C23
4	D	801	CHD	C17-C20-C22-C23
3	D	703	PP9	C2D-C3D-CAD-CBD
3	D	703	PP9	C2B-C3B-CAB-CBB
3	A	701	PP9	C3D-CAD-CBD-CGD
3	A	701	PP9	C4B-C3B-CAB-CBB
3	D	704	PP9	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	703	PP9	CAD-CBD-CGD-O2D
4	D	802	CHD	C20-C22-C23-C24
3	D	704	PP9	CAA-CBA-CGA-O2A
4	D	802	CHD	C22-C23-C24-O25
3	D	703	PP9	CAD-CBD-CGD-O1D
4	D	802	CHD	C22-C23-C24-O26
3	A	701	PP9	C2B-C3B-CAB-CBB
3	D	704	PP9	CAD-CBD-CGD-O2D
3	D	704	PP9	CAD-CBD-CGD-O1D
3	D	703	PP9	C4B-C3B-CAB-CBB
3	D	706	PP9	CAA-CBA-CGA-O2A
3	D	703	PP9	CAA-CBA-CGA-O1A
3	D	703	PP9	CAA-CBA-CGA-O2A
3	C	705	PP9	CAD-CBD-CGD-O2D
4	D	802	CHD	C17-C20-C22-C23
3	C	705	PP9	CAD-CBD-CGD-O1D

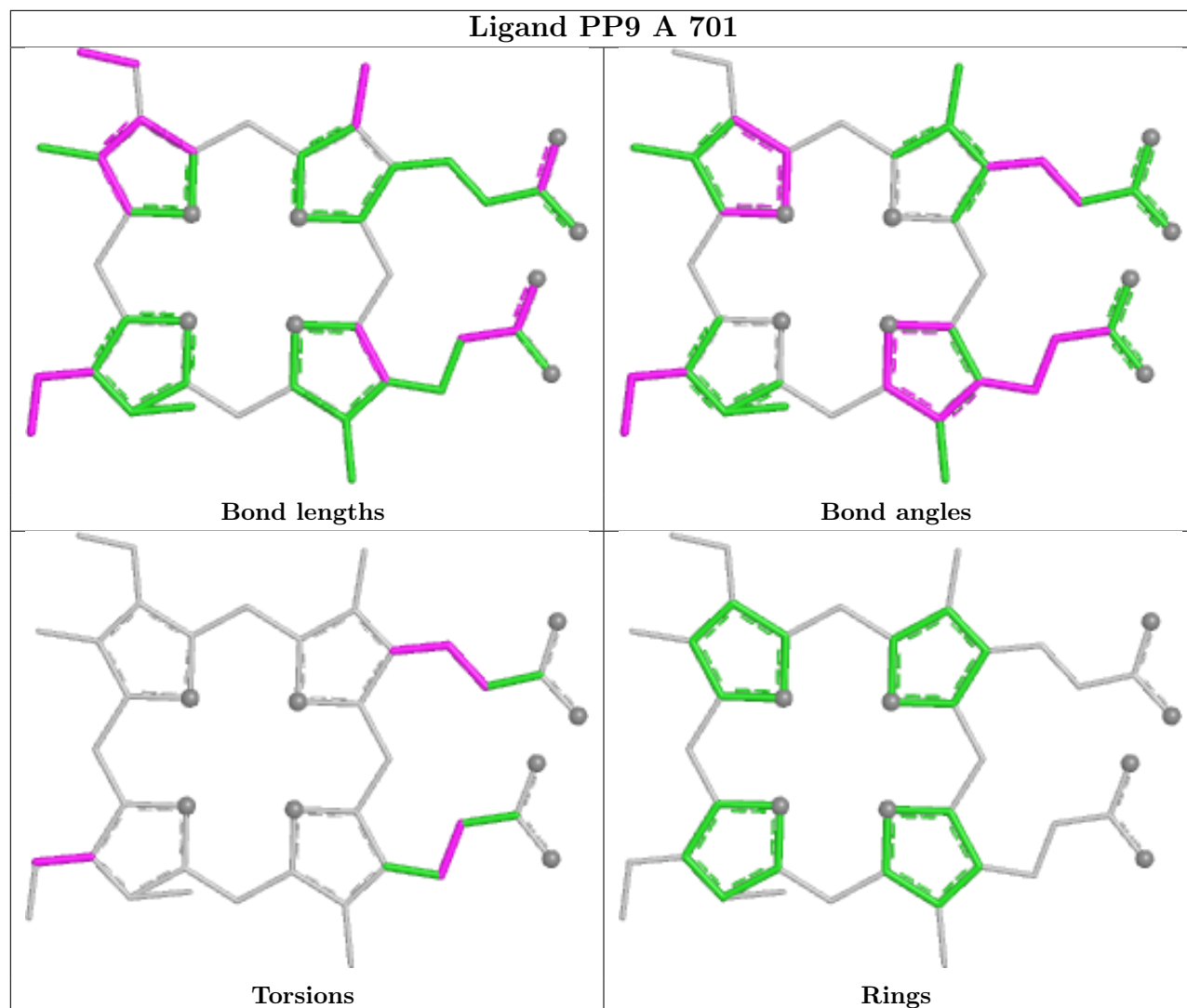
There are no ring outliers.

8 monomers are involved in 38 short contacts:

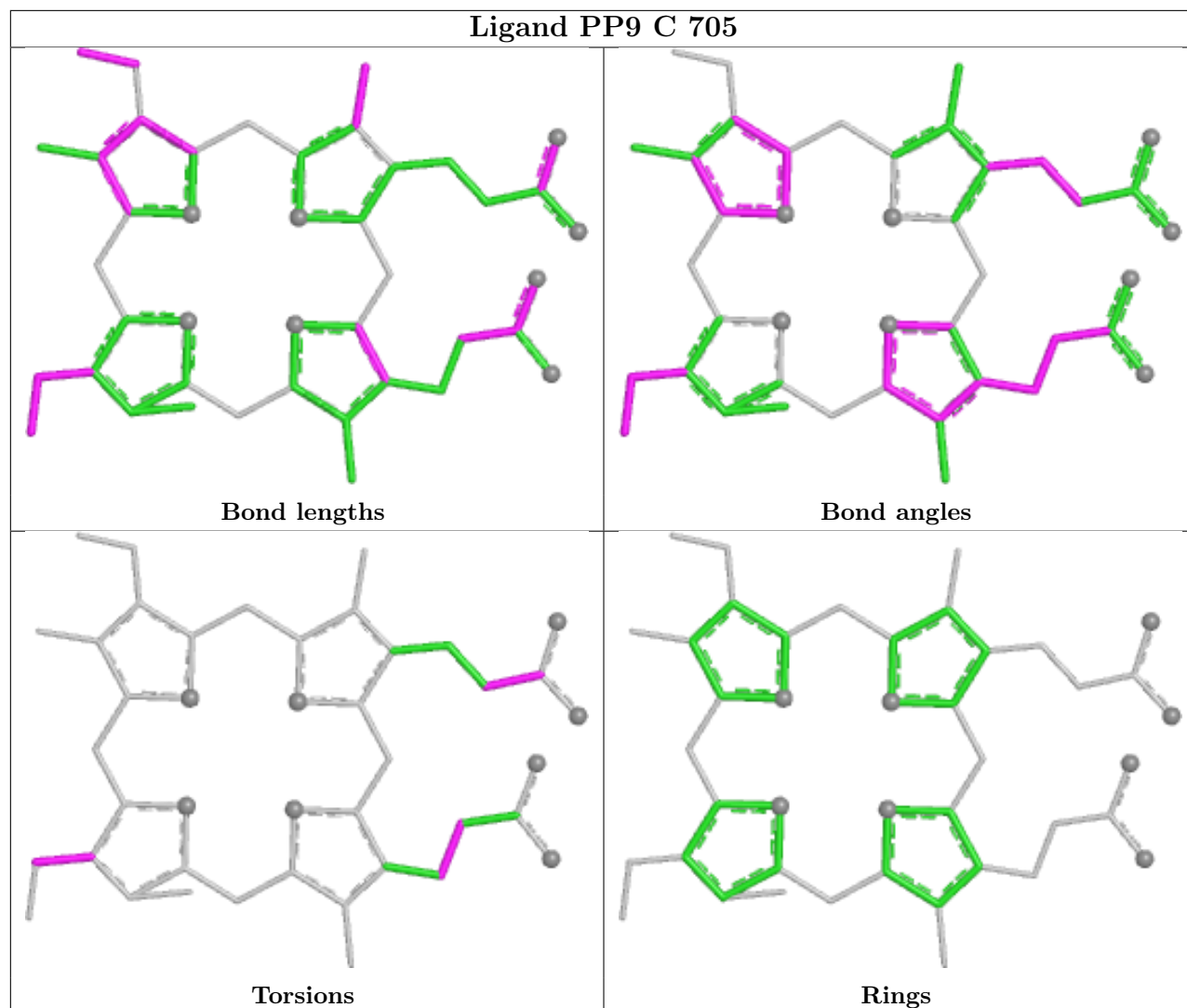
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	PP9	5	0
3	C	705	PP9	14	0
3	B	702	PP9	9	0
3	D	704	PP9	3	0
3	D	706	PP9	4	0
4	D	801	CHD	1	0
4	D	802	CHD	1	0
3	D	703	PP9	4	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

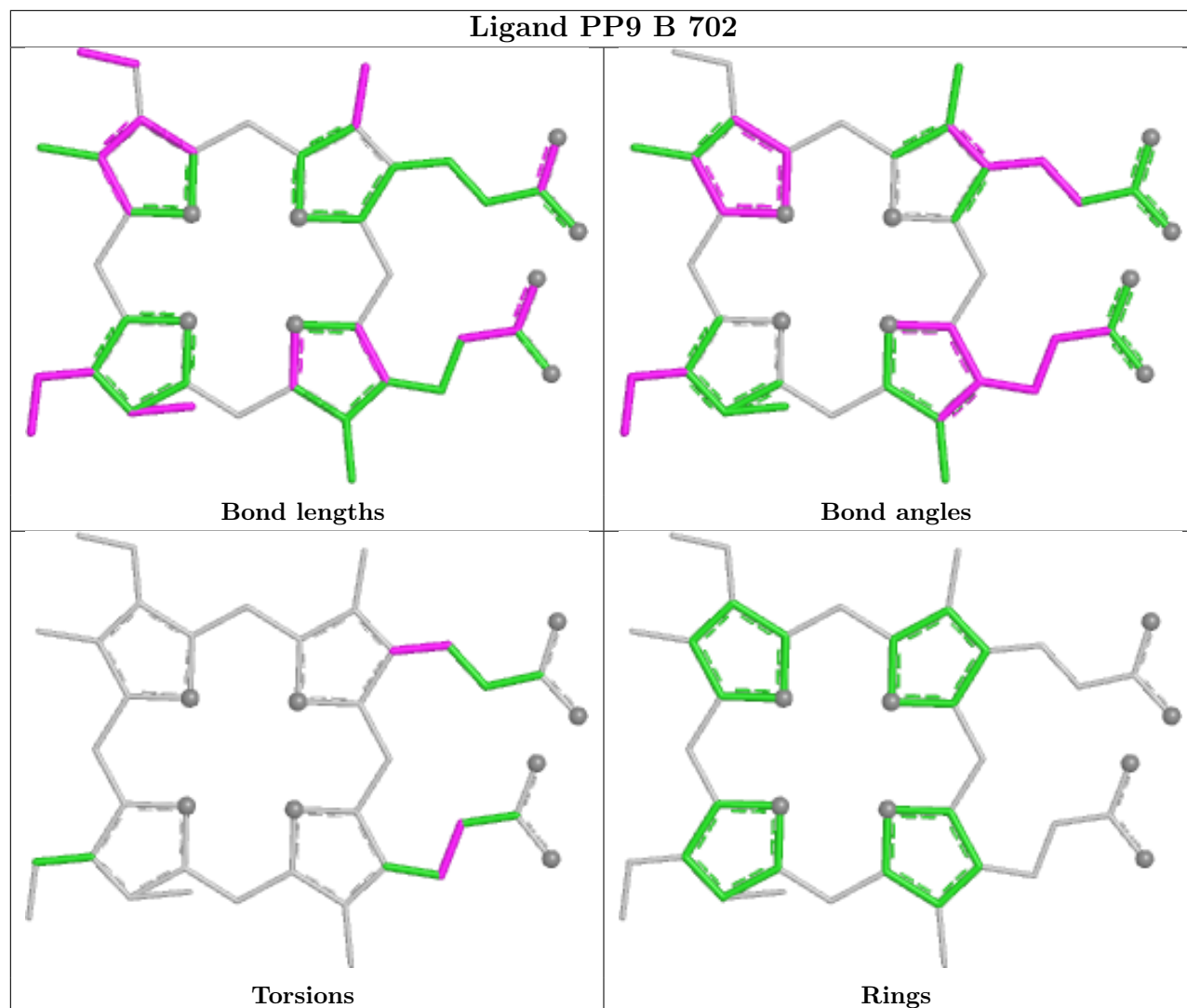
Ligand PP9 A 701



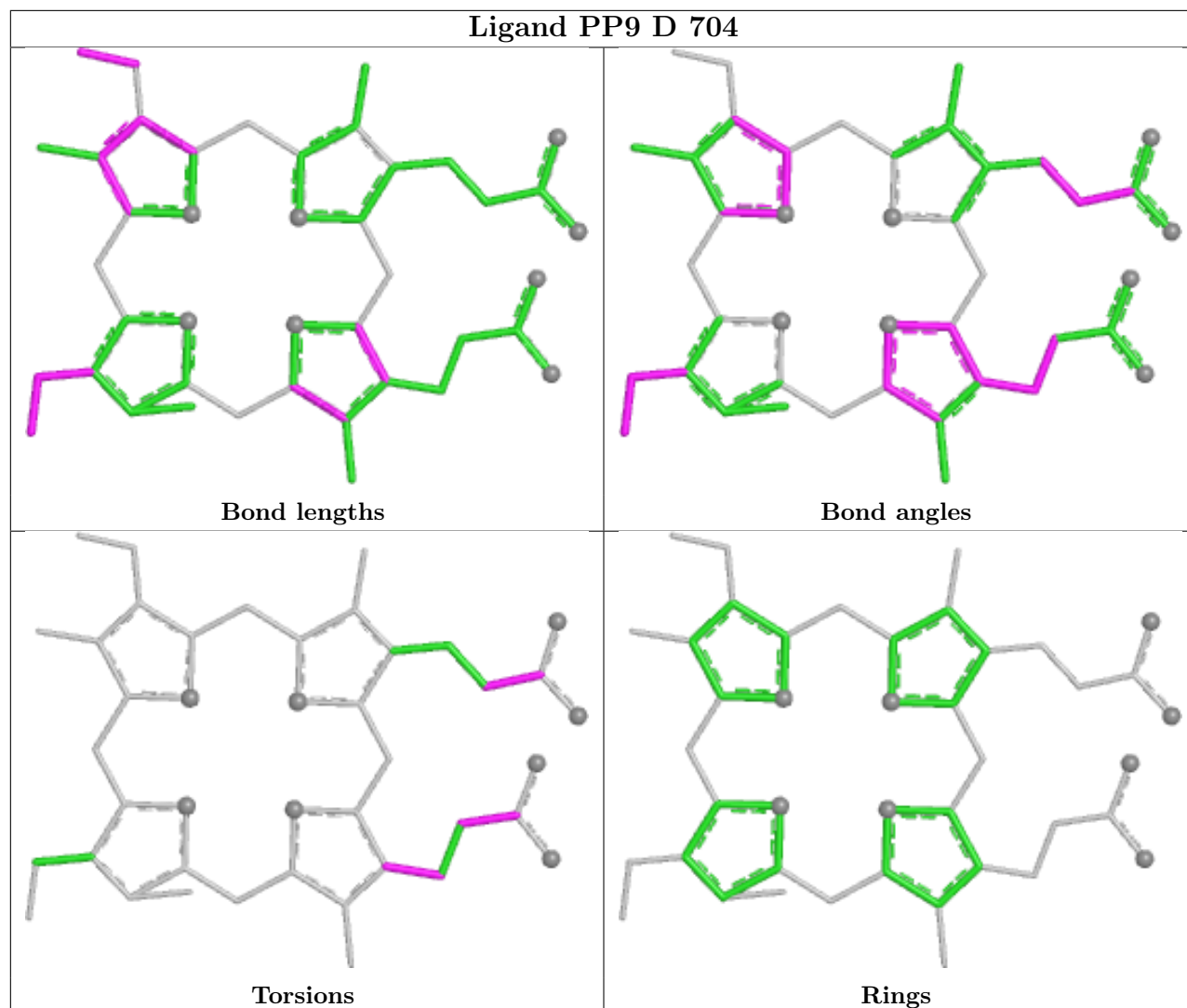
Ligand PP9 C 705



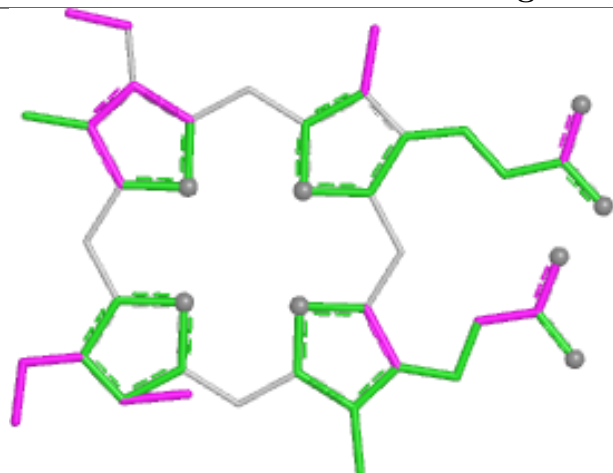
Ligand PP9 B 702



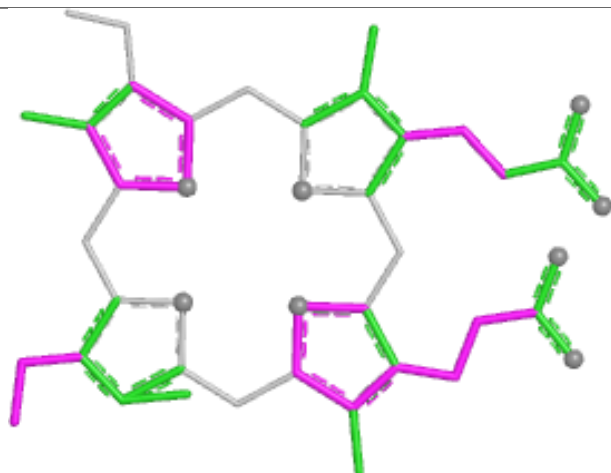
Ligand PP9 D 704



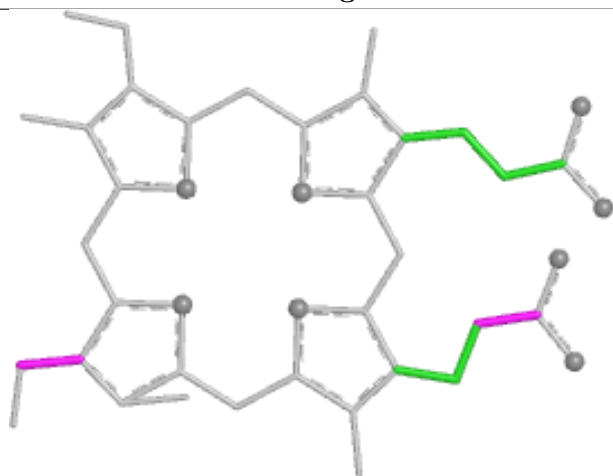
Ligand PP9 D 706



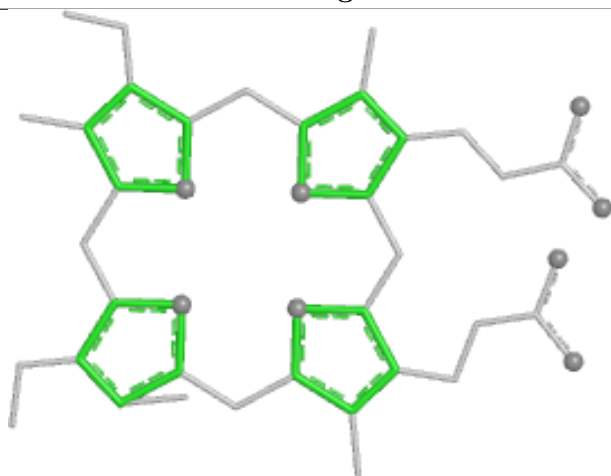
Bond lengths



Bond angles

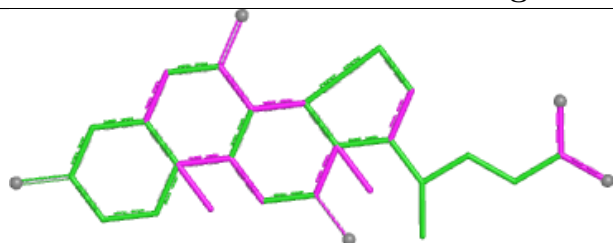


Torsions

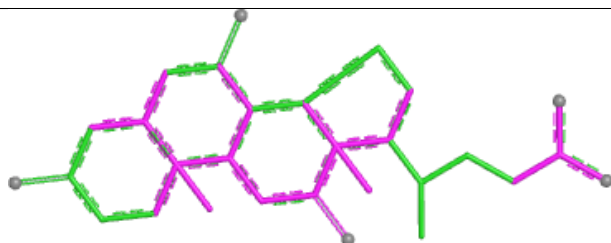


Rings

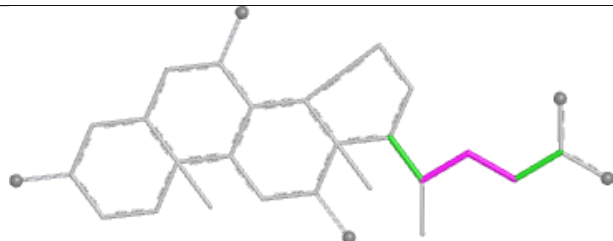
Ligand CHD D 801



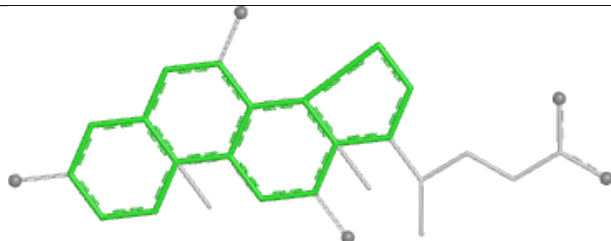
Bond lengths



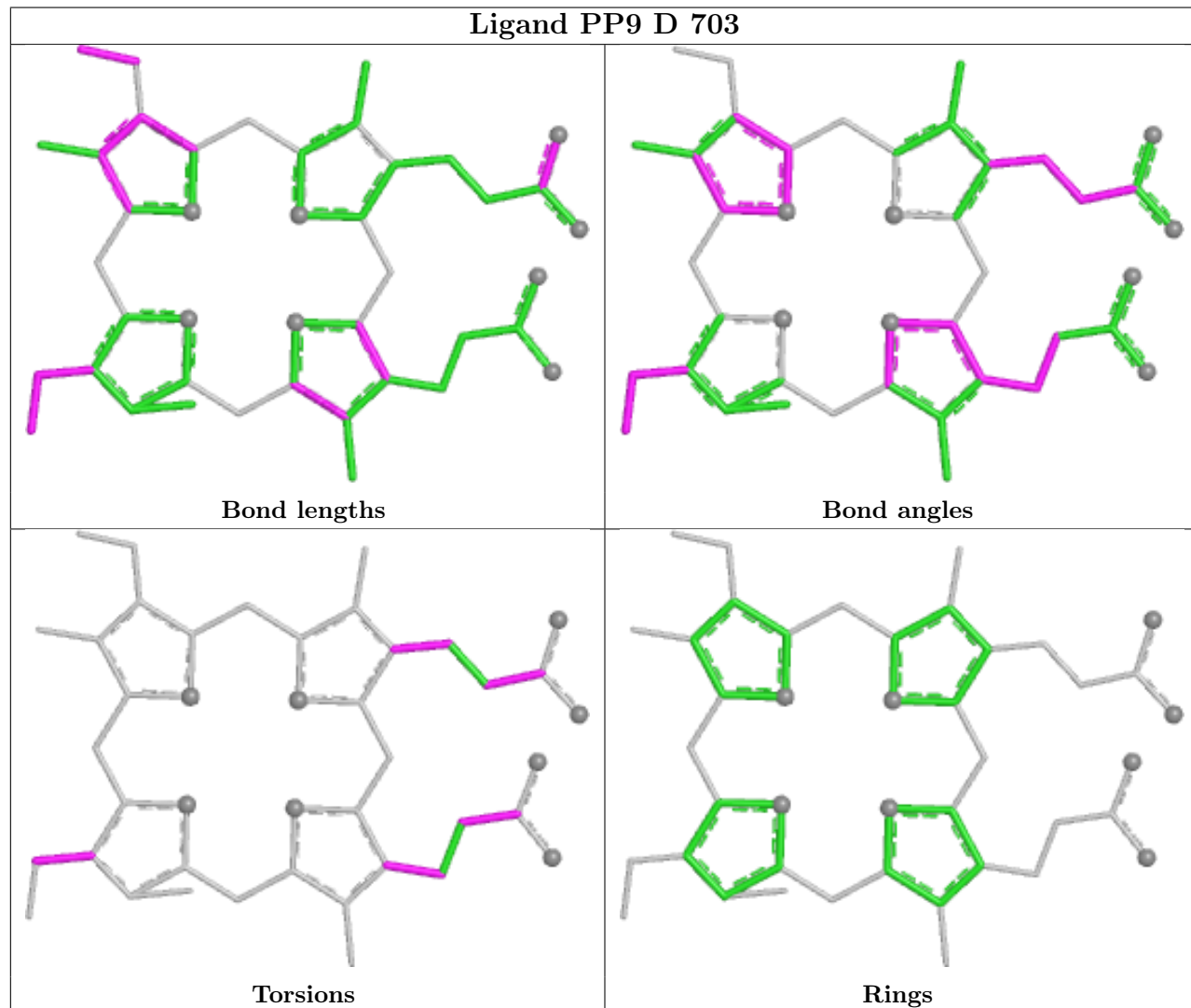
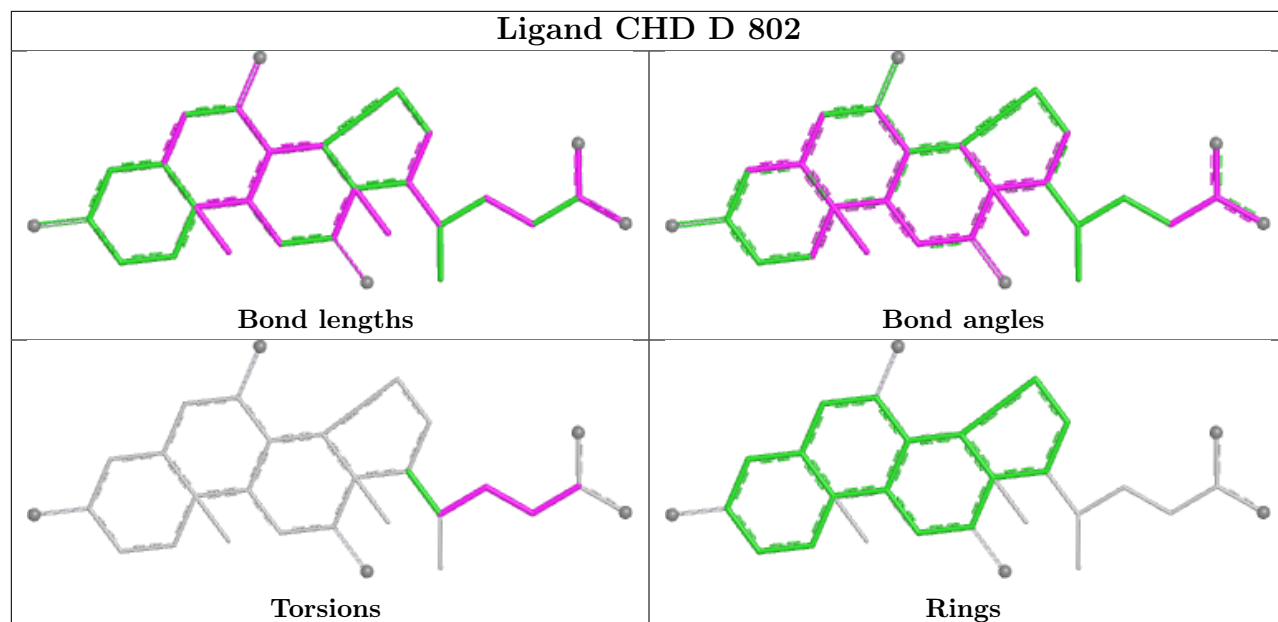
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	359/359 (100%)	0.59	26 (7%)	21 18	14, 25, 41, 67	0
1	B	359/359 (100%)	0.59	22 (6%)	27 24	9, 26, 43, 70	4 (1%)
1	C	359/359 (100%)	0.70	33 (9%)	14 12	11, 26, 45, 73	2 (0%)
1	D	359/359 (100%)	0.61	25 (6%)	22 19	10, 25, 44, 70	4 (1%)
All	All	1436/1436 (100%)	0.62	106 (7%)	20 18	9, 26, 44, 73	10 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	155	ALA	6.7
1	B	420	SER	6.3
1	C	423	LEU	6.1
1	A	155	ALA	5.7
1	C	253[A]	ARG	5.4
1	B	155	ALA	5.2
1	D	360	CYS	5.2
1	C	155	ALA	5.1
1	D	423	LEU	4.8
1	C	421	GLN	4.4
1	B	423	LEU	4.4
1	C	360	CYS	4.2
1	C	420	SER	3.9
1	A	422	GLN	3.7
1	D	65	ARG	3.7
1	D	154	THR	3.7
1	D	422	GLN	3.5
1	B	421	GLN	3.5
1	D	420	SER	3.4
1	C	358	LYS	3.4
1	B	359	GLU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	422	GLN	3.4
1	C	255	GLU	3.3
1	C	359	GLU	3.3
1	C	419	THR	3.3
1	D	213	VAL	3.3
1	A	423	LEU	3.2
1	C	308	MET	3.2
1	A	421	GLN	3.2
1	A	420	SER	3.2
1	D	419	THR	3.1
1	B	393	GLU	3.1
1	C	363	GLU	3.1
1	D	418	PHE	3.0
1	A	359	GLU	3.0
1	C	154	THR	3.0
1	B	422	GLN	2.9
1	D	183	GLU	2.9
1	C	65	ARG	2.9
1	C	251	GLU	2.9
1	C	357	ALA	2.8
1	A	66	LYS	2.8
1	D	421	GLN	2.8
1	A	251	GLU	2.8
1	C	418	PHE	2.8
1	C	254	SER	2.7
1	B	66	LYS	2.7
1	D	403	CYS	2.7
1	B	392	ASN	2.7
1	B	419	THR	2.7
1	D	359	GLU	2.7
1	A	212	GLN	2.7
1	A	149	GLU	2.6
1	B	100	THR	2.6
1	D	151	SER	2.6
1	A	403	CYS	2.6
1	C	407	VAL	2.6
1	A	375	PRO	2.5
1	A	154	THR	2.5
1	C	149	GLU	2.5
1	B	375	PRO	2.5
1	C	179	ARG	2.5
1	C	356	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	392	ASN	2.5
1	B	390	GLN	2.5
1	A	100	THR	2.4
1	D	150	LEU	2.4
1	D	407	VAL	2.4
1	B	415	LYS	2.4
1	D	308	MET	2.4
1	A	65	ARG	2.4
1	C	212	GLN	2.4
1	C	361	GLY	2.4
1	C	151	SER	2.3
1	A	360	CYS	2.3
1	A	171	GLU	2.3
1	B	179	ARG	2.3
1	C	364	ASN	2.3
1	A	407	VAL	2.3
1	D	362	VAL	2.3
1	A	176	GLU	2.2
1	B	251	GLU	2.2
1	D	255	GLU	2.2
1	A	419	THR	2.2
1	A	410	VAL	2.2
1	C	362	VAL	2.2
1	C	323	CYS	2.2
1	D	323	CYS	2.2
1	A	247	HIS	2.2
1	C	96	ARG	2.2
1	C	250	LEU	2.2
1	D	412	ARG	2.2
1	B	289	GLU	2.2
1	A	323	CYS	2.2
1	D	66	LYS	2.1
1	D	324	GLU	2.1
1	A	392	ASN	2.1
1	B	141	GLU	2.1
1	B	213	VAL	2.1
1	C	256	VAL	2.1
1	D	179	ARG	2.1
1	A	179	ARG	2.1
1	A	180	ASP	2.0
1	B	156	PRO	2.0
1	B	255	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	152	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

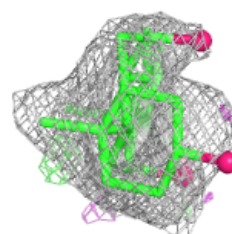
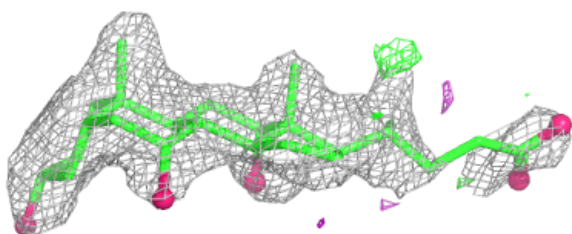
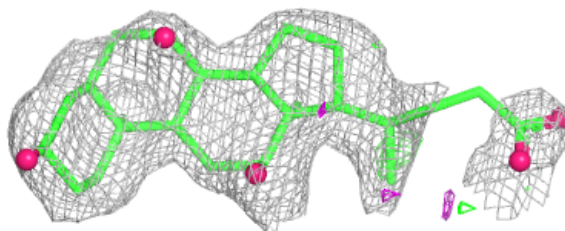
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	IMD	D	901	5/5	0.76	0.16	26,27,27,28	0
4	CHD	D	801	29/29	0.77	0.18	48,49,53,54	0
4	CHD	D	802	29/29	0.78	0.16	42,43,45,46	0
3	PP9	D	704	42/42	0.84	0.16	43,47,52,54	0
3	PP9	D	703	42/42	0.86	0.14	38,41,48,50	0
3	PP9	C	705	42/42	0.86	0.12	13,16,22,26	0
3	PP9	D	706	42/42	0.86	0.13	16,18,21,23	0
3	PP9	A	701	42/42	0.88	0.11	17,18,21,24	0
3	PP9	B	702	42/42	0.89	0.12	20,21,23,24	0
2	FES	D	1004	4/4	0.96	0.10	27,28,28,28	0
2	FES	C	1003	4/4	0.97	0.08	28,28,28,29	0
2	FES	B	1002	4/4	0.98	0.10	31,31,31,31	0
2	FES	A	1001	4/4	0.98	0.09	30,30,31,31	0

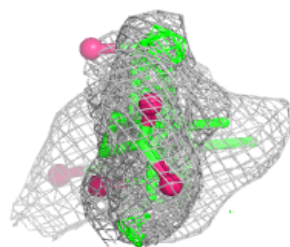
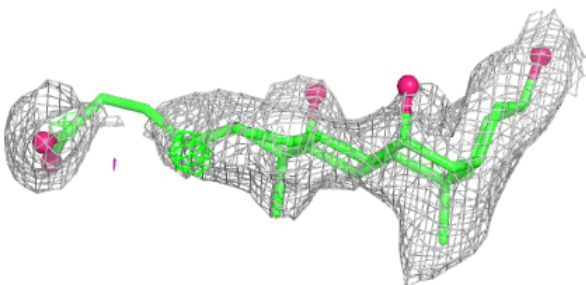
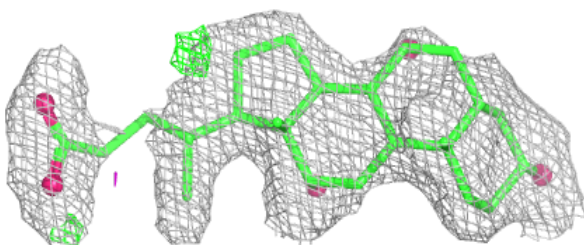
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CHD D 801:

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

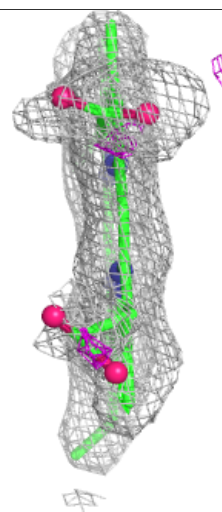
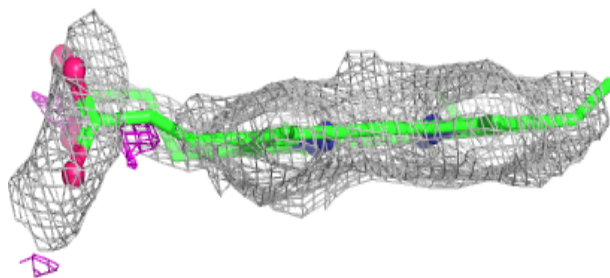
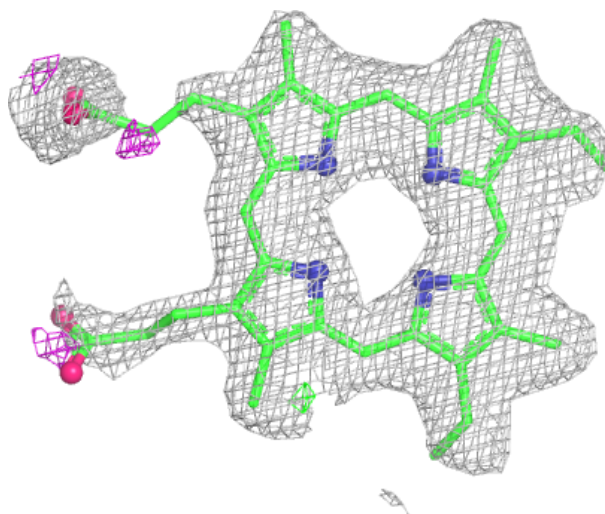
**Electron density around CHD D 802:**

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



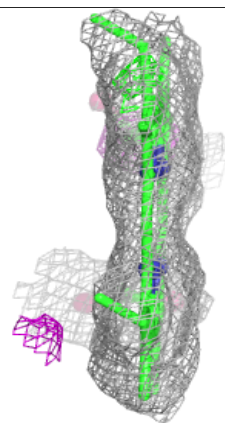
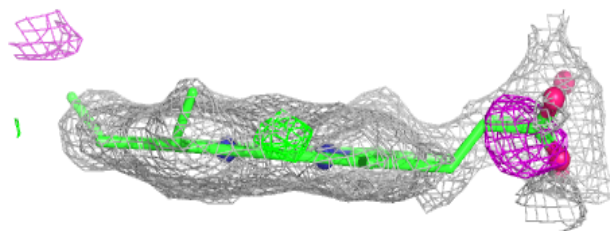
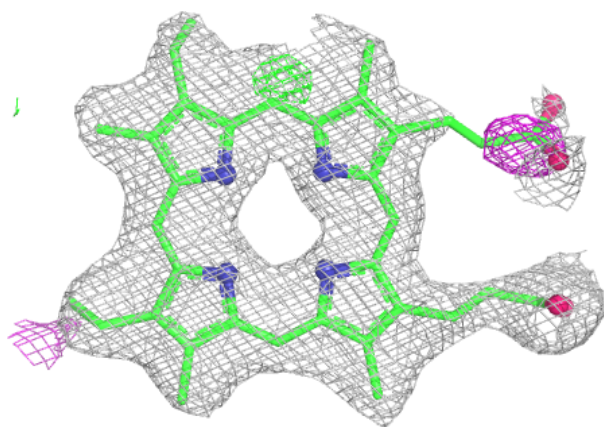
Electron density around PP9 D 704:

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



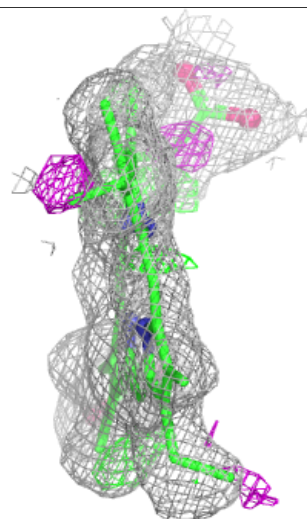
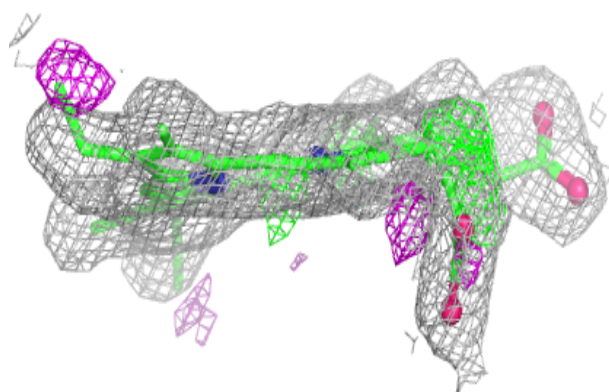
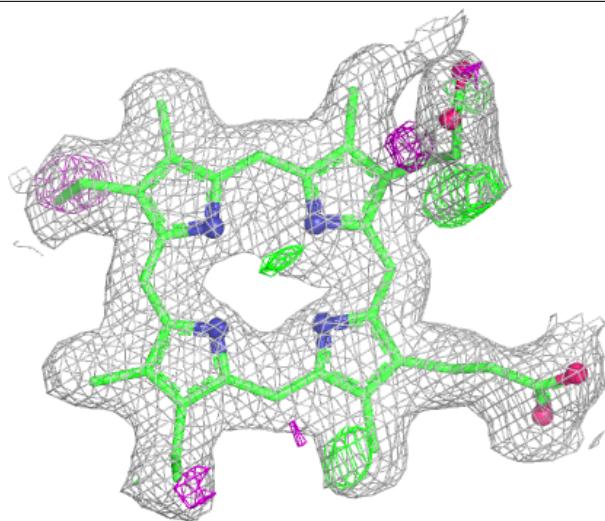
Electron density around PP9 D 703:

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



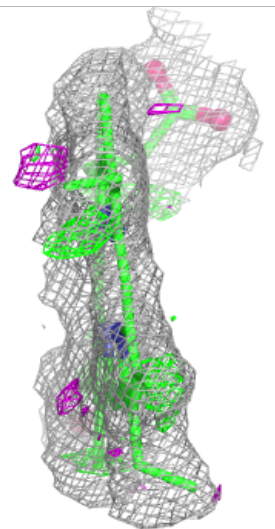
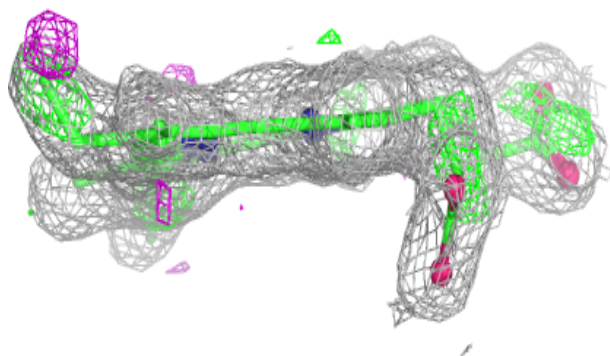
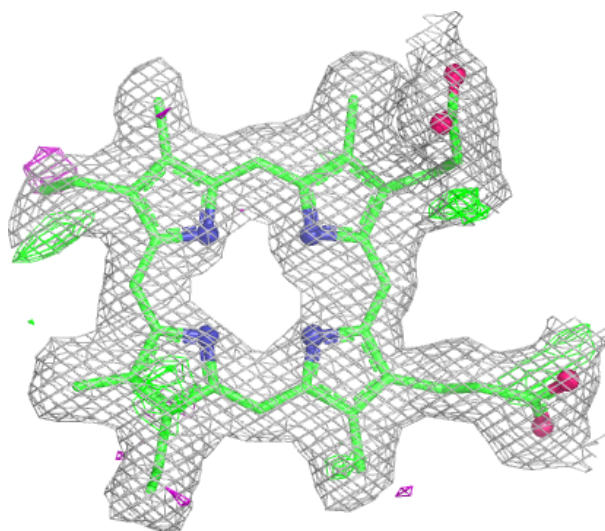
Electron density around PP9 C 705:

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



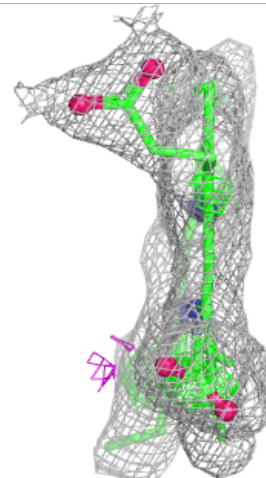
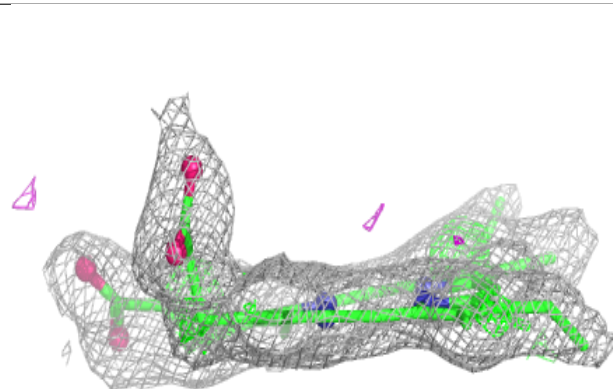
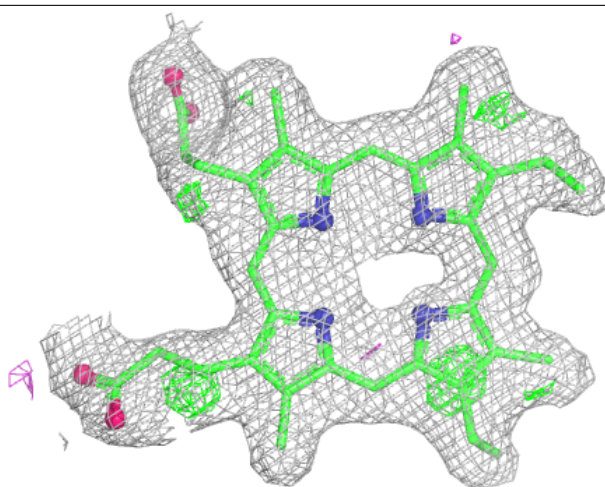
Electron density around PP9 D 706:

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



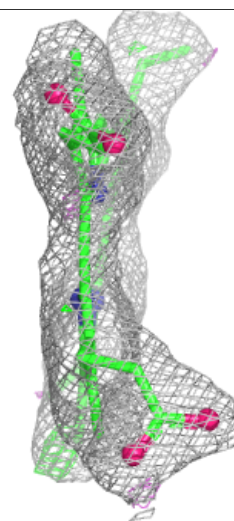
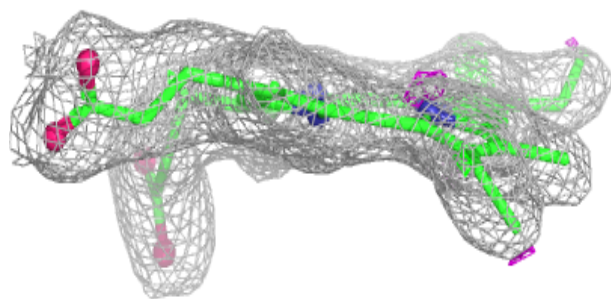
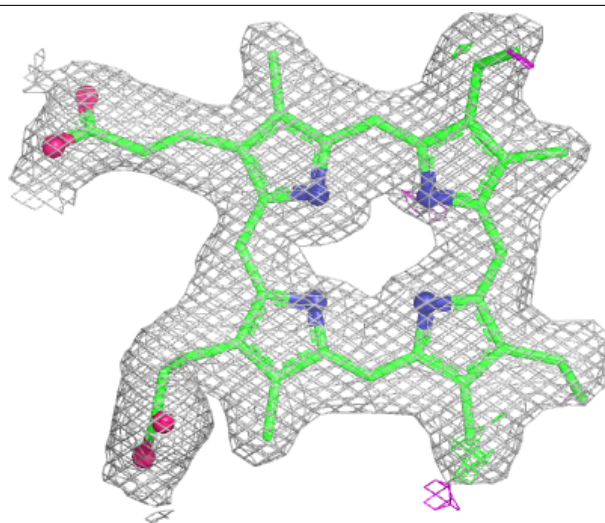
Electron density around PP9 A 701:

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



Electron density around PP9 B 702:

$2mF_o-DF_c$ (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.