



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 05:46 PM JST

PDB ID : 5XZN  
Title : CATPO mutant - V228C  
Authors : Yuzugullu Karakus, Y.; Balci, S.; Goc, G.; Pearson, A.R.; Yorke, B.  
Deposited on : 2017-07-13  
Resolution : 1.47 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

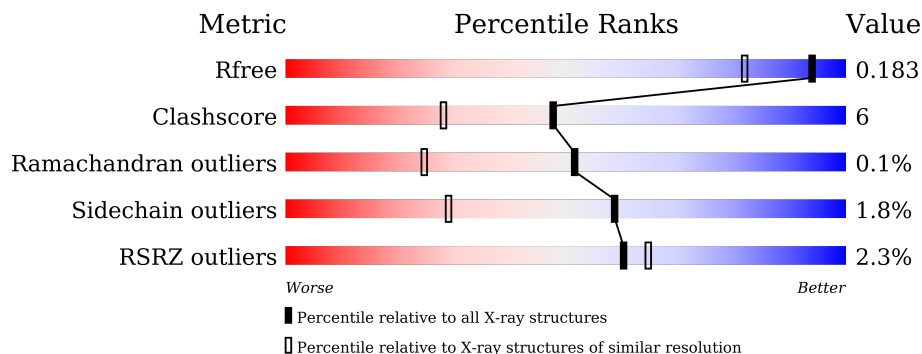
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.47 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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  $\geq 3$ , 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	 4% 92% 8%
1	B	678	 4% 91% 9%
1	C	678	 89% 10%
1	D	678	 90% 9%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	1PE	C	706[B]	-	-	X	-
4	1PE	D	705[B]	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25490 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.

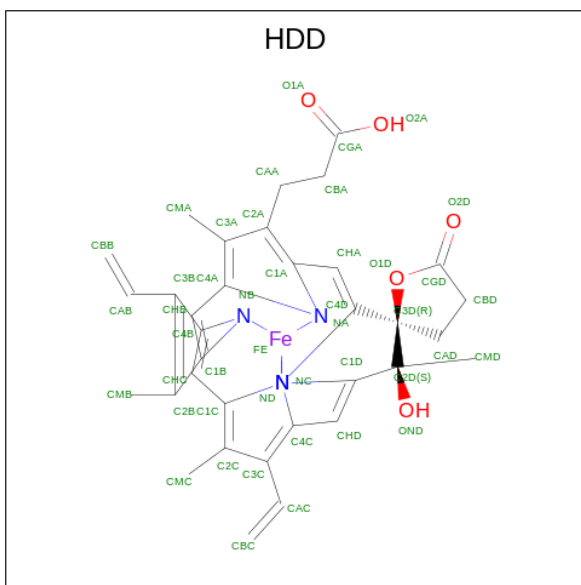
- Molecule 1 is a protein called Catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	678	5661	3550	1003	1094	14	0	45	0
1	B	678	5671	3561	1002	1095	13	0	46	0
1	C	675	5648	3545	998	1090	15	0	45	0
1	D	678	5659	3554	1002	1089	14	0	42	0

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).

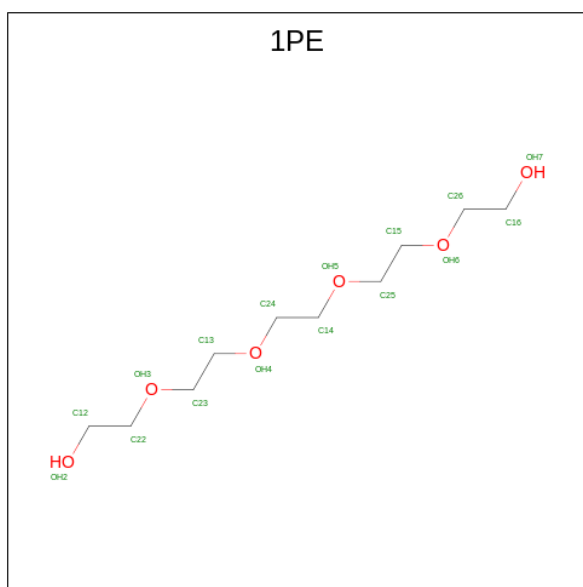


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	C	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	D	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Ca	0	0
			5	5		
3	B	2	Total	Ca	0	0
			2	2		
3	C	1	Total	Ca	0	0
			1	1		
3	D	2	Total	Ca	0	0
			2	2		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	C O	0	0
			16	10 6		
4	B	1	Total	C O	0	0
			16	10 6		
4	B	1	Total	C O	0	0
			16	10 6		
4	C	1	Total	C O	0	0
			16	10 6		
4	C	1	Total	C O	0	0
			16	10 6		
4	C	1	Total	C O	0	0
			16	10 6		
4	C	1	Total	C O	0	1
			32	20 12		
4	D	1	Total	C O	0	0
			16	10 6		
4	D	1	Total	C O	0	1
			32	20 12		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	616	Total	O	0	0
			616	616		
5	B	590	Total	O	0	0
			590	590		
5	C	668	Total	O	0	0
			668	668		

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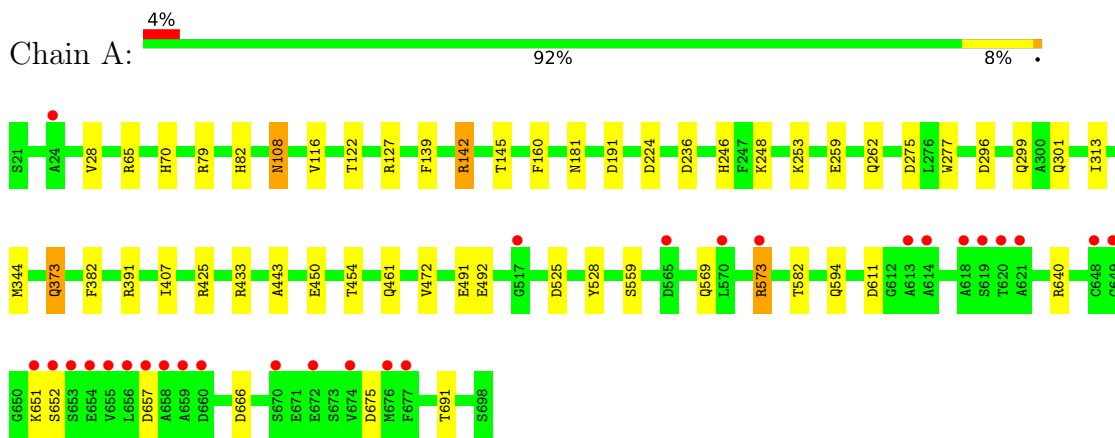
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	D	615	Total 615	O 615	0	0

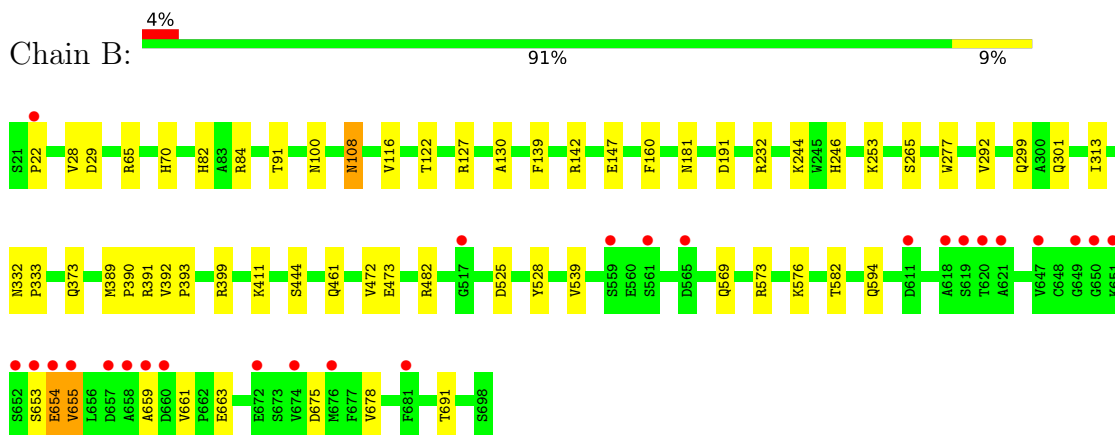
### 3 Residue-property plots [i](#)

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

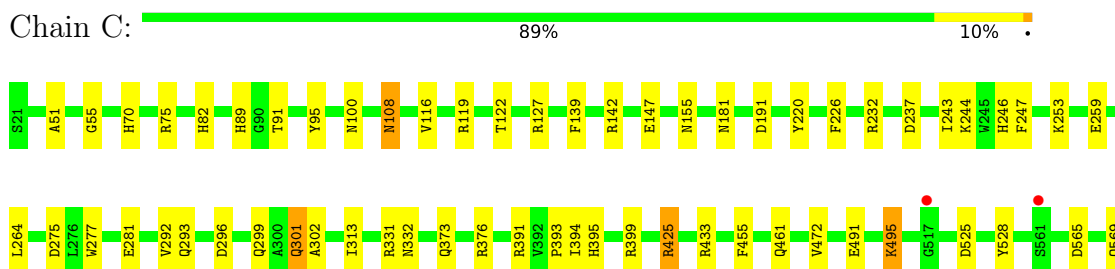
- Molecule 1: Catalase



- Molecule 1: Catalase



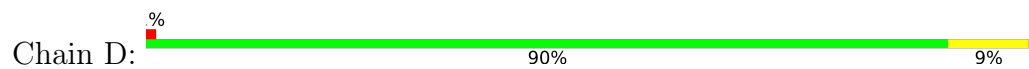
- Molecule 1: Catalase







● Molecule 1: Catalase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.12Å 121.08Å 185.12Å 90.00° 101.96° 90.00°	Depositor
Resolution (Å)	55.25 – 1.47 55.19 – 1.47	Depositor EDS
% Data completeness (in resolution range)	99.4 (55.25-1.47) 99.4 (55.19-1.47)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 1.47Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.149 , 0.175 0.159 , 0.183	Depositor DCC
$R_{free}$ test set	22662 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.8	Xtrriage
Anisotropy	0.078	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	25490	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.33 % 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 5.9365e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.75	0/5802	0.92	6/7877 (0.1%)
1	B	0.74	0/5812	0.91	6/7891 (0.1%)
1	C	0.74	2/5785 (0.0%)	0.94	17/7851 (0.2%)
1	D	0.75	0/5797	0.93	10/7867 (0.1%)
All	All	0.75	2/23196 (0.0%)	0.92	39/31486 (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	C	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	259[A]	GLU	CD-OE1	5.93	1.32	1.25
1	C	259[B]	GLU	CD-OE1	5.93	1.32	1.25

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	425	ARG	NE-CZ-NH1	10.90	125.75	120.30
1	D	399	ARG	NE-CZ-NH2	-9.99	115.31	120.30
1	C	425[A]	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	C	425[B]	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	D	232	ARG	NE-CZ-NH1	7.67	124.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	425	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	A	79	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	B	399	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	C	399	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	D	425	ARG	CD-NE-CZ	6.26	132.36	123.60
1	B	84	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	482	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	425[A]	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	A	425[B]	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	B	232	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	425[A]	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	C	425[B]	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	482	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	D	142	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	C	247	PHE	CB-CG-CD1	5.74	124.82	120.80
1	C	391[A]	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	391[B]	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	232	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	B	65	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	D	698	SER	CA-C-O	-5.60	108.34	120.10
1	C	376	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	D	399	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	79	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	D	232	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	D	220	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	C	232	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	301	GLN	CB-CA-C	5.21	120.83	110.40
1	A	142	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	C	425[A]	ARG	CD-NE-CZ	5.16	130.82	123.60
1	C	425[B]	ARG	CD-NE-CZ	5.16	130.82	123.60
1	C	119	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	65	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	C	220	TYR	CB-CG-CD1	5.04	124.02	121.00
1	C	455	PHE	CB-CG-CD1	5.01	124.31	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	75	ARG	Sidechain
1	D	75	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5661	0	5378	67	0
1	B	5671	0	5400	68	0
1	C	5648	0	5367	58	0
1	D	5659	0	5396	65	0
2	A	44	0	31	2	0
2	B	44	0	31	2	0
2	C	44	0	31	3	0
2	D	44	0	31	3	0
3	A	5	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	B	48	0	66	1	0
4	C	80	0	110	25	0
4	D	48	0	66	16	0
5	A	616	0	0	19	0
5	B	590	0	0	23	0
5	C	668	0	0	24	0
5	D	615	0	0	33	0
All	All	25490	0	21907	277	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 6.

All (277) 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:253[C]:LYS:HG2	5:D:1314:HOH:O	1.37	1.17
1:D:296[B]:ASP:OD2	5:D:803:HOH:O	1.60	1.17
1:A:491[A]:GLU:OE2	5:A:803:HOH:O	1.63	1.15
1:B:573[B]:ARG:HH21	1:B:573[B]:ARG:CG	1.63	1.10
1:D:394:ILE:H	4:D:705[B]:1PE:H151	1.10	1.09
1:D:253[C]:LYS:CG	5:D:1314:HOH:O	1.96	1.09
1:A:573[A]:ARG:HE	1:A:573[A]:ARG:HA	1.09	1.08
1:C:127[B]:ARG:NH2	5:C:803:HOH:O	1.84	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389[B]:MET:HE2	1:B:390:PRO:HD2	1.13	1.06
1:A:573[A]:ARG:HA	1:A:573[A]:ARG:NE	1.71	1.04
1:D:253[A]:LYS:HG2	5:D:1314:HOH:O	1.60	1.02
1:B:573[B]:ARG:HG2	1:B:573[B]:ARG:NH2	1.51	1.00
1:A:127[A]:ARG:NH1	5:A:804:HOH:O	1.93	0.99
1:D:127[A]:ARG:NH1	5:D:804:HOH:O	1.98	0.97
1:A:313:ILE:H	1:A:461:GLN:HE22	1.14	0.95
1:B:576[B]:LYS:HE2	5:B:1212:HOH:O	1.66	0.95
1:C:127[B]:ARG:CZ	5:C:803:HOH:O	2.16	0.93
1:B:29[A]:ASP:OD2	5:B:803:HOH:O	1.86	0.93
1:B:389[B]:MET:HE2	1:B:390:PRO:CD	1.98	0.93
1:A:127[A]:ARG:NH2	5:A:804:HOH:O	1.99	0.93
1:C:127[B]:ARG:NH1	5:C:803:HOH:O	2.03	0.92
1:B:28:VAL:HG13	4:C:706[B]:1PE:H232	1.48	0.92
1:C:313:ILE:H	1:C:461:GLN:HE22	1.13	0.91
1:D:253[B]:LYS:NZ	5:D:805:HOH:O	2.03	0.91
1:B:313:ILE:H	1:B:461:GLN:HE22	1.15	0.91
1:B:127[A]:ARG:NH1	5:B:804:HOH:O	2.03	0.89
1:C:299[A]:GLN:OE1	5:C:804:HOH:O	1.92	0.88
1:A:640[A]:ARG:HG2	5:A:1253:HOH:O	1.74	0.87
1:B:389[B]:MET:CE	1:B:390:PRO:HD2	2.03	0.86
1:D:313:ILE:H	1:D:461:GLN:HE22	1.20	0.86
1:C:91[B]:THR:HG21	5:C:1221:HOH:O	1.75	0.85
1:D:127[A]:ARG:NH2	5:D:804:HOH:O	2.10	0.85
5:B:1034:HOH:O	4:C:706[B]:1PE:H262	1.77	0.85
1:D:246[A]:HIS:CD2	5:D:814:HOH:O	2.29	0.85
1:B:389[B]:MET:HE3	1:B:389[B]:MET:HA	1.59	0.84
1:B:576[B]:LYS:CE	5:B:1212:HOH:O	2.21	0.84
1:C:246[A]:HIS:CD2	5:C:806:HOH:O	2.31	0.83
1:D:160:PHE:CD1	5:D:1319:HOH:O	2.32	0.83
1:C:491[A]:GLU:O	1:C:495[A]:LYS:HD3	1.79	0.82
1:B:160:PHE:CE1	5:B:1315:HOH:O	2.30	0.82
1:A:640[B]:ARG:NH1	5:A:807:HOH:O	2.14	0.80
1:A:246[B]:HIS:CD2	1:A:248:LYS:CD	2.65	0.80
1:D:160:PHE:CE1	5:D:1319:HOH:O	2.35	0.79
1:B:28:VAL:HG13	4:C:706[B]:1PE:C23	2.12	0.79
1:A:573[A]:ARG:NE	1:A:573[A]:ARG:CA	2.44	0.79
1:B:127[B]:ARG:NH1	5:B:808:HOH:O	2.16	0.78
1:A:246[B]:HIS:NE2	1:A:248:LYS:CD	2.47	0.78
1:D:394:ILE:H	4:D:705[B]:1PE:C15	1.94	0.78
1:A:299[B]:GLN:NE2	5:A:805:HOH:O	2.04	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127[A]:ARG:CZ	5:A:804:HOH:O	2.22	0.78
1:B:573[B]:ARG:HH21	1:B:573[B]:ARG:HG2	0.70	0.78
1:D:394:ILE:N	4:D:705[B]:1PE:H151	1.94	0.78
1:D:127[A]:ARG:CZ	5:D:804:HOH:O	2.29	0.77
1:B:573[A]:ARG:HG3	1:B:678:VAL:HG11	1.66	0.77
1:B:91[B]:THR:HG22	5:B:1252:HOH:O	1.85	0.76
1:A:127[B]:ARG:NH1	5:A:808:HOH:O	2.18	0.76
1:A:246[B]:HIS:CD2	1:A:248:LYS:HD2	2.21	0.75
1:A:246[B]:HIS:CD2	1:A:248:LYS:HD3	2.22	0.75
1:B:299[A]:GLN:OE1	5:B:805:HOH:O	2.04	0.74
1:A:675[B]:ASP:OD1	1:A:675[B]:ASP:O	2.06	0.74
1:D:663[B]:GLU:HG2	5:D:1221:HOH:O	1.88	0.74
1:D:393:PRO:HA	4:D:705[B]:1PE:H152	1.70	0.74
1:B:127[A]:ARG:NH2	5:B:804:HOH:O	2.21	0.73
1:C:127[A]:ARG:NH2	5:C:805:HOH:O	2.20	0.73
1:A:160:PHE:CD1	5:A:1259:HOH:O	2.41	0.72
1:D:274[B]:GLN:NE2	5:D:810:HOH:O	2.22	0.72
1:D:395:HIS:CE1	4:D:705[B]:1PE:H162	2.24	0.72
1:D:394:ILE:O	4:D:705[B]:1PE:H261	1.89	0.72
1:B:246[A]:HIS:CE1	5:B:839:HOH:O	2.43	0.72
1:A:160:PHE:CE1	5:A:1259:HOH:O	2.43	0.71
1:B:160:PHE:CD1	5:B:1315:HOH:O	2.42	0.71
1:B:389[B]:MET:CE	1:B:389[B]:MET:HA	2.19	0.71
1:A:246[B]:HIS:NE2	1:A:248:LYS:NZ	2.38	0.71
1:A:450[B]:GLU:OE2	5:A:806:HOH:O	2.10	0.70
4:D:705[A]:1PE:H232	5:D:866:HOH:O	1.91	0.70
5:B:1148:HOH:O	4:C:706[B]:1PE:H121	1.90	0.70
1:D:259[B]:GLU:OE2	5:D:806:HOH:O	2.08	0.70
1:C:393:PRO:HB3	4:C:706[B]:1PE:H221	1.76	0.68
1:C:394:ILE:O	4:C:706[B]:1PE:H231	1.92	0.68
1:A:246[B]:HIS:CE1	1:A:248:LYS:HZ2	2.12	0.68
1:B:301:GLN:OE1	5:B:806:HOH:O	2.11	0.67
1:A:246[B]:HIS:CE1	1:A:248:LYS:NZ	2.63	0.67
2:A:701:HDD:HMB1	2:A:701:HDD:HBB1	1.76	0.67
1:C:393:PRO:HB3	4:C:706[B]:1PE:C22	2.25	0.66
1:A:492[B]:GLU:HG2	5:A:902:HOH:O	1.95	0.66
1:D:127[B]:ARG:NH1	5:D:811:HOH:O	2.27	0.66
4:D:705[B]:1PE:H131	5:D:866:HOH:O	1.95	0.66
1:D:21:SER:N	5:D:813:HOH:O	2.29	0.65
1:B:100:ASN:OD1	5:B:807:HOH:O	2.15	0.64
5:B:1034:HOH:O	4:C:706[B]:1PE:C26	2.40	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:NZ	5:A:809:HOH:O	2.29	0.64
1:D:253[B]:LYS:HG3	5:D:1171:HOH:O	1.99	0.63
1:C:246[A]:HIS:NE2	5:C:806:HOH:O	2.28	0.63
1:D:394:ILE:O	4:D:705[B]:1PE:C26	2.46	0.63
1:A:582:THR:HG21	1:A:594[A]:GLN:HE21	1.64	0.63
1:B:373:GLN:HE21	1:B:373:GLN:HA	1.64	0.61
1:B:127[A]:ARG:CZ	5:B:804:HOH:O	2.41	0.61
1:A:28:VAL:HG22	4:D:705[B]:1PE:H141	1.82	0.61
1:A:492[B]:GLU:CG	5:A:902:HOH:O	2.49	0.61
1:B:253:LYS:HG2	5:B:1287:HOH:O	2.00	0.61
1:A:373:GLN:HA	1:A:373:GLN:HE21	1.65	0.61
1:B:472[A]:VAL:HG11	1:B:691:THR:HB	1.83	0.60
1:B:573[B]:ARG:CG	1:B:573[B]:ARG:NH2	2.35	0.60
1:A:246[B]:HIS:NE2	1:A:248:LYS:HD3	2.15	0.60
1:B:389[B]:MET:CE	1:B:390:PRO:CD	2.73	0.60
2:D:701:HDD:HMB1	2:D:701:HDD:HBB1	1.83	0.59
1:B:277[A]:TRP:CZ3	1:D:181:ASN:HB3	2.38	0.59
1:D:373:GLN:HA	1:D:373:GLN:HE21	1.66	0.59
1:D:299[A]:GLN:OE1	5:D:808:HOH:O	2.16	0.59
1:D:253[C]:LYS:HG3	5:D:1314:HOH:O	1.80	0.58
4:D:705[B]:1PE:H141	4:D:705[B]:1PE:H232	1.84	0.58
1:C:253:LYS:HG2	5:C:1249:HOH:O	2.03	0.58
1:A:253:LYS:HG2	5:A:1273:HOH:O	2.04	0.57
2:B:701:HDD:HMB1	2:B:701:HDD:HBB1	1.86	0.57
1:D:331[B]:ARG:NH1	5:D:807:HOH:O	2.09	0.57
1:A:246[B]:HIS:CE1	1:A:248:LYS:HD3	2.39	0.57
1:A:277[A]:TRP:CZ3	1:C:181:ASN:HB3	2.40	0.57
1:A:573[B]:ARG:CG	1:A:573[B]:ARG:HH21	2.18	0.57
1:B:277[A]:TRP:CE3	1:D:181:ASN:HB3	2.40	0.57
1:C:100[B]:ASN:H	1:C:100[B]:ASN:HD22	1.52	0.57
1:D:582:THR:HG21	1:D:594[B]:GLN:HE21	1.70	0.56
1:A:246[B]:HIS:NE2	1:A:248:LYS:HD2	2.18	0.56
1:D:472[A]:VAL:HG11	1:D:691:THR:HB	1.86	0.56
1:B:147[B]:GLU:OE1	5:B:809:HOH:O	2.18	0.56
1:A:640[A]:ARG:CG	5:A:1253:HOH:O	2.40	0.56
1:D:246[A]:HIS:NE2	5:D:814:HOH:O	2.33	0.55
1:B:313:ILE:N	1:B:461:GLN:HE22	1.96	0.55
1:C:395:HIS:CE1	4:C:706[B]:1PE:H222	2.42	0.55
1:B:389[B]:MET:HE1	5:C:1139:HOH:O	2.06	0.55
1:C:640[A]:ARG:CG	5:C:851:HOH:O	2.55	0.55
1:C:313:ILE:N	1:C:461:GLN:HE22	1.94	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246[B]:HIS:HD2	5:D:814:HOH:O	1.90	0.54
5:B:1148:HOH:O	4:C:706[B]:1PE:C12	2.52	0.54
1:A:296[B]:ASP:H	1:A:299[B]:GLN:HE21	1.56	0.54
1:D:633[A]:GLN:NE2	5:D:816:HOH:O	2.40	0.54
1:A:108:ASN:C	1:A:108:ASN:HD22	2.12	0.53
1:C:373:GLN:HE21	1:C:373:GLN:HA	1.72	0.53
1:C:108:ASN:C	1:C:108:ASN:HD22	2.12	0.53
1:A:246[B]:HIS:CG	1:A:248:LYS:HD3	2.44	0.53
1:B:473:GLU:HG3	1:B:539:VAL:CG2	2.39	0.52
1:C:281[B]:GLU:HG3	5:C:950:HOH:O	2.09	0.52
1:A:181:ASN:HB3	1:C:277[B]:TRP:CE3	2.44	0.52
1:B:22:PRO:HD2	1:B:391[A]:ARG:NE	2.23	0.52
2:C:701:HDD:HMB1	2:C:701:HDD:HBB1	1.91	0.52
1:A:313:ILE:N	1:A:461:GLN:HE22	1.94	0.52
1:B:108:ASN:C	1:B:108:ASN:HD22	2.12	0.52
1:A:525:ASP:HA	1:A:528:TYR:CD2	2.45	0.52
1:A:472[B]:VAL:HG11	1:A:691:THR:HB	1.92	0.52
1:B:573[B]:ARG:NH2	1:B:675:ASP:OD1	2.43	0.52
1:D:241:LYS:NZ	1:D:296[A]:ASP:OD1	2.37	0.52
1:D:253[B]:LYS:HE3	1:D:541:SER:HB3	1.92	0.51
1:A:472[A]:VAL:HG11	1:A:691:THR:HB	1.91	0.51
1:B:392[B]:VAL:HG13	1:B:393:PRO:HD2	1.90	0.51
1:C:565[A]:ASP:O	1:C:569[A]:GLN:HG3	2.10	0.51
1:D:108:ASN:C	1:D:108:ASN:HD22	2.13	0.51
1:A:181:ASN:HB3	1:C:277[B]:TRP:CZ3	2.45	0.51
1:C:277[B]:TRP:CZ3	1:C:332:ASN:HB3	2.46	0.51
1:D:253[B]:LYS:CG	5:D:1171:HOH:O	2.55	0.51
1:B:659:ALA:HB1	1:B:661:VAL:HG23	1.93	0.51
1:C:147:GLU:OE2	1:C:433[B]:ARG:HD3	2.11	0.51
1:B:181:ASN:HB3	1:D:277[B]:TRP:CZ3	2.46	0.50
2:D:701:HDD:HMC1	2:D:701:HDD:HBC1	1.94	0.50
1:B:392[B]:VAL:CG1	1:B:393:PRO:HD2	2.42	0.50
1:C:226:PHE:CE1	1:C:246[B]:HIS:CD2	3.00	0.50
1:D:21:SER:HB3	1:D:331[A]:ARG:NH1	2.26	0.50
1:A:666:ASP:HB2	5:A:810:HOH:O	2.12	0.49
1:C:301:GLN:HG2	5:C:1345:HOH:O	2.12	0.49
1:A:262[B]:GLN:NE2	5:A:812:HOH:O	2.41	0.49
1:A:573[A]:ARG:HE	1:A:573[A]:ARG:CA	1.99	0.49
1:D:301:GLN:NE2	1:D:454:THR:HG21	2.28	0.48
1:D:492[A]:GLU:CD	5:D:899:HOH:O	2.51	0.48
1:C:95:TYR:CD1	4:C:705:1PE:H141	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277[A]:TRP:CE3	1:C:181:ASN:HB3	2.49	0.48
1:B:573[B]:ARG:HD2	1:B:576[B]:LYS:HZ1	1.78	0.48
1:B:663[B]:GLU:H	1:B:663[B]:GLU:HG2	1.41	0.48
4:C:706[B]:1PE:H122	5:C:817:HOH:O	2.12	0.48
1:B:525:ASP:HA	1:B:528:TYR:CD2	2.49	0.48
2:B:701:HDD:HMC1	2:B:701:HDD:HBC1	1.96	0.48
1:D:82:HIS:CE1	1:D:123:VAL:HG22	2.48	0.48
1:A:28:VAL:HG22	4:D:705[B]:1PE:C14	2.44	0.48
1:D:469:LEU:HB3	1:D:473:GLU:HB3	1.95	0.48
1:C:253:LYS:HE2	5:C:916:HOH:O	2.14	0.48
1:A:259:GLU:HA	1:A:262[B]:GLN:HE21	1.79	0.48
4:D:705[B]:1PE:H232	4:D:705[B]:1PE:H252	1.96	0.47
1:C:237:ASP:HB2	4:C:703:1PE:H231	1.96	0.47
1:C:582:THR:HG21	1:C:594[B]:GLN:HE21	1.79	0.47
1:A:573[B]:ARG:HH21	1:A:573[B]:ARG:HG2	1.80	0.47
1:B:181:ASN:HB3	1:D:277[B]:TRP:CE3	2.50	0.47
2:A:701:HDD:HMC1	2:A:701:HDD:HBC1	1.96	0.47
1:C:95:TYR:HD1	4:C:705:1PE:H141	1.80	0.47
1:A:573[B]:ARG:CG	1:A:573[B]:ARG:NH2	2.76	0.46
1:B:22:PRO:HG2	5:B:877:HOH:O	2.15	0.46
1:B:244:LYS:O	1:B:292:VAL:HA	2.14	0.46
1:C:281[B]:GLU:CG	5:C:1186:HOH:O	2.63	0.46
4:C:706[A]:1PE:H161	4:C:706[A]:1PE:H151	1.57	0.46
1:B:277[A]:TRP:CH2	1:B:332:ASN:HB3	2.50	0.46
1:C:569[B]:GLN:NE2	5:C:819:HOH:O	2.49	0.46
1:C:640[A]:ARG:NH1	5:C:811:HOH:O	2.49	0.46
1:B:582:THR:HG21	1:B:594[A]:GLN:HE21	1.81	0.45
4:C:705:1PE:C15	5:C:1375:HOH:O	2.64	0.45
1:C:393:PRO:HB3	4:C:706[B]:1PE:H222	1.98	0.45
4:C:705:1PE:H152	5:C:1375:HOH:O	2.17	0.45
1:A:313:ILE:H	1:A:461:GLN:NE2	1.97	0.45
1:B:82:HIS:HA	1:B:122:THR:O	2.17	0.45
1:D:82:HIS:HA	1:D:122:THR:O	2.16	0.45
1:A:569:GLN:NE2	1:A:573[B]:ARG:HH12	2.14	0.45
1:D:331[B]:ARG:NH2	5:D:807:HOH:O	2.44	0.45
1:C:91[B]:THR:HG23	5:C:834:HOH:O	2.16	0.45
1:C:525:ASP:HA	1:C:528:TYR:CD2	2.52	0.45
1:C:116:VAL:HA	1:C:142:ARG:O	2.17	0.45
1:D:243:ILE:HA	1:D:293:GLN:O	2.17	0.44
1:C:640[A]:ARG:HG2	5:C:851:HOH:O	2.17	0.44
1:D:244:LYS:O	1:D:292:VAL:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:GLU:O	1:B:655:VAL:HB	2.17	0.44
1:B:659:ALA:CB	1:B:661:VAL:HG23	2.47	0.44
1:D:248[B]:LYS:HD3	5:D:995:HOH:O	2.17	0.44
1:C:640[A]:ARG:CG	1:C:640[A]:ARG:O	2.66	0.44
1:A:236:ASP:CG	1:A:433[B]:ARG:HH22	2.21	0.44
2:C:701:HDD:HMC1	2:C:701:HDD:HBC1	2.00	0.44
1:D:525:ASP:HA	1:D:528:TYR:CD2	2.53	0.44
4:C:706[B]:1PE:H221	4:C:706[B]:1PE:H132	1.03	0.44
1:A:391[B]:ARG:HE	1:A:391[B]:ARG:HB3	1.48	0.44
1:A:407:ILE:O	1:D:27:GLU:HA	2.18	0.43
1:C:155:ASN:CG	2:C:701:HDD:HMB2	2.38	0.43
1:C:237:ASP:N	4:C:703:1PE:H262	2.33	0.43
1:A:253:LYS:HG3	5:A:1274:HOH:O	2.18	0.43
1:A:301:GLN:NE2	1:A:454:THR:HG21	2.33	0.43
1:D:616[A]:LEU:N	1:D:616[A]:LEU:HD12	2.32	0.43
1:A:443:ALA:O	1:B:444[B]:SER:HA	2.18	0.43
1:C:51:ALA:O	1:C:55:GLY:HA3	2.18	0.43
1:B:130:ALA:CB	1:B:265[B]:SER:HB2	2.49	0.43
1:D:115:PRO:HG2	1:D:391[B]:ARG:CZ	2.49	0.43
2:D:701:HDD:HMB1	2:D:701:HDD:CBB	2.49	0.43
1:B:277[A]:TRP:CZ3	1:B:333:PRO:HD2	2.54	0.43
4:C:706[B]:1PE:H262	4:C:706[B]:1PE:H252	1.28	0.43
1:D:640[B]:ARG:HE	1:D:640[B]:ARG:HB2	1.40	0.43
1:B:373:GLN:HA	1:B:373:GLN:NE2	2.33	0.42
1:B:573[A]:ARG:CG	1:B:678:VAL:HG21	2.50	0.42
1:B:392[B]:VAL:CG1	1:B:393:PRO:CD	2.97	0.42
1:B:576[B]:LYS:HE3	1:B:576[B]:LYS:HB2	1.84	0.42
1:B:573[A]:ARG:HG2	1:B:678:VAL:HG21	2.02	0.42
1:C:82:HIS:HA	1:C:122:THR:O	2.20	0.42
1:C:89:HIS:HB2	1:C:331:ARG:HB3	2.02	0.42
4:C:706[A]:1PE:H141	4:C:706[A]:1PE:H132	1.32	0.42
1:A:116:VAL:HA	1:A:142:ARG:O	2.20	0.42
1:B:277[A]:TRP:CZ3	1:B:332:ASN:HB3	2.55	0.42
1:A:344:MET:SD	1:A:382:PHE:HB2	2.60	0.41
1:A:569:GLN:HE21	1:A:573[B]:ARG:HH12	1.67	0.41
4:C:703:1PE:H261	5:C:1395:HOH:O	2.20	0.41
1:D:344:MET:SD	1:D:382:PHE:HB2	2.60	0.41
1:D:530:ASN:ND2	5:D:832:HOH:O	2.53	0.41
1:B:116:VAL:HA	1:B:142:ARG:O	2.21	0.41
1:B:472[B]:VAL:HG11	1:B:691:THR:HB	2.02	0.41
1:C:299[B]:GLN:HE21	1:C:302:ALA:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274[B]:GLN:OE1	5:D:809:HOH:O	2.21	0.41
1:D:472[B]:VAL:HG11	1:D:691:THR:HB	2.03	0.41
1:B:569[B]:GLN:HE21	1:B:569[B]:GLN:HB3	1.63	0.41
1:C:472:VAL:HG11	1:C:691:THR:HB	2.02	0.41
1:A:301:GLN:HE22	1:A:454:THR:HG21	1.85	0.41
1:D:393:PRO:HA	4:D:705[B]:1PE:C15	2.46	0.41
1:A:82:HIS:HA	1:A:122:THR:O	2.21	0.41
1:C:243:ILE:HA	1:C:293:GLN:O	2.21	0.41
4:C:706[B]:1PE:C12	5:C:817:HOH:O	2.68	0.41
1:C:656:LEU:CD1	1:C:663[B]:GLU:HG3	2.51	0.41
1:D:277[B]:TRP:CH2	1:D:332:ASN:HB3	2.56	0.41
4:D:705[B]:1PE:H231	4:D:705[B]:1PE:H121	1.14	0.41
1:C:394:ILE:H	4:C:706[B]:1PE:C13	2.34	0.41
1:D:472[B]:VAL:HG13	5:D:1325:HOH:O	2.20	0.41
1:A:224:ASP:OD2	1:A:248:LYS:NZ	2.54	0.40
1:C:108:ASN:C	1:C:108:ASN:ND2	2.75	0.40
1:C:244:LYS:O	1:C:292:VAL:HA	2.21	0.40
1:C:264:LEU:HD13	1:C:602:THR:HB	2.03	0.40
1:C:299[B]:GLN:HE21	1:C:302:ALA:CB	2.35	0.40
4:D:705[B]:1PE:C13	5:D:866:HOH:O	2.63	0.40
1:B:391[B]:ARG:NE	5:B:828:HOH:O	2.53	0.40
1:D:135:ASP:O	1:D:137:HIS:CE1	2.74	0.40
4:B:706:1PE:H132	5:B:831:HOH:O	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	721/678 (106%)	700 (97%)	21 (3%)	0	100 100
1	B	722/678 (106%)	698 (97%)	22 (3%)	2 (0%)	41 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	716/678 (106%)	698 (98%)	18 (2%)	0	100	100
1	D	720/678 (106%)	704 (98%)	16 (2%)	0	100	100
All	All	2879/2712 (106%)	2800 (97%)	77 (3%)	2 (0%)	51	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	653	SER
1	B	655	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	606/562 (108%)	591 (98%)	15 (2%)	47	16
1	B	607/562 (108%)	600 (99%)	7 (1%)	71	46
1	C	604/562 (108%)	590 (98%)	14 (2%)	50	19
1	D	605/562 (108%)	595 (98%)	10 (2%)	60	31
All	All	2422/2248 (108%)	2376 (98%)	46 (2%)	59	26

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	108	ASN
1	A	139	PHE
1	A	145	THR
1	A	191	ASP
1	A	275	ASP
1	A	373	GLN
1	A	559[A]	SER
1	A	559[B]	SER
1	A	573[A]	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	573[B]	ARG
1	A	611	ASP
1	A	651	LYS
1	A	652	SER
1	A	657	ASP
1	B	70	HIS
1	B	108	ASN
1	B	139	PHE
1	B	191	ASP
1	B	411[A]	LYS
1	B	411[B]	LYS
1	B	654	GLU
1	C	70	HIS
1	C	108	ASN
1	C	139	PHE
1	C	191	ASP
1	C	275	ASP
1	C	296	ASP
1	C	425[A]	ARG
1	C	425[B]	ARG
1	C	495[A]	LYS
1	C	495[B]	LYS
1	C	572[A]	THR
1	C	572[B]	THR
1	C	653	SER
1	C	660	ASP
1	D	21	SER
1	D	70	HIS
1	D	108	ASN
1	D	139	PHE
1	D	145	THR
1	D	191	ASP
1	D	275	ASP
1	D	425	ARG
1	D	530	ASN
1	D	620	THR

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	108	ASN
1	A	167	GLN

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Mol	Chain	Res	Type
1	A	301	GLN
1	A	373	GLN
1	A	375	ASN
1	A	461	GLN
1	A	569	GLN
1	B	108	ASN
1	B	167	GLN
1	B	301	GLN
1	B	373	GLN
1	B	375	ASN
1	B	461	GLN
1	C	108	ASN
1	C	167	GLN
1	C	301	GLN
1	C	373	GLN
1	C	375	ASN
1	C	461	GLN
1	D	108	ASN
1	D	167	GLN
1	D	301	GLN
1	D	373	GLN
1	D	375	ASN
1	D	461	GLN
1	D	530	ASN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 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	705	-	15,15,15	0.37	0	14,14,14	0.24	0
4	1PE	C	706[A]	-	15,15,15	0.27	0	14,14,14	0.27	0
2	HDD	D	701	1	41,52,52	1.33	6 (14%)	31,89,89	2.11	8 (25%)
2	HDD	A	701	1	41,52,52	1.27	7 (17%)	31,89,89	2.10	12 (38%)
4	1PE	C	704	-	15,15,15	0.29	0	14,14,14	0.18	0
4	1PE	D	705[A]	-	15,15,15	0.34	0	14,14,14	0.46	0
2	HDD	C	701	1	41,52,52	1.41	6 (14%)	31,89,89	2.01	10 (32%)
4	1PE	D	704	-	15,15,15	0.39	0	14,14,14	0.24	0
4	1PE	C	703	-	15,15,15	0.79	1 (6%)	14,14,14	0.75	1 (7%)
4	1PE	B	706	-	15,15,15	0.40	0	14,14,14	0.26	0
4	1PE	D	705[B]	-	15,15,15	0.41	0	14,14,14	0.37	0
2	HDD	B	701	1	41,52,52	1.58	12 (29%)	31,89,89	2.38	12 (38%)
4	1PE	C	706[B]	-	15,15,15	0.46	0	14,14,14	0.60	0
4	1PE	C	705	-	15,15,15	0.49	0	14,14,14	0.74	0
4	1PE	B	704	-	15,15,15	0.26	0	14,14,14	0.18	0

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	705	-	-	1/13/13/13	-
4	1PE	C	706[A]	-	-	8/13/13/13	-
2	HDD	D	701	1	-	2/5/89/89	0/1/9/9
2	HDD	A	701	1	-	2/5/89/89	0/1/9/9
4	1PE	C	704	-	-	4/13/13/13	-
4	1PE	D	705[A]	-	-	8/13/13/13	-
2	HDD	C	701	1	-	2/5/89/89	0/1/9/9
4	1PE	D	704	-	-	10/13/13/13	-
4	1PE	C	703	-	-	7/13/13/13	-
4	1PE	B	706	-	-	5/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1PE	D	705[B]	-	-	9/13/13/13	-
2	HDD	B	701	1	-	2/5/89/89	0/1/9/9
4	1PE	C	706[B]	-	-	9/13/13/13	-
4	1PE	C	705	-	-	7/13/13/13	-
4	1PE	B	704	-	-	6/13/13/13	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	HDD	O1D-C3D	3.57	1.52	1.46
2	C	701	HDD	C3B-C2B	3.33	1.45	1.40
2	D	701	HDD	O1D-C3D	3.05	1.51	1.46
2	C	701	HDD	CBD-CGD	-2.76	1.44	1.50
2	D	701	HDD	CBD-CGD	-2.73	1.44	1.50
2	B	701	HDD	CAA-C2A	-2.72	1.48	1.52
2	C	701	HDD	OND-C2D	2.69	1.48	1.42
2	B	701	HDD	O1D-C3D	2.67	1.51	1.46
2	B	701	HDD	C1D-ND	-2.63	1.33	1.37
2	A	701	HDD	C3B-C2B	2.59	1.44	1.40
2	B	701	HDD	C2B-C1B	2.57	1.48	1.42
2	D	701	HDD	C3C-C2C	2.57	1.43	1.40
2	C	701	HDD	C1A-CHA	2.55	1.48	1.41
2	D	701	HDD	CAA-C2A	-2.47	1.48	1.52
2	A	701	HDD	CHA-C4D	-2.46	1.32	1.36
2	B	701	HDD	OND-C2D	2.45	1.47	1.42
4	C	703	1PE	OH7-C16	2.37	1.54	1.42
2	A	701	HDD	C3C-CAC	-2.31	1.43	1.47
2	B	701	HDD	C3B-C2B	2.31	1.43	1.40
2	A	701	HDD	OND-C2D	2.29	1.47	1.42
2	B	701	HDD	C1A-CHA	2.26	1.47	1.41
2	B	701	HDD	CBD-CGD	-2.26	1.45	1.50
2	B	701	HDD	C4C-NC	-2.21	1.31	1.36
2	D	701	HDD	C2A-C3A	2.21	1.44	1.37
2	A	701	HDD	C1A-CHA	2.21	1.47	1.41
2	B	701	HDD	FE-ND	2.17	2.04	1.95
2	C	701	HDD	CMD-C2D	-2.17	1.50	1.53
2	A	701	HDD	O1A-CGA	2.15	1.29	1.22
2	B	701	HDD	CMA-C3A	-2.12	1.47	1.51
2	D	701	HDD	C3B-C2B	2.09	1.43	1.40
2	A	701	HDD	CMD-C2D	-2.01	1.50	1.53
2	B	701	HDD	CMD-C2D	-2.01	1.50	1.53

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	HDD	OND-C2D-CMD	-6.31	97.97	109.59
2	B	701	HDD	C2B-C3B-C4B	6.22	111.24	106.90
2	C	701	HDD	C4A-C3A-C2A	-5.40	103.24	107.00
2	B	701	HDD	OND-C2D-CMD	-4.86	100.64	109.59
2	D	701	HDD	C4A-C3A-C2A	-4.40	103.94	107.00
2	A	701	HDD	C4A-C3A-C2A	-4.34	103.97	107.00
2	A	701	HDD	OND-C2D-CMD	-4.33	101.62	109.59
2	D	701	HDD	O1D-CGD-O2D	4.29	124.63	120.80
2	B	701	HDD	C4A-C3A-C2A	-4.11	104.13	107.00
2	A	701	HDD	C2D-C1D-CHD	-4.02	117.65	124.28
2	B	701	HDD	C2D-C1D-CHD	-3.99	117.69	124.28
2	C	701	HDD	OND-C2D-CMD	-3.63	102.91	109.59
2	B	701	HDD	CMB-C2B-C3B	3.49	131.20	124.68
2	C	701	HDD	O1D-CGD-CBD	3.46	113.67	110.19
2	A	701	HDD	CMC-C2C-C3C	3.34	130.93	124.68
2	C	701	HDD	C2D-C1D-CHD	-3.26	118.90	124.28
2	A	701	HDD	C4C-CHD-C1D	-3.13	123.93	130.12
2	C	701	HDD	C4C-CHD-C1D	-3.07	124.04	130.12
2	B	701	HDD	O1D-CGD-CBD	-3.06	107.11	110.19
2	D	701	HDD	C4C-CHD-C1D	-2.85	124.47	130.12
2	B	701	HDD	CMC-C2C-C3C	2.80	129.92	124.68
2	D	701	HDD	C2D-C1D-CHD	-2.75	119.74	124.28
2	A	701	HDD	O1D-C3D-CAD	-2.72	97.89	103.01
2	B	701	HDD	CAA-CBA-CGA	-2.70	106.19	113.76
2	D	701	HDD	CAA-CBA-CGA	-2.66	106.31	113.76
2	C	701	HDD	O1D-CGD-O2D	2.64	123.16	120.80
2	A	701	HDD	CAA-CBA-CGA	-2.60	106.47	113.76
2	C	701	HDD	C1A-CHA-C4D	-2.45	125.26	130.12
2	B	701	HDD	O2A-CGA-CBA	2.42	121.81	114.03
2	C	701	HDD	CMB-C2B-C3B	2.33	129.03	124.68
2	C	701	HDD	CMC-C2C-C3C	2.31	129.01	124.68
2	B	701	HDD	CMA-C3A-C2A	2.29	129.27	124.94
2	A	701	HDD	C1A-CHA-C4D	-2.28	125.59	130.12
2	A	701	HDD	O1D-CGD-O2D	-2.23	118.81	120.80
4	C	703	1PE	OH6-C26-C16	2.21	119.76	110.07
2	B	701	HDD	C1A-CHA-C4D	-2.14	125.87	130.12
2	A	701	HDD	C3D-C4D-CHA	-2.13	118.01	124.34
2	A	701	HDD	CMA-C3A-C2A	2.12	128.94	124.94
2	D	701	HDD	CHD-C1D-ND	2.11	127.30	124.20
2	D	701	HDD	C3C-C4C-NC	2.09	111.91	109.21
2	A	701	HDD	CMB-C2B-C3B	2.09	128.59	124.68
2	B	701	HDD	O1D-C3D-CAD	-2.07	99.11	103.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	HDD	CAA-CBA-CGA	-2.06	107.97	113.76

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	706[B]	1PE	C13-C23-OH3-C22
4	C	706[B]	1PE	C25-C15-OH6-C26
4	C	706[A]	1PE	C14-C24-OH4-C13
4	D	705[A]	1PE	C24-C14-OH5-C25
4	D	705[B]	1PE	C12-C22-OH3-C23
4	D	705[A]	1PE	OH2-C12-C22-OH3
4	D	704	1PE	C25-C15-OH6-C26
4	C	704	1PE	OH6-C15-C25-OH5
4	C	706[A]	1PE	C16-C26-OH6-C15
4	C	703	1PE	C12-C22-OH3-C23
4	C	706[A]	1PE	OH5-C14-C24-OH4
4	C	706[A]	1PE	OH6-C15-C25-OH5
4	D	704	1PE	OH5-C14-C24-OH4
4	C	705	1PE	OH4-C13-C23-OH3
4	D	704	1PE	OH6-C15-C25-OH5
4	C	705	1PE	C13-C23-OH3-C22
4	B	706	1PE	OH4-C13-C23-OH3
4	C	706[A]	1PE	OH7-C16-C26-OH6
4	D	704	1PE	OH2-C12-C22-OH3
4	C	706[B]	1PE	OH5-C14-C24-OH4
4	D	705[B]	1PE	OH5-C14-C24-OH4
4	C	706[B]	1PE	C23-C13-OH4-C24
4	B	704	1PE	OH2-C12-C22-OH3
4	C	703	1PE	OH7-C16-C26-OH6
4	B	704	1PE	OH5-C14-C24-OH4
4	C	704	1PE	OH7-C16-C26-OH6
4	C	705	1PE	C16-C26-OH6-C15
4	C	706[B]	1PE	OH6-C15-C25-OH5
4	C	706[B]	1PE	OH2-C12-C22-OH3
4	D	705[A]	1PE	OH7-C16-C26-OH6
4	C	703	1PE	C25-C15-OH6-C26
4	D	704	1PE	OH7-C16-C26-OH6
4	C	706[B]	1PE	OH4-C13-C23-OH3
4	C	706[B]	1PE	OH7-C16-C26-OH6
4	C	705	1PE	C25-C15-OH6-C26
4	B	706	1PE	OH7-C16-C26-OH6

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Mol	Chain	Res	Type	Atoms
4	B	704	1PE	C12-C22-OH3-C23
4	B	706	1PE	C14-C24-OH4-C13
4	D	705[B]	1PE	C15-C25-OH5-C14
4	D	704	1PE	C14-C24-OH4-C13
4	B	706	1PE	C23-C13-OH4-C24
4	C	706[A]	1PE	C12-C22-OH3-C23
4	B	704	1PE	OH7-C16-C26-OH6
4	D	705[A]	1PE	C25-C15-OH6-C26
4	C	706[A]	1PE	C13-C23-OH3-C22
4	D	705[B]	1PE	OH4-C13-C23-OH3
4	C	704	1PE	OH4-C13-C23-OH3
4	D	704	1PE	C23-C13-OH4-C24
4	C	704	1PE	C15-C25-OH5-C14
4	D	705[B]	1PE	OH2-C12-C22-OH3
4	D	705[B]	1PE	C16-C26-OH6-C15
4	D	705[A]	1PE	OH5-C14-C24-OH4
4	B	704	1PE	OH4-C13-C23-OH3
4	C	703	1PE	C23-C13-OH4-C24
4	D	705[B]	1PE	C13-C23-OH3-C22
4	D	705[B]	1PE	C14-C24-OH4-C13
4	B	704	1PE	C13-C23-OH3-C22
2	C	701	HDD	CAA-CBA-CGA-O2A
2	C	701	HDD	CAA-CBA-CGA-O1A
2	D	701	HDD	CAA-CBA-CGA-O1A
4	D	705[A]	1PE	C13-C23-OH3-C22
2	D	701	HDD	CAA-CBA-CGA-O2A
2	A	701	HDD	CAA-CBA-CGA-O2A
2	B	701	HDD	CAA-CBA-CGA-O1A
4	D	705[A]	1PE	OH4-C13-C23-OH3
2	B	701	HDD	CAA-CBA-CGA-O2A
4	C	703	1PE	OH5-C14-C24-OH4
4	C	705	1PE	C23-C13-OH4-C24
2	A	701	HDD	CAA-CBA-CGA-O1A
4	C	705	1PE	C24-C14-OH5-C25
4	C	703	1PE	OH6-C15-C25-OH5
4	C	705	1PE	OH6-C15-C25-OH5
4	D	704	1PE	C24-C14-OH5-C25
4	C	703	1PE	OH4-C13-C23-OH3
4	D	705[B]	1PE	C24-C14-OH5-C25
4	D	704	1PE	C13-C23-OH3-C22
4	B	705	1PE	C25-C15-OH6-C26
4	D	704	1PE	OH4-C13-C23-OH3

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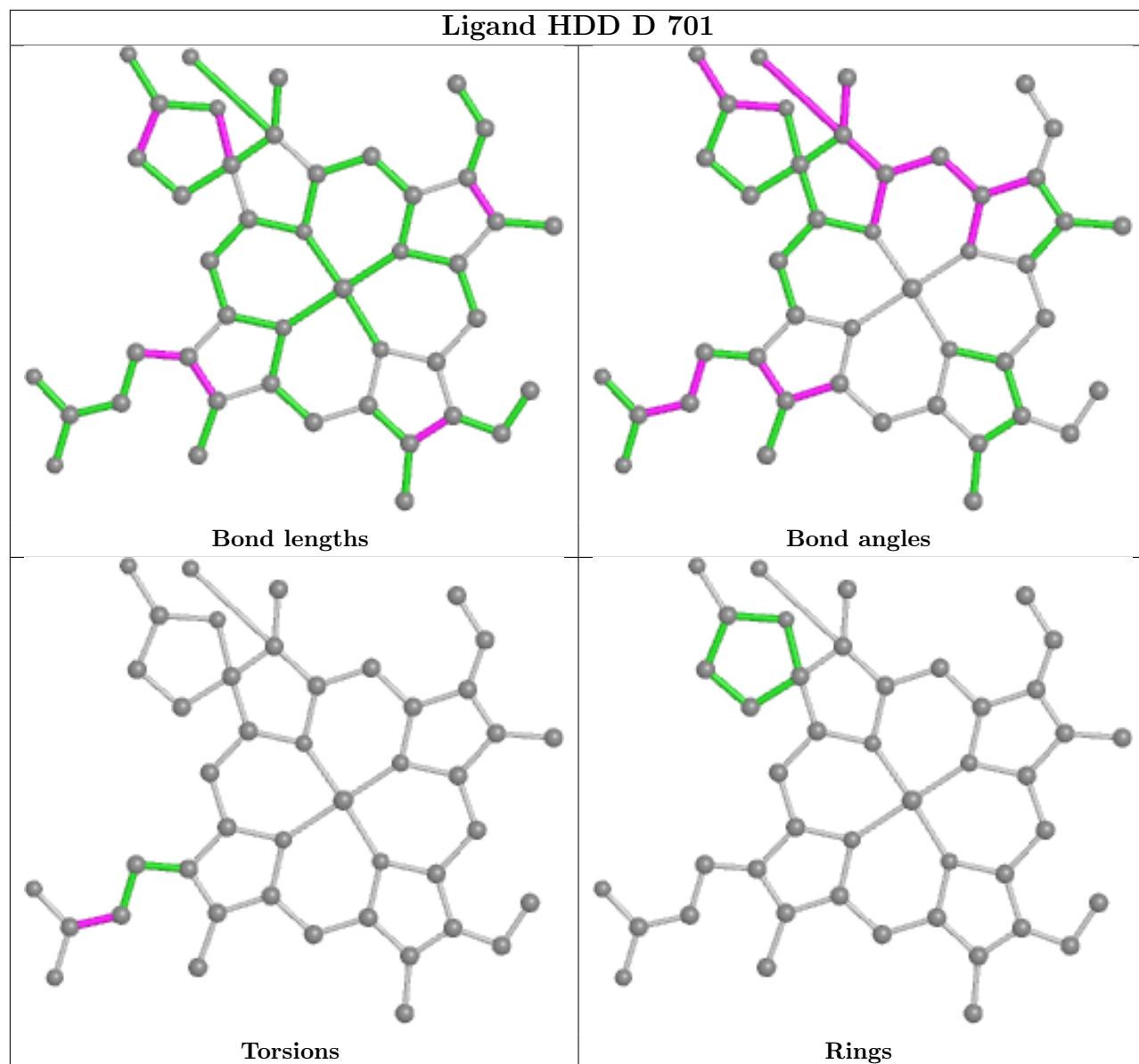
Mol	Chain	Res	Type	Atoms
4	C	706[A]	1PE	OH4-C13-C23-OH3
4	B	706	1PE	OH6-C15-C25-OH5
4	D	705[A]	1PE	OH6-C15-C25-OH5
4	C	706[B]	1PE	C12-C22-OH3-C23

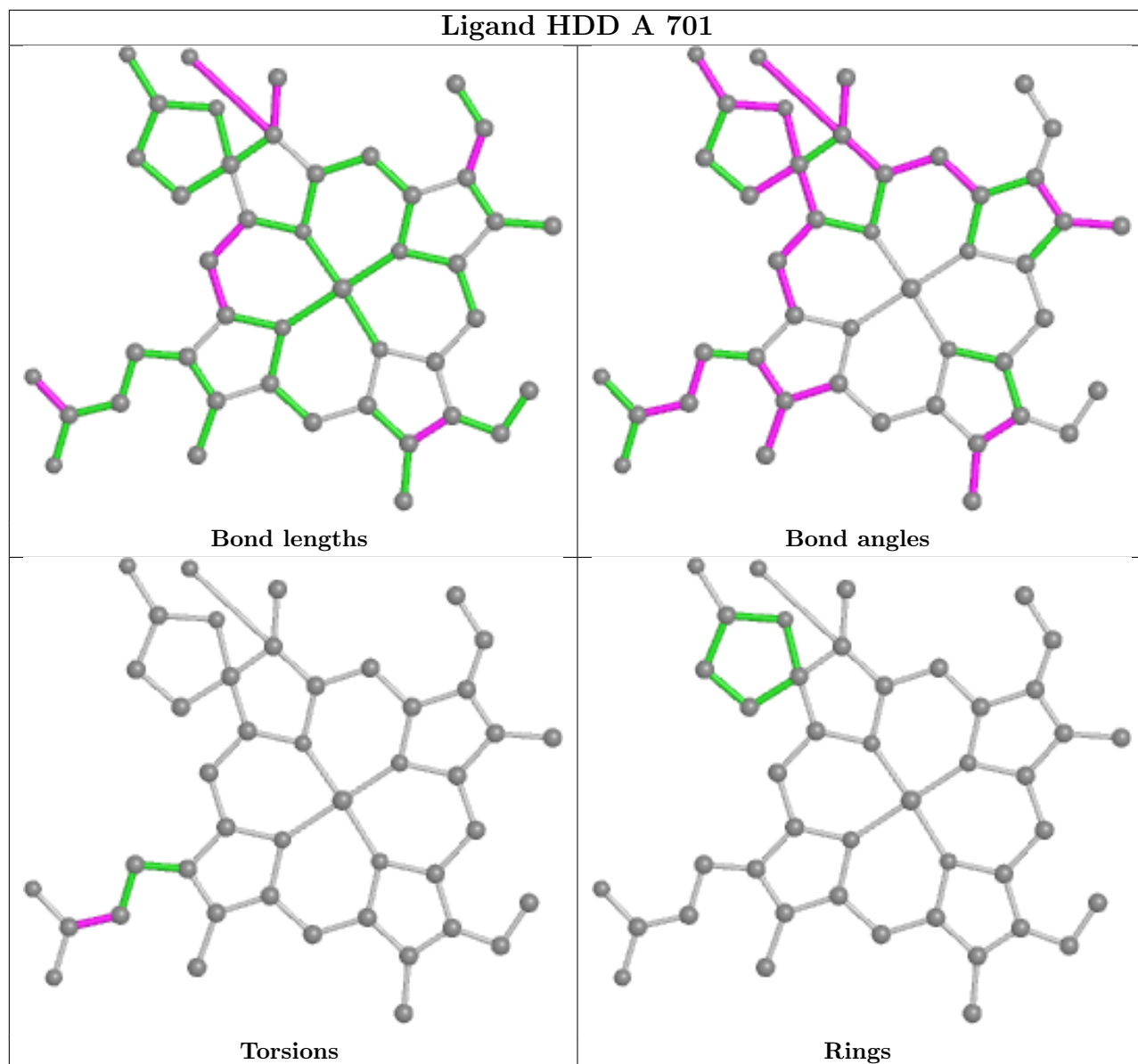
There are no ring outliers.

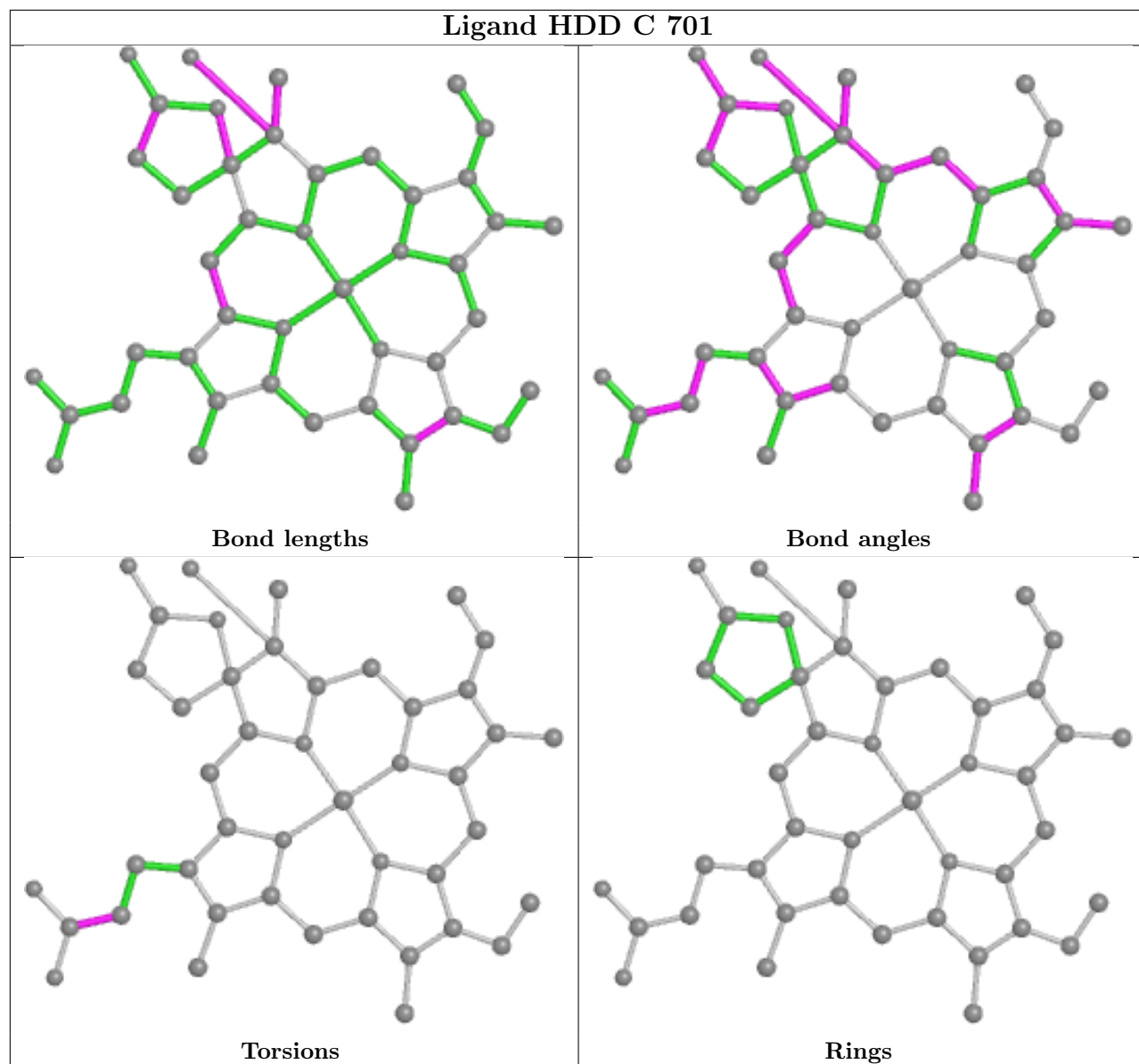
11 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	706[A]	1PE	2	0
2	D	701	HDD	3	0
2	A	701	HDD	2	0
4	D	705[A]	1PE	1	0
2	C	701	HDD	3	0
4	C	703	1PE	3	0
4	B	706	1PE	1	0
4	D	705[B]	1PE	15	0
2	B	701	HDD	2	0
4	C	706[B]	1PE	16	0
4	C	705	1PE	4	0

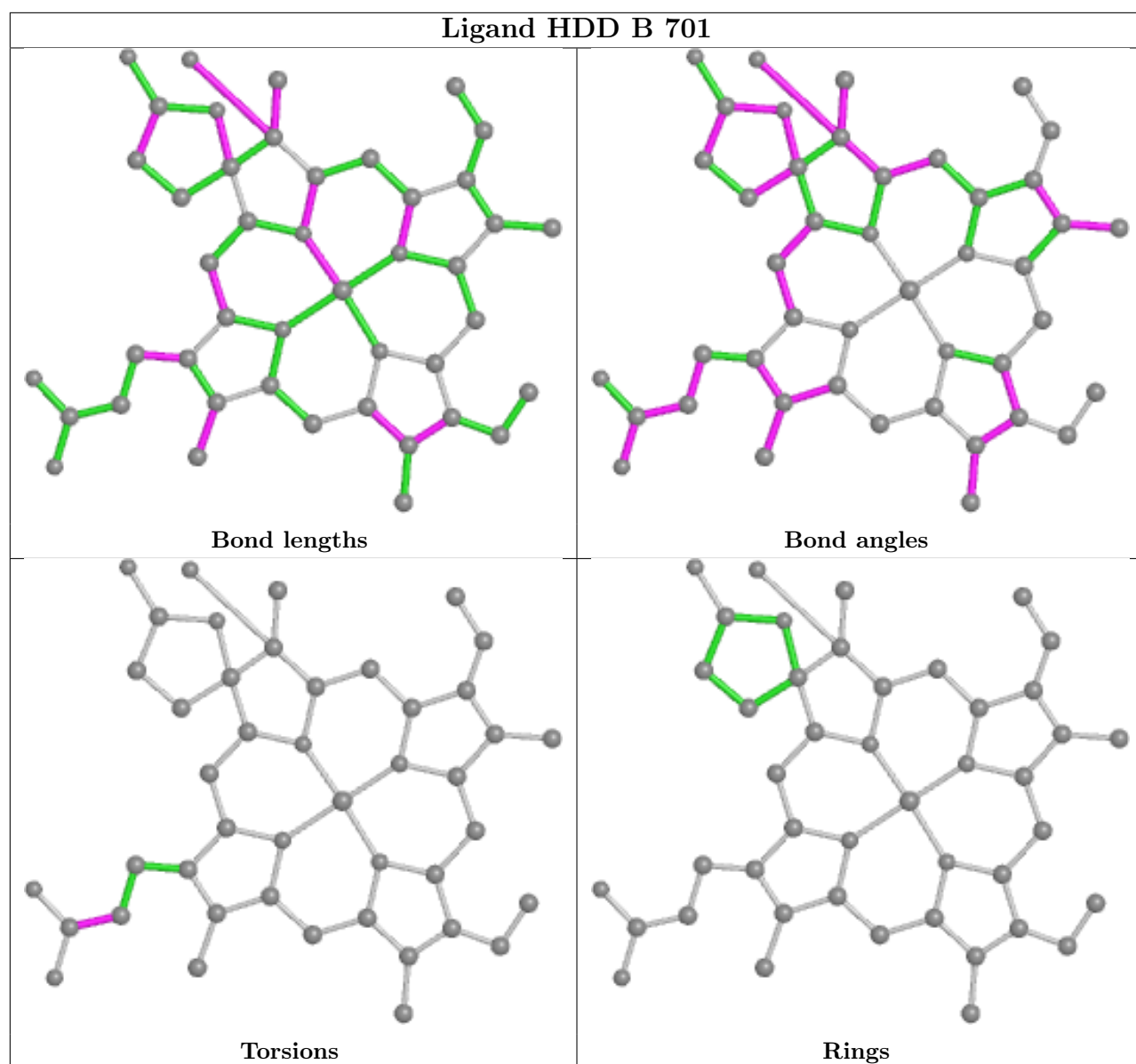
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	678/678 (100%)	-0.20	28 (4%) 37 40	6, 12, 32, 91	0
1	B	678/678 (100%)	-0.23	26 (3%) 40 44	5, 12, 32, 68	0
1	C	675/678 (99%)	-0.45	3 (0%) 92 94	5, 11, 21, 46	0
1	D	678/678 (100%)	-0.31	6 (0%) 84 86	6, 13, 26, 47	0
All	All	2709/2712 (99%)	-0.30	63 (2%) 60 65	5, 12, 28, 91	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	619	SER	5.6
1	B	655	VAL	5.4
1	B	653	SER	5.3
1	A	653	SER	5.0
1	A	651	LYS	4.8
1	A	655	VAL	4.6
1	D	620	THR	4.5
1	A	618	ALA	4.4
1	A	652	SER	4.4
1	B	652	SER	4.4
1	C	618	ALA	4.3
1	D	621	ALA	4.3
1	A	649	GLY	4.2
1	A	620	THR	4.0
1	A	573[A]	ARG	3.8
1	A	621	ALA	3.8
1	D	618	ALA	3.8
1	D	517	GLY	3.8
1	A	619	SER	3.7
1	B	657	ASP	3.6
1	B	658	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	654	GLU	3.4
1	B	649	GLY	3.4
1	B	651	LYS	3.3
1	A	672	GLU	3.3
1	B	561	SER	3.2
1	B	22	PRO	3.2
1	B	659	ALA	3.2
1	A	654	GLU	3.2
1	B	619	SER	3.1
1	B	660	ASP	3.0
1	B	611	ASP	2.9
1	A	676[A]	MET	2.9
1	A	648	CYS	2.9
1	B	620	THR	2.9
1	B	672	GLU	2.8
1	B	676	MET	2.8
1	C	561	SER	2.8
1	B	565[A]	ASP	2.7
1	B	650	GLY	2.6
1	A	657	ASP	2.6
1	A	24	ALA	2.5
1	B	681	PHE	2.4
1	A	658	ALA	2.4
1	B	674	VAL	2.3
1	A	660[A]	ASP	2.3
1	B	647	VAL	2.3
1	A	670[A]	SER	2.2
1	A	659	ALA	2.2
1	B	621	ALA	2.2
1	C	517	GLY	2.2
1	A	614	ALA	2.1
1	A	674	VAL	2.1
1	A	517	GLY	2.1
1	D	674	VAL	2.1
1	A	565	ASP	2.1
1	A	570	LEU	2.1
1	B	618	ALA	2.0
1	A	677	PHE	2.0
1	A	656	LEU	2.0
1	B	517	GLY	2.0
1	B	559[A]	SER	2.0
1	A	613	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

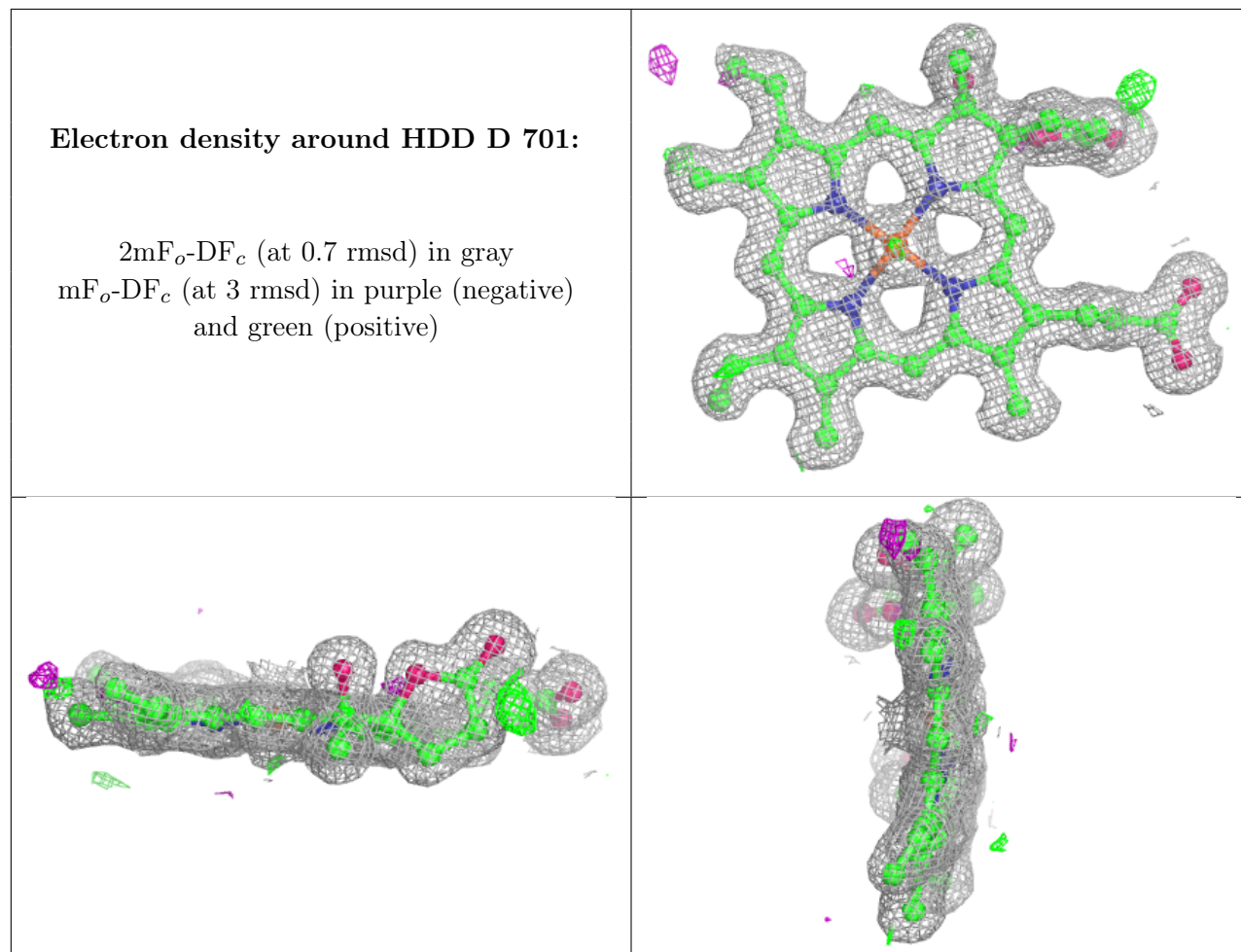
## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	1PE	D	705[A]	16/16	0.61	0.28	22,24,28,29	16
4	1PE	D	705[B]	16/16	0.61	0.28	18,33,38,38	16
4	1PE	C	706[A]	16/16	0.67	0.26	20,28,32,33	16
4	1PE	C	706[B]	16/16	0.67	0.26	14,24,32,33	16
4	1PE	B	706	16/16	0.68	0.26	46,61,80,83	0
4	1PE	D	704	16/16	0.75	0.24	44,62,75,77	0
4	1PE	C	705	16/16	0.76	0.27	35,39,62,68	0
4	1PE	B	704	16/16	0.78	0.21	46,62,77,84	0
4	1PE	B	705	16/16	0.80	0.26	34,45,58,59	0
4	1PE	C	704	16/16	0.82	0.25	41,50,75,75	0
4	1PE	C	703	16/16	0.85	0.17	17,23,39,42	0
3	CA	D	703	1/1	0.98	0.08	15,15,15,15	1
3	CA	B	703	1/1	0.98	0.04	26,26,26,26	0
2	HDD	D	701	44/44	0.99	0.08	7,9,13,17	0
3	CA	A	703	1/1	0.99	0.08	10,10,10,10	1
3	CA	A	704	1/1	0.99	0.04	16,16,16,16	1
3	CA	A	705	1/1	0.99	0.04	11,11,11,11	1
3	CA	A	706	1/1	0.99	0.04	21,21,21,21	0
3	CA	B	702	1/1	0.99	0.08	8,8,8,8	1
2	HDD	A	701	44/44	0.99	0.07	7,8,13,18	0
3	CA	C	702	1/1	0.99	0.06	14,14,14,14	1
2	HDD	B	701	44/44	0.99	0.07	7,9,13,17	0
2	HDD	C	701	44/44	0.99	0.08	5,8,12,15	0
3	CA	A	702	1/1	1.00	0.02	10,10,10,10	0
3	CA	D	702	1/1	1.00	0.02	14,14,14,14	0

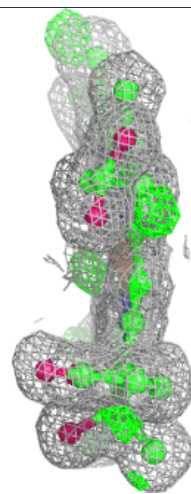
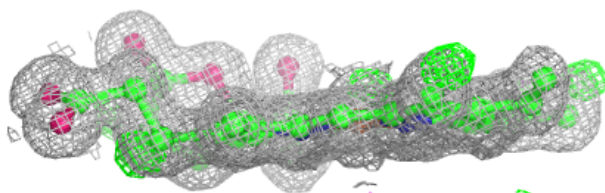
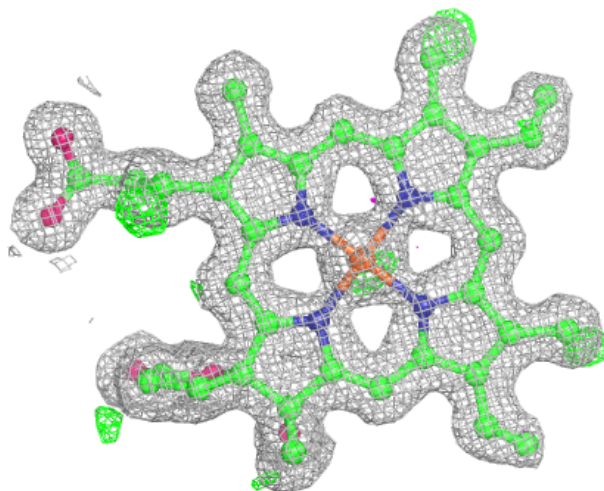
The following is a graphical depiction of the model fit to experimental electron density of all

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.



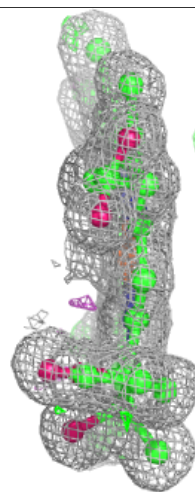
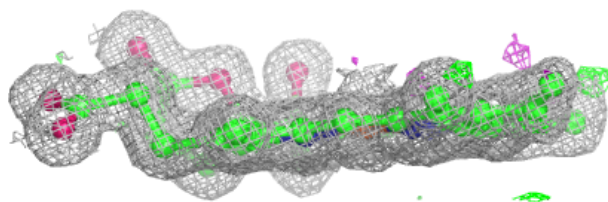
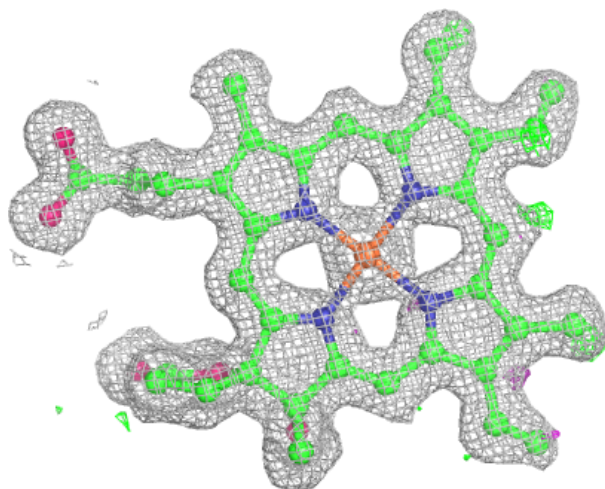
**Electron density around HDD A 701:**

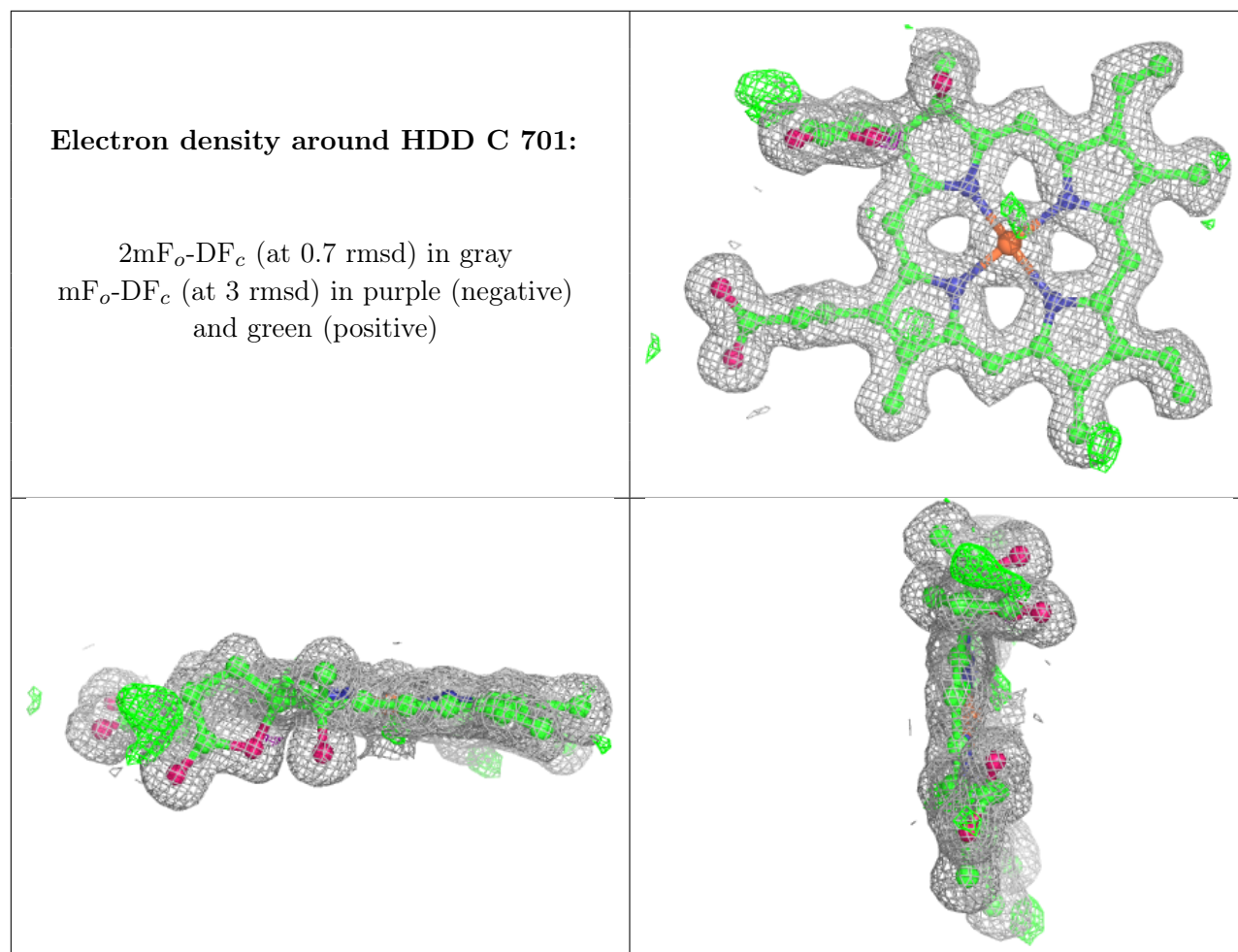
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.