



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 11:24 AM JST

PDB ID : 5ZZ1 / pdb_00005zz1
Title : Probing the active center of catalase-phenol oxidase from *Scytalidium thermophilum*
Authors : Yuzugullu Karakus, Y.; Trinh, C.H.; Pearson, A.R.; Ogel, Z.B.; McPherson, M.J.
Deposited on : 2018-05-29
Resolution : 1.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

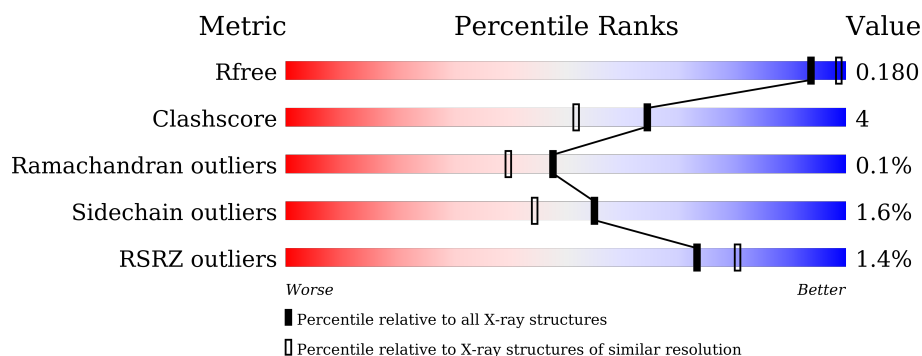
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	719	2% 83% 10% 6%
1	B	719	2% 86% 7% 6%
1	C	719	0% 84% 9% 6%
1	D	719	0% 86% 8% 6%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HDD	A	701	X	-	-	-
2	HDD	C	701	X	-	-	-
2	HDD	D	701	X	-	-	-
3	3TR	A	703	-	X	-	-
3	3TR	B	1704	-	X	-	-
3	3TR	B	1706	-	X	-	-
3	3TR	C	703	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23217 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	677	Total	C	N	O	S	0	14	0
			5372	3397	940	1023	12			
1	B	678	Total	C	N	O	S	0	4	0
			5314	3356	930	1017	11			
1	C	678	Total	C	N	O	S	0	6	0
			5327	3365	931	1019	12			
1	D	678	Total	C	N	O	S	0	7	0
			5329	3363	932	1022	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	GLY	-	expression tag	UNP M4GGR7
A	-19	SER	-	expression tag	UNP M4GGR7
A	-18	SER	-	expression tag	UNP M4GGR7
A	-17	HIS	-	expression tag	UNP M4GGR7
A	-16	HIS	-	expression tag	UNP M4GGR7
A	-15	HIS	-	expression tag	UNP M4GGR7
A	-14	HIS	-	expression tag	UNP M4GGR7
A	-13	HIS	-	expression tag	UNP M4GGR7
A	-12	HIS	-	expression tag	UNP M4GGR7
A	-11	SER	-	expression tag	UNP M4GGR7
A	-10	SER	-	expression tag	UNP M4GGR7
A	-9	GLY	-	expression tag	UNP M4GGR7
A	-8	GLU	-	expression tag	UNP M4GGR7
A	-7	ASN	-	expression tag	UNP M4GGR7
A	-6	LEU	-	expression tag	UNP M4GGR7
A	-5	TYR	-	expression tag	UNP M4GGR7
A	-4	PHE	-	expression tag	UNP M4GGR7
A	-3	GLN	-	expression tag	UNP M4GGR7
A	-2	GLY	-	expression tag	UNP M4GGR7
A	-1	HIS	-	expression tag	UNP M4GGR7
B	-20	GLY	-	expression tag	UNP M4GGR7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	SER	-	expression tag	UNP M4GGR7
B	-18	SER	-	expression tag	UNP M4GGR7
B	-17	HIS	-	expression tag	UNP M4GGR7
B	-16	HIS	-	expression tag	UNP M4GGR7
B	-15	HIS	-	expression tag	UNP M4GGR7
B	-14	HIS	-	expression tag	UNP M4GGR7
B	-13	HIS	-	expression tag	UNP M4GGR7
B	-12	HIS	-	expression tag	UNP M4GGR7
B	-11	SER	-	expression tag	UNP M4GGR7
B	-10	SER	-	expression tag	UNP M4GGR7
B	-9	GLY	-	expression tag	UNP M4GGR7
B	-8	GLU	-	expression tag	UNP M4GGR7
B	-7	ASN	-	expression tag	UNP M4GGR7
B	-6	LEU	-	expression tag	UNP M4GGR7
B	-5	TYR	-	expression tag	UNP M4GGR7
B	-4	PHE	-	expression tag	UNP M4GGR7
B	-3	GLN	-	expression tag	UNP M4GGR7
B	-2	GLY	-	expression tag	UNP M4GGR7
B	-1	HIS	-	expression tag	UNP M4GGR7
C	-20	GLY	-	expression tag	UNP M4GGR7
C	-19	SER	-	expression tag	UNP M4GGR7
C	-18	SER	-	expression tag	UNP M4GGR7
C	-17	HIS	-	expression tag	UNP M4GGR7
C	-16	HIS	-	expression tag	UNP M4GGR7
C	-15	HIS	-	expression tag	UNP M4GGR7
C	-14	HIS	-	expression tag	UNP M4GGR7
C	-13	HIS	-	expression tag	UNP M4GGR7
C	-12	HIS	-	expression tag	UNP M4GGR7
C	-11	SER	-	expression tag	UNP M4GGR7
C	-10	SER	-	expression tag	UNP M4GGR7
C	-9	GLY	-	expression tag	UNP M4GGR7
C	-8	GLU	-	expression tag	UNP M4GGR7
C	-7	ASN	-	expression tag	UNP M4GGR7
C	-6	LEU	-	expression tag	UNP M4GGR7
C	-5	TYR	-	expression tag	UNP M4GGR7
C	-4	PHE	-	expression tag	UNP M4GGR7
C	-3	GLN	-	expression tag	UNP M4GGR7
C	-2	GLY	-	expression tag	UNP M4GGR7
C	-1	HIS	-	expression tag	UNP M4GGR7
D	-20	GLY	-	expression tag	UNP M4GGR7
D	-19	SER	-	expression tag	UNP M4GGR7
D	-18	SER	-	expression tag	UNP M4GGR7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	HIS	-	expression tag	UNP M4GGR7
D	-16	HIS	-	expression tag	UNP M4GGR7
D	-15	HIS	-	expression tag	UNP M4GGR7
D	-14	HIS	-	expression tag	UNP M4GGR7
D	-13	HIS	-	expression tag	UNP M4GGR7
D	-12	HIS	-	expression tag	UNP M4GGR7
D	-11	SER	-	expression tag	UNP M4GGR7
D	-10	SER	-	expression tag	UNP M4GGR7
D	-9	GLY	-	expression tag	UNP M4GGR7
D	-8	GLU	-	expression tag	UNP M4GGR7
D	-7	ASN	-	expression tag	UNP M4GGR7
D	-6	LEU	-	expression tag	UNP M4GGR7
D	-5	TYR	-	expression tag	UNP M4GGR7
D	-4	PHE	-	expression tag	UNP M4GGR7
D	-3	GLN	-	expression tag	UNP M4GGR7
D	-2	GLY	-	expression tag	UNP M4GGR7
D	-1	HIS	-	expression tag	UNP M4GGR7

- # HDD
-

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

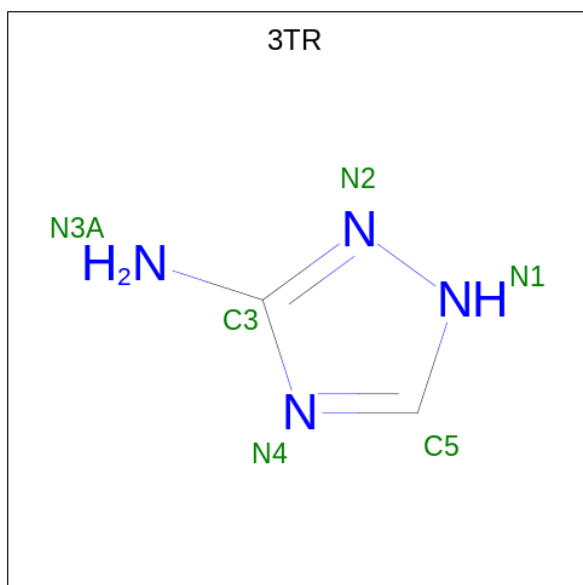


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PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 3-AMINO-1,2,4-TRIAZOLE (CCD ID: 3TR) (formula: C₂H₄N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			6	2	4		
3	A	1	Total	C	N	0	0
			6	2	4		
3	B	1	Total	C	N	0	0
			6	2	4		
3	B	1	Total	C	N	0	0
			6	2	4		
3	C	1	Total	C	N	0	0
			6	2	4		
3	C	1	Total	C	N	0	0
			6	2	4		
3	D	1	Total	C	N	0	0
			6	2	4		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

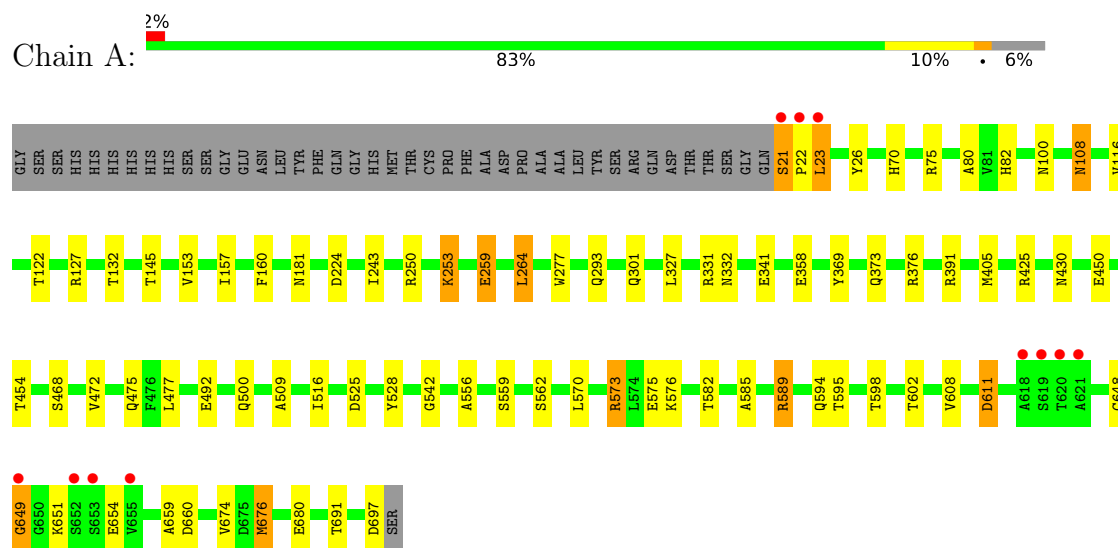
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	409	Total 409	O 409	0	0
5	B	411	Total 411	O 411	0	0
5	C	432	Total 432	O 432	0	0
5	D	394	Total 394	O 394	0	0

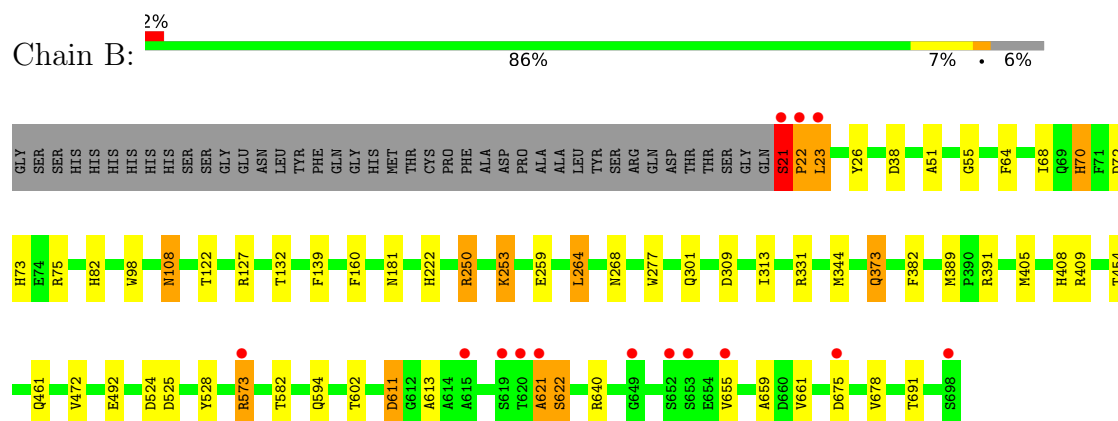
3 Residue-property plots

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.

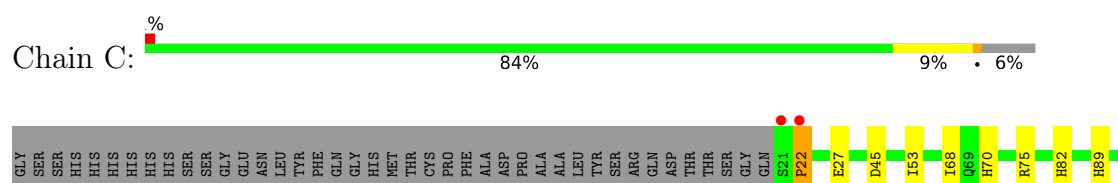
• Molecule 1: Catalase

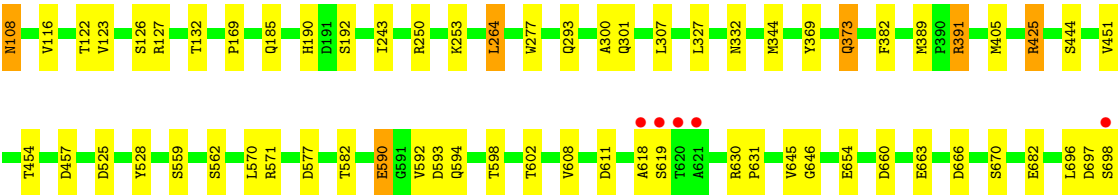


• Molecule 1: Catalase

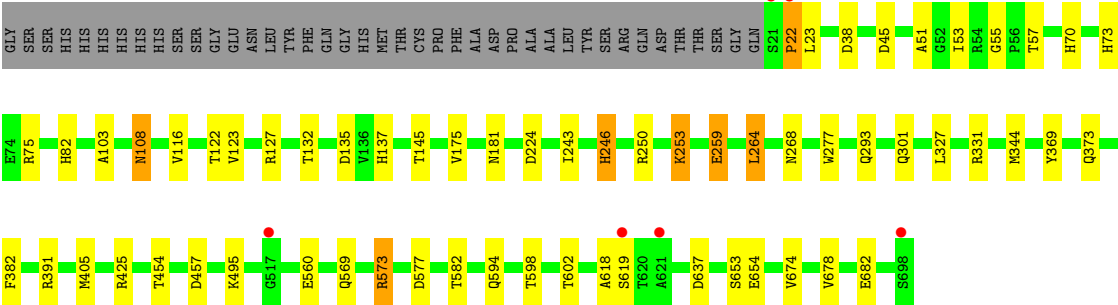
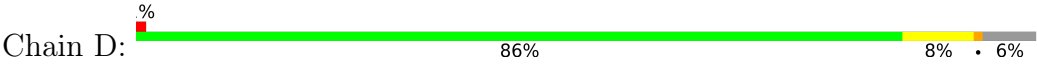


• Molecule 1: Catalase





● 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	125.53Å 121.68Å 185.45Å 90.00° 102.16° 90.00°	Depositor
Resolution (Å)	29.40 – 1.91 29.40 – 1.91	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.40-1.91) 98.8 (29.40-1.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 1.92Å)	Xtrriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.142 , 0.174 0.152 , 0.180	Depositor DCC
R_{free} test set	10381 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtrriage
Anisotropy	0.068	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	23217	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 38.66 % 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 3.5656e-04. 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, HDD, 3TR

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	1.09	12/5539 (0.2%)	1.11	10/7530 (0.1%)
1	B	1.08	8/5457 (0.1%)	1.13	13/7420 (0.2%)
1	C	1.14	15/5473 (0.3%)	1.14	10/7443 (0.1%)
1	D	1.10	10/5476 (0.2%)	1.12	8/7445 (0.1%)
All	All	1.10	45/21945 (0.2%)	1.12	41/29838 (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	6
1	B	0	6
1	C	0	4
1	D	0	3
All	All	0	19

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	621	ALA	C-O	-8.95	1.12	1.24
1	D	73	HIS	CE1-NE2	7.10	1.39	1.32
1	B	73	HIS	CE1-NE2	6.95	1.39	1.32
1	C	618	ALA	N-CA	6.83	1.55	1.46
1	D	618	ALA	N-CA	6.79	1.54	1.46
1	A	542	GLY	N-CA	6.74	1.53	1.44
1	C	89	HIS	CE1-NE2	6.61	1.39	1.32
1	D	23	LEU	N-CA	-6.45	1.38	1.46
1	A	516	ILE	C-O	-6.42	1.14	1.24
1	B	622	SER	N-CA	6.41	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	268	ASN	C-O	6.35	1.29	1.23
1	A	576	LYS	C-O	-6.31	1.16	1.24
1	C	190	HIS	CE1-NE2	6.23	1.38	1.32
1	A	80	ALA	N-CA	6.16	1.54	1.46
1	C	590	GLU	C-O	-5.86	1.16	1.23
1	C	169	PRO	C-O	5.82	1.30	1.24
1	B	222	HIS	CE1-NE2	5.75	1.38	1.32
1	C	619	SER	N-CA	5.73	1.53	1.46
1	D	103	ALA	C-O	-5.67	1.16	1.24
1	C	592	VAL	C-O	-5.55	1.18	1.24
1	B	72	ASP	CG-OD2	5.54	1.35	1.25
1	C	68	ILE	C-O	-5.53	1.17	1.24
1	A	509	ALA	C-O	-5.44	1.17	1.24
1	A	153	VAL	N-CA	-5.33	1.39	1.46
1	C	192	SER	N-CA	5.32	1.52	1.46
1	C	451	VAL	C-O	-5.31	1.18	1.24
1	D	246	HIS	CE1-NE2	-5.30	1.27	1.32
1	B	250	ARG	C-O	-5.30	1.17	1.24
1	B	408	HIS	CE1-NE2	5.27	1.37	1.32
1	B	268	ASN	C-O	5.27	1.28	1.23
1	A	575	GLU	C-O	-5.23	1.17	1.24
1	C	696	LEU	C-O	-5.22	1.17	1.23
1	A	430	ASN	C-O	-5.22	1.17	1.24
1	A	556	ALA	N-CA	-5.21	1.39	1.46
1	A	468	SER	C-O	-5.19	1.17	1.24
1	C	646	GLY	N-CA	-5.18	1.40	1.45
1	D	619	SER	N-CA	5.18	1.52	1.46
1	D	137	HIS	C-O	-5.17	1.17	1.24
1	D	637	ASP	C-O	-5.13	1.18	1.24
1	A	341	GLU	CD-OE2	5.12	1.35	1.25
1	C	645	VAL	C-O	5.11	1.29	1.24
1	C	22	PRO	C-O	-5.07	1.17	1.24
1	A	674	VAL	N-CA	-5.06	1.40	1.46
1	D	57	THR	C-O	5.06	1.30	1.23
1	C	660	ASP	C-O	-5.06	1.17	1.23

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	611	ASP	CA-CB-CG	9.21	121.81	112.60
1	D	259	GLU	CB-CG-CD	9.16	128.17	112.60
1	B	21	SER	O-C-N	-8.37	109.61	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	590	GLU	CB-CG-CD	8.32	126.74	112.60
1	D	674	VAL	N-CA-CB	7.61	118.96	110.51
1	A	21	SER	O-C-N	-7.25	111.40	123.00
1	A	259	GLU	CB-CG-CD	6.84	124.23	112.60
1	C	22	PRO	O-C-N	6.44	129.97	122.17
1	B	259	GLU	CB-CG-CD	6.36	123.42	112.60
1	B	21	SER	CA-CB-OG	-6.34	98.42	111.10
1	B	22	PRO	CB-CA-C	-6.21	101.31	111.56
1	D	45	ASP	CA-CB-CG	6.20	118.80	112.60
1	C	425	ARG	CG-CD-NE	-6.18	98.41	112.00
1	D	135	ASP	CA-CB-CG	6.08	118.68	112.60
1	C	611	ASP	CA-CB-CG	6.04	118.64	112.60
1	C	654	GLU	CB-CA-C	-5.92	100.78	110.85
1	D	224	ASP	CA-CB-CG	5.92	118.52	112.60
1	D	259	GLU	CB-CA-C	-5.78	99.93	110.63
1	B	611	ASP	CA-CB-CG	5.71	118.31	112.60
1	C	22	PRO	CB-CA-C	-5.69	102.76	112.26
1	A	23	LEU	N-CA-C	-5.67	105.18	111.36
1	B	21	SER	CA-C-O	5.67	130.43	120.80
1	D	22	PRO	CB-CA-C	-5.65	103.40	112.21
1	A	157	ILE	CB-CA-C	5.63	115.59	110.13
1	A	358	GLU	CB-CG-CD	5.57	122.07	112.60
1	B	139	PHE	CA-CB-CG	5.53	119.33	113.80
1	C	559	SER	CB-CA-C	-5.50	101.34	110.68
1	C	697	ASP	CA-C-O	-5.45	115.77	121.55
1	A	500	GLN	CB-CG-CD	5.39	121.77	112.60
1	B	492	GLU	CB-CG-CD	5.37	121.73	112.60
1	A	391	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	C	45	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	391	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	B	309	ASP	CB-CA-C	5.22	115.34	110.17
1	B	573	ARG	N-CA-CB	-5.21	102.46	110.12
1	A	654	GLU	N-CA-CB	-5.09	102.39	110.28
1	B	98	TRP	CA-C-N	5.09	127.36	120.38
1	B	98	TRP	C-N-CA	5.09	127.36	120.38
1	A	224	ASP	CA-CB-CG	5.08	117.68	112.60
1	D	674	VAL	CB-CA-C	-5.04	105.43	111.88
1	C	391	ARG	NE-CZ-NH2	5.03	123.73	119.20

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	250	ARG	Sidechain
1	A	425[A]	ARG	Sidechain
1	A	573	ARG	Sidechain
1	A	589[A]	ARG	Sidechain
1	A	589[B]	ARG	Sidechain
1	A	75	ARG	Sidechain
1	B	21	SER	Peptide
1	B	250	ARG	Sidechain
1	B	331	ARG	Sidechain
1	B	409	ARG	Sidechain
1	B	640	ARG	Sidechain
1	B	75	ARG	Sidechain
1	C	127[A]	ARG	Sidechain
1	C	250	ARG	Sidechain
1	C	425	ARG	Sidechain
1	C	75	ARG	Sidechain
1	D	250	ARG	Sidechain
1	D	425	ARG	Sidechain
1	D	75	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	5372	0	5178	53	0
1	B	5314	0	5094	39	1
1	C	5327	0	5108	40	0
1	D	5329	0	5113	34	0
2	A	44	0	31	4	0
2	B	44	0	31	0	0
2	C	44	0	31	0	0
2	D	44	0	31	1	0
3	A	12	0	8	0	0
3	B	18	0	12	0	0
3	C	12	0	8	1	0
3	D	6	0	4	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
5	A	409	0	0	17	0
5	B	411	0	0	10	0
5	C	432	0	0	8	0
5	D	394	0	0	9	0
All	All	23217	0	20649	164	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 (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589[B]:ARG:HH11	1:A:589[B]:ARG:CG	1.42	1.26
1:B:127[B]:ARG:NH2	5:B:1802:HOH:O	1.65	1.26
1:B:21:SER:HA	5:B:2086:HOH:O	1.41	1.20
1:A:589[B]:ARG:HG2	1:A:589[B]:ARG:NH1	1.27	1.19
1:D:127[A]:ARG:O	5:D:801:HOH:O	1.77	1.03
1:B:389:MET:SD	5:B:2144:HOH:O	2.19	1.00
1:B:313:ILE:H	1:B:461:GLN:HE22	1.20	0.88
1:C:663:GLU:OE1	5:C:801:HOH:O	1.91	0.88
2:A:701:HDD:HBD2	5:A:803:HOH:O	1.73	0.88
1:A:676:MET:SD	5:A:983:HOH:O	2.36	0.84
2:A:701:HDD:CGD	5:A:803:HOH:O	2.26	0.83
1:A:648:CYS:SG	5:A:873:HOH:O	2.35	0.83
2:A:701:HDD:CBD	5:A:803:HOH:O	2.27	0.82
3:C:703:3TR:H5	5:C:1071:HOH:O	1.79	0.81
1:C:253:LYS:HD2	5:C:1203:HOH:O	1.82	0.80
1:A:253:LYS:HG2	5:A:1109:HOH:O	1.83	0.79
1:A:475:GLN:NE2	1:A:697:ASP:H	1.81	0.78
1:A:127[B]:ARG:O	5:A:802:HOH:O	2.02	0.77
1:A:160:PHE:CD1	5:A:1167:HOH:O	2.38	0.75
1:B:70:HIS:CD2	5:B:1863:HOH:O	2.38	0.75
1:B:253:LYS:HE3	5:B:1955:HOH:O	1.88	0.74
1:D:253:LYS:HG3	5:D:1138:HOH:O	1.87	0.74
1:B:655:VAL:HG23	5:B:2065:HOH:O	1.89	0.73
1:B:264:LEU:HG	1:B:602:THR:HB	1.72	0.72
1:D:22:PRO:HB3	1:D:391:ARG:NH2	2.05	0.72
1:A:264:LEU:HG	1:A:602:THR:HB	1.73	0.70
1:C:373:GLN:HE21	1:C:373:GLN:HA	1.57	0.69
1:A:582:THR:HG21	1:A:594:GLN:HE21	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589[B]:ARG:CG	1:A:589[B]:ARG:NH1	2.14	0.69
1:B:373:GLN:HE21	1:B:373:GLN:HA	1.56	0.69
1:D:654:GLU:OE1	5:D:802:HOH:O	2.11	0.68
1:C:22:PRO:HB3	1:C:391:ARG:NH2	2.10	0.66
1:C:253:LYS:HG2	5:C:1202:HOH:O	1.96	0.66
1:B:38:ASP:OD2	1:B:70:HIS:HE1	1.76	0.66
1:B:389:MET:HE3	5:B:2211:HOH:O	1.95	0.66
1:A:100:ASN:HB2	5:A:1183:HOH:O	1.96	0.65
1:D:264:LEU:HG	1:D:602:THR:HB	1.78	0.65
1:A:373:GLN:HE21	1:A:373:GLN:HA	1.61	0.64
1:A:160:PHE:CE1	5:A:1167:HOH:O	2.51	0.64
1:B:22:PRO:O	1:B:26:TYR:HD2	1.82	0.62
1:C:126:SER:H	1:C:185:GLN:HE22	1.49	0.61
1:C:264:LEU:HG	1:C:602:THR:HB	1.81	0.60
1:C:570:LEU:HD11	1:C:608:VAL:HG11	1.84	0.60
1:B:160:PHE:CE1	5:B:2186:HOH:O	2.54	0.60
1:C:70:HIS:CE1	5:C:805:HOH:O	2.55	0.59
1:C:253:LYS:CG	5:C:1202:HOH:O	2.50	0.59
1:B:277[A]:TRP:CZ3	1:D:181:ASN:HB3	2.39	0.58
1:D:582:THR:HG21	1:D:594:GLN:HE21	1.69	0.58
1:B:160:PHE:CD1	5:B:2186:HOH:O	2.53	0.57
1:A:108:ASN:C	1:A:108:ASN:HD22	2.13	0.57
1:A:676:MET:HE2	1:A:676:MET:HA	1.86	0.57
1:A:181:ASN:HB3	1:C:277[A]:TRP:CZ3	2.40	0.56
1:A:611:ASP:CG	1:A:649:GLY:HA3	2.30	0.56
1:B:181:ASN:HB3	1:D:277:TRP:CZ3	2.40	0.56
1:B:38:ASP:OD2	1:B:70:HIS:CE1	2.58	0.56
1:B:573:ARG:HG3	1:B:678:VAL:HG11	1.86	0.55
1:B:132:THR:HG21	1:B:264:LEU:HD13	1.89	0.54
1:B:277[A]:TRP:CE3	1:D:181:ASN:HB3	2.42	0.54
1:C:132:THR:HG21	1:C:264:LEU:HD13	1.89	0.54
1:D:132:THR:HG21	1:D:264:LEU:HD13	1.89	0.54
1:A:259:GLU:HG3	5:A:1097:HOH:O	2.06	0.54
1:C:126:SER:H	1:C:185:GLN:NE2	2.05	0.54
1:B:108:ASN:C	1:B:108:ASN:HD22	2.16	0.54
1:A:680:GLU:HG3	5:A:894:HOH:O	2.07	0.54
1:D:560:GLU:CD	5:D:957:HOH:O	2.51	0.54
1:B:253:LYS:HD2	5:B:2182:HOH:O	2.07	0.53
1:A:132:THR:HG21	1:A:264:LEU:HD13	1.91	0.53
1:D:301:GLN:HE22	1:D:454:THR:HG21	1.73	0.52
1:C:22:PRO:CB	1:C:391:ARG:NH2	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PRO:O	1:A:26:TYR:HD2	1.94	0.51
1:B:405:MET:HE2	1:C:405:MET:HE2	1.92	0.51
1:C:82:HIS:HA	1:C:122:THR:O	2.11	0.51
1:C:108:ASN:C	1:C:108:ASN:HD22	2.18	0.51
1:C:301:GLN:HE22	1:C:454:THR:HG21	1.76	0.50
1:A:475:GLN:HE22	1:A:697:ASP:H	1.54	0.50
1:D:108:ASN:HD22	1:D:108:ASN:C	2.21	0.49
1:A:525:ASP:HA	1:A:528:TYR:CD2	2.47	0.49
1:A:376:ARG:CD	5:A:803:HOH:O	2.61	0.49
1:A:582:THR:HG21	1:A:594:GLN:NE2	2.28	0.48
1:A:82:HIS:HA	1:A:122:THR:O	2.13	0.48
1:C:27:GLU:OE2	5:C:802:HOH:O	2.20	0.48
1:C:594:GLN:HG3	1:C:598:THR:OG1	2.14	0.48
1:C:670:SER:HB2	5:C:1122:HOH:O	2.14	0.48
1:D:82:HIS:HA	1:D:122:THR:O	2.14	0.48
1:B:301:GLN:HE22	1:B:454:THR:HG21	1.79	0.48
1:D:82:HIS:CE1	1:D:123:VAL:HG22	2.48	0.48
1:C:373:GLN:HE21	1:C:373:GLN:CA	2.22	0.47
1:A:181:ASN:HB3	1:C:277[A]:TRP:CE3	2.50	0.47
1:B:373:GLN:HA	1:B:373:GLN:NE2	2.27	0.47
1:A:570:LEU:HD11	1:A:608:VAL:HG11	1.95	0.47
1:B:313:ILE:N	1:B:461:GLN:HE22	1.99	0.47
1:D:51:ALA:O	1:D:55:GLY:HA3	2.14	0.47
1:A:450[B]:GLU:HB2	1:C:53:ILE:CD1	2.45	0.47
1:B:82:HIS:HA	1:B:122:THR:O	2.14	0.47
1:C:82:HIS:CE1	1:C:123:VAL:HG22	2.49	0.47
1:C:300:ALA:HA	1:C:307:LEU:HD12	1.97	0.47
1:D:331:ARG:HD3	5:D:1122:HOH:O	2.14	0.47
1:C:389[B]:MET:HE3	1:C:389[B]:MET:HB3	1.76	0.47
2:D:701:HDD:HMD3	2:D:701:HDD:HAD2	1.78	0.46
1:D:243:ILE:HA	1:D:293:GLN:O	2.15	0.46
1:A:659:ALA:O	1:A:660:ASP:HB2	2.15	0.46
1:C:577:ASP:OD2	1:C:682:GLU:OE2	2.33	0.46
1:A:100:ASN:CB	5:A:1183:HOH:O	2.60	0.46
1:A:676:MET:O	1:A:680:GLU:HG2	2.14	0.46
1:B:472:VAL:HG11	1:B:691:THR:HB	1.98	0.46
1:A:277[A]:TRP:CH2	1:A:332:ASN:HB3	2.51	0.46
1:A:680:GLU:HA	1:A:680:GLU:OE1	2.16	0.46
1:A:594:GLN:HG3	1:A:598:THR:OG1	2.16	0.45
1:C:457:ASP:OD1	1:C:457:ASP:C	2.59	0.45
1:A:116:VAL:HG21	1:A:327[A]:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:ASP:HA	1:B:528:TYR:CD2	2.51	0.45
1:A:277[A]:TRP:CZ3	1:A:332:ASN:HB3	2.52	0.45
1:B:23:LEU:N	1:B:23:LEU:HD23	2.31	0.45
1:D:246:HIS:HD2	5:D:1091:HOH:O	1.99	0.45
1:D:573[B]:ARG:NH1	1:D:577:ASP:OD2	2.45	0.45
1:A:108:ASN:C	1:A:108:ASN:ND2	2.74	0.45
1:A:369:TYR:O	1:A:373:GLN:HG2	2.17	0.45
1:D:344:MET:SD	1:D:382:PHE:HB2	2.57	0.45
1:D:457:ASP:C	1:D:457:ASP:OD1	2.59	0.45
1:A:373:GLN:HA	1:A:373:GLN:NE2	2.31	0.44
1:D:495:LYS:HE2	5:D:1180:HOH:O	2.17	0.44
1:A:585:ALA:O	1:A:595:THR:HA	2.18	0.44
1:B:51:ALA:O	1:B:55:GLY:HA3	2.18	0.44
1:C:369:TYR:O	1:C:373:GLN:HG2	2.18	0.44
1:A:376:ARG:HD2	5:A:803:HOH:O	2.17	0.44
1:C:571:ARG:NH2	1:C:593:ASP:OD2	2.38	0.44
1:D:38:ASP:OD2	1:D:70:HIS:NE2	2.49	0.44
1:B:573:ARG:HG2	1:B:678:VAL:HG21	2.00	0.44
1:C:373:GLN:HA	1:C:373:GLN:NE2	2.29	0.44
1:D:253:LYS:CG	5:D:1138:HOH:O	2.55	0.43
2:A:701:HDD:O2D	5:A:803:HOH:O	2.21	0.43
1:A:243:ILE:HA	1:A:293:GLN:O	2.18	0.43
1:D:175:VAL:HB	5:D:829:HOH:O	2.17	0.43
1:D:301:GLN:NE2	1:D:454:THR:HG21	2.33	0.43
1:B:344:MET:SD	1:B:382:PHE:HB2	2.58	0.43
1:B:659:ALA:HB1	1:B:661:VAL:HG23	2.00	0.43
1:D:577:ASP:OD2	1:D:682:GLU:OE2	2.37	0.42
1:B:582:THR:HG21	1:B:594:GLN:HE21	1.84	0.42
1:C:630:ARG:HB3	1:C:631:PRO:HD3	2.01	0.42
1:D:22:PRO:CB	1:D:391:ARG:NH2	2.78	0.42
1:C:116:VAL:HG21	1:C:327:LEU:HD11	2.00	0.42
1:D:594:GLN:HG3	1:D:598:THR:OG1	2.18	0.42
1:A:301:GLN:NE2	1:A:454:THR:HG21	2.34	0.42
1:C:277[A]:TRP:CZ3	1:C:332:ASN:HB3	2.54	0.42
1:C:582:THR:HG21	1:C:594:GLN:HE21	1.83	0.42
1:A:331[B]:ARG:HH21	1:A:331[B]:ARG:HD3	1.66	0.42
1:A:405:MET:HE2	1:D:405:MET:HE2	2.01	0.42
1:D:369:TYR:O	1:D:373:GLN:HG2	2.20	0.41
1:B:611:ASP:C	1:B:613:ALA:H	2.29	0.41
1:A:492[A]:GLU:CG	5:A:838:HOH:O	2.67	0.41
1:C:373:GLN:CA	1:C:373:GLN:NE2	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:VAL:HG21	1:D:327:LEU:HD11	2.02	0.41
1:B:108:ASN:C	1:B:108:ASN:ND2	2.77	0.41
1:A:477:LEU:HD23	1:A:477:LEU:C	2.46	0.41
1:C:525:ASP:HA	1:C:528:TYR:CD2	2.56	0.41
1:A:472:VAL:HG11	1:A:691:THR:HB	2.02	0.41
1:C:243:ILE:HA	1:C:293:GLN:O	2.21	0.41
1:D:573[B]:ARG:HG3	1:D:678:VAL:HG11	2.02	0.41
1:B:64:PHE:CZ	1:B:68:ILE:HG13	2.56	0.40
1:B:573:ARG:CG	1:B:678:VAL:HG21	2.52	0.40
1:A:589[B]:ARG:HH11	1:A:589[B]:ARG:HG2	0.48	0.40
1:C:344:MET:SD	1:C:382:PHE:HB2	2.61	0.40
1:A:331[A]:ARG:NH2	1:A:331[A]:ARG:HG2	2.36	0.40
1:A:301:GLN:HE22	1:A:454:THR:HG21	1.86	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:21:SER:OG	1:B:675:ASP:OD2[2_555]	1.72	0.48

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	689/719 (96%)	671 (97%)	17 (2%)	1 (0%)	48	40
1	B	680/719 (95%)	656 (96%)	22 (3%)	2 (0%)	36	26
1	C	682/719 (95%)	661 (97%)	21 (3%)	0	100	100
1	D	683/719 (95%)	665 (97%)	18 (3%)	0	100	100
All	All	2734/2876 (95%)	2653 (97%)	78 (3%)	3 (0%)	48	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	622	SER
1	B	621	ALA
1	A	649	GLY

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	574/596 (96%)	562 (98%)	12 (2%)	47	33
1	B	565/596 (95%)	558 (99%)	7 (1%)	63	57
1	C	567/596 (95%)	559 (99%)	8 (1%)	59	50
1	D	568/596 (95%)	558 (98%)	10 (2%)	51	39
All	All	2274/2384 (95%)	2237 (98%)	37 (2%)	55	44

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	23	LEU
1	A	70	HIS
1	A	108	ASN
1	A	145	THR
1	A	253	LYS
1	A	264	LEU
1	A	559	SER
1	A	562	SER
1	A	573	ARG
1	A	651	LYS
1	A	676	MET
1	B	23	LEU
1	B	70	HIS
1	B	108	ASN
1	B	253	LYS
1	B	264	LEU
1	B	373	GLN
1	B	524	ASP

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Mol	Chain	Res	Type
1	C	108	ASN
1	C	264	LEU
1	C	373	GLN
1	C	444	SER
1	C	562	SER
1	C	590	GLU
1	C	666	ASP
1	C	698	SER
1	D	53	ILE
1	D	108	ASN
1	D	145	THR
1	D	253	LYS
1	D	259	GLU
1	D	264	LEU
1	D	569	GLN
1	D	573[A]	ARG
1	D	573[B]	ARG
1	D	653	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	301	GLN
1	A	346	GLN
1	A	373	GLN
1	A	475	GLN
1	A	594	GLN
1	B	70	HIS
1	B	108	ASN
1	B	167	GLN
1	B	301	GLN
1	B	342	GLN
1	B	346	GLN
1	B	373	GLN
1	B	375	ASN
1	B	461	GLN
1	B	594	GLN
1	C	46	GLN
1	C	108	ASN
1	C	185	GLN
1	C	301	GLN

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Mol	Chain	Res	Type
1	C	342	GLN
1	C	373	GLN
1	C	375	ASN
1	C	429	GLN
1	C	594	GLN
1	D	108	ASN
1	D	113	GLN
1	D	246	HIS
1	D	293	GLN
1	D	301	GLN
1	D	375	ASN
1	D	594	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](#)

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HDD	C	701	1,5	50,52,52	2.46	21 (42%)	56,89,89	2.39	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	3TR	C	702	-	6,6,6	1.37	1 (16%)	7,7,7	0.80	0
3	3TR	A	702	-	6,6,6	1.82	3 (50%)	7,7,7	0.78	0
3	3TR	B	1706	-	6,6,6	3.14	5 (83%)	7,7,7	1.89	3 (42%)
3	3TR	B	1703	-	6,6,6	2.09	3 (50%)	7,7,7	0.82	0
2	HDD	B	1702	1	50,52,52	2.37	23 (46%)	56,89,89	2.59	16 (28%)
2	HDD	D	701	1,5	50,52,52	2.31	21 (42%)	56,89,89	2.72	21 (37%)
3	3TR	B	1704	-	6,6,6	3.43	5 (83%)	7,7,7	1.50	2 (28%)
3	3TR	C	703	-	6,6,6	3.46	5 (83%)	7,7,7	2.36	2 (28%)
2	HDD	A	701	1,5	50,52,52	2.32	19 (38%)	56,89,89	2.43	20 (35%)
3	3TR	A	703	-	6,6,6	3.32	4 (66%)	7,7,7	1.73	2 (28%)
3	3TR	D	702	-	6,6,6	1.46	1 (16%)	7,7,7	1.30	1 (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
2	HDD	C	701	1,5	1/1/8/14	2/9/89/89	0/1/9/9
3	3TR	C	702	-	-	-	0/1/1/1
3	3TR	A	702	-	-	-	0/1/1/1
3	3TR	B	1706	-	-	-	0/1/1/1
3	3TR	B	1703	-	-	-	0/1/1/1
2	HDD	B	1702	1	-	2/9/89/89	0/1/9/9
2	HDD	D	701	1,5	1/1/8/14	2/9/89/89	0/1/9/9
3	3TR	B	1704	-	-	-	0/1/1/1
3	3TR	C	703	-	-	-	0/1/1/1
2	HDD	A	701	1,5	1/1/8/14	2/9/89/89	0/1/9/9
3	3TR	A	703	-	-	-	0/1/1/1
3	3TR	D	702	-	-	-	0/1/1/1

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	3TR	C3-N2	6.04	1.40	1.33
3	B	1706	3TR	C3-N2	5.90	1.40	1.33
3	C	703	3TR	C3-N2	5.84	1.40	1.33
2	C	701	HDD	C4A-NA	-5.47	1.29	1.39
2	A	701	HDD	CHD-C4C	5.09	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1704	3TR	C3-N2	5.02	1.39	1.33
2	D	701	HDD	OND-C2D	4.94	1.52	1.42
2	B	1702	HDD	C3B-C2B	4.82	1.47	1.37
2	B	1702	HDD	CHC-C4B	4.64	1.49	1.39
2	C	701	HDD	CHA-C1A	4.55	1.49	1.39
2	C	701	HDD	CHC-C1C	4.53	1.47	1.38
2	C	701	HDD	C1C-NC	-4.30	1.31	1.39
2	A	701	HDD	C3C-C2C	4.30	1.46	1.37
2	B	1702	HDD	FE-NB	4.27	2.08	1.94
2	C	701	HDD	C1B-NB	-4.26	1.33	1.40
2	C	701	HDD	FE-NB	4.25	2.08	1.94
2	B	1702	HDD	CHA-C1A	4.18	1.48	1.39
2	A	701	HDD	CHA-C1A	4.18	1.48	1.39
2	A	701	HDD	FE-NC	4.16	2.09	1.95
2	D	701	HDD	FE-NB	4.14	2.07	1.94
2	A	701	HDD	FE-NB	4.09	2.07	1.94
2	A	701	HDD	CHB-C1B	4.08	1.46	1.38
2	D	701	HDD	C1A-NA	-4.05	1.31	1.39
2	C	701	HDD	CHD-C4C	4.01	1.46	1.38
2	C	701	HDD	FE-NC	4.00	2.08	1.95
2	A	701	HDD	C3B-C2B	4.00	1.45	1.37
2	A	701	HDD	C4C-NC	-3.99	1.32	1.39
2	B	1702	HDD	FE-NA	3.94	2.08	1.95
2	D	701	HDD	C1B-NB	-3.90	1.33	1.40
3	B	1704	3TR	N1-N2	3.89	1.42	1.36
2	C	701	HDD	C1A-NA	-3.76	1.32	1.39
2	B	1702	HDD	FE-NC	3.74	2.07	1.95
2	C	701	HDD	CHB-C4A	3.73	1.47	1.39
2	A	701	HDD	CHC-C1C	3.69	1.45	1.38
2	D	701	HDD	C4A-NA	-3.68	1.32	1.39
3	B	1704	3TR	C5-N1	3.67	1.41	1.32
2	D	701	HDD	CHD-C4C	3.66	1.45	1.38
2	D	701	HDD	CHA-C1A	3.66	1.47	1.39
2	A	701	HDD	C1A-NA	-3.65	1.32	1.39
2	A	701	HDD	OND-C2D	3.50	1.49	1.42
3	C	703	3TR	C3-N3A	3.46	1.44	1.34
2	D	701	HDD	C3B-C2B	3.45	1.44	1.37
2	B	1702	HDD	CHC-C1C	3.41	1.45	1.38
2	D	701	HDD	CHD-C1D	-3.38	1.31	1.41
2	B	1702	HDD	O1D-CGD	3.37	1.41	1.35
2	D	701	HDD	CHB-C4A	3.37	1.47	1.39
2	D	701	HDD	C3C-C2C	3.37	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	703	3TR	N1-N2	3.36	1.41	1.36
2	C	701	HDD	C3B-C2B	3.35	1.44	1.37
2	C	701	HDD	OND-C2D	3.35	1.49	1.42
2	D	701	HDD	C4C-NC	-3.31	1.33	1.39
2	B	1702	HDD	CHD-C4C	3.27	1.44	1.38
3	A	703	3TR	N1-N2	3.25	1.41	1.36
2	B	1702	HDD	C4A-NA	-3.25	1.33	1.39
2	C	701	HDD	CMD-C2D	-3.21	1.48	1.53
2	D	701	HDD	C4B-NB	-3.20	1.32	1.38
2	D	701	HDD	FE-NC	3.18	2.05	1.95
2	B	1702	HDD	OND-C2D	3.16	1.48	1.42
2	D	701	HDD	CBD-CGD	-3.10	1.43	1.50
2	A	701	HDD	C1C-NC	-3.10	1.33	1.39
2	A	701	HDD	CHD-C1D	-3.08	1.32	1.41
2	B	1702	HDD	C1C-NC	-3.07	1.33	1.39
2	B	1702	HDD	C4C-NC	-3.04	1.33	1.39
2	C	701	HDD	FE-NA	3.03	2.05	1.95
3	B	1703	3TR	C5-N4	3.02	1.40	1.33
3	B	1703	3TR	C3-N2	3.01	1.37	1.33
2	B	1702	HDD	C1A-NA	-2.99	1.34	1.39
3	B	1704	3TR	C3-N4	2.88	1.41	1.37
2	A	701	HDD	FE-NA	2.86	2.04	1.95
2	C	701	HDD	CHB-C1B	2.85	1.44	1.38
3	B	1706	3TR	C5-N1	2.83	1.39	1.32
2	D	701	HDD	CHB-C1B	2.82	1.44	1.38
2	C	701	HDD	CHC-C4B	2.80	1.45	1.39
3	A	703	3TR	C5-N1	2.79	1.39	1.32
2	B	1702	HDD	CHB-C1B	2.79	1.44	1.38
2	B	1702	HDD	FE-ND	2.77	2.03	1.94
3	A	702	3TR	C3-N4	-2.76	1.33	1.37
2	D	701	HDD	FE-NA	2.75	2.04	1.95
2	D	701	HDD	CMB-C2B	-2.71	1.45	1.50
2	C	701	HDD	C4C-NC	-2.70	1.34	1.39
3	C	703	3TR	C3-N4	2.69	1.41	1.37
3	B	1704	3TR	C3-N3A	2.68	1.42	1.34
3	A	703	3TR	C3-N3A	2.61	1.41	1.34
3	B	1706	3TR	N1-N2	2.60	1.40	1.36
2	A	701	HDD	FE-ND	2.57	2.02	1.94
2	D	701	HDD	CHC-C4B	2.55	1.45	1.39
2	A	701	HDD	C1B-NB	-2.55	1.35	1.40
2	B	1702	HDD	CMD-C2D	-2.55	1.49	1.53
2	C	701	HDD	CBD-CGD	-2.51	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	HDD	CHD-C1D	-2.49	1.34	1.41
2	A	701	HDD	C1D-ND	2.43	1.37	1.35
2	D	701	HDD	CHC-C1C	2.40	1.43	1.38
2	A	701	HDD	C4A-NA	-2.39	1.35	1.39
2	B	1702	HDD	CBA-CGA	2.29	1.55	1.50
2	B	1702	HDD	C1B-C2B	2.28	1.49	1.44
2	B	1702	HDD	CHB-C4A	2.26	1.44	1.39
3	B	1703	3TR	N1-N2	2.24	1.39	1.36
3	A	702	3TR	N1-N2	2.23	1.39	1.36
3	B	1706	3TR	C5-N4	2.21	1.38	1.33
3	C	703	3TR	C5-N1	2.20	1.38	1.32
2	B	1702	HDD	O1D-C3D	2.18	1.50	1.46
2	C	701	HDD	O1D-CGD	2.13	1.39	1.35
2	C	701	HDD	O1A-CGA	2.13	1.29	1.22
2	B	1702	HDD	C3C-C4C	2.13	1.49	1.46
2	A	701	HDD	CHB-C4A	2.09	1.44	1.39
3	A	702	3TR	C3-N2	2.06	1.35	1.33
3	D	702	3TR	C5-N1	2.06	1.37	1.32
2	D	701	HDD	FE-ND	2.04	2.01	1.94
2	B	1702	HDD	O1A-CGA	2.04	1.28	1.22
3	C	702	3TR	N1-N2	2.00	1.39	1.36
3	B	1706	3TR	C3-N3A	2.00	1.40	1.34

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1702	HDD	C3B-C2B-C1B	-10.03	99.04	106.49
2	A	701	HDD	C3C-C2C-C1C	-8.94	98.54	107.08
2	D	701	HDD	C3C-C2C-C1C	-8.31	99.14	107.08
2	D	701	HDD	C3B-C2B-C1B	-7.60	100.85	106.49
2	B	1702	HDD	C3C-C2C-C1C	-7.09	100.30	107.08
2	D	701	HDD	O1D-CGD-CBD	-6.74	103.39	110.19
2	C	701	HDD	C3C-C2C-C1C	-6.46	100.91	107.08
2	A	701	HDD	C3B-C2B-C1B	-6.43	101.71	106.49
2	B	1702	HDD	O1D-CGD-CBD	-6.08	104.05	110.19
2	C	701	HDD	OND-C2D-CMD	-5.79	98.92	109.59
2	C	701	HDD	C3B-C2B-C1B	-5.44	102.45	106.49
2	B	1702	HDD	O1D-CGD-O2D	5.34	125.57	120.80
2	C	701	HDD	C2B-C1B-NB	5.33	116.16	109.84
3	C	703	3TR	N3A-C3-N4	5.32	129.53	121.47
2	C	701	HDD	O1D-CGD-O2D	5.19	125.43	120.80
2	D	701	HDD	C2B-C1B-NB	5.12	115.91	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	HDD	C2B-C1B-NB	4.88	115.62	109.84
2	B	1702	HDD	C2B-C1B-NB	4.87	115.61	109.84
2	D	701	HDD	O1D-CGD-O2D	4.79	125.08	120.80
2	D	701	HDD	C4A-C3A-C2A	-4.59	101.46	106.83
2	D	701	HDD	OND-C2D-CMD	-4.26	101.75	109.59
2	B	1702	HDD	C2C-C1C-NC	4.23	117.50	109.69
2	A	701	HDD	C2C-C1C-NC	3.92	116.92	109.69
2	B	1702	HDD	CAA-CBA-CGA	-3.87	105.28	113.60
2	A	701	HDD	OND-C2D-CMD	-3.86	102.48	109.59
2	C	701	HDD	C4B-C3B-C2B	-3.80	104.10	107.11
2	D	701	HDD	CMB-C2B-C1B	3.76	130.76	125.04
2	C	701	HDD	O1D-CGD-CBD	-3.73	106.43	110.19
2	C	701	HDD	CAD-CBD-CGD	3.66	110.22	104.56
2	D	701	HDD	C2D-C1D-CHD	-3.61	117.62	123.33
2	C	701	HDD	C2C-C1C-NC	3.59	116.31	109.69
2	D	701	HDD	CAA-CBA-CGA	-3.43	106.22	113.60
2	D	701	HDD	CAD-CBD-CGD	3.38	109.79	104.56
2	A	701	HDD	CAA-C2A-C1A	3.34	131.47	124.89
2	D	701	HDD	C2C-C1C-NC	3.33	115.83	109.69
2	A	701	HDD	CMC-C2C-C1C	3.28	130.50	124.71
2	D	701	HDD	C3A-C4A-NA	3.28	115.07	110.08
2	B	1702	HDD	OND-C2D-CMD	-3.28	103.56	109.59
2	B	1702	HDD	CHC-C1C-C2C	-3.26	118.64	125.48
2	C	701	HDD	C2D-C1D-CHD	-3.20	118.27	123.33
2	A	701	HDD	CHC-C1C-C2C	-3.17	118.83	125.48
2	C	701	HDD	C1A-C2A-C3A	-3.13	101.97	106.89
2	A	701	HDD	O1D-CGD-CBD	-3.04	107.12	110.19
2	A	701	HDD	CHB-C1B-NB	-2.93	120.76	124.37
2	A	701	HDD	C2D-C1D-CHD	-2.79	118.92	123.33
2	A	701	HDD	C4A-C3A-C2A	-2.74	103.62	106.83
2	D	701	HDD	CHB-C4A-C3A	-2.73	119.52	127.24
2	D	701	HDD	C4C-C3C-C2C	2.70	108.97	106.75
3	B	1706	3TR	N1-C5-N4	-2.69	105.90	110.78
3	A	703	3TR	N1-C5-N4	-2.66	105.94	110.78
2	C	701	HDD	CHB-C4A-C3A	-2.65	119.75	127.24
2	C	701	HDD	CAA-C2A-C1A	2.61	130.03	124.89
2	C	701	HDD	CHB-C1B-NB	-2.61	121.16	124.37
2	C	701	HDD	CAA-CBA-CGA	-2.58	108.05	113.60
2	D	701	HDD	CMA-C3A-C4A	2.57	129.28	125.37
2	B	1702	HDD	CMB-C2B-C1B	2.55	128.93	125.04
2	B	1702	HDD	C2D-C1D-CHD	-2.55	119.30	123.33
2	D	701	HDD	CMC-C2C-C1C	2.54	129.18	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1702	HDD	C4A-NA-C1A	2.51	107.80	105.35
2	A	701	HDD	CAA-CBA-CGA	-2.49	108.24	113.60
2	A	701	HDD	CHB-C4A-C3A	-2.47	120.26	127.24
3	D	702	3TR	N3A-C3-N4	-2.45	117.75	121.47
3	B	1704	3TR	N1-C5-N4	-2.42	106.37	110.78
2	C	701	HDD	C3A-C4A-NA	2.42	113.77	110.08
3	B	1706	3TR	N3A-C3-N4	-2.42	117.81	121.47
2	C	701	HDD	C2A-C1A-NA	2.41	112.84	110.15
2	C	701	HDD	CMB-C2B-C1B	2.41	128.71	125.04
2	A	701	HDD	C4B-C3B-C2B	-2.37	105.23	107.11
2	D	701	HDD	C4B-C3B-C2B	-2.36	105.24	107.11
2	A	701	HDD	CAC-C3C-C4C	-2.36	119.20	124.90
3	C	703	3TR	N3A-C3-N2	-2.35	119.33	123.48
2	A	701	HDD	O1A-CGA-CBA	-2.33	115.60	123.08
2	A	701	HDD	O1D-C3D-CAD	-2.26	98.77	103.01
2	C	701	HDD	CHC-C1C-C2C	-2.24	120.79	125.48
3	B	1704	3TR	C5-N4-C3	2.22	106.83	102.10
2	B	1702	HDD	CAA-C2A-C1A	2.19	129.21	124.89
2	B	1702	HDD	CHB-C1B-NB	-2.18	121.69	124.37
3	B	1706	3TR	N3A-C3-N2	2.15	127.27	123.48
2	A	701	HDD	C2A-C1A-NA	2.12	112.52	110.15
2	B	1702	HDD	O1D-C3D-CAD	-2.08	99.10	103.01
2	B	1702	HDD	CAC-C3C-C4C	-2.08	119.87	124.90
2	D	701	HDD	CAC-C3C-C4C	-2.07	119.90	124.90
2	D	701	HDD	CHC-C1C-C2C	-2.06	121.16	125.48
2	A	701	HDD	C3A-C4A-NA	2.06	113.22	110.08
2	D	701	HDD	C2A-C1A-NA	2.02	112.40	110.15
3	A	703	3TR	C5-N4-C3	2.00	106.37	102.10

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	701	HDD	NC
2	C	701	HDD	NC
2	D	701	HDD	NC

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1702	HDD	CAA-CBA-CGA-O2A
2	C	701	HDD	CAA-CBA-CGA-O2A
2	A	701	HDD	CAA-CBA-CGA-O2A

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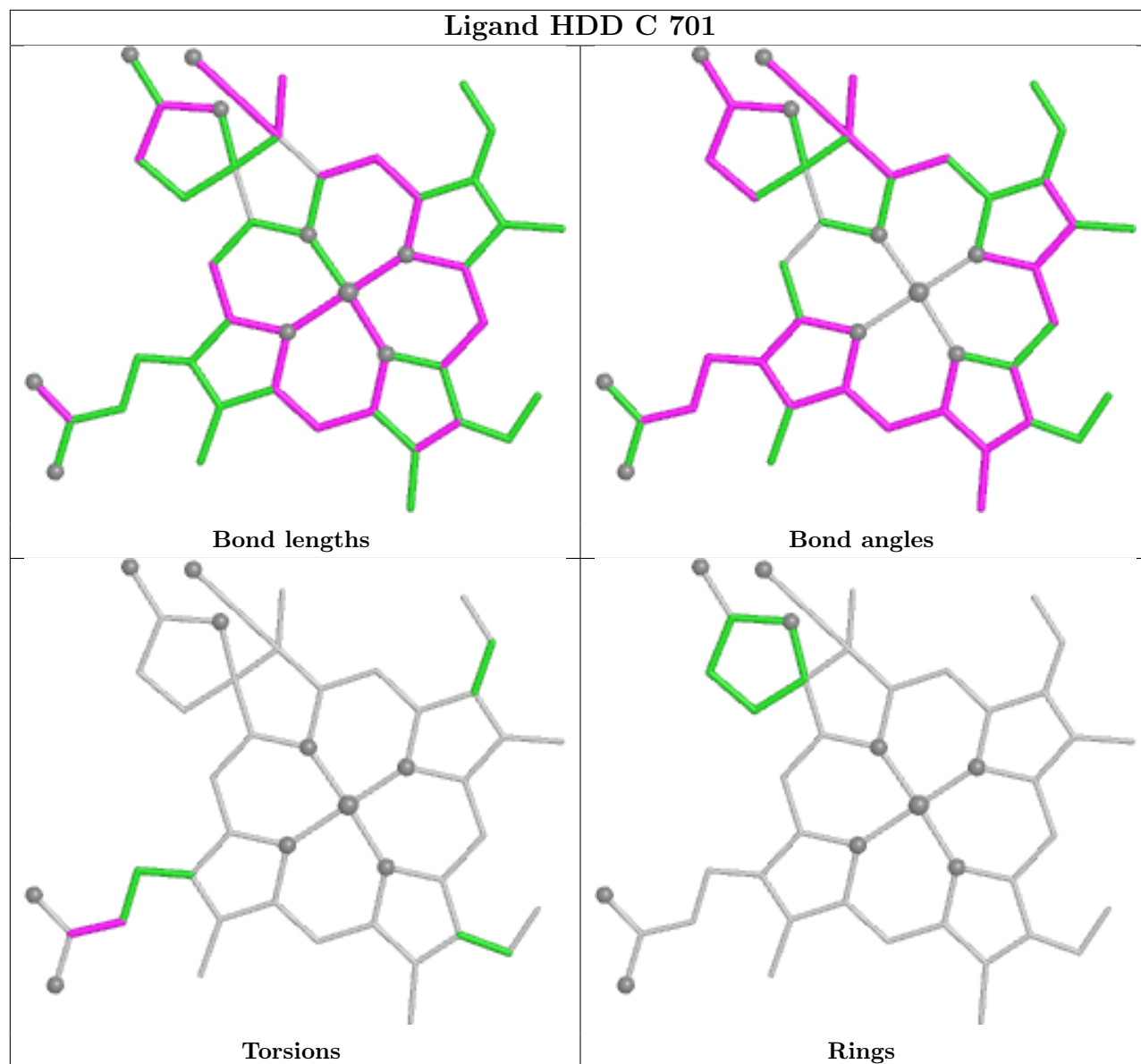
Mol	Chain	Res	Type	Atoms
2	D	701	HDD	CAA-CBA-CGA-O2A
2	D	701	HDD	CAA-CBA-CGA-O1A
2	C	701	HDD	CAA-CBA-CGA-O1A
2	B	1702	HDD	CAA-CBA-CGA-O1A
2	A	701	HDD	CAA-CBA-CGA-O1A

There are no ring outliers.

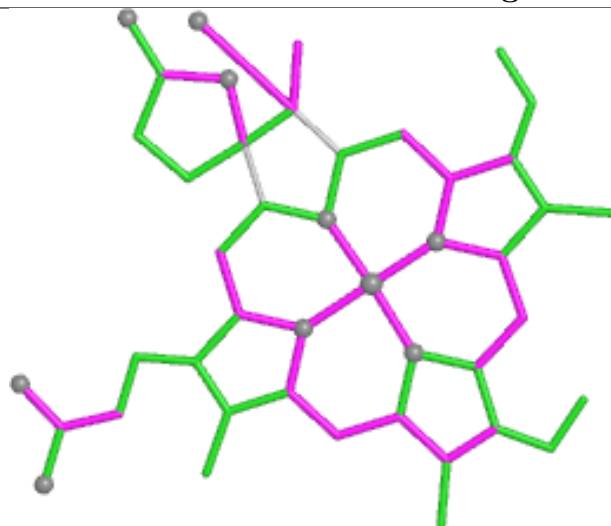
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	HDD	1	0
3	C	703	3TR	1	0
2	A	701	HDD	4	0

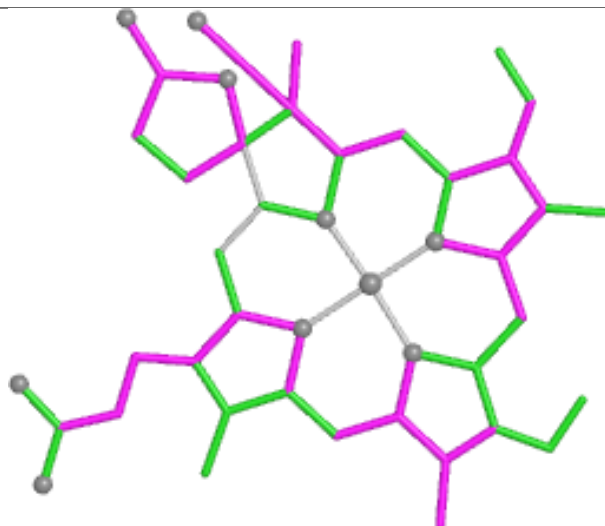
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



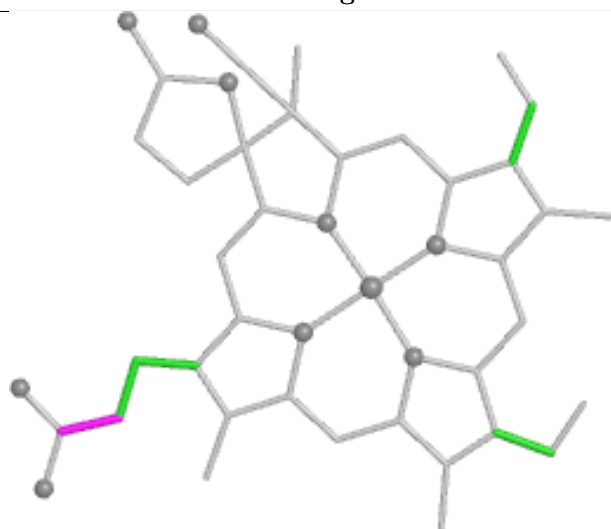
Ligand HDD B 1702



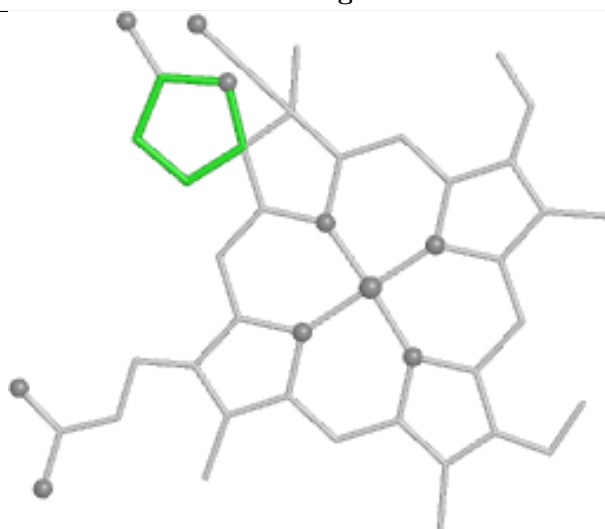
Bond lengths



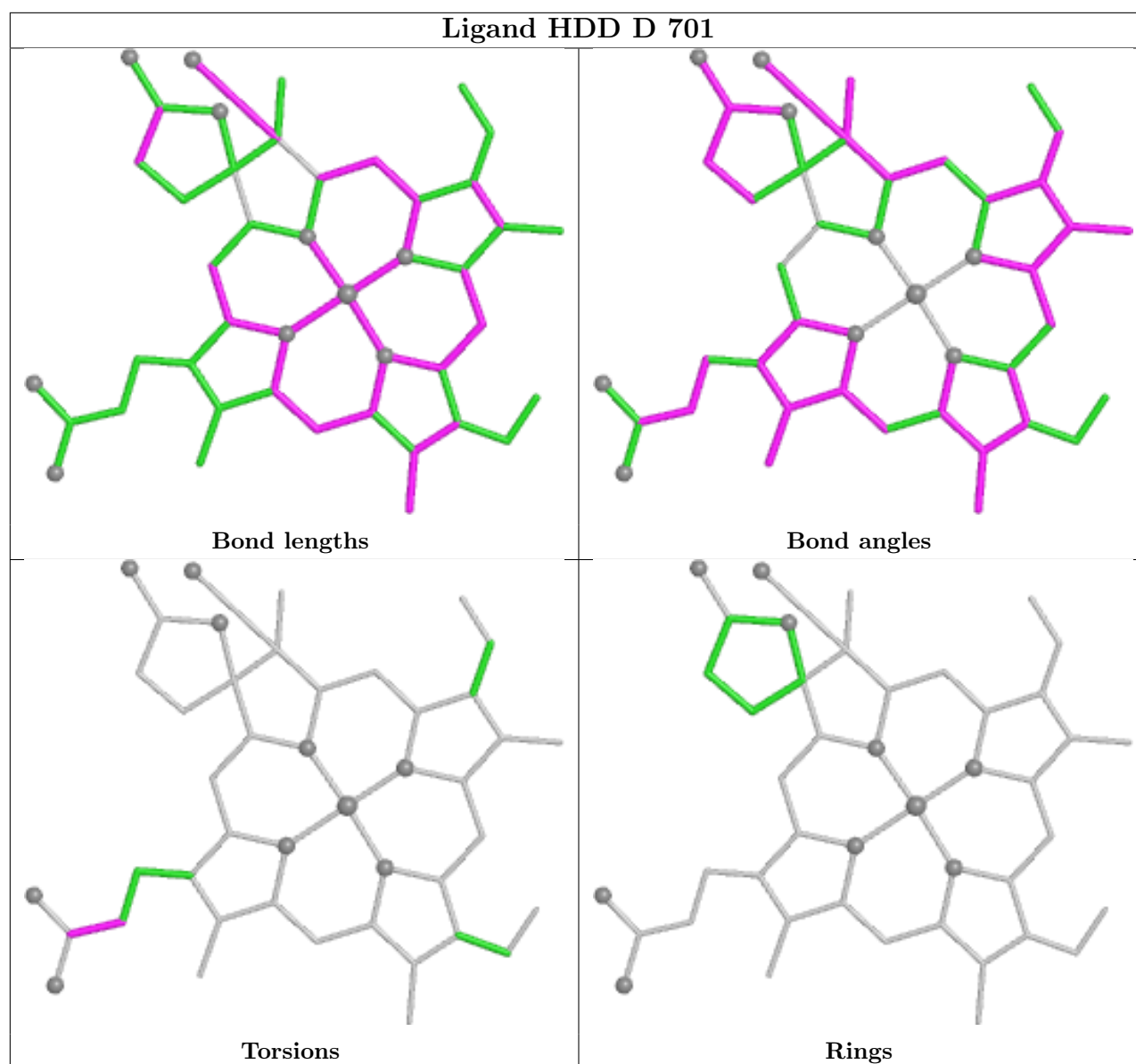
Bond angles

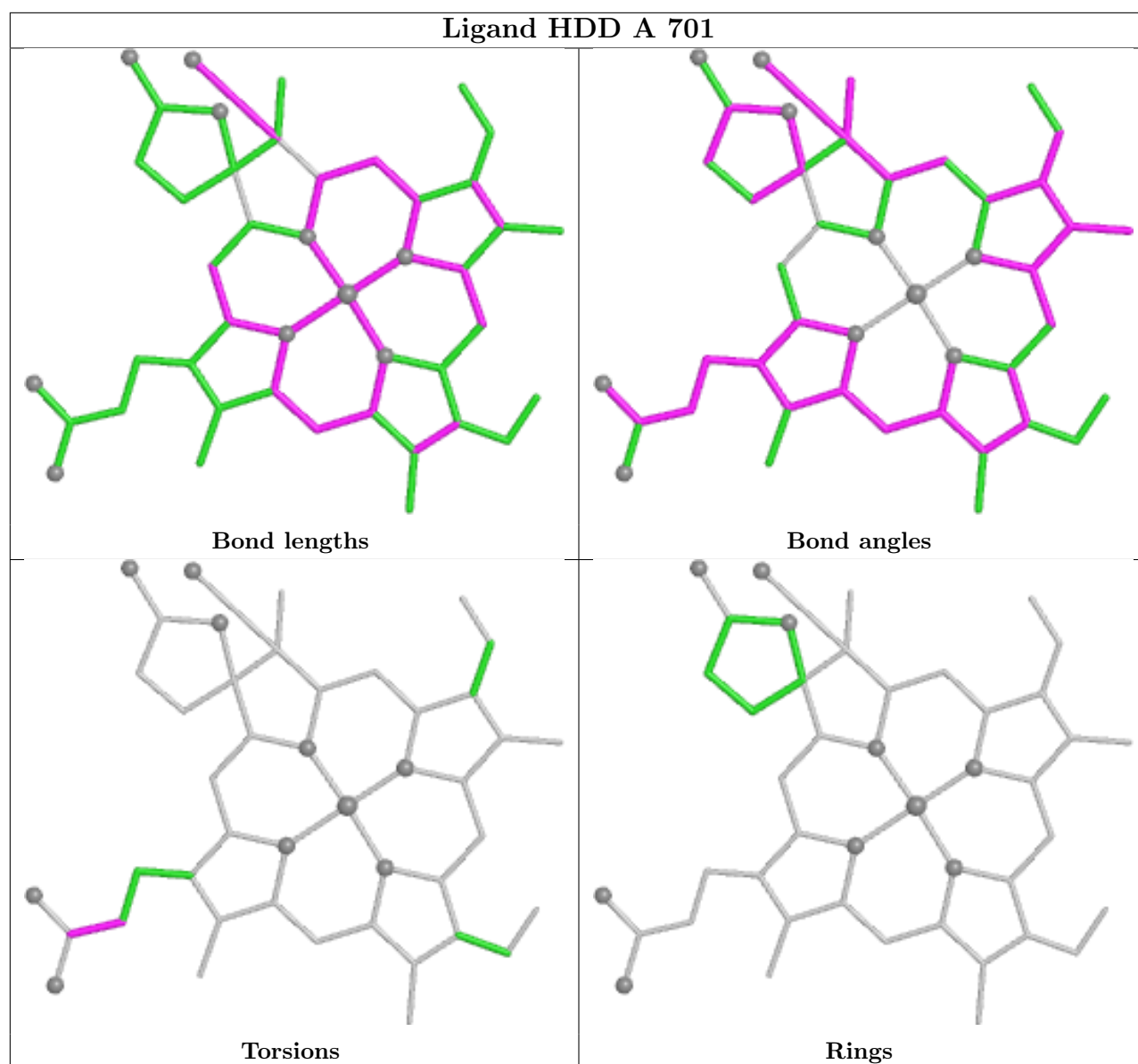


Torsions



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	677/719 (94%)	-0.44	11 (1%) 70 77	7, 18, 46, 90	14 (2%)
1	B	678/719 (94%)	-0.41	14 (2%) 63 70	7, 20, 49, 89	4 (0%)
1	C	678/719 (94%)	-0.56	7 (1%) 79 85	6, 17, 34, 84	6 (0%)
1	D	678/719 (94%)	-0.49	6 (0%) 81 86	7, 20, 39, 66	7 (1%)
All	All	2711/2876 (94%)	-0.47	38 (1%) 73 80	6, 19, 41, 90	31 (1%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	SER	9.1
1	B	22	PRO	7.0
1	A	22	PRO	6.2
1	A	21	SER	5.9
1	D	22	PRO	5.3
1	C	22	PRO	4.3
1	C	698	SER	4.1
1	D	21	SER	3.7
1	D	698	SER	3.4
1	C	618	ALA	3.3
1	B	652	SER	3.2
1	B	621	ALA	3.1
1	B	23	LEU	3.0
1	A	649	GLY	3.0
1	A	652	SER	2.9
1	B	655	VAL	2.9
1	B	653	SER	2.9
1	B	675	ASP	2.8
1	A	621	ALA	2.7
1	B	615	ALA	2.7
1	B	649	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	21	SER	2.6
1	B	620	THR	2.6
1	A	653	SER	2.6
1	B	698	SER	2.6
1	A	23	LEU	2.5
1	C	619	SER	2.5
1	C	621	ALA	2.4
1	A	655	VAL	2.4
1	C	620	THR	2.3
1	A	619	SER	2.3
1	B	573	ARG	2.3
1	D	619	SER	2.2
1	A	620	THR	2.2
1	B	619	SER	2.2
1	D	517	GLY	2.1
1	D	621	ALA	2.1
1	A	618	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 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.

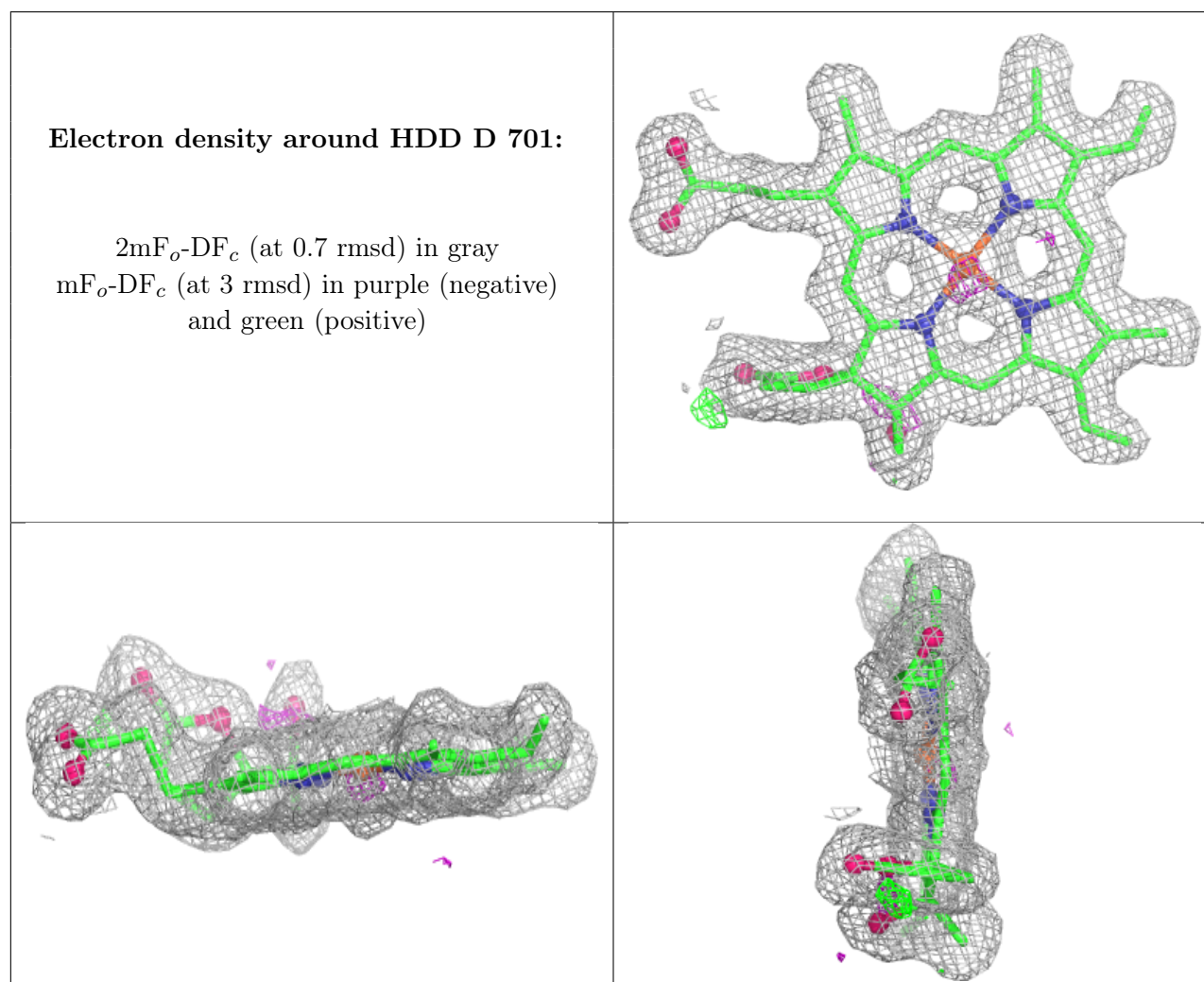
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	3TR	B	1704	6/6	0.86	0.13	33,35,35,35	0
3	3TR	B	1706	6/6	0.87	0.12	29,31,32,32	0
3	3TR	A	703	6/6	0.88	0.14	32,35,36,37	0
3	3TR	C	703	6/6	0.88	0.12	29,29,30,32	0
3	3TR	B	1703	6/6	0.94	0.09	24,25,25,26	0
3	3TR	C	702	6/6	0.97	0.06	22,22,22,22	0

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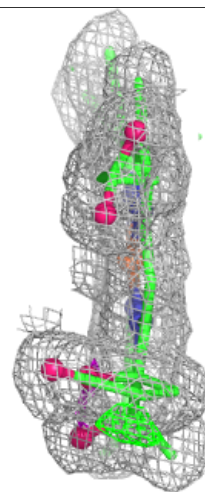
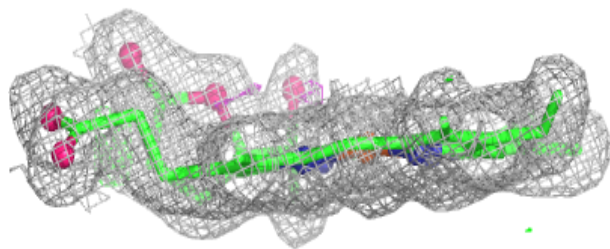
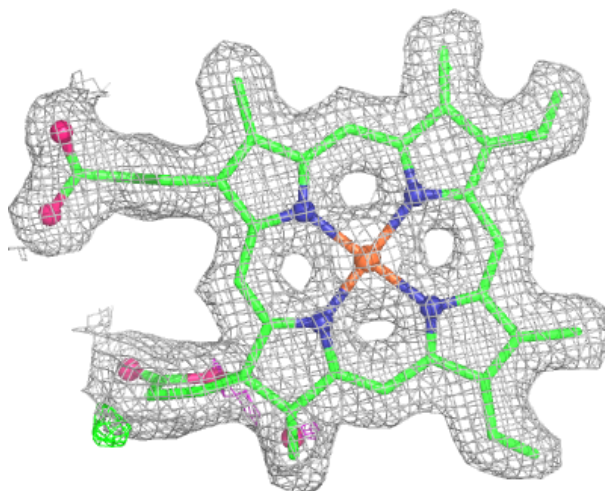
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	3TR	A	702	6/6	0.97	0.07	21,22,23,23	0
3	3TR	D	702	6/6	0.97	0.10	22,23,24,24	0
2	HDD	D	701	44/44	0.98	0.05	11,13,16,20	0
4	CA	B	1701	1/1	0.98	0.13	44,44,44,44	0
2	HDD	B	1702	44/44	0.99	0.05	10,12,16,20	0
2	HDD	C	701	44/44	0.99	0.05	9,12,15,19	0
2	HDD	A	701	44/44	0.99	0.05	10,12,16,20	0
4	CA	C	704	1/1	0.99	0.10	24,24,24,24	0
4	CA	D	703	1/1	0.99	0.08	24,24,24,24	0
4	CA	A	704	1/1	1.00	0.06	19,19,19,19	0
4	CA	B	1705	1/1	1.00	0.07	23,23,23,23	0

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



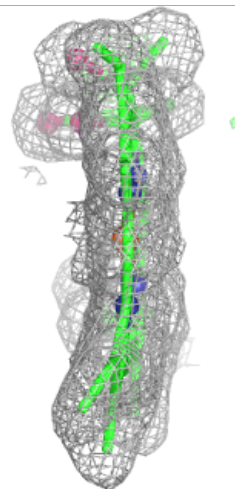
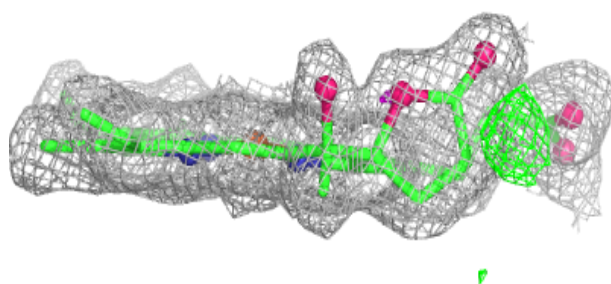
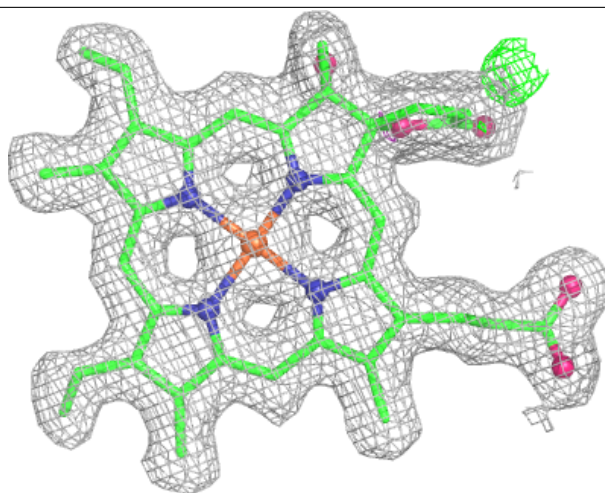
Electron density around HDD B 1702:

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



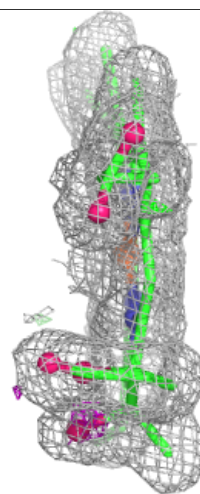
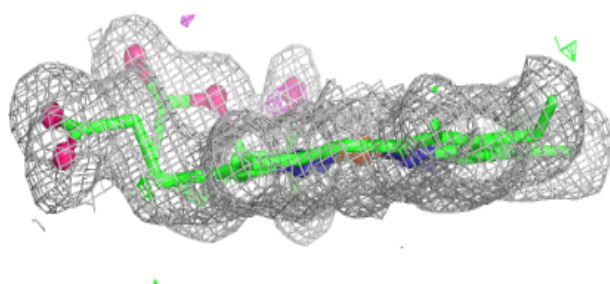
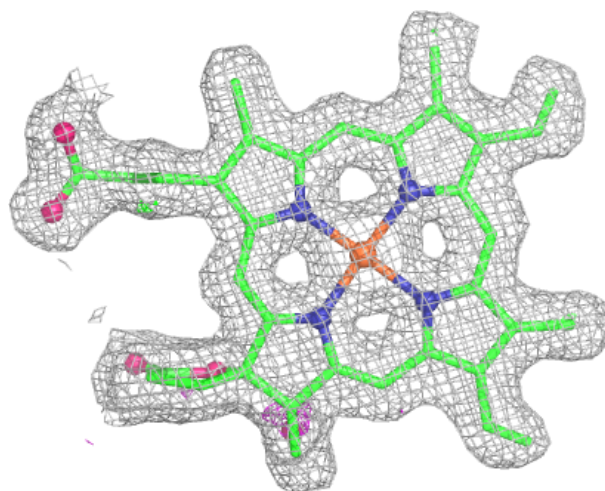
Electron density around HDD C 701:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.