



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:16 PM UTC

PDB ID : 5XZM / pdb_00005xzm
Title : CATPO mutant - V228I
Authors : Yuzugullu Karakus, Y.; Balci, S.; Goc, G.; Pearson, A.R.; Yorke, B.
Deposited on : 2017-07-12
Resolution : 1.41 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

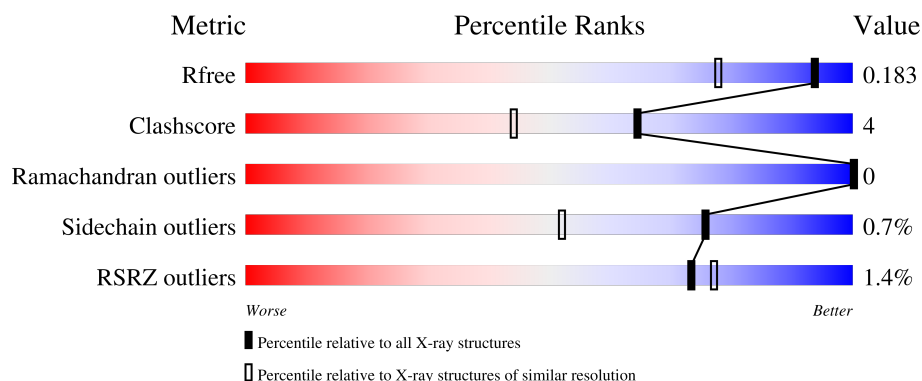
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.41 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	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (1.44-1.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	678	
1	B	678	
1	C	678	
1	D	678	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24285 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.

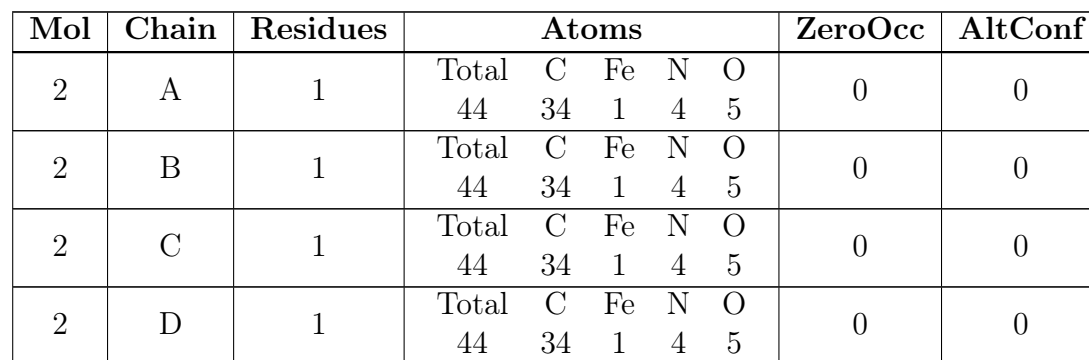
- Molecule 1 is a protein called Catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	31	0
			5524	3477	976	1059	12			
1	B	678	Total	C	N	O	S	0	28	0
			5515	3470	965	1069	11			
1	C	675	Total	C	N	O	S	0	22	0
			5451	3433	963	1043	12			
1	D	673	Total	C	N	O	S	0	20	0
			5415	3416	952	1035	12			

There are 4 discrepancies between the modelled and reference sequences:

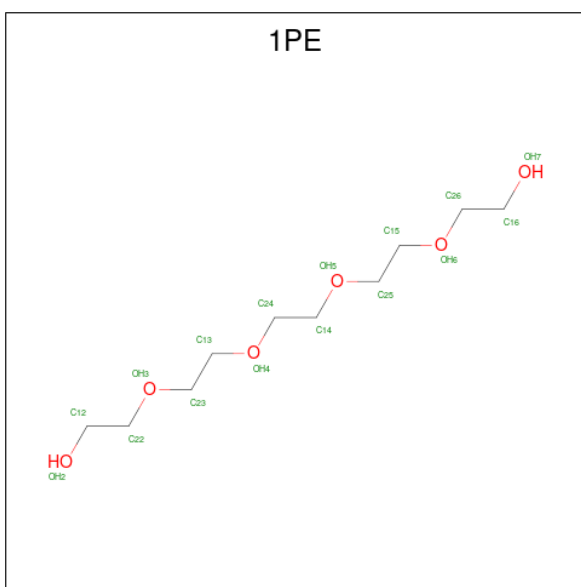
Chain	Residue	Modelled	Actual	Comment	Reference
A	228	ILE	VAL	engineered mutation	UNP M4GGR7
B	228	ILE	VAL	engineered mutation	UNP M4GGR7
C	228	ILE	VAL	engineered mutation	UNP M4GGR7
D	228	ILE	VAL	engineered mutation	UNP M4GGR7

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: C₃₄H₃₂FeN₄O₅).



- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3 | A | 5 | Total Ca
5 5 | 0 | 0 |
| 3 | B | 2 | Total Ca
2 2 | 0 | 0 |
| 3 | C | 2 | Total Ca
2 2 | 0 | 0 |
| 3 | D | 2 | Total Ca
2 2 | 0 | 0 |

- 



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	A	1	Total	C	O	0	0
			16	10	6		
4	A	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			16	10	6		
4	D	1	Total	C	O	0	0
			16	10	6		

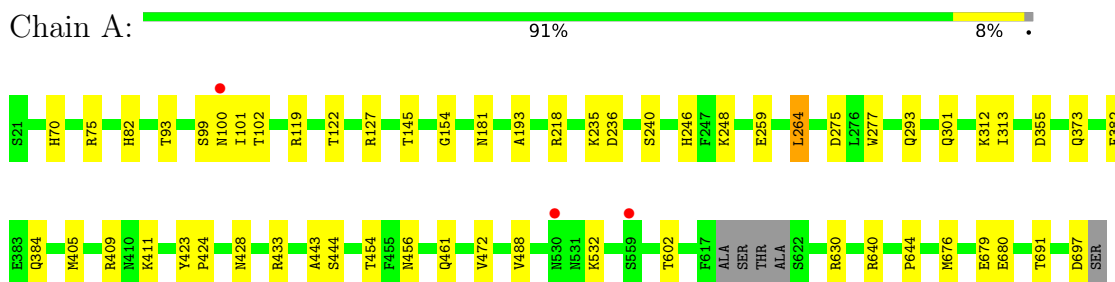
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	511	Total	O	0	0
			511	511		
5	B	555	Total	O	0	0
			555	555		
5	C	522	Total	O	0	0
			522	522		
5	D	525	Total	O	0	0
			525	525		

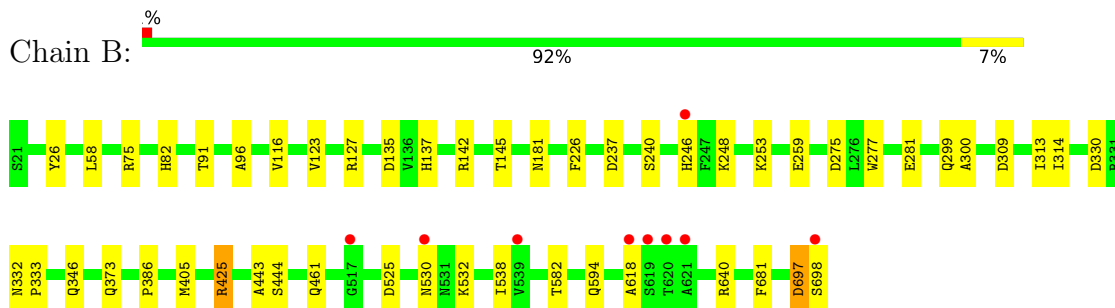
3 Residue-property plots

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.

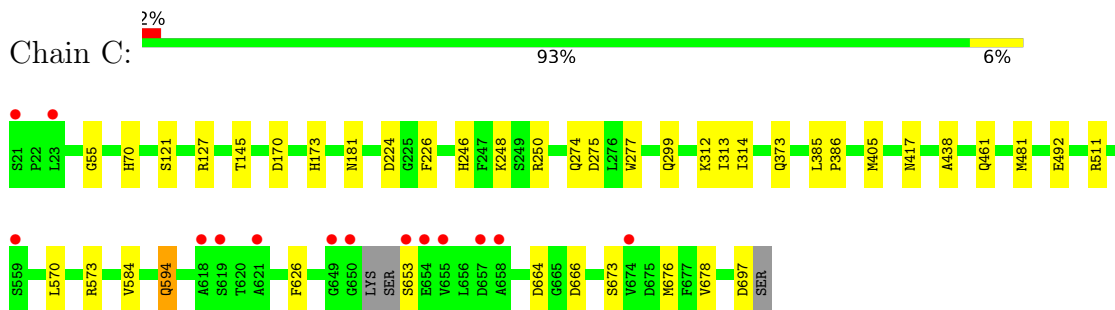
• Molecule 1: Catalase



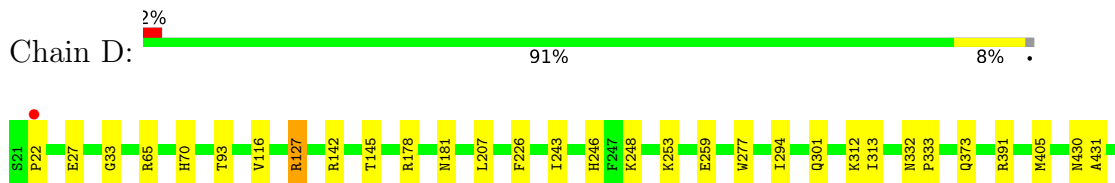
• Molecule 1: Catalase

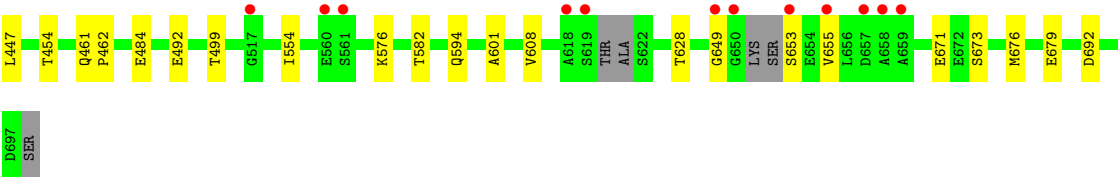


• Molecule 1: Catalase



• Molecule 1: Catalase





4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.47Å 120.25Å 183.66Å 90.00° 101.97° 90.00°	Depositor
Resolution (Å)	112.84 – 1.41 112.83 – 1.41	Depositor EDS
% Data completeness (in resolution range)	99.2 (112.84-1.41) 99.2 (112.83-1.41)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.41Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.158 , 0.182 0.158 , 0.183	Depositor DCC
R_{free} test set	25280 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	11.2	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	24285	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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 65.88 % 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 6.6011e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 1PE, HDD

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	1.38	16/5661 (0.3%)	1.20	6/7686 (0.1%)
1	B	1.33	12/5656 (0.2%)	1.17	10/7686 (0.1%)
1	C	1.34	8/5588 (0.1%)	1.19	7/7594 (0.1%)
1	D	1.35	14/5554 (0.3%)	1.17	5/7547 (0.1%)
All	All	1.35	50/22459 (0.2%)	1.18	28/30513 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	2
All	All	0	4

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	649	GLY	N-CA	9.57	1.53	1.45
1	A	102	THR	N-CA	7.25	1.54	1.46
1	B	538	ILE	C-O	-7.14	1.16	1.23
1	B	58	LEU	N-CA	-7.03	1.36	1.46
1	D	430	ASN	C-O	7.02	1.33	1.24
1	B	137	HIS	CA-C	-6.88	1.44	1.52
1	D	178	ARG	CA-C	6.82	1.60	1.53
1	B	532	LYS	CA-C	-6.62	1.44	1.52
1	D	430	ASN	N-CA	6.30	1.53	1.46
1	A	100	ASN	N-CA	6.10	1.54	1.46
1	A	101	ILE	N-CA	-6.09	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	LEU	N-CA	-5.98	1.39	1.46
1	D	431	ALA	CA-C	-5.91	1.45	1.52
1	D	462	PRO	N-CA	-5.86	1.39	1.47
1	D	447	LEU	N-CA	5.82	1.53	1.46
1	A	355	ASP	CA-C	-5.78	1.45	1.52
1	A	293	GLN	CA-CB	-5.75	1.45	1.53
1	A	488	VAL	C-O	5.74	1.29	1.24
1	D	207	LEU	C-O	-5.74	1.17	1.24
1	C	417	ASN	C-O	5.71	1.31	1.23
1	D	93	THR	N-CA	5.63	1.52	1.46
1	C	170	ASP	C-O	-5.60	1.17	1.24
1	D	601	ALA	N-CA	-5.54	1.39	1.46
1	A	154	GLY	CA-C	-5.53	1.46	1.52
1	B	240	SER	CA-C	-5.46	1.46	1.52
1	A	235	LYS	CA-C	-5.45	1.45	1.53
1	B	96	ALA	CA-C	-5.44	1.46	1.52
1	B	330	ASP	CA-C	-5.42	1.46	1.52
1	D	679	GLU	CA-C	5.41	1.59	1.52
1	C	250	ARG	CD-NE	-5.39	1.38	1.46
1	B	681	PHE	N-CA	5.35	1.52	1.46
1	A	428	ASN	C-O	-5.31	1.19	1.24
1	C	511	ARG	CZ-NH2	-5.26	1.26	1.33
1	B	309	ASP	C-N	5.24	1.38	1.33
1	D	671	GLU	N-CA	5.24	1.52	1.46
1	D	576	LYS	C-O	5.24	1.30	1.24
1	A	630	ARG	N-CA	5.23	1.51	1.46
1	B	618	ALA	N-CA	5.22	1.52	1.45
1	A	99	SER	N-CA	5.18	1.52	1.46
1	B	135	ASP	CA-C	-5.18	1.46	1.52
1	A	119	ARG	CA-C	-5.16	1.46	1.52
1	D	655	VAL	C-O	5.13	1.30	1.24
1	A	93	THR	C-O	-5.13	1.18	1.24
1	C	173	HIS	N-CA	5.12	1.52	1.46
1	C	481	MET	N-CA	-5.10	1.40	1.46
1	C	121	SER	N-CA	5.08	1.52	1.46
1	B	237	ASP	N-CA	5.07	1.52	1.46
1	A	680	GLU	CA-C	5.04	1.59	1.52
1	C	385	LEU	CA-C	-5.03	1.48	1.53
1	A	644	PRO	C-O	5.00	1.29	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	425	ARG	NE-CZ-NH1	8.18	129.68	121.50
1	C	697	ASP	CA-C-O	-8.06	107.09	120.80
1	B	425	ARG	CD-NE-CZ	8.05	135.67	124.40
1	A	697	ASP	CA-C-O	-7.79	107.56	120.80
1	D	492	GLU	CB-CG-CD	7.34	125.07	112.60
1	D	649	GLY	N-CA-C	6.95	119.10	112.08
1	B	697	ASP	CA-C-N	-6.89	109.30	121.70
1	B	697	ASP	C-N-CA	-6.89	109.30	121.70
1	C	314	ILE	CA-C-O	6.62	122.83	119.12
1	A	456	ASN	N-CA-C	5.79	120.19	113.18
1	B	697	ASP	N-CA-C	-5.77	102.36	110.50
1	B	425	ARG	NE-CZ-NH2	-5.55	114.21	119.20
1	A	382	PHE	N-CA-C	5.48	119.22	112.54
1	B	346	GLN	CA-C-N	-5.37	114.29	119.87
1	B	346	GLN	C-N-CA	-5.37	114.29	119.87
1	C	570	LEU	N-CA-C	-5.35	105.36	111.14
1	D	430	ASN	N-CA-CB	-5.35	102.37	111.20
1	A	240	SER	N-CA-C	5.26	117.39	109.23
1	D	484	GLU	N-CA-C	5.16	116.59	111.07
1	C	626	PHE	N-CA-C	5.15	112.86	108.22
1	A	193	ALA	O-C-N	5.15	127.37	122.07
1	B	525	ASP	N-CA-C	5.14	119.26	113.15
1	C	438	ALA	CA-C-N	-5.13	114.50	120.04
1	C	438	ALA	C-N-CA	-5.13	114.50	120.04
1	D	33	GLY	N-CA-C	5.12	118.02	112.29
1	B	314	ILE	CB-CA-C	-5.11	105.03	110.95
1	C	55	GLY	O-C-N	5.04	126.81	121.77
1	A	218	ARG	NE-CZ-NH2	5.04	123.74	119.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	75	ARG	Sidechain
1	B	75	ARG	Sidechain
1	D	127[A]	ARG	Sidechain
1	D	65	ARG	Sidechain

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	5524	0	5267	50	0
1	B	5515	0	5242	46	1
1	C	5451	0	5201	32	1
1	D	5415	0	5175	53	0
2	A	44	0	31	0	0
2	B	44	0	31	0	0
2	C	44	0	31	0	0
2	D	44	0	31	0	0
3	A	5	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	48	0	66	2	0
4	B	16	0	22	0	0
4	D	16	0	22	2	0
5	A	511	0	0	9	0
5	B	555	0	0	10	0
5	C	522	0	0	9	0
5	D	525	0	0	15	0
All	All	24285	0	21119	168	1

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 4.

All (168) 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:127[B]:ARG:O	5:B:801:HOH:O	1.54	1.25
1:A:259[A]:GLU:HG3	5:A:951:HOH:O	1.39	1.22
1:A:246[B]:HIS:CD2	1:A:248[B]:LYS:CD	2.29	1.15
1:A:246[B]:HIS:CD2	1:A:248[B]:LYS:HD2	1.84	1.11
1:D:405[B]:MET:CE	5:D:891:HOH:O	1.98	1.09
1:D:259[A]:GLU:HG3	5:D:808:HOH:O	1.55	1.04
1:A:246[B]:HIS:CE1	1:A:248[B]:LYS:NZ	2.26	1.03
1:A:246[B]:HIS:CD2	1:A:248[B]:LYS:HD3	1.93	1.02
1:B:259[A]:GLU:HG3	5:D:939:HOH:O	1.58	1.00
1:A:246[B]:HIS:NE2	1:A:248[B]:LYS:NZ	2.09	1.00
1:A:246[B]:HIS:NE2	1:A:248[B]:LYS:CD	2.25	1.00
1:D:246[B]:HIS:CD2	1:D:248:LYS:HD3	2.04	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ILE:H	1:C:461:GLN:HE22	1.17	0.93
1:B:277[B]:TRP:CH2	1:B:281[B]:GLU:OE1	2.24	0.90
1:A:259[A]:GLU:OE1	1:A:640[A]:ARG:NE	2.05	0.90
1:D:313:ILE:H	1:D:461:GLN:HE22	1.20	0.89
1:A:313:ILE:H	1:A:461:GLN:HE22	1.20	0.88
1:D:246[B]:HIS:CD2	1:D:248:LYS:CD	2.57	0.87
1:B:313:ILE:H	1:B:461:GLN:HE22	1.19	0.86
1:A:246[B]:HIS:CE1	1:A:248[B]:LYS:HZ3	1.96	0.84
1:A:246[B]:HIS:CG	1:A:248[B]:LYS:HD3	2.12	0.84
1:A:246[B]:HIS:CE1	1:A:248[B]:LYS:HZ2	1.93	0.83
1:B:127[A]:ARG:NH1	5:B:802:HOH:O	2.10	0.83
1:D:246[B]:HIS:NE2	1:D:248:LYS:NZ	2.25	0.82
1:D:253:LYS:HG2	5:D:1159:HOH:O	1.80	0.81
1:A:127[A]:ARG:NH2	5:A:803:HOH:O	2.13	0.81
1:B:127[A]:ARG:NH2	5:B:802:HOH:O	2.11	0.81
1:C:246[B]:HIS:CE1	1:C:248:LYS:HZ3	1.99	0.81
1:A:127[B]:ARG:NH2	5:A:804:HOH:O	2.13	0.80
1:C:664:ASP:CG	5:C:805:HOH:O	2.25	0.80
1:D:127[A]:ARG:NH1	5:D:804:HOH:O	2.14	0.79
1:B:253:LYS:HG2	5:B:1193:HOH:O	1.83	0.78
1:D:127[B]:ARG:NH2	5:D:805:HOH:O	2.15	0.78
1:B:226:PHE:HE1	1:B:246[A]:HIS:CE1	2.04	0.76
1:C:127[B]:ARG:NH2	5:C:804:HOH:O	2.17	0.76
1:C:246[B]:HIS:CE1	1:C:248:LYS:NZ	2.54	0.75
1:D:405[B]:MET:HE2	5:D:891:HOH:O	1.74	0.75
1:C:127[A]:ARG:NH1	5:C:803:HOH:O	2.09	0.75
1:B:226:PHE:CE1	1:B:246[A]:HIS:CE1	2.74	0.75
1:A:246[B]:HIS:NE2	1:A:248[B]:LYS:HD2	1.96	0.73
1:B:127[A]:ARG:CZ	5:B:802:HOH:O	2.37	0.73
1:D:127[B]:ARG:NH1	5:D:805:HOH:O	2.19	0.72
1:B:246[A]:HIS:CE1	1:B:248:LYS:NZ	2.59	0.71
1:A:246[B]:HIS:CE1	1:A:248[B]:LYS:HD3	2.26	0.70
1:C:299[A]:GLN:OE1	5:C:802:HOH:O	2.09	0.70
1:D:673:SER:HB3	1:D:676:MET:HE3	1.74	0.69
1:D:246[B]:HIS:CD2	1:D:248:LYS:HD2	2.27	0.69
1:B:640[B]:ARG:HG2	5:B:827:HOH:O	1.93	0.69
1:C:127[A]:ARG:NH2	5:C:803:HOH:O	2.23	0.69
1:D:673:SER:CB	1:D:676:MET:HE3	2.23	0.69
1:A:640[A]:ARG:HG2	5:A:930:HOH:O	1.93	0.68
1:D:692:ASP:OD1	5:D:803:HOH:O	2.12	0.67
1:D:226:PHE:CE1	1:D:246[B]:HIS:CD2	2.83	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127[A]:ARG:NH1	5:A:803:HOH:O	2.23	0.66
1:D:127[B]:ARG:CZ	5:D:805:HOH:O	2.44	0.66
1:A:246[B]:HIS:NE2	1:A:248[B]:LYS:CE	2.60	0.65
1:C:226:PHE:CE1	1:C:246[B]:HIS:CE1	2.84	0.64
1:C:492[A]:GLU:HG3	5:C:1193:HOH:O	1.97	0.64
1:C:127[A]:ARG:CZ	5:C:803:HOH:O	2.44	0.64
1:B:246[A]:HIS:CE1	1:B:248:LYS:CD	2.81	0.64
1:B:246[A]:HIS:CE1	1:B:248:LYS:HD3	2.32	0.63
1:D:246[B]:HIS:CE1	1:D:248:LYS:HZ3	2.15	0.63
1:A:246[B]:HIS:NE2	1:A:248[B]:LYS:HD3	2.04	0.63
1:A:246[B]:HIS:CE1	1:A:248[B]:LYS:CD	2.82	0.62
1:A:301[B]:GLN:O	1:A:301[B]:GLN:HG3	1.97	0.62
1:B:127[B]:ARG:NH1	5:B:803:HOH:O	2.32	0.61
1:B:246[A]:HIS:ND1	1:B:248:LYS:HD3	2.15	0.60
1:D:405[B]:MET:HE3	5:D:891:HOH:O	1.80	0.60
1:C:246[B]:HIS:CE1	1:C:248:LYS:CD	2.85	0.60
1:C:246[B]:HIS:CE1	1:C:248:LYS:HD3	2.37	0.60
1:D:313:ILE:N	1:D:461:GLN:HE22	1.97	0.59
1:B:246[A]:HIS:CE1	1:B:248:LYS:HZ3	2.19	0.58
1:C:573[A]:ARG:HG3	1:C:678:VAL:HG11	1.86	0.57
1:D:246[B]:HIS:CG	1:D:248:LYS:HD3	2.38	0.57
1:D:582:THR:HG21	1:D:594[A]:GLN:HE21	1.69	0.57
1:B:405:MET:HE2	1:C:405[B]:MET:HE2	1.87	0.57
1:C:226:PHE:HE1	1:C:246[B]:HIS:CE1	2.23	0.57
1:C:246[B]:HIS:HE1	1:C:248:LYS:NZ	1.99	0.57
1:B:640[B]:ARG:CG	5:B:827:HOH:O	2.53	0.57
1:D:246[B]:HIS:NE2	1:D:248:LYS:CD	2.67	0.56
1:A:373:GLN:HE21	1:A:373:GLN:HA	1.70	0.56
1:B:253:LYS:CG	5:B:1193:HOH:O	2.49	0.55
1:B:246[A]:HIS:HE1	1:B:248:LYS:NZ	2.04	0.55
1:B:246[A]:HIS:ND1	1:B:248:LYS:CD	2.70	0.55
1:A:676[B]:MET:HE2	1:A:679[B]:GLU:HB3	1.88	0.55
1:B:373:GLN:HE21	1:B:373:GLN:HA	1.72	0.54
1:C:274[B]:GLN:NE2	5:C:807:HOH:O	2.41	0.54
1:B:181:ASN:HB3	1:D:277[A]:TRP:CZ3	2.43	0.54
1:A:411[B]:LYS:HE2	5:D:1105:HOH:O	2.08	0.53
4:A:707:1PE:H231	5:A:1200:HOH:O	2.08	0.53
1:B:277[A]:TRP:CE3	1:D:181:ASN:HB3	2.43	0.53
1:C:246[B]:HIS:ND1	1:C:248:LYS:HD3	2.24	0.53
1:A:246[B]:HIS:HE1	1:A:248[B]:LYS:HZ3	1.52	0.53
1:D:22:PRO:HD2	1:D:391[B]:ARG:NE	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246[B]:HIS:NE2	1:D:248:LYS:HD3	2.24	0.52
1:A:532:LYS:NZ	5:A:806:HOH:O	2.26	0.52
1:B:226:PHE:CE1	1:B:246[A]:HIS:ND1	2.78	0.51
1:A:246[B]:HIS:CE1	1:A:248[B]:LYS:CE	2.92	0.51
1:D:22:PRO:CD	1:D:391[B]:ARG:NE	2.74	0.51
1:C:313:ILE:N	1:C:461:GLN:HE22	1.96	0.51
1:A:181:ASN:HB3	1:C:277[A]:TRP:CZ3	2.45	0.50
1:A:127[A]:ARG:CZ	5:A:803:HOH:O	2.47	0.50
1:C:224:ASP:OD2	1:C:248:LYS:NZ	2.41	0.50
1:B:697:ASP:O	1:B:698:SER:C	2.49	0.50
1:B:313:ILE:N	1:B:461:GLN:HE22	1.99	0.49
1:D:22:PRO:HD3	1:D:391[B]:ARG:CD	2.43	0.49
1:B:277[A]:TRP:CZ3	1:D:181:ASN:HB3	2.48	0.49
1:B:181:ASN:HB3	1:D:277[A]:TRP:CE3	2.48	0.49
1:B:246[A]:HIS:HE1	1:B:248:LYS:HZ2	1.61	0.49
1:D:301:GLN:NE2	1:D:454:THR:HG21	2.28	0.49
1:A:236:ASP:CG	1:A:433[B]:ARG:HH22	2.21	0.48
1:A:640[A]:ARG:CG	5:A:930:HOH:O	2.56	0.48
1:B:277[B]:TRP:CZ3	1:B:281[B]:GLU:OE1	2.66	0.48
1:D:554:ILE:HG12	1:D:608[B]:VAL:CG2	2.44	0.48
1:C:226:PHE:CE1	1:C:246[B]:HIS:ND1	2.83	0.47
1:C:246[B]:HIS:ND1	1:C:248:LYS:CD	2.78	0.47
1:D:373:GLN:HE21	1:D:373:GLN:HA	1.79	0.47
1:A:384:GLN:O	1:D:405[B]:MET:HE1	2.15	0.46
1:A:443:ALA:O	1:B:444[B]:SER:HA	2.15	0.46
1:B:640[B]:ARG:CB	1:B:640[B]:ARG:NH1	2.78	0.46
1:C:373:GLN:HE21	1:C:373:GLN:HA	1.79	0.46
1:C:584:VAL:HA	1:C:594[A]:GLN:O	2.15	0.46
1:D:277[A]:TRP:CZ3	1:D:332:ASN:HB3	2.51	0.46
1:A:181:ASN:HB3	1:C:277[A]:TRP:CE3	2.50	0.46
1:B:640[B]:ARG:HD3	1:D:628:THR:O	2.15	0.46
4:A:707:1PE:H232	5:D:1080:HOH:O	2.16	0.46
1:D:226:PHE:HE1	1:D:246[B]:HIS:CD2	2.29	0.45
1:B:582:THR:HG21	1:B:594:GLN:HE21	1.81	0.45
1:B:640[B]:ARG:NH1	1:B:640[B]:ARG:HB3	2.31	0.45
1:A:409[B]:ARG:NE	1:D:27:GLU:OE1	2.50	0.45
1:B:277[A]:TRP:CZ3	1:B:332:ASN:HB3	2.52	0.45
1:A:444[B]:SER:HA	1:B:443:ALA:O	2.17	0.45
1:A:277[A]:TRP:CE3	1:C:181:ASN:HB3	2.52	0.45
1:A:264:LEU:HD13	1:A:602:THR:HB	1.99	0.45
1:C:492[A]:GLU:CG	5:C:1193:HOH:O	2.59	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277[A]:TRP:CH2	1:D:332:ASN:HB3	2.52	0.44
1:A:246[B]:HIS:ND1	1:A:248[B]:LYS:HD3	2.30	0.44
1:D:499:THR:OG1	4:D:704:1PE:C12	2.66	0.44
1:D:248:LYS:NZ	5:D:806:HOH:O	2.34	0.44
1:D:499:THR:OG1	4:D:704:1PE:H121	2.17	0.44
1:A:82:HIS:HA	1:A:122:THR:O	2.18	0.43
1:B:91[B]:THR:HG22	5:B:807:HOH:O	2.18	0.43
1:B:116:VAL:HA	1:B:142:ARG:O	2.19	0.43
1:D:277[A]:TRP:CZ3	1:D:333:PRO:HD2	2.53	0.43
1:D:246[B]:HIS:NE2	1:D:248:LYS:CE	2.82	0.43
1:D:243:ILE:HG22	1:D:294[A]:ILE:HG23	2.01	0.42
1:A:373:GLN:HA	1:A:373:GLN:NE2	2.34	0.42
1:A:277[A]:TRP:CZ3	1:C:181:ASN:HB3	2.54	0.42
1:B:277[A]:TRP:CZ3	1:B:333:PRO:HD2	2.54	0.42
1:A:313:ILE:N	1:A:461:GLN:HE22	2.02	0.42
1:A:312:LYS:HA	1:A:461:GLN:NE2	2.35	0.42
1:A:301[B]:GLN:O	1:A:301[B]:GLN:CG	2.60	0.42
1:C:312:LYS:HA	1:C:461:GLN:NE2	2.34	0.42
1:C:673:SER:HB3	1:C:676:MET:HE3	2.02	0.42
1:D:253:LYS:CG	5:D:1159:HOH:O	2.51	0.42
1:D:391[A]:ARG:HH11	1:D:391[A]:ARG:HD2	1.73	0.41
1:D:582:THR:HG21	1:D:594[A]:GLN:NE2	2.34	0.41
1:A:405:MET:HG3	1:D:405[B]:MET:HE2	2.02	0.41
1:B:373:GLN:HA	1:B:373:GLN:NE2	2.35	0.41
1:D:116:VAL:HA	1:D:142:ARG:O	2.21	0.41
1:A:472:VAL:HG11	1:A:691:THR:HB	2.01	0.41
1:B:82:HIS:CE1	1:B:123:VAL:HG22	2.56	0.41
1:D:312:LYS:HA	1:D:461:GLN:NE2	2.35	0.41
1:B:299[A]:GLN:O	1:B:300:ALA:C	2.62	0.40
1:A:423:TYR:HA	1:A:424:PRO:C	2.45	0.40
1:A:301[A]:GLN:NE2	1:A:454:THR:HG21	2.36	0.40
1:B:26:TYR:CD1	1:B:386:PRO:HG3	2.56	0.40
1:D:22:PRO:CD	1:D:391[B]:ARG:CD	3.00	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:ASN:OD1	1:C:666:ASP:OD1[3_545]	1.98	0.22

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	700/678 (103%)	686 (98%)	14 (2%)	0	100	100
1	B	704/678 (104%)	687 (98%)	17 (2%)	0	100	100
1	C	693/678 (102%)	676 (98%)	17 (2%)	0	100	100
1	D	687/678 (101%)	671 (98%)	16 (2%)	0	100	100
All	All	2784/2712 (103%)	2720 (98%)	64 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	589/562 (105%)	586 (100%)	3 (0%)	81	62
1	B	589/562 (105%)	586 (100%)	3 (0%)	81	62
1	C	580/562 (103%)	573 (99%)	7 (1%)	63	32
1	D	577/562 (103%)	574 (100%)	3 (0%)	81	62
All	All	2335/2248 (104%)	2319 (99%)	16 (1%)	76	52

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	145	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	275	ASP
1	B	145	THR
1	B	275	ASP
1	B	425	ARG
1	C	70	HIS
1	C	145	THR
1	C	275	ASP
1	C	386	PRO
1	C	594[A]	GLN
1	C	594[B]	GLN
1	C	653	SER
1	D	70	HIS
1	D	145	THR
1	D	653	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	113	GLN
1	A	346	GLN
1	A	373	GLN
1	A	375	ASN
1	A	461	GLN
1	A	530	ASN
1	B	301	GLN
1	B	346	GLN
1	B	373	GLN
1	B	375	ASN
1	B	461	GLN
1	B	594	GLN
1	C	113	GLN
1	C	346	GLN
1	C	373	GLN
1	C	375	ASN
1	C	429	GLN
1	C	461	GLN
1	C	530	ASN
1	D	262	GLN
1	D	301	GLN
1	D	373	GLN
1	D	375	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	398	ASN
1	D	461	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 11 are monoatomic - leaving 9 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
4	1PE	B	704	-	15,15,15	0.76	0	14,14,14	0.79	0
4	1PE	A	709	-	15,15,15	0.83	0	14,14,14	0.83	0
4	1PE	D	704	-	15,15,15	0.94	0	14,14,14	1.15	1 (7%)
2	HDD	B	701	1,5	46,52,52	1.63	11 (23%)	62,89,89	1.57	16 (25%)
4	1PE	A	708	-	15,15,15	0.60	0	14,14,14	0.54	0
2	HDD	D	701	1,5	46,52,52	1.74	13 (28%)	62,89,89	1.86	14 (22%)
2	HDD	C	701	1,5	46,52,52	1.80	14 (30%)	62,89,89	1.67	13 (20%)
2	HDD	A	701	1	46,52,52	1.52	10 (21%)	62,89,89	1.58	14 (22%)
4	1PE	A	707	-	15,15,15	0.74	0	14,14,14	1.53	2 (14%)

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
4	1PE	B	704	-	-	6/13/13/13	-
4	1PE	A	709	-	-	7/13/13/13	-
4	1PE	D	704	-	-	4/13/13/13	-
2	HDD	B	701	1,5	-	2/9/89/89	0/1/9/9
4	1PE	A	708	-	-	4/13/13/13	-
2	HDD	D	701	1,5	-	2/9/89/89	0/1/9/9
2	HDD	C	701	1,5	-	2/9/89/89	0/1/9/9
2	HDD	A	701	1	-	2/9/89/89	0/1/9/9
4	1PE	A	707	-	-	5/13/13/13	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	HDD	O1D-C3D	4.28	1.53	1.46
2	C	701	HDD	CHA-C1A	4.13	1.48	1.39
2	D	701	HDD	CHD-C4C	3.88	1.48	1.39
2	B	701	HDD	CHB-C4A	3.81	1.48	1.39
2	B	701	HDD	C1B-NB	-3.59	1.32	1.39
2	A	701	HDD	CBD-CGD	-3.45	1.43	1.50
2	C	701	HDD	CHB-C1B	3.44	1.45	1.38
2	D	701	HDD	C4A-NA	-3.39	1.33	1.39
2	A	701	HDD	C1A-NA	-3.37	1.33	1.39
2	A	701	HDD	CHB-C4A	3.35	1.46	1.39
2	B	701	HDD	C1A-NA	-3.24	1.33	1.39
2	D	701	HDD	C1A-NA	-3.22	1.33	1.39
2	D	701	HDD	CHA-C1A	3.19	1.46	1.39
2	C	701	HDD	C4C-NC	-3.16	1.33	1.39
2	D	701	HDD	O1D-C3D	3.15	1.51	1.46
2	B	701	HDD	C4C-NC	-3.14	1.33	1.39
2	D	701	HDD	CBD-CGD	-3.13	1.44	1.50
2	C	701	HDD	CHD-C4C	3.05	1.46	1.39
2	C	701	HDD	OND-C2D	2.99	1.48	1.42
2	B	701	HDD	CHD-C4C	2.94	1.46	1.39
2	D	701	HDD	CHB-C4A	2.87	1.45	1.39
2	C	701	HDD	C1B-NB	-2.81	1.34	1.39
2	C	701	HDD	C1C-NC	-2.77	1.34	1.39
2	A	701	HDD	CHD-C4C	2.74	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	HDD	CHB-C1B	2.71	1.43	1.38
2	A	701	HDD	C4A-NA	-2.71	1.34	1.39
2	B	701	HDD	C1C-NC	-2.71	1.34	1.39
2	C	701	HDD	CBD-CGD	-2.70	1.44	1.50
2	D	701	HDD	CHC-C4B	2.66	1.43	1.38
2	B	701	HDD	O1D-C3D	2.65	1.51	1.46
2	D	701	HDD	CAD-CBD	-2.65	1.46	1.52
2	C	701	HDD	C3B-C2B	2.55	1.42	1.37
2	D	701	HDD	C1C-NC	-2.47	1.35	1.39
2	B	701	HDD	C4B-NB	-2.26	1.35	1.39
2	A	701	HDD	CHA-C1A	2.24	1.44	1.39
2	A	701	HDD	CHB-C1B	2.18	1.42	1.38
2	C	701	HDD	C1A-C2A	2.17	1.48	1.44
2	A	701	HDD	CMD-C2D	-2.13	1.50	1.53
2	C	701	HDD	CAD-CBD	-2.13	1.48	1.52
2	A	701	HDD	OND-C2D	2.13	1.46	1.42
2	B	701	HDD	CAD-CBD	-2.11	1.48	1.52
2	B	701	HDD	O1A-CGA	2.09	1.28	1.22
2	C	701	HDD	C4B-NB	-2.07	1.35	1.39
2	D	701	HDD	C4D-ND	-2.06	1.34	1.37
2	C	701	HDD	CAD-C3D	-2.06	1.49	1.53
2	D	701	HDD	CAC-C3C	-2.04	1.41	1.47
2	A	701	HDD	C1C-NC	-2.01	1.35	1.39
2	D	701	HDD	C4C-NC	-2.01	1.35	1.39

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	HDD	CBD-CAD-C3D	5.28	111.51	103.98
2	B	701	HDD	C3B-C2B-C1B	-4.68	102.62	107.05
2	D	701	HDD	OND-C2D-CMD	-4.53	100.68	109.45
2	C	701	HDD	OND-C2D-CMD	-4.50	100.75	109.45
2	D	701	HDD	C2A-C1A-NA	4.48	115.12	110.15
2	C	701	HDD	O1D-CGD-O2D	-4.47	117.04	120.81
2	A	701	HDD	C3D-O1D-CGD	4.02	114.89	111.14
4	A	707	1PE	C24-OH4-C13	3.99	130.73	113.26
2	D	701	HDD	CMC-C2C-C1C	3.90	131.35	125.42
2	C	701	HDD	CBD-CAD-C3D	3.82	109.42	103.98
2	A	701	HDD	C2D-C1D-CHD	-3.68	118.55	124.27
2	D	701	HDD	CAA-C2A-C1A	3.54	131.86	124.94
2	A	701	HDD	O1D-CGD-CBD	-3.48	107.00	110.17
2	A	701	HDD	CHC-C4B-NB	3.40	128.15	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	HDD	C2D-C1D-CHD	-3.37	119.03	124.27
2	D	701	HDD	C3C-C2C-C1C	-3.33	103.24	107.17
2	A	701	HDD	O1D-CGD-O2D	3.15	123.46	120.81
2	D	701	HDD	CHC-C1C-C2C	-3.14	118.31	127.43
2	D	701	HDD	C2C-C1C-NC	3.04	115.02	110.14
4	A	707	1PE	OH3-C23-C13	3.04	124.19	110.35
2	D	701	HDD	C1A-C2A-C3A	-2.96	102.29	106.87
2	B	701	HDD	OND-C2D-CMD	-2.90	103.85	109.45
2	D	701	HDD	CHA-C4D-ND	2.90	128.28	124.28
2	D	701	HDD	CAA-CBA-CGA	-2.85	106.12	113.67
2	B	701	HDD	CMC-C2C-C1C	2.77	129.63	125.42
2	C	701	HDD	C3C-C2C-C1C	-2.77	103.91	107.17
2	C	701	HDD	C3A-C4A-NA	2.76	114.56	110.14
2	B	701	HDD	CAA-CBA-CGA	-2.75	106.36	113.67
2	A	701	HDD	C3C-C2C-C1C	-2.72	103.96	107.17
2	B	701	HDD	C3C-C2C-C1C	-2.61	104.09	107.17
2	D	701	HDD	O1D-C3D-CAD	-2.55	98.34	103.06
2	C	701	HDD	C2A-C1A-NA	2.53	112.96	110.15
2	B	701	HDD	CHB-C4A-C3A	-2.51	120.15	127.43
2	B	701	HDD	O2A-CGA-CBA	2.46	121.78	114.00
2	A	701	HDD	CAA-C2A-C1A	2.45	129.73	124.94
2	C	701	HDD	C3C-C4C-NC	2.45	111.86	109.80
2	B	701	HDD	CMA-C3A-C4A	2.44	129.13	125.42
2	D	701	HDD	C3C-C4C-NC	2.36	111.79	109.80
2	C	701	HDD	C4B-C3B-C2B	-2.34	104.79	106.81
2	B	701	HDD	CHA-C4D-ND	2.32	127.48	124.28
2	B	701	HDD	C2B-C1B-NB	2.31	113.91	109.64
2	B	701	HDD	C3A-C4A-NA	2.28	113.80	110.14
2	B	701	HDD	O1A-CGA-CBA	-2.27	115.88	123.09
2	D	701	HDD	O1A-CGA-CBA	-2.27	115.88	123.09
2	C	701	HDD	CHB-C4A-C3A	-2.23	120.95	127.43
2	A	701	HDD	C3B-C2B-C1B	-2.22	104.95	107.05
2	C	701	HDD	C4A-NA-C1A	-2.20	102.24	105.82
2	B	701	HDD	C2D-C1D-CHD	-2.19	120.86	124.27
2	B	701	HDD	C2A-C1A-NA	2.15	112.54	110.15
2	C	701	HDD	C1C-CHC-C4B	2.15	131.29	124.66
2	B	701	HDD	CAD-CBD-CGD	2.11	107.62	104.48
4	D	704	1PE	OH6-C26-C16	-2.11	100.83	110.11
2	A	701	HDD	CHB-C4A-C3A	-2.09	121.36	127.43
2	B	701	HDD	C4A-C3A-C2A	-2.06	104.45	106.82
2	A	701	HDD	CAA-CBA-CGA	-2.05	108.23	113.67
2	C	701	HDD	CMA-C3A-C4A	2.03	128.51	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	HDD	CMA-C3A-C4A	2.03	128.50	125.42
2	A	701	HDD	C1A-C2A-C3A	-2.02	103.74	106.87
2	A	701	HDD	CHD-C4C-NC	2.01	127.51	123.86
2	A	701	HDD	OND-C2D-CMD	-2.01	105.56	109.45

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	707	1PE	OH4-C13-C23-OH3
4	A	709	1PE	OH4-C13-C23-OH3
4	D	704	1PE	OH7-C16-C26-OH6
4	B	704	1PE	OH4-C13-C23-OH3
4	B	704	1PE	OH2-C12-C22-OH3
4	A	707	1PE	OH7-C16-C26-OH6
4	A	707	1PE	OH5-C14-C24-OH4
4	B	704	1PE	OH6-C15-C25-OH5
4	A	707	1PE	OH2-C12-C22-OH3
4	D	704	1PE	OH2-C12-C22-OH3
4	A	708	1PE	OH5-C14-C24-OH4
4	A	708	1PE	C23-C13-OH4-C24
4	A	709	1PE	C14-C24-OH4-C13
4	A	708	1PE	C16-C26-OH6-C15
4	B	704	1PE	C16-C26-OH6-C15
4	A	709	1PE	C12-C22-OH3-C23
4	A	709	1PE	OH6-C15-C25-OH5
4	B	704	1PE	C24-C14-OH5-C25
4	B	704	1PE	C13-C23-OH3-C22
4	A	709	1PE	OH7-C16-C26-OH6
4	A	709	1PE	C13-C23-OH3-C22
4	D	704	1PE	C23-C13-OH4-C24
4	A	709	1PE	C25-C15-OH6-C26
4	A	707	1PE	C25-C15-OH6-C26
2	C	701	HDD	CAA-CBA-CGA-O2A
4	A	708	1PE	C14-C24-OH4-C13
2	A	701	HDD	CAA-CBA-CGA-O1A
2	A	701	HDD	CAA-CBA-CGA-O2A
2	B	701	HDD	CAA-CBA-CGA-O1A
2	D	701	HDD	CAA-CBA-CGA-O1A
2	D	701	HDD	CAA-CBA-CGA-O2A
4	D	704	1PE	C13-C23-OH3-C22
2	B	701	HDD	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

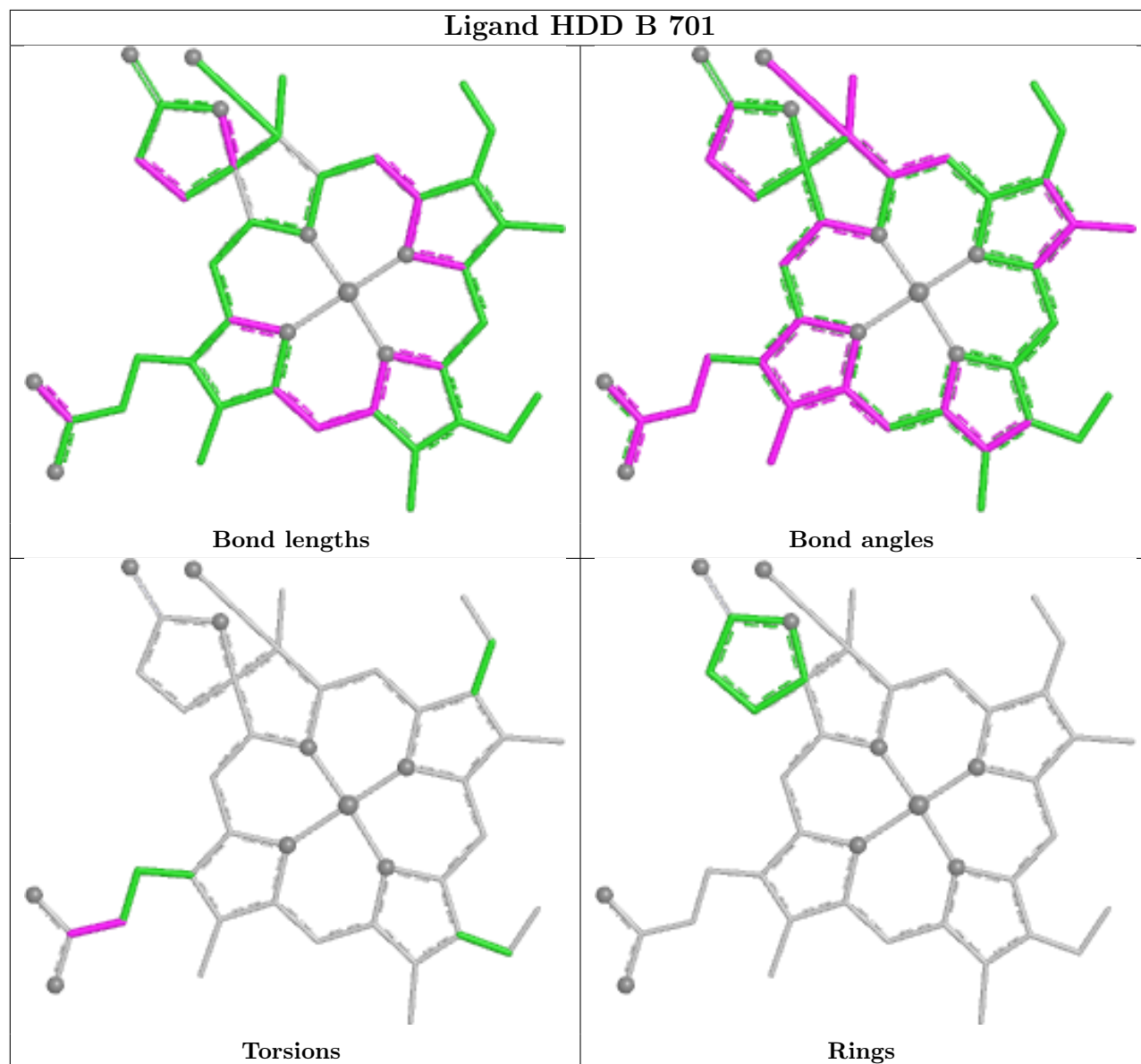
Mol	Chain	Res	Type	Atoms
2	C	701	HDD	CAA-CBA-CGA-O1A

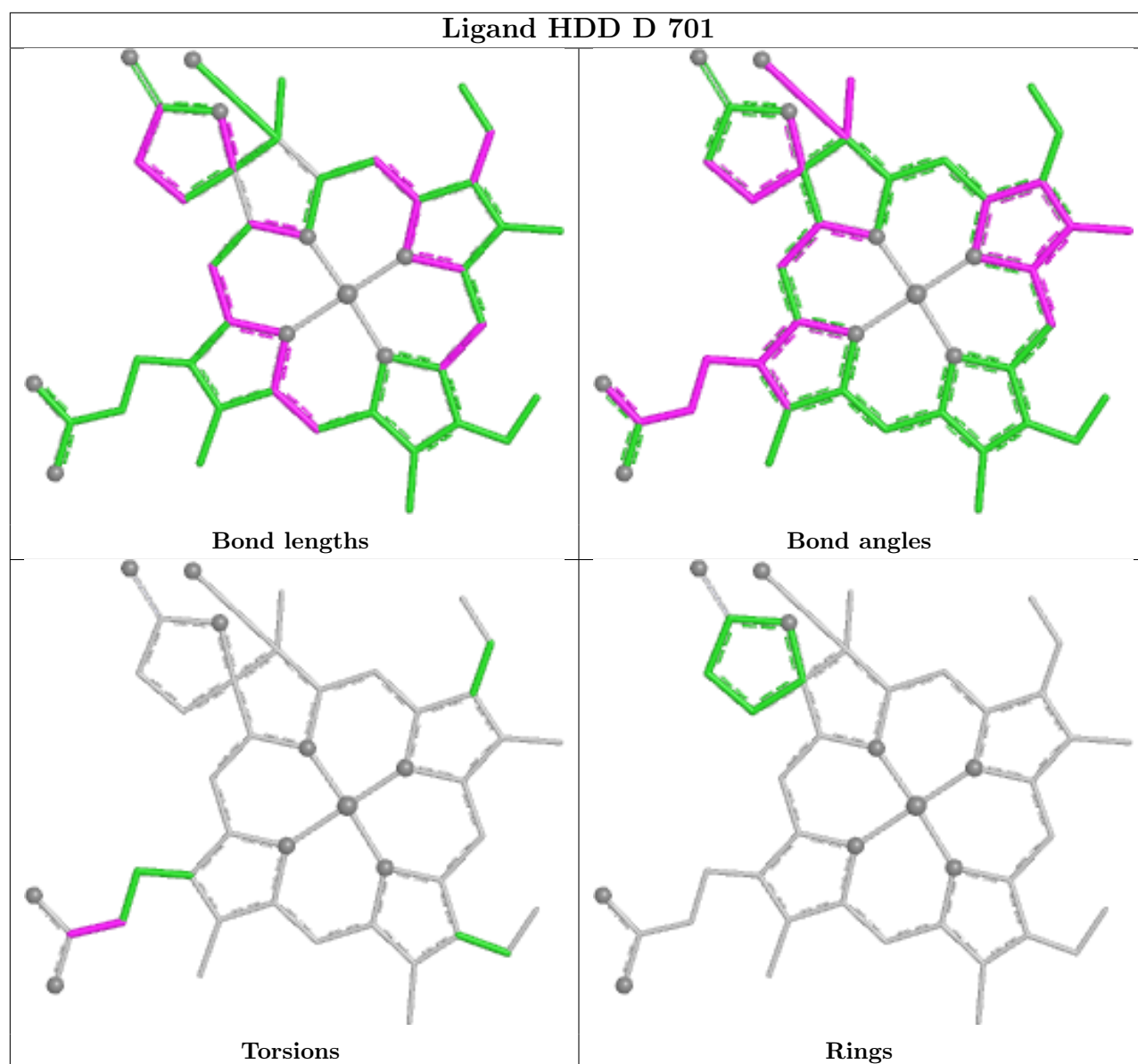
There are no ring outliers.

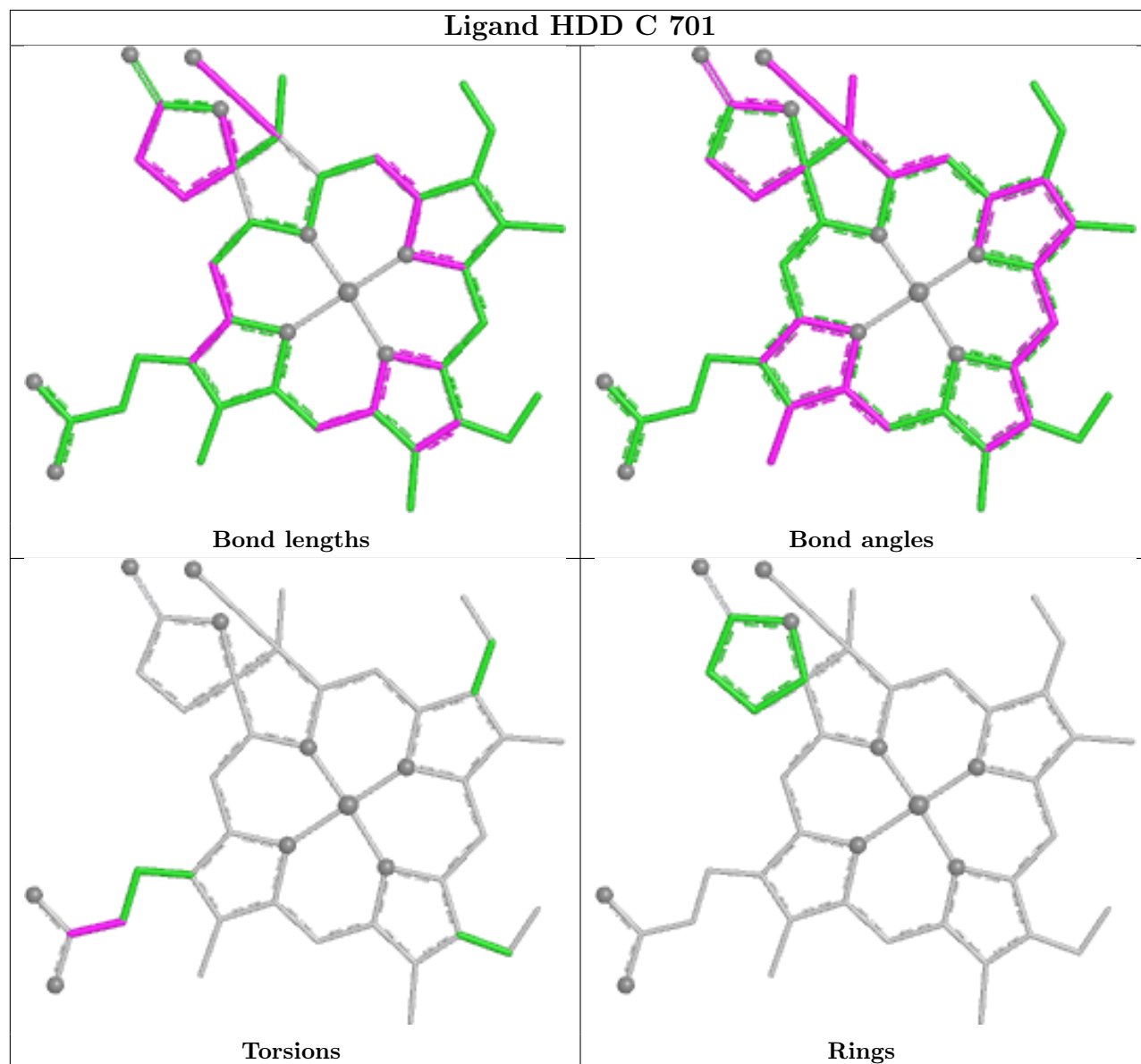
2 monomers are involved in 4 short contacts:

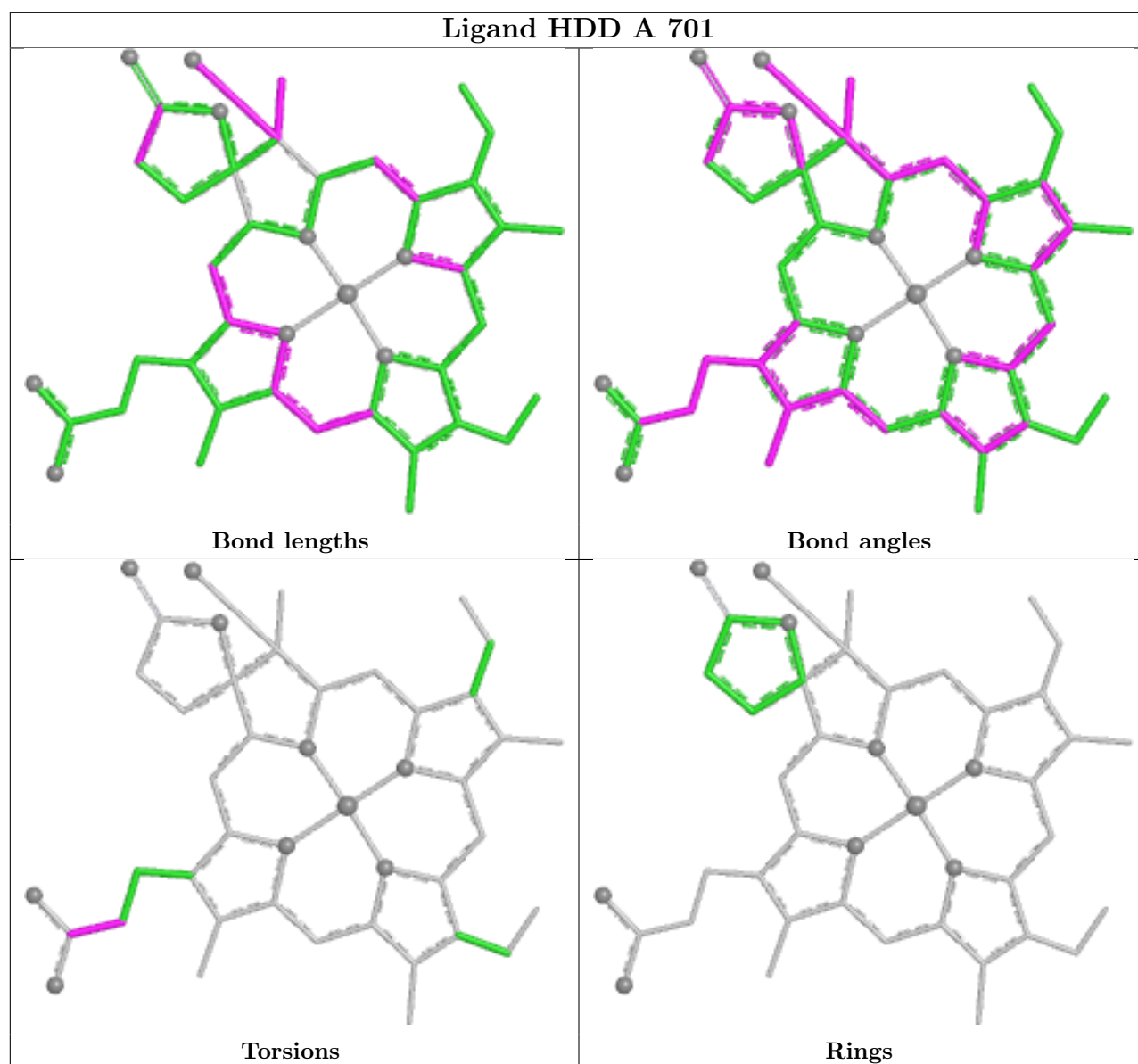
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	704	1PE	2	0
4	A	707	1PE	2	0

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









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	673/678 (99%)	-0.30	3 (0%) 88 91	4, 13, 25, 35	31 (4%)
1	B	678/678 (100%)	-0.36	9 (1%) 75 79	4, 12, 25, 45	28 (4%)
1	C	675/678 (99%)	-0.26	14 (2%) 63 67	4, 13, 30, 65	22 (3%)
1	D	673/678 (99%)	-0.30	13 (1%) 66 70	4, 13, 27, 56	20 (2%)
All	All	2699/2712 (99%)	-0.30	39 (1%) 73 77	4, 13, 27, 65	101 (3%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	620	THR	4.3
1	C	655	VAL	4.1
1	C	618	ALA	3.7
1	B	619	SER	3.4
1	A	559[A]	SER	3.4
1	D	650	GLY	3.4
1	B	618	ALA	3.4
1	B	621	ALA	3.3
1	C	658	ALA	3.2
1	C	650	GLY	3.0
1	D	653	SER	3.0
1	D	619	SER	2.9
1	C	621	ALA	2.8
1	B	517	GLY	2.8
1	B	539	VAL	2.8
1	D	618	ALA	2.8
1	D	517	GLY	2.8
1	D	561	SER	2.7
1	A	100	ASN	2.7
1	C	21	SER	2.7
1	D	658	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	698	SER	2.7
1	D	655	VAL	2.6
1	B	530	ASN	2.6
1	D	657	ASP	2.5
1	B	246[A]	HIS	2.5
1	C	674	VAL	2.4
1	C	559[A]	SER	2.4
1	C	654	GLU	2.4
1	C	23	LEU	2.4
1	C	653	SER	2.4
1	C	649	GLY	2.3
1	C	657	ASP	2.3
1	D	22	PRO	2.3
1	A	530	ASN	2.2
1	D	659	ALA	2.1
1	D	649	GLY	2.1
1	D	560	GLU	2.1
1	C	619	SER	2.1

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(Å ²)	Q<0.9
4	1PE	A	708	16/16	0.67	0.22	43,59,84,85	0
4	1PE	A	709	16/16	0.73	0.19	49,54,69,76	0
4	1PE	B	704	16/16	0.77	0.17	43,48,56,60	0
4	1PE	D	704	16/16	0.77	0.19	29,43,57,57	0
4	1PE	A	707	16/16	0.82	0.17	32,39,47,48	0

Continued on next page...

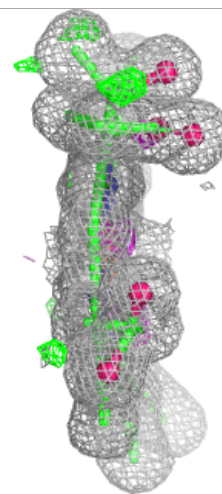
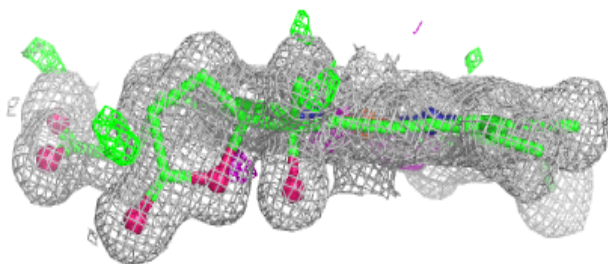
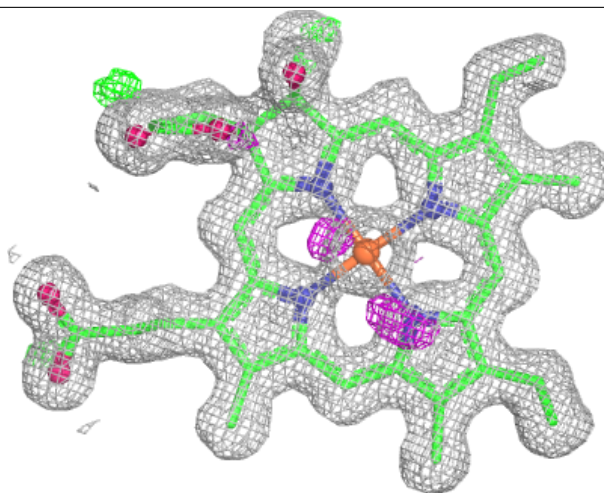
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	C	703	1/1	0.98	0.11	26,26,26,26	0
3	CA	A	706	1/1	0.98	0.05	18,18,18,18	1
3	CA	A	705	1/1	0.99	0.05	13,13,13,13	1
2	HDD	A	701	44/44	0.99	0.05	7,9,12,13	0
3	CA	B	702	1/1	0.99	0.05	14,14,14,14	0
3	CA	B	703	1/1	0.99	0.11	23,23,23,23	0
3	CA	C	702	1/1	0.99	0.05	14,14,14,14	0
2	HDD	B	701	44/44	0.99	0.04	6,9,11,15	0
3	CA	D	703	1/1	0.99	0.09	23,23,23,23	0
2	HDD	C	701	44/44	0.99	0.04	8,9,12,15	0
2	HDD	D	701	44/44	0.99	0.04	7,8,10,13	0
3	CA	A	702	1/1	0.99	0.08	13,13,13,13	1
3	CA	A	703	1/1	0.99	0.06	15,15,15,15	0
3	CA	A	704	1/1	0.99	0.10	25,25,25,25	0
3	CA	D	702	1/1	1.00	0.04	12,12,12,12	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.

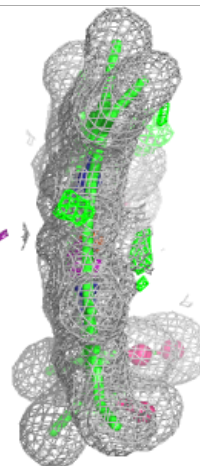
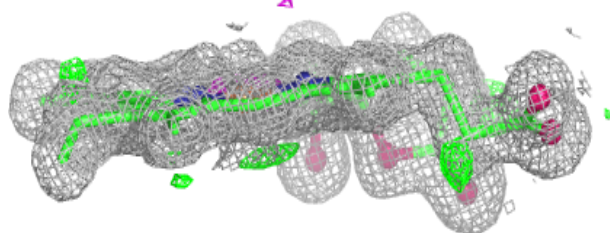
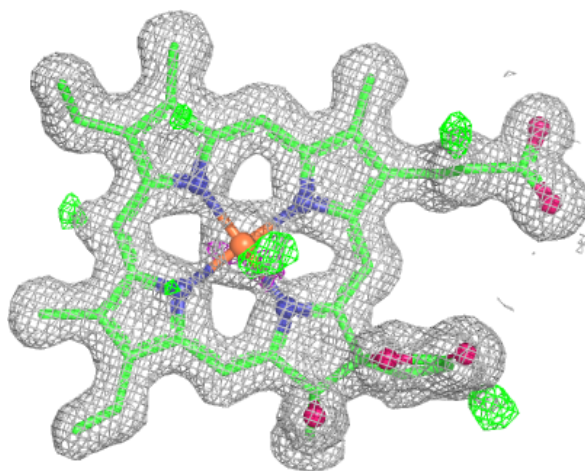
Electron density around HDD A 701:

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



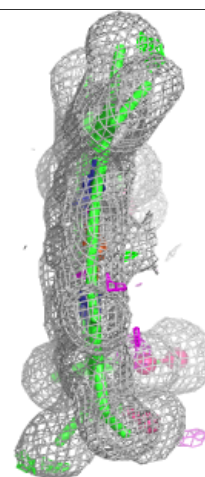
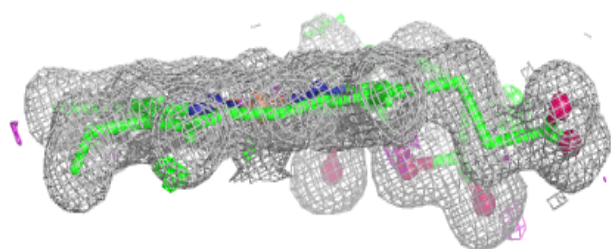
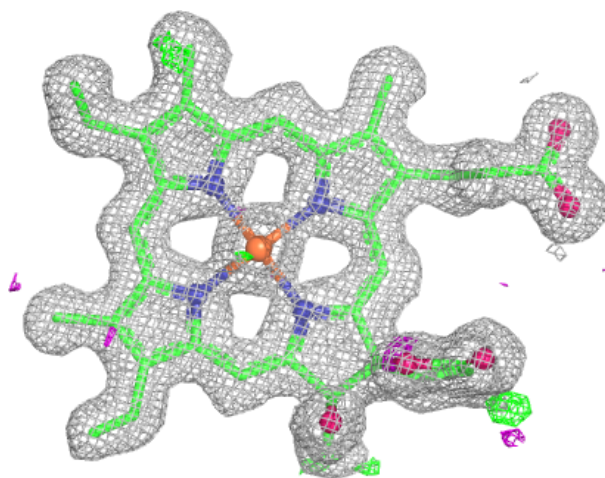
Electron density around HDD B 701:

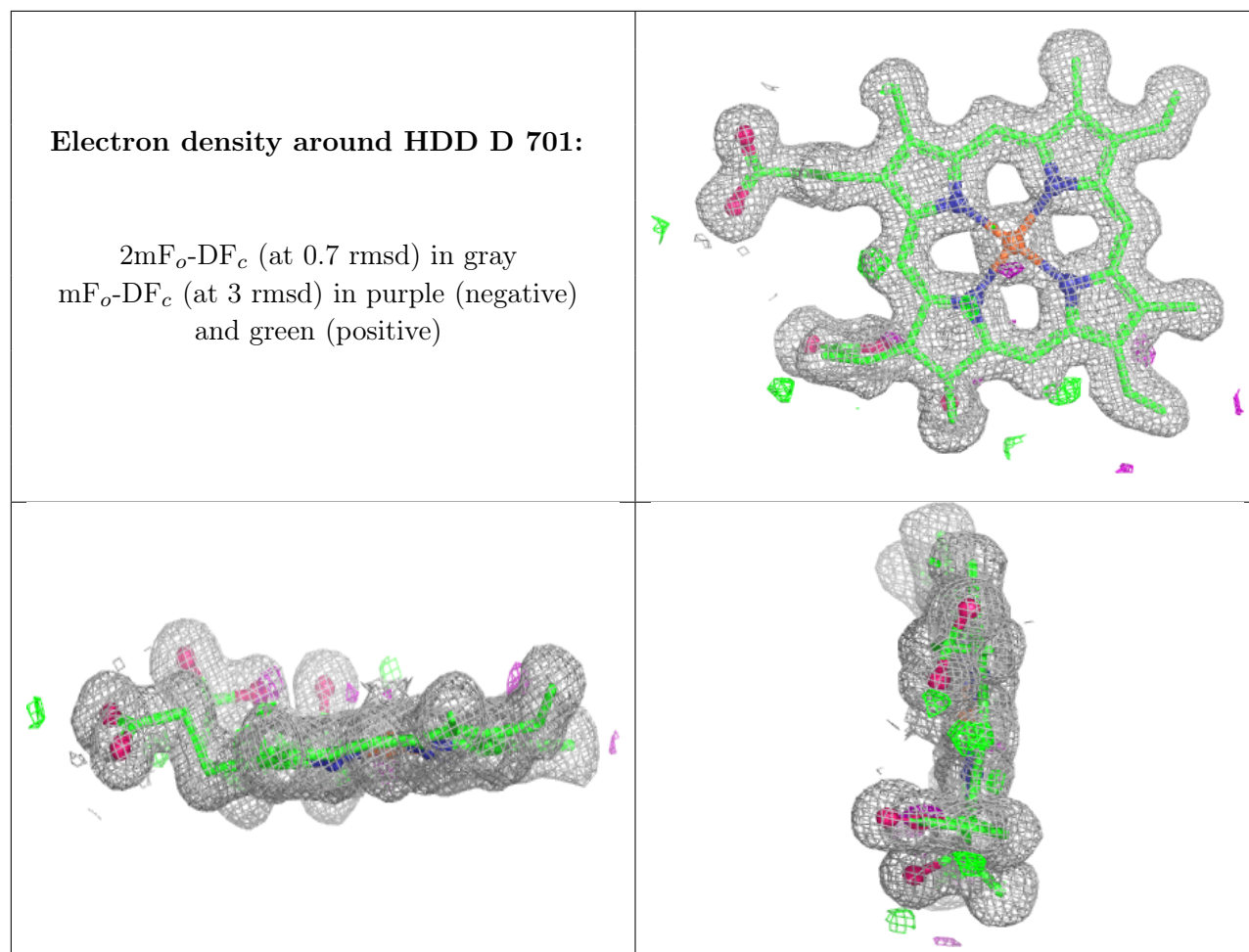
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HDD C 701:

$2mF_o-DF_c$ (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.