Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 10:24 PM EDT

PDB ID	:	4ENQ / pdb_00004enq
Title	:	Structure of E530D variant E. coli KatE
Authors	:	Loewen, P.C.; Jha, V.
Deposited on	:	2012-04-13
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

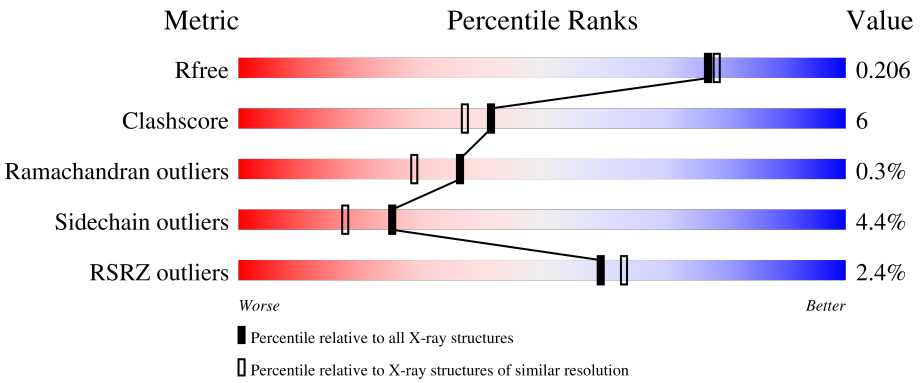
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	753	% 83% 12% • •
1	B	753	5% 80% 13% • •
1	C	753	2% 77% 16% • •
1	D	753	82% 12% • •

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	C	801	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26319 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.

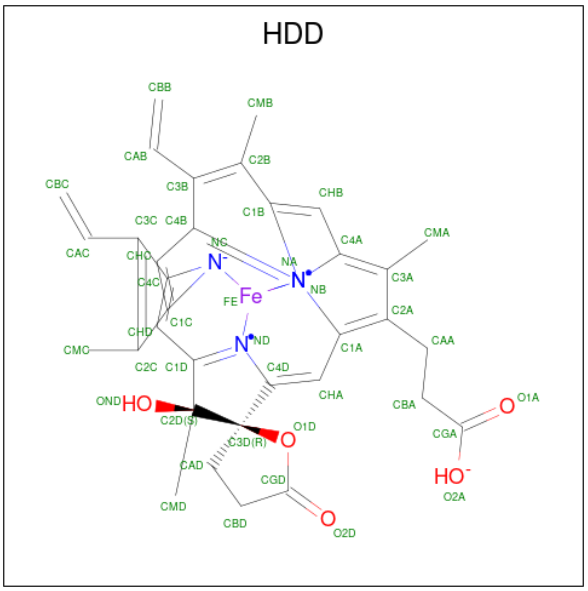
- Molecule 1 is a protein called Catalase HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	725	5742	3643	1005	1082	12	0	3	0
1	B	725	5746	3645	1006	1083	12	0	3	0
1	C	725	5742	3643	1005	1082	12	0	3	0
1	D	725	5746	3645	1006	1083	12	0	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	530	ASP	GLU	engineered mutation	UNP P21179
B	530	ASP	GLU	engineered mutation	UNP P21179
C	530	ASP	GLU	engineered mutation	UNP P21179
D	530	ASP	GLU	engineered mutation	UNP P21179

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



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

- Molecule 3 is water.

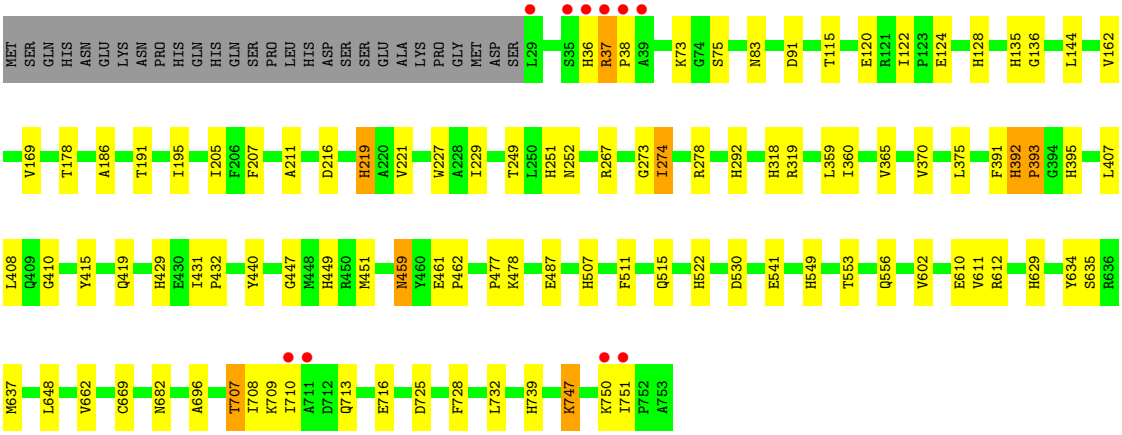
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	852	Total	O	0	0
			852	852		
3	B	705	Total	O	0	0
			705	705		
3	C	766	Total	O	0	0
			766	766		
3	D	844	Total	O	0	0
			844	844		

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.

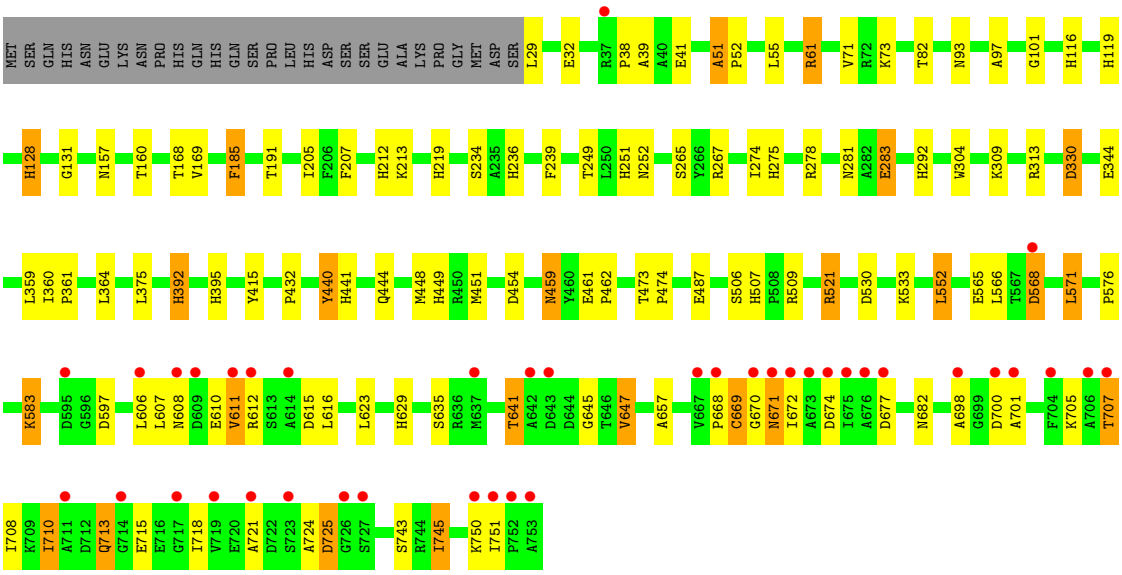
- Molecule 1: Catalase HPII

Chain A:



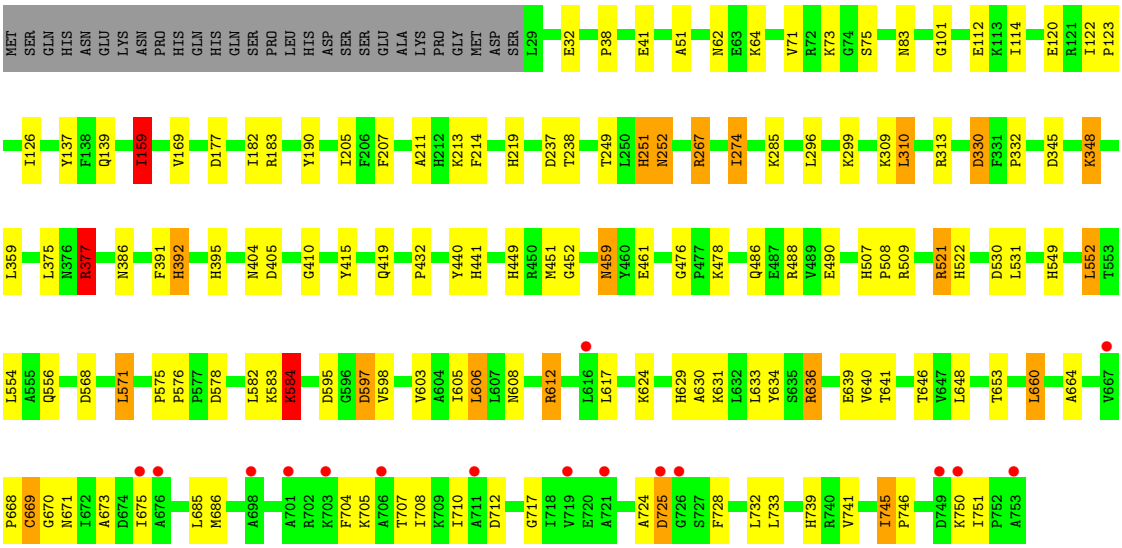
- Molecule 1: Catalase HPII

Chain B:



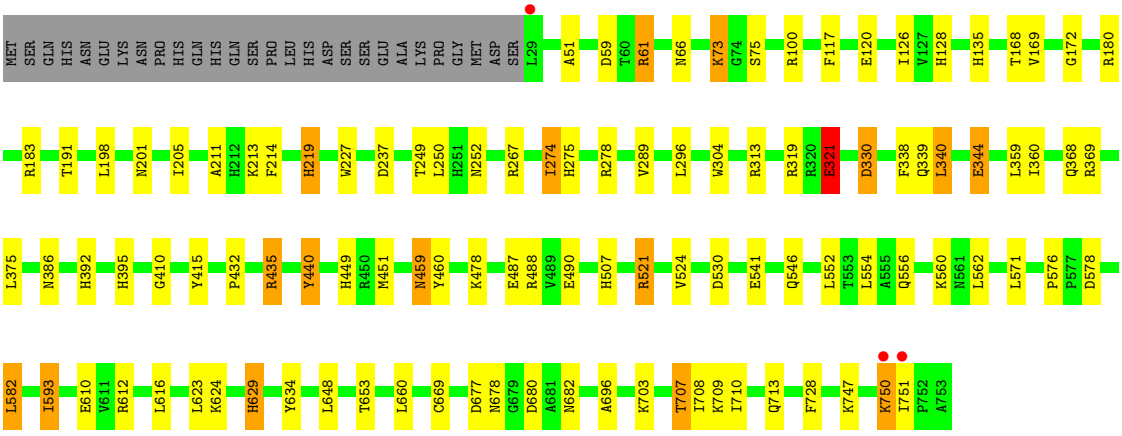
- Molecule 1: Catalase HPII

Chain C:



- Molecule 1: Catalase HPII

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.38Å 133.09Å 122.34Å 90.00° 109.68° 90.00°	Depositor
Resolution (Å)	40.51 – 1.90 40.51 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.1 (40.51-1.90) 92.1 (40.51-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.158 , 0.207 0.158 , 0.206	Depositor DCC
R_{free} test set	10269 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	13.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26319	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.37	23/5903 (0.4%)	1.16	15/8024 (0.2%)
1	B	1.31	21/5903 (0.4%)	1.16	13/8024 (0.2%)
1	C	1.30	14/5903 (0.2%)	1.18	19/8024 (0.2%)
1	D	1.32	15/5903 (0.3%)	1.17	16/8024 (0.2%)
All	All	1.33	73/23612 (0.3%)	1.17	63/32096 (0.2%)

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

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	HIS	CE1-NE2	8.05	1.40	1.32
1	C	126	ILE	N-CA	7.16	1.54	1.46
1	A	274	ILE	N-CA	6.76	1.54	1.46
1	B	441	HIS	ND1-CE1	6.70	1.39	1.32
1	B	119	HIS	CG-CD2	6.61	1.43	1.35
1	C	575	PRO	CA-C	6.60	1.55	1.51
1	D	274	ILE	N-CA	6.28	1.54	1.46
1	C	392	HIS	ND1-CE1	6.26	1.38	1.32
1	D	360	ILE	CA-C	6.17	1.58	1.53
1	B	236	HIS	ND1-CE1	6.16	1.38	1.32
1	B	128	HIS	CB-CG	6.11	1.58	1.50
1	C	114	ILE	N-CA	5.95	1.53	1.46
1	A	178	THR	N-CA	5.95	1.53	1.46
1	B	392	HIS	ND1-CE1	5.91	1.38	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	ILE	N-CA	-5.88	1.41	1.46
1	A	83	ASN	C-O	5.80	1.31	1.24
1	D	180	ARG	C-O	5.79	1.31	1.24
1	D	219	HIS	CE1-NE2	5.79	1.38	1.32
1	C	522	HIS	CG-CD2	5.75	1.42	1.35
1	B	474	PRO	CA-C	5.75	1.55	1.51
1	B	395	HIS	ND1-CE1	5.70	1.38	1.32
1	D	172	GLY	N-CA	5.69	1.52	1.45
1	D	330	ASP	CA-CB	5.69	1.60	1.52
1	A	522	HIS	CG-CD2	5.67	1.42	1.35
1	D	395	HIS	ND1-CE1	5.67	1.38	1.32
1	C	490	GLU	C-O	5.66	1.30	1.23
1	B	119	HIS	CE1-NE2	5.62	1.38	1.32
1	B	116	HIS	CE1-NE2	5.58	1.38	1.32
1	A	739	HIS	ND1-CE1	5.56	1.38	1.32
1	C	391	PHE	N-CA	5.52	1.52	1.45
1	C	395	HIS	CG-CD2	5.51	1.42	1.35
1	B	444	GLN	C-O	5.47	1.30	1.23
1	C	441	HIS	CE1-NE2	5.45	1.38	1.32
1	D	275	HIS	CG-CD2	5.45	1.41	1.35
1	A	395	HIS	ND1-CE1	5.44	1.38	1.32
1	A	391	PHE	N-CA	5.43	1.52	1.45
1	B	275	HIS	CE1-NE2	5.42	1.38	1.32
1	D	214	PHE	C-O	-5.41	1.19	1.24
1	B	185	PHE	CA-C	5.39	1.58	1.53
1	A	115	THR	N-CA	5.39	1.52	1.46
1	B	292	HIS	CG-CD2	5.38	1.41	1.35
1	A	292	HIS	C-O	5.37	1.30	1.23
1	A	135	HIS	CG-CD2	5.35	1.41	1.35
1	D	395	HIS	CA-C	-5.34	1.46	1.53
1	C	251	HIS	ND1-CE1	5.32	1.37	1.32
1	C	71	VAL	CA-CB	5.29	1.60	1.54
1	C	112	GLU	N-CA	5.28	1.52	1.46
1	C	739	HIS	N-CA	5.27	1.52	1.46
1	B	160	THR	C-O	-5.24	1.18	1.24
1	B	71	VAL	CA-CB	5.24	1.60	1.54
1	D	435	ARG	N-CA	5.24	1.52	1.45
1	A	229	ILE	N-CA	5.23	1.53	1.46
1	D	629	HIS	CE1-NE2	5.23	1.37	1.32
1	A	186	ALA	N-CA	5.22	1.52	1.46
1	B	131	GLY	N-CA	5.22	1.50	1.45
1	A	318	HIS	CE1-NE2	5.21	1.37	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	739	HIS	CG-CD2	5.17	1.41	1.35
1	A	393	PRO	N-CA	5.16	1.54	1.47
1	D	321	GLU	C-O	5.14	1.30	1.24
1	A	522	HIS	ND1-CE1	5.12	1.37	1.32
1	A	221	VAL	N-CA	5.11	1.53	1.46
1	B	93	ASN	CA-C	-5.11	1.46	1.52
1	D	135	HIS	CG-CD2	5.09	1.41	1.35
1	A	549	HIS	ND1-CE1	5.08	1.37	1.32
1	A	392	HIS	CG-ND1	-5.07	1.32	1.38
1	D	219	HIS	CG-CD2	5.05	1.41	1.35
1	B	473	THR	C-N	5.05	1.38	1.33
1	B	441	HIS	CG-CD2	5.04	1.41	1.35
1	C	214	PHE	C-O	-5.04	1.19	1.24
1	A	216	ASP	C-O	5.04	1.29	1.24
1	B	212	HIS	ND1-CE1	5.03	1.37	1.32
1	B	745	ILE	CA-CB	5.03	1.56	1.54
1	A	359	LEU	N-CA	5.02	1.51	1.45

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	61	ARG	NE-CZ-NH2	9.23	127.51	119.20
1	C	169	VAL	CB-CA-C	-7.73	104.17	111.05
1	C	330	ASP	CB-CA-C	-7.65	101.10	111.88
1	B	51	ALA	CA-C-N	7.20	127.64	119.93
1	B	51	ALA	C-N-CA	7.20	127.64	119.93
1	C	139	GLN	CA-C-N	-6.82	113.62	120.31
1	C	139	GLN	C-N-CA	-6.82	113.62	120.31
1	C	177	ASP	N-CA-C	6.80	118.48	111.14
1	D	126	ILE	CB-CA-C	-6.79	102.97	112.14
1	C	377	ARG	NE-CZ-NH1	-6.45	115.05	121.50
1	B	330	ASP	CB-CA-C	-6.43	102.82	111.88
1	D	330	ASP	CB-CA-C	-6.35	101.77	112.00
1	A	365	VAL	CA-C-N	-6.28	114.16	120.31
1	A	365	VAL	C-N-CA	-6.28	114.16	120.31
1	D	61	ARG	NE-CZ-NH1	-6.22	115.28	121.50
1	D	183	ARG	NE-CZ-NH2	6.18	124.76	119.20
1	D	524	VAL	N-CA-C	-6.15	104.51	110.42
1	B	360	ILE	N-CA-C	-6.05	101.56	107.55
1	A	408	LEU	N-CA-C	-6.00	104.65	111.07
1	D	249	THR	N-CA-C	5.88	119.72	112.54
1	C	120	GLU	N-CA-C	5.87	117.67	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	553	THR	N-CA-C	-5.84	104.99	111.36
1	C	101	GLY	CA-C-N	-5.84	114.58	120.31
1	C	101	GLY	C-N-CA	-5.84	114.58	120.31
1	B	55	LEU	N-CA-C	-5.80	106.33	113.41
1	C	267	ARG	N-CA-C	5.80	119.17	111.75
1	B	304	TRP	N-CA-C	5.79	118.06	111.11
1	A	447	GLY	N-CA-C	-5.75	105.53	112.48
1	C	745	ILE	O-C-N	5.73	124.09	120.42
1	C	159	ILE	CB-CG1-CD1	-5.68	101.88	113.80
1	C	237	ASP	N-CA-C	5.56	120.54	111.37
1	A	648	LEU	CA-C-N	-5.55	114.25	120.14
1	A	648	LEU	C-N-CA	-5.55	114.25	120.14
1	C	745	ILE	N-CA-CB	5.52	114.22	110.52
1	A	37	ARG	CA-C-N	5.50	125.51	119.90
1	A	37	ARG	C-N-CA	5.50	125.51	119.90
1	C	159	ILE	CA-CB-CG2	5.49	119.83	110.50
1	A	273	GLY	N-CA-C	-5.46	108.17	115.32
1	B	444	GLN	N-CA-C	-5.37	101.79	110.32
1	D	747	LYS	N-CA-C	5.35	119.07	112.54
1	D	237	ASP	N-CA-C	5.31	116.75	111.07
1	B	168	THR	CA-C-N	-5.27	117.57	123.16
1	B	168	THR	C-N-CA	-5.27	117.57	123.16
1	A	747	LYS	N-CA-C	5.23	119.38	112.89
1	A	120	GLU	N-CA-C	5.23	116.98	111.28
1	B	82	THR	N-CA-C	-5.23	103.98	110.41
1	C	639	GLU	N-CA-C	5.20	116.75	108.79
1	D	576	PRO	CA-C-N	5.18	125.12	119.78
1	D	576	PRO	C-N-CA	5.18	125.12	119.78
1	A	360	ILE	CA-C-N	-5.18	114.58	119.76
1	A	360	ILE	C-N-CA	-5.18	114.58	119.76
1	B	454	ASP	N-CA-C	5.14	117.68	109.96
1	C	41	GLU	CA-C-N	5.13	125.38	119.83
1	C	41	GLU	C-N-CA	5.13	125.38	119.83
1	D	344	GLU	CA-CB-CG	5.11	124.33	114.10
1	D	623	LEU	N-CA-C	-5.11	105.62	111.14
1	D	51	ALA	N-CA-C	5.11	114.17	108.25
1	B	657	ALA	CA-C-N	5.10	125.38	119.92
1	B	657	ALA	C-N-CA	5.10	125.38	119.92
1	D	593	ILE	CB-CA-C	-5.10	105.32	111.18
1	D	304	TRP	N-CA-C	5.08	117.21	111.11
1	C	348	LYS	CA-CB-CG	-5.02	104.06	114.10
1	A	124	GLU	N-CA-C	-5.00	104.07	110.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	724	ALA	Peptide

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	5742	0	5571	53	0
1	B	5746	0	5575	84	0
1	C	5742	0	5572	88	0
1	D	5746	0	5574	81	0
2	A	44	0	31	4	0
2	B	44	0	31	2	0
2	C	44	0	31	2	0
2	D	44	0	31	4	0
3	A	852	0	0	11	0
3	B	705	0	0	20	0
3	C	766	0	0	18	0
3	D	844	0	0	30	0
All	All	26319	0	22416	292	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 (292) 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:392:HIS:ND1	1:D:415:TYR:CB	1.70	1.50
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.71	1.50
1:A:392:HIS:ND1	1:A:415:TYR:CB	1.77	1.47
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.77	1.45
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.69	1.27
1:B:392:HIS:CE1	1:B:415:TYR:HB2	1.71	1.24
1:D:546:GLN:HG3	3:D:1588:HOH:O	1.39	1.22
1:D:369:ARG:HD2	3:D:1742:HOH:O	1.35	1.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:HIS:CE1	1:A:415:TYR:HB2	1.78	1.19
1:D:392:HIS:ND1	1:D:415:TYR:HB2	0.84	1.16
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.83	1.16
3:B:1481:HOH:O	1:D:73:LYS:HD3	1.41	1.15
1:A:392:HIS:ND1	1:A:415:TYR:HB2	0.83	1.15
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.80	1.12
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.84	1.11
1:B:451:MET:HE2	1:D:451:MET:HE2	1.15	1.06
1:A:716:GLU:HG2	3:A:1685:HOH:O	1.54	1.05
1:D:709:LYS:HG3	1:D:750:LYS:HE3	1.38	1.04
1:C:267:ARG:HG3	3:C:1573:HOH:O	1.59	1.00
1:D:321:GLU:HG2	3:D:1424:HOH:O	1.58	1.00
1:A:451:MET:HE2	1:C:451:MET:HE2	1.46	0.97
1:C:73:LYS:HD2	3:C:1537:HOH:O	1.62	0.97
1:A:267:ARG:HG3	3:A:1730:HOH:O	1.66	0.94
1:D:321:GLU:CG	3:D:1424:HOH:O	2.17	0.89
1:A:612:ARG:HG3	3:A:1597:HOH:O	1.74	0.88
1:A:392:HIS:CG	1:A:415:TYR:HB2	2.04	0.87
1:C:486:GLN:OE1	3:C:1570:HOH:O	1.94	0.86
1:B:61:ARG:CG	1:B:61:ARG:HH11	1.91	0.83
1:D:392:HIS:ND1	1:D:415:TYR:HB3	1.95	0.81
1:D:330:ASP:HA	3:D:1400:HOH:O	1.81	0.80
1:D:541:GLU:HG2	3:D:1684:HOH:O	1.83	0.78
1:A:278:ARG:HH12	1:A:487:GLU:CD	1.92	0.77
1:B:73:LYS:HE3	1:D:440:TYR:O	1.85	0.77
1:B:583:LYS:NZ	1:B:583:LYS:H	1.81	0.77
1:B:61:ARG:HH11	1:B:61:ARG:HG3	1.49	0.76
1:D:267:ARG:HG3	3:D:1366:HOH:O	1.86	0.76
1:C:488:ARG:NH1	1:D:490:GLU:OE1	2.19	0.75
1:B:583:LYS:H	1:B:583:LYS:HZ2	1.34	0.75
1:D:703:LYS:HE2	3:D:1589:HOH:O	1.85	0.74
1:D:629:HIS:HD2	3:D:1255:HOH:O	1.70	0.74
1:B:267:ARG:HG3	3:B:1370:HOH:O	1.88	0.73
1:B:451:MET:HE2	1:D:451:MET:CE	2.08	0.73
1:B:710:ILE:HD12	1:B:718:ILE:HG13	1.71	0.71
1:C:392:HIS:CG	1:C:415:TYR:HB2	2.08	0.71
1:B:392:HIS:ND1	1:B:415:TYR:HB3	2.00	0.71
1:D:578:ASP:HB3	1:D:582:LEU:O	1.90	0.71
1:B:629:HIS:HD2	3:B:1166:HOH:O	1.73	0.70
1:B:724:ALA:O	1:B:725:ASP:O	2.10	0.69
1:C:137:TYR:HB2	1:C:159:ILE:HD11	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:GLN:NE2	3:A:1503:HOH:O	2.25	0.68
1:B:41:GLU:OE1	3:B:1485:HOH:O	2.10	0.68
1:B:73:LYS:CE	1:D:440:TYR:O	2.41	0.68
1:B:721:ALA:HB2	3:B:1258:HOH:O	1.93	0.68
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.01	0.67
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.25	0.67
1:D:61:ARG:NH1	3:D:1713:HOH:O	2.27	0.67
1:B:521:ARG:HH21	1:B:521:ARG:HG3	1.59	0.67
1:A:392:HIS:ND1	1:A:415:TYR:CG	2.62	0.66
1:B:521:ARG:HE	1:B:745:ILE:HG21	1.62	0.65
1:C:704:PHE:O	1:C:707:THR:HG22	1.97	0.65
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.78	0.64
1:C:309:LYS:HE3	3:C:1175:HOH:O	1.98	0.63
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.28	0.63
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.81	0.62
1:C:478:LYS:HB2	3:C:1613:HOH:O	1.97	0.62
1:B:671:ASN:O	1:B:674:ASP:HB3	2.00	0.62
1:C:746:PRO:HG2	3:C:1521:HOH:O	2.00	0.61
1:C:274:ILE:HD12	2:C:801:HDD:HMB3	1.84	0.60
1:C:578:ASP:HB2	1:C:582:LEU:O	2.02	0.60
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.43	0.59
1:C:313:ARG:HD2	3:C:1254:HOH:O	2.01	0.59
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.85	0.58
1:B:533:LYS:HE3	3:B:1259:HOH:O	2.02	0.58
1:D:541:GLU:CG	3:D:1684:HOH:O	2.45	0.58
1:D:521:ARG:HD3	3:D:1705:HOH:O	2.04	0.57
1:B:61:ARG:HG3	1:B:61:ARG:NH1	2.15	0.57
1:B:610:GLU:HB3	1:B:671:ASN:HB2	1.87	0.57
1:D:250:LEU:HD11	1:D:546:GLN:HE21	1.70	0.57
1:A:73:LYS:HE2	3:C:1142:HOH:O	2.04	0.56
1:C:629:HIS:HD2	3:C:1209:HOH:O	1.88	0.56
1:C:38:PRO:HG2	1:C:51:ALA:HB2	1.87	0.56
1:D:330:ASP:CA	3:D:1400:HOH:O	2.43	0.56
1:D:624:LYS:O	1:D:624:LYS:HD3	2.05	0.56
1:D:488:ARG:NE	3:D:1571:HOH:O	1.93	0.56
1:C:476:GLY:HA3	3:C:1281:HOH:O	2.04	0.56
1:D:338:PHE:HB3	1:D:340:LEU:HD13	1.87	0.56
1:B:610:GLU:HB3	1:B:671:ASN:CB	2.35	0.56
1:B:708:ILE:HD12	1:B:710:ILE:HD11	1.88	0.55
1:D:313:ARG:HG3	1:D:660:LEU:HD12	1.89	0.55
1:A:725:ASP:H	1:A:728:PHE:HB3	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1481:HOH:O	1:D:73:LYS:CD	2.19	0.55
1:C:392:HIS:ND1	1:C:415:TYR:CG	2.70	0.55
1:D:624:LYS:HD3	1:D:624:LYS:C	2.31	0.55
1:A:274:ILE:HD12	2:A:801:HDD:HMB3	1.89	0.54
1:C:521:ARG:HG2	3:C:1575:HOH:O	2.06	0.54
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.88	0.54
1:C:636:ARG:NH1	3:C:1629:HOH:O	2.40	0.54
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.22	0.54
1:C:345:ASP:HA	1:C:348:LYS:HD2	1.89	0.54
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.68	0.54
1:C:725:ASP:HA	1:C:728:PHE:HB3	1.90	0.53
1:C:62:ASN:OD1	1:C:62:ASN:C	2.51	0.53
1:C:359:LEU:H	1:C:507:HIS:HD2	1.57	0.53
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.91	0.53
1:D:556:GLN:NE2	3:D:1592:HOH:O	2.42	0.53
1:B:278:ARG:HH22	1:B:487:GLU:CD	2.17	0.53
3:B:1338:HOH:O	1:D:449[A]:HIS:HE1	1.92	0.53
1:C:415:TYR:O	1:C:419:GLN:HG2	2.08	0.53
1:B:669:OCS:OD1	1:B:700:ASP:HB2	2.08	0.53
1:B:713:GLN:CD	1:B:713:GLN:H	2.16	0.52
1:B:533:LYS:HE2	3:B:1550:HOH:O	2.09	0.52
1:B:29:LEU:N	3:B:1601:HOH:O	2.41	0.52
1:B:615:ASP:HA	1:B:724:ALA:HB3	1.90	0.52
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.75	0.52
1:A:751:ILE:HD12	1:A:751:ILE:O	2.08	0.52
1:C:313:ARG:HG3	1:C:660:LEU:HD23	1.92	0.52
1:B:612:ARG:O	1:B:615:ASP:HB2	2.11	0.51
1:B:698:ALA:H	1:B:701:ALA:HB3	1.74	0.51
1:C:267:ARG:HD3	1:C:332:PRO:HG3	1.92	0.51
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.91	0.51
1:B:281:ASN:OD1	1:B:283:GLU:HG3	2.10	0.51
1:C:73:LYS:CD	3:C:1537:HOH:O	2.39	0.51
1:B:207:PHE:O	1:B:249:THR:HA	2.11	0.51
1:C:32:GLU:HB2	3:C:1578:HOH:O	2.11	0.51
1:D:267:ARG:CG	3:D:1366:HOH:O	2.52	0.51
1:B:61:ARG:HH11	1:B:61:ARG:HG2	1.72	0.50
1:B:267:ARG:CG	3:B:1370:HOH:O	2.55	0.50
1:B:606:LEU:O	1:B:668:PRO:HD2	2.10	0.50
1:C:597:ASP:OD2	1:C:597:ASP:C	2.54	0.50
1:D:61:ARG:NH1	1:D:66:ASN:HA	2.27	0.50
1:B:97:ALA:O	1:B:101:GLY:HA3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:ILE:HG23	1:B:715:GLU:HB2	1.95	0.49
1:B:39:ALA:HB1	1:B:41:GLU:HG2	1.93	0.49
1:C:705:LYS:NZ	1:C:712:ASP:HA	2.27	0.49
1:D:368:GLN:HB3	3:D:1572:HOH:O	2.12	0.49
1:C:608:ASN:HA	1:C:634:TYR:HE1	1.77	0.49
1:B:29:LEU:HG	3:B:1601:HOH:O	2.13	0.48
1:A:393:PRO:HD2	1:A:415:TYR:CD2	2.48	0.48
1:C:251:HIS:HA	1:C:508:PRO:HG3	1.96	0.48
1:D:560:LYS:HD3	3:D:1717:HOH:O	2.14	0.48
1:B:52:PRO:HG3	3:D:1189:HOH:O	2.12	0.48
1:C:583:LYS:O	1:C:584:LYS:HB3	2.14	0.48
1:C:671:ASN:HD21	1:C:673:ALA:HB3	1.79	0.48
1:B:721:ALA:HB1	3:B:1555:HOH:O	2.13	0.48
1:C:299:LYS:HE3	1:C:595:ASP:OD1	2.14	0.48
1:A:319:ARG:HD3	1:D:227:TRP:O	2.13	0.47
1:A:511:PHE:O	1:A:515:GLN:HG2	2.14	0.47
1:C:745:ILE:HD13	3:C:1575:HOH:O	2.13	0.47
1:A:461:GLU:HA	1:A:462:PRO:C	2.38	0.47
1:D:330:ASP:CB	3:D:1400:HOH:O	2.62	0.47
1:D:634:TYR:O	1:D:653:THR:HA	2.14	0.47
1:A:73:LYS:HD2	1:C:452:GLY:HA3	1.95	0.47
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.70	0.47
1:C:705:LYS:HZ3	1:C:712:ASP:HA	1.79	0.47
1:B:608:ASN:O	1:B:611:VAL:HG23	2.15	0.47
2:B:801:HDD:HBD2	3:B:1047:HOH:O	2.14	0.47
1:C:392:HIS:CG	1:C:415:TYR:CB	2.84	0.47
1:C:605:ILE:HD12	1:C:630:ALA:HB1	1.97	0.47
2:C:801:HDD:HBD2	3:C:1088:HOH:O	2.14	0.47
1:D:321:GLU:HG3	3:D:1424:HOH:O	2.03	0.47
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.50	0.47
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.50	0.46
1:C:309:LYS:HB3	1:C:660:LEU:HD21	1.97	0.46
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.50	0.46
1:B:309:LYS:CE	3:B:1132:HOH:O	2.64	0.46
1:C:669:OCS:SG	1:C:670:GLY:N	2.89	0.46
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.30	0.46
1:D:359:LEU:H	1:D:507:HIS:HD2	1.63	0.46
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.98	0.46
1:D:392:HIS:CG	1:D:415:TYR:CB	2.82	0.46
1:D:488:ARG:NH2	3:D:1571:HOH:O	2.48	0.46
1:A:392:HIS:CE1	1:A:415:TYR:CB	2.68	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ILE:HD12	2:B:801:HDD:HMB3	1.98	0.46
1:B:448:MET:HG3	1:B:449[B]:HIS:CD2	2.50	0.46
1:C:64:LYS:HE2	1:C:190:TYR:CE1	2.51	0.46
1:A:716:GLU:CG	3:A:1685:HOH:O	2.34	0.45
2:A:801:HDD:HBD2	3:A:996:HOH:O	2.16	0.45
1:A:629:HIS:HE1	3:A:1495:HOH:O	1.98	0.45
1:B:610:GLU:O	1:B:670:GLY:HA3	2.15	0.45
1:B:521:ARG:HH21	1:B:521:ARG:CG	2.27	0.45
1:D:59:ASP:HB2	3:D:1318:HOH:O	2.15	0.45
1:A:429:HIS:CD2	1:C:83:ASN:HB3	2.52	0.45
1:C:207:PHE:CD2	1:C:252:ASN:HB3	2.51	0.45
1:C:359:LEU:H	1:C:507:HIS:CD2	2.35	0.45
1:D:750:LYS:HD3	1:D:751:ILE:HG12	1.97	0.45
1:B:392:HIS:ND1	1:B:415:TYR:CA	2.69	0.45
1:C:386:ASN:C	1:C:386:ASN:OD1	2.59	0.45
1:B:359:LEU:H	1:B:507:HIS:HD2	1.65	0.45
1:A:207:PHE:O	1:A:249:THR:HA	2.17	0.44
1:D:201:ASN:CG	2:D:801:HDD:HMB2	2.41	0.44
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.53	0.44
1:C:597:ASP:OD2	1:C:598:VAL:N	2.50	0.44
1:B:506[B]:SER:OG	1:B:576:PRO:HB2	2.18	0.44
1:C:267:ARG:CD	1:C:332:PRO:HG3	2.47	0.44
1:A:392:HIS:CG	1:A:415:TYR:CB	2.83	0.44
1:C:207:PHE:O	1:C:249:THR:HA	2.18	0.44
1:D:435:ARG:HD3	3:D:1293:HOH:O	2.18	0.44
1:D:369:ARG:CD	3:D:1742:HOH:O	2.21	0.44
1:C:549:HIS:O	1:C:576:PRO:HD3	2.17	0.44
1:C:603:VAL:HG22	1:C:664:ALA:HB3	2.00	0.43
1:C:686:MET:CB	1:C:751:ILE:HD11	2.48	0.43
1:A:637:MET:HB2	1:D:562:LEU:HA	2.01	0.43
1:B:670:GLY:O	1:B:672:ILE:N	2.51	0.43
1:C:708:ILE:HG13	1:C:710:ILE:HG12	2.00	0.43
1:A:431:ILE:HG13	1:C:449[A]:HIS:CE1	2.53	0.43
1:B:32:GLU:OE1	1:B:32:GLU:HA	2.18	0.43
1:B:647:VAL:O	1:B:647:VAL:HG12	2.18	0.43
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.99	0.43
1:A:602:VAL:HG13	1:A:662:VAL:HA	1.99	0.43
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.48	0.43
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.33	0.43
1:C:182:ILE:HG22	1:C:183:ARG:N	2.33	0.43
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:LEU:O	1:C:668:PRO:HD2	2.19	0.43
1:B:682:ASN:HB3	1:B:707:THR:HG21	2.00	0.43
1:B:698:ALA:N	1:B:701:ALA:HB3	2.33	0.43
1:C:313:ARG:HG3	1:C:660:LEU:CD2	2.49	0.43
1:C:612:ARG:HD2	3:C:1610:HOH:O	2.17	0.43
2:D:801:HDD:HAD2	2:D:801:HDD:HMD3	1.68	0.43
1:A:278:ARG:HH21	1:A:278:ARG:HD2	1.70	0.43
1:D:117:PHE:HA	1:D:120:GLU:HG3	2.01	0.43
1:D:459:ASN:C	1:D:459:ASN:HD22	2.27	0.42
1:A:407:LEU:HD11	2:A:801:HDD:HMC1	2.01	0.42
1:B:73:LYS:HE2	1:D:440:TYR:O	2.17	0.42
1:C:238:THR:HB	1:D:460:TYR:CE2	2.54	0.42
1:C:330:ASP:OD1	1:C:629:HIS:HE1	2.02	0.42
1:D:296:LEU:HD23	1:D:296:LEU:HA	1.84	0.42
1:D:521:ARG:HG2	3:D:1629:HOH:O	2.19	0.42
1:A:91:ASP:OD1	1:C:461:GLU:OE1	2.36	0.42
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.50	0.42
1:B:38:PRO:HG2	1:B:51:ALA:HB2	2.00	0.42
1:B:672:ILE:HG13	1:B:700:ASP:CB	2.49	0.42
1:D:682:ASN:HB3	1:D:707:THR:HG21	2.01	0.42
2:D:801:HDD:HBD2	3:D:1139:HOH:O	2.19	0.42
1:A:708:ILE:HG13	1:A:710:ILE:HG12	2.01	0.42
1:B:234:SER:HB2	1:B:239:PHE:CD2	2.54	0.42
1:B:440:TYR:CD2	1:B:440:TYR:C	2.98	0.42
1:D:478:LYS:NZ	3:D:994:HOH:O	2.48	0.42
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.55	0.42
1:A:36:HIS:HE1	3:A:1363:HOH:O	2.02	0.42
1:B:671:ASN:ND2	1:B:674:ASP:HB2	2.34	0.42
1:C:64:LYS:HE2	1:C:190:TYR:CZ	2.55	0.42
1:C:122:ILE:O	1:C:123:PRO:C	2.62	0.42
1:D:274:ILE:HD12	2:D:801:HDD:HMB1	2.02	0.42
1:A:136:GLY:C	1:A:162:VAL:HG22	2.44	0.42
2:A:801:HDD:HMD3	2:A:801:HDD:HAD2	1.71	0.42
1:B:267:ARG:NH1	3:B:1140:HOH:O	2.53	0.42
1:B:361:PRO:HD2	1:B:364:LEU:HD12	2.02	0.42
1:A:37:ARG:HA	1:A:38:PRO:HD2	1.83	0.41
1:A:634:TYR:CG	1:A:635:SER:N	2.88	0.41
3:A:1172:HOH:O	1:D:100:ARG:HG3	2.18	0.41
1:C:671:ASN:ND2	1:C:673:ALA:HB3	2.35	0.41
1:A:477:PRO:C	1:A:478:LYS:HG3	2.45	0.41
1:B:509:ARG:HD2	1:B:576:PRO:HD2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:ASN:O	1:C:405:ASP:C	2.62	0.41
1:B:157:ASN:HB2	3:B:1554:HOH:O	2.19	0.41
1:A:459:ASN:HD22	1:A:459:ASN:C	2.27	0.41
1:C:578:ASP:HB3	3:C:1574:HOH:O	2.20	0.41
1:C:717:GLY:HA3	1:C:741:VAL:HG11	2.02	0.41
1:D:578:ASP:HB2	3:D:1419:HOH:O	2.20	0.41
1:B:330:ASP:OD1	1:B:629:HIS:HE1	2.03	0.41
1:B:713:GLN:H	1:B:713:GLN:NE2	2.18	0.41
1:B:607:LEU:HD22	1:B:611:VAL:HG21	2.03	0.41
1:B:623:LEU:HD23	1:B:623:LEU:HA	1.73	0.41
1:C:686:MET:HB3	1:C:751:ILE:HD11	2.02	0.41
1:D:128:HIS:HA	1:D:168:THR:O	2.20	0.41
1:D:678:ASN:OD1	1:D:680:ASP:HB2	2.21	0.41
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.55	0.41
1:A:610:GLU:HG3	3:A:1563:HOH:O	2.19	0.41
1:B:461:GLU:HA	1:B:462:PRO:C	2.44	0.41
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.56	0.41
1:D:521:ARG:CG	3:D:1629:HOH:O	2.68	0.41
1:A:541:GLU:CD	3:A:1735:HOH:O	2.63	0.41
1:B:743:SER:OG	3:B:1265:HOH:O	1.95	0.41
1:C:641:THR:HA	1:C:646:THR:O	2.21	0.41
1:B:313:ARG:HD2	3:B:1212:HOH:O	2.20	0.40
1:B:616:LEU:HD23	1:B:616:LEU:HA	1.74	0.40
3:B:1481:HOH:O	1:D:73:LYS:CG	2.64	0.40
1:A:415:TYR:O	1:A:419:GLN:HG2	2.20	0.40
1:A:610:GLU:OE1	1:A:610:GLU:HA	2.21	0.40
1:D:386:ASN:OD1	1:D:386:ASN:C	2.64	0.40
1:C:296:LEU:HD23	1:C:296:LEU:HA	1.90	0.40
1:C:310:LEU:HD13	1:C:660:LEU:HB3	2.03	0.40
1:C:377:ARG:HH11	1:C:377:ARG:HD3	1.65	0.40
1:C:732:LEU:C	1:C:732:LEU:HD13	2.46	0.40
1:D:289:VAL:HA	1:D:339:GLN:O	2.21	0.40
1:A:227:TRP:O	1:D:319:ARG:HD3	2.22	0.40
1:C:451:MET:HE3	1:C:451:MET:HB3	1.78	0.40
1:C:509:ARG:HD3	1:C:576:PRO:HG2	2.02	0.40
1:B:641:THR:CG2	1:B:645:GLY:HA2	2.51	0.40
1:C:634:TYR:O	1:C:653:THR:HA	2.21	0.40
1:D:392:HIS:CE1	1:D:415:TYR:CB	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	725/753 (96%)	700 (97%)	24 (3%)	1 (0%)	48	40
1	B	725/753 (96%)	700 (97%)	21 (3%)	4 (1%)	21	13
1	C	725/753 (96%)	697 (96%)	24 (3%)	4 (1%)	21	13
1	D	725/753 (96%)	706 (97%)	18 (2%)	1 (0%)	48	40
All	All	2900/3012 (96%)	2803 (97%)	87 (3%)	10 (0%)	36	29

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	B	671	ASN
1	A	75	SER
1	B	705	LYS
1	C	75	SER
1	C	725	ASP
1	B	568	ASP
1	C	584	LYS
1	D	75	SER
1	C	274	ILE

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	612/635 (96%)	596 (97%)	16 (3%)	40	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	612/635 (96%)	580 (95%)	32 (5%)	21	13
1	C	612/635 (96%)	578 (94%)	34 (6%)	19	11
1	D	612/635 (96%)	586 (96%)	26 (4%)	26	19
All	All	2448/2540 (96%)	2340 (96%)	108 (4%)	25	17

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	THR
1	A	195	ILE
1	A	205	ILE
1	A	252	ASN
1	A	375	LEU
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	530	ASP
1	A	611	VAL
1	A	707	THR
1	A	709	LYS
1	A	713	GLN
1	A	732	LEU
1	A	747	LYS
1	A	750	LYS
1	B	61	ARG
1	B	185	PHE
1	B	191	THR
1	B	205	ILE
1	B	213	LYS
1	B	252	ASN
1	B	265	SER
1	B	283	GLU
1	B	344	GLU
1	B	375	LEU
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	521	ARG
1	B	530	ASP
1	B	552	LEU
1	B	565	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	597	ASP
1	B	611	VAL
1	B	635	SER
1	B	641	THR
1	B	647	VAL
1	B	677	ASP
1	B	707	THR
1	B	710	ILE
1	B	713	GLN
1	B	750	LYS
1	B	751	ILE
1	C	159	ILE
1	C	205	ILE
1	C	213	LYS
1	C	252	ASN
1	C	285	LYS
1	C	310	LEU
1	C	375	LEU
1	C	377	ARG
1	C	432	PRO
1	C	440	TYR
1	C	459	ASN
1	C	521	ARG
1	C	530	ASP
1	C	531	LEU
1	C	552	LEU
1	C	554	LEU
1	C	568	ASP
1	C	571	LEU
1	C	584	LYS
1	C	597	ASP
1	C	606	LEU
1	C	612	ARG
1	C	617	LEU
1	C	624	LYS
1	C	631	LYS
1	C	633	LEU
1	C	636	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	640	VAL
1	C	648	LEU
1	C	660	LEU
1	C	675	ILE
1	C	685	LEU
1	C	733	LEU
1	C	750	LYS
1	D	73	LYS
1	D	191	THR
1	D	198	LEU
1	D	205	ILE
1	D	213	LYS
1	D	252	ASN
1	D	321	GLU
1	D	340	LEU
1	D	344	GLU
1	D	375	LEU
1	D	432	PRO
1	D	440	TYR
1	D	459	ASN
1	D	521	ARG
1	D	530	ASP
1	D	554	LEU
1	D	582	LEU
1	D	593	ILE
1	D	610	GLU
1	D	612	ARG
1	D	616	LEU
1	D	648	LEU
1	D	677	ASP
1	D	707	THR
1	D	713	GLN
1	D	750	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	368	GLN
1	A	459	ASN
1	A	515	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	556	GLN
1	B	157	ASN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	B	671	ASN
1	B	713	GLN
1	C	77	ASN
1	C	252	ASN
1	C	459	ASN
1	C	486	GLN
1	C	507	HIS
1	C	546	GLN
1	C	556	GLN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	77	ASN
1	D	246	GLN
1	D	252	ASN
1	D	459	ASN
1	D	507	HIS
1	D	556	GLN
1	D	629	HIS
1	D	671	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OCS	C	669	1	6,8,9	1.96	1 (16%)	7,11,13	2.80	3 (42%)
1	OCS	D	669	1	6,8,9	1.62	1 (16%)	7,11,13	1.96	3 (42%)
1	OCS	B	669	1	6,8,9	1.91	1 (16%)	7,11,13	3.05	2 (28%)
1	OCS	A	669	1	6,8,9	1.96	1 (16%)	7,11,13	2.40	2 (28%)

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
1	OCS	C	669	1	-	4/4/7/9	-
1	OCS	D	669	1	-	3/4/7/9	-
1	OCS	B	669	1	-	4/4/7/9	-
1	OCS	A	669	1	-	1/4/7/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	669	OCS	OD2-SG	4.43	1.63	1.47
1	B	669	OCS	OD2-SG	4.36	1.63	1.47
1	A	669	OCS	OD2-SG	4.19	1.63	1.47
1	D	669	OCS	OD2-SG	3.83	1.61	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	669	OCS	OD1-SG-CB	6.12	115.89	106.76
1	C	669	OCS	OD2-SG-CB	5.24	116.10	105.97
1	A	669	OCS	OD1-SG-CB	4.56	113.56	106.76
1	B	669	OCS	CA-CB-SG	4.48	120.27	113.61
1	C	669	OCS	CA-CB-SG	4.01	119.56	113.61
1	A	669	OCS	OD2-SG-OD3	-3.76	101.98	111.40
1	D	669	OCS	OD1-SG-CB	3.59	112.12	106.76
1	D	669	OCS	CA-CB-SG	2.42	117.21	113.61
1	D	669	OCS	OD3-SG-CB	-2.29	103.34	106.76
1	C	669	OCS	OD3-SG-OD1	-2.11	106.96	113.82

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	669	OCS	N-CA-CB-SG
1	B	669	OCS	N-CA-CB-SG
1	C	669	OCS	N-CA-CB-SG
1	D	669	OCS	N-CA-CB-SG
1	D	669	OCS	CA-CB-SG-OD2
1	C	669	OCS	CA-CB-SG-OD3
1	B	669	OCS	CA-CB-SG-OD1
1	D	669	OCS	CA-CB-SG-OD1
1	B	669	OCS	CA-CB-SG-OD2
1	C	669	OCS	CA-CB-SG-OD2
1	B	669	OCS	CA-CB-SG-OD3
1	C	669	OCS	CA-CB-SG-OD1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	669	OCS	1	0
1	B	669	OCS	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HDD	D	801	1	49,52,52	2.50	17 (34%)	62,89,89	2.94	24 (38%)
2	HDD	A	801	3,1	49,52,52	2.55	17 (34%)	62,89,89	3.23	22 (35%)
2	HDD	C	801	3,1	49,52,52	2.54	20 (40%)	62,89,89	2.93	23 (37%)
2	HDD	B	801	3,1	49,52,52	2.55	19 (38%)	62,89,89	3.12	24 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HDD	D	801	1	-	4/9/89/89	0/1/9/9
2	HDD	A	801	3,1	-	2/9/89/89	0/1/9/9
2	HDD	C	801	3,1	1/1/8/14	4/9/89/89	0/1/9/9
2	HDD	B	801	3,1	-	4/9/89/89	0/1/9/9

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HDD	O1D-CGD	6.97	1.46	1.35
2	D	801	HDD	O1D-CGD	6.67	1.46	1.35
2	C	801	HDD	C3C-C2C	6.34	1.50	1.37
2	D	801	HDD	C3B-C2B	5.92	1.49	1.37
2	B	801	HDD	O1D-C3D	5.85	1.56	1.46
2	C	801	HDD	FE-NB	5.80	2.12	1.94
2	B	801	HDD	C3B-C2B	5.52	1.48	1.37
2	A	801	HDD	CHC-C1C	5.29	1.48	1.38
2	B	801	HDD	CHD-C4C	5.27	1.48	1.38
2	D	801	HDD	CHD-C4C	5.05	1.48	1.38
2	A	801	HDD	FE-NB	5.00	2.10	1.94
2	A	801	HDD	CHB-C1B	4.91	1.48	1.38
2	D	801	HDD	O1D-C3D	4.79	1.54	1.46
2	A	801	HDD	CHD-C4C	4.77	1.47	1.38
2	B	801	HDD	O1D-CGD	4.73	1.43	1.35
2	B	801	HDD	C3C-C2C	4.63	1.46	1.37
2	C	801	HDD	CHA-C1A	4.61	1.49	1.39
2	C	801	HDD	CHD-C4C	4.56	1.47	1.38
2	B	801	HDD	CHC-C4B	4.54	1.49	1.39
2	B	801	HDD	FE-NB	4.46	2.08	1.94
2	C	801	HDD	CHC-C1C	4.40	1.47	1.38
2	A	801	HDD	CHA-C1A	4.36	1.49	1.39
2	C	801	HDD	O1D-CGD	4.33	1.42	1.35
2	C	801	HDD	C3B-C2B	4.28	1.45	1.37
2	A	801	HDD	FE-NA	4.26	2.09	1.95
2	B	801	HDD	FE-NC	4.17	2.08	1.95
2	A	801	HDD	C3B-C2B	4.17	1.45	1.37
2	C	801	HDD	CHB-C1B	4.15	1.46	1.38
2	D	801	HDD	FE-NC	4.07	2.08	1.95
2	A	801	HDD	FE-NC	3.88	2.08	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	HDD	CHB-C4A	3.84	1.48	1.39
2	D	801	HDD	FE-NA	3.82	2.07	1.95
2	D	801	HDD	C3C-C2C	3.75	1.44	1.37
2	C	801	HDD	FE-NA	3.74	2.07	1.95
2	D	801	HDD	CHC-C1C	3.62	1.45	1.38
2	B	801	HDD	FE-NA	3.57	2.06	1.95
2	B	801	HDD	CHB-C4A	3.56	1.47	1.39
2	C	801	HDD	CHC-C4B	3.55	1.47	1.39
2	C	801	HDD	O1D-C3D	3.52	1.52	1.46
2	B	801	HDD	CHC-C1C	3.50	1.45	1.38
2	D	801	HDD	C4A-NA	-3.41	1.33	1.39
2	A	801	HDD	C3C-C2C	3.40	1.44	1.37
2	D	801	HDD	FE-NB	3.39	2.05	1.94
2	C	801	HDD	C2A-C3A	3.18	1.47	1.38
2	B	801	HDD	C1A-NA	-3.03	1.33	1.39
2	B	801	HDD	CHA-C1A	3.03	1.46	1.39
2	C	801	HDD	FE-NC	3.03	2.05	1.95
2	D	801	HDD	C4C-NC	-3.01	1.33	1.39
2	D	801	HDD	CHB-C4A	3.00	1.46	1.39
2	D	801	HDD	CHB-C1B	2.96	1.44	1.38
2	D	801	HDD	CHC-C4B	2.86	1.45	1.39
2	A	801	HDD	CHC-C4B	2.80	1.45	1.39
2	B	801	HDD	C4B-NB	-2.80	1.33	1.38
2	B	801	HDD	C4A-NA	-2.77	1.34	1.39
2	A	801	HDD	C1A-NA	-2.74	1.34	1.39
2	A	801	HDD	C1A-C2A	2.74	1.50	1.44
2	A	801	HDD	C2A-C3A	2.66	1.45	1.38
2	D	801	HDD	C4B-NB	-2.66	1.33	1.38
2	B	801	HDD	C4C-NC	-2.62	1.34	1.39
2	B	801	HDD	CHB-C1B	2.62	1.43	1.38
2	A	801	HDD	CMC-C2C	2.57	1.56	1.50
2	B	801	HDD	CHD-C1D	-2.51	1.33	1.41
2	A	801	HDD	CHB-C4A	2.40	1.44	1.39
2	D	801	HDD	OND-C2D	2.31	1.47	1.42
2	C	801	HDD	C4B-NB	-2.28	1.34	1.38
2	B	801	HDD	C4A-C3A	2.25	1.48	1.43
2	D	801	HDD	C1A-NA	-2.10	1.35	1.39
2	C	801	HDD	O2A-CGA	-2.09	1.23	1.30
2	C	801	HDD	C1A-NA	-2.08	1.35	1.39
2	C	801	HDD	FE-ND	2.07	2.01	1.94
2	C	801	HDD	C4A-NA	-2.01	1.35	1.39
2	A	801	HDD	O1D-C3D	2.00	1.49	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	HDD	CHD-C1D	-2.00	1.35	1.41

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	HDD	O1D-CGD-O2D	12.81	131.60	120.81
2	C	801	HDD	C3B-C2B-C1B	-10.08	98.84	106.41
2	A	801	HDD	O1D-CGD-O2D	9.89	129.15	120.81
2	B	801	HDD	C3B-C2B-C1B	-9.00	99.66	106.41
2	A	801	HDD	C3B-C2B-C1B	-8.93	99.70	106.41
2	A	801	HDD	C3D-O1D-CGD	8.76	119.31	111.14
2	D	801	HDD	C3B-C2B-C1B	-8.63	99.93	106.41
2	B	801	HDD	C3C-C2C-C1C	-8.30	99.20	107.05
2	D	801	HDD	O1D-CGD-O2D	8.25	127.76	120.81
2	D	801	HDD	C3C-C2C-C1C	-7.94	99.53	107.05
2	C	801	HDD	C3C-C2C-C1C	-7.18	100.25	107.05
2	A	801	HDD	C2B-C1B-NB	6.85	117.71	109.84
2	C	801	HDD	O1D-CGD-O2D	6.82	126.55	120.81
2	A	801	HDD	C3C-C2C-C1C	-6.64	100.76	107.05
2	A	801	HDD	O1D-CGD-CBD	-6.56	104.19	110.17
2	A	801	HDD	CBD-CAD-C3D	6.19	112.81	103.98
2	D	801	HDD	C3B-C4B-NB	5.83	113.66	109.47
2	C	801	HDD	C2B-C1B-NB	5.75	116.45	109.84
2	C	801	HDD	C3D-O1D-CGD	5.59	116.35	111.14
2	D	801	HDD	OND-C2D-CMD	-5.55	98.73	109.45
2	C	801	HDD	OND-C2D-CMD	-5.51	98.80	109.45
2	C	801	HDD	O1D-CGD-CBD	-5.40	105.25	110.17
2	D	801	HDD	C2B-C1B-NB	5.36	116.00	109.84
2	A	801	HDD	OND-C2D-CMD	-5.30	99.19	109.45
2	D	801	HDD	CBD-CAD-C3D	5.12	111.28	103.98
2	A	801	HDD	C3B-C4B-NB	4.99	113.06	109.47
2	B	801	HDD	C2B-C1B-NB	4.99	115.57	109.84
2	B	801	HDD	OND-C2D-CMD	-4.90	99.98	109.45
2	B	801	HDD	CAA-CBA-CGA	-4.52	101.69	113.67
2	A	801	HDD	CMB-C2B-C1B	4.47	132.02	125.03
2	B	801	HDD	C3B-C4B-NB	4.45	112.66	109.47
2	D	801	HDD	CMC-C2C-C1C	4.30	132.30	124.73
2	A	801	HDD	O1D-C3D-CAD	-4.28	95.13	103.06
2	B	801	HDD	O1D-CGD-CBD	-4.25	106.29	110.17
2	C	801	HDD	CBD-CAD-C3D	4.14	109.89	103.98
2	C	801	HDD	CMB-C2B-C1B	4.10	131.44	125.03
2	B	801	HDD	C4A-C3A-C2A	-4.06	102.17	106.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801	HDD	CMC-C2C-C1C	4.02	131.81	124.73
2	C	801	HDD	C3B-C4B-NB	3.96	112.31	109.47
2	C	801	HDD	C4A-C3A-C2A	-3.93	102.31	106.82
2	B	801	HDD	CMB-C2B-C1B	3.91	131.15	125.03
2	B	801	HDD	C2C-C1C-NC	3.89	116.82	109.64
2	D	801	HDD	O1D-CGD-CBD	-3.88	106.64	110.17
2	C	801	HDD	CAA-CBA-CGA	-3.83	103.49	113.67
2	D	801	HDD	C3D-O1D-CGD	3.79	114.68	111.14
2	A	801	HDD	C4A-C3A-C2A	-3.77	102.50	106.82
2	D	801	HDD	CAA-CBA-CGA	-3.71	103.84	113.67
2	A	801	HDD	CMC-C2C-C1C	3.69	131.23	124.73
2	B	801	HDD	CBD-CAD-C3D	3.66	109.20	103.98
2	D	801	HDD	CMB-C2B-C1B	3.65	130.74	125.03
2	C	801	HDD	C2A-C1A-NA	3.47	114.00	110.15
2	D	801	HDD	C2C-C1C-NC	3.44	116.00	109.64
2	A	801	HDD	CBC-CAC-C3C	-3.43	110.40	127.53
2	B	801	HDD	C3D-O1D-CGD	3.41	114.33	111.14
2	A	801	HDD	CAA-CBA-CGA	-3.38	104.71	113.67
2	D	801	HDD	C2D-C1D-CHD	-3.32	118.05	123.28
2	C	801	HDD	C3A-C4A-NA	3.23	115.33	110.14
2	D	801	HDD	C4A-C3A-C2A	-3.15	103.20	106.82
2	A	801	HDD	CMA-C3A-C4A	3.15	130.21	125.42
2	D	801	HDD	C3A-C4A-NA	3.10	115.12	110.14
2	C	801	HDD	O1D-C3D-CAD	-2.94	97.63	103.06
2	C	801	HDD	C2C-C1C-NC	2.93	115.06	109.64
2	B	801	HDD	C2A-C1A-NA	2.90	113.37	110.15
2	B	801	HDD	CMD-C2D-C3D	2.90	122.73	115.11
2	A	801	HDD	C1B-NB-C4B	-2.87	101.81	105.21
2	B	801	HDD	CHD-C4C-NC	-2.83	121.37	124.45
2	B	801	HDD	C3A-C4A-NA	2.72	114.51	110.14
2	B	801	HDD	C2D-C1D-CHD	-2.71	119.01	123.28
2	D	801	HDD	CMA-C3A-C4A	2.71	129.54	125.42
2	D	801	HDD	CBC-CAC-C3C	-2.69	114.07	127.53
2	C	801	HDD	CMA-C3A-C2A	2.69	131.34	125.62
2	C	801	HDD	CMD-C2D-C3D	2.68	122.17	115.11
2	D	801	HDD	CHD-C4C-NC	-2.68	121.53	124.45
2	C	801	HDD	CBB-CAB-C3B	-2.67	114.20	127.53
2	D	801	HDD	C2A-C1A-NA	2.61	113.05	110.15
2	A	801	HDD	C3A-C4A-NA	2.57	114.26	110.14
2	A	801	HDD	CHB-C1B-C2B	-2.48	119.90	126.95
2	B	801	HDD	CHB-C1B-C2B	-2.45	119.98	126.95
2	B	801	HDD	CHC-C1C-C2C	-2.40	120.49	125.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	HDD	OND-C2D-C3D	-2.39	104.86	110.46
2	C	801	HDD	CHB-C1B-C2B	-2.38	120.18	126.95
2	A	801	HDD	C2C-C1C-NC	2.32	113.92	109.64
2	D	801	HDD	C4B-C3B-C2B	-2.30	105.17	107.28
2	D	801	HDD	CHC-C1C-NC	-2.27	121.98	124.45
2	A	801	HDD	C4C-C3C-C2C	2.21	108.73	106.81
2	C	801	HDD	CHB-C4A-C3A	-2.20	121.03	127.43
2	B	801	HDD	CAD-CBD-CGD	2.16	107.68	104.48
2	B	801	HDD	CHC-C1C-NC	-2.11	122.16	124.45
2	B	801	HDD	CBA-CAA-C2A	-2.08	106.79	112.53
2	C	801	HDD	CBA-CAA-C2A	-2.06	106.83	112.53
2	A	801	HDD	CHB-C1B-NB	-2.04	121.84	124.37
2	D	801	HDD	CHC-C1C-C2C	-2.02	121.30	125.49
2	D	801	HDD	CHB-C1B-C2B	-2.00	121.25	126.95

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	801	HDD	NC

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	HDD	C2C-C3C-CAC-CBC
2	C	801	HDD	C2B-C3B-CAB-CBB
2	D	801	HDD	C2C-C3C-CAC-CBC
2	B	801	HDD	C4C-C3C-CAC-CBC
2	A	801	HDD	CAA-CBA-CGA-O2A
2	B	801	HDD	CAA-CBA-CGA-O1A
2	C	801	HDD	CAA-CBA-CGA-O2A
2	D	801	HDD	CAA-CBA-CGA-O2A
2	C	801	HDD	CAA-CBA-CGA-O1A
2	B	801	HDD	CAA-CBA-CGA-O2A
2	A	801	HDD	CAA-CBA-CGA-O1A
2	D	801	HDD	CAA-CBA-CGA-O1A
2	C	801	HDD	C4B-C3B-CAB-CBB
2	D	801	HDD	C4C-C3C-CAC-CBC

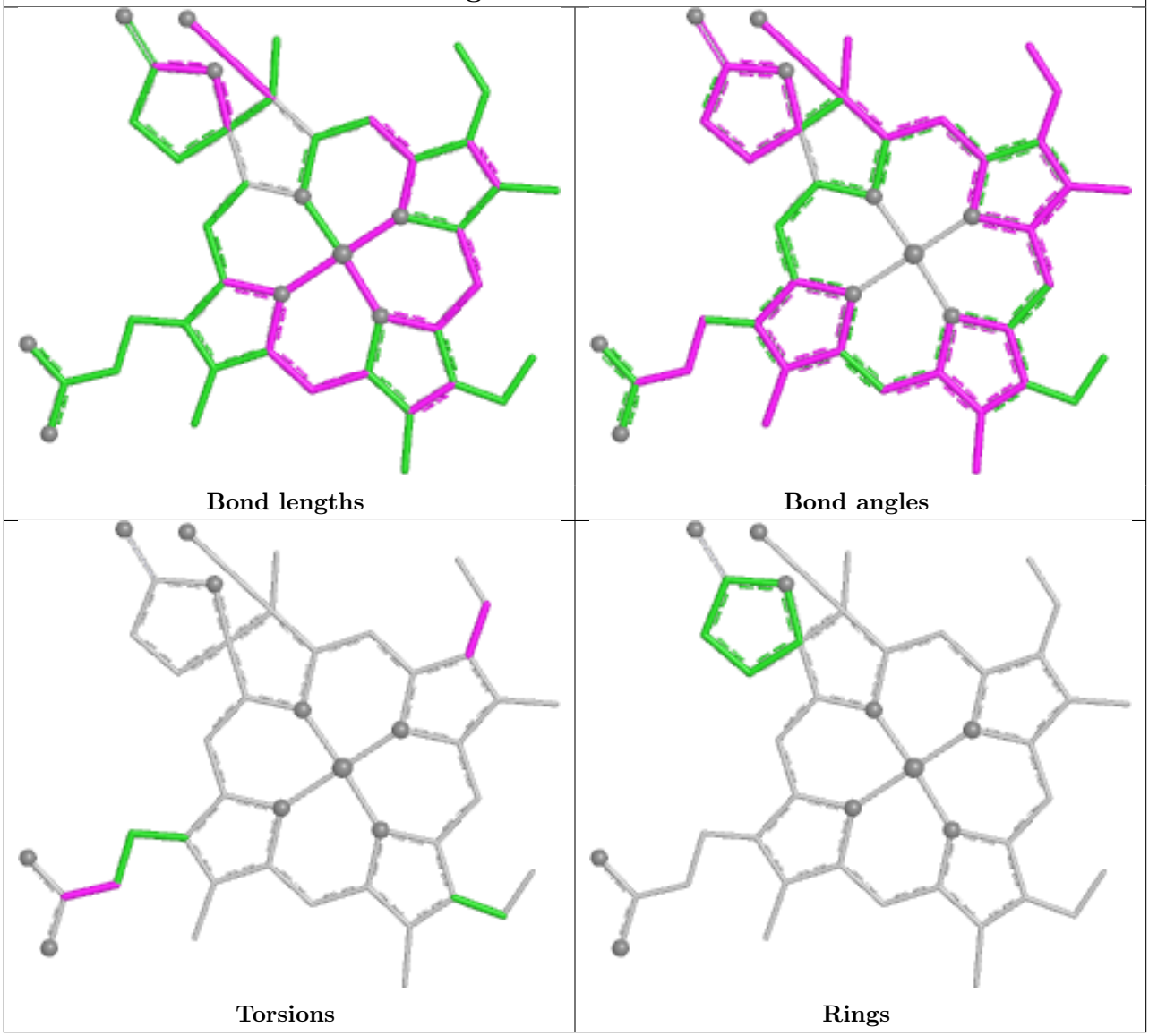
There are no ring outliers.

4 monomers are involved in 12 short contacts:

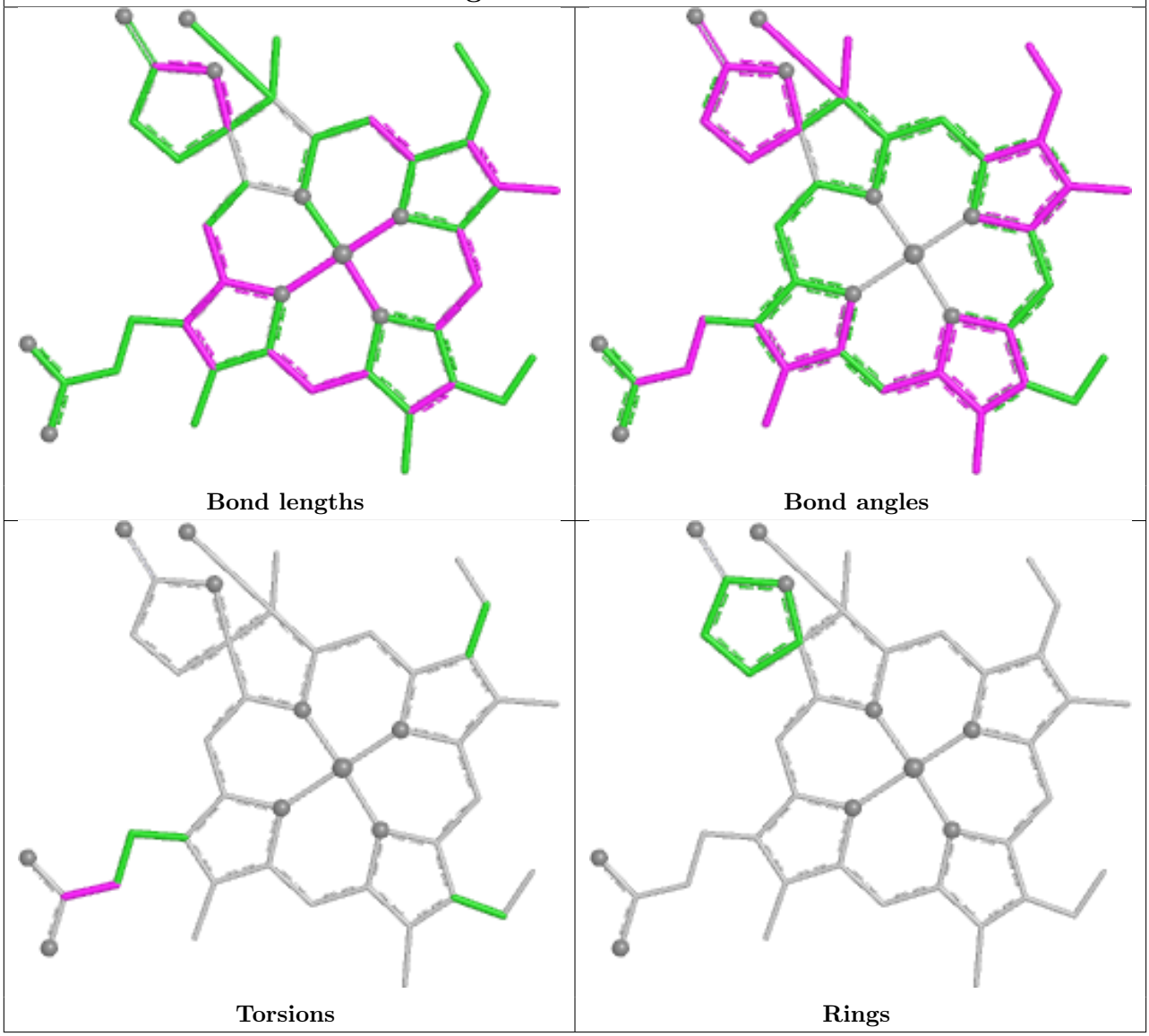
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	HDD	4	0
2	A	801	HDD	4	0
2	C	801	HDD	2	0
2	B	801	HDD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

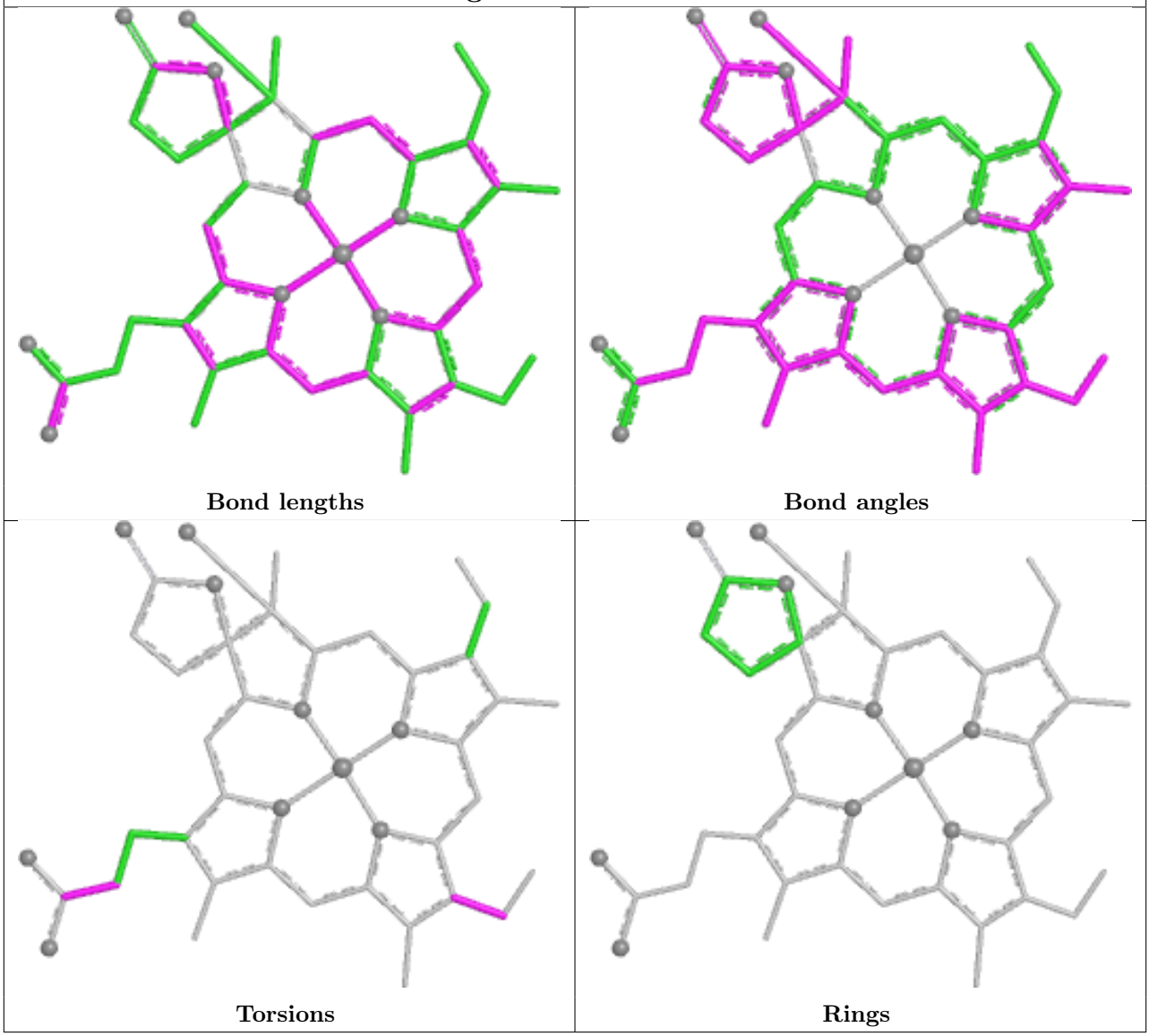
Ligand HDD D 801



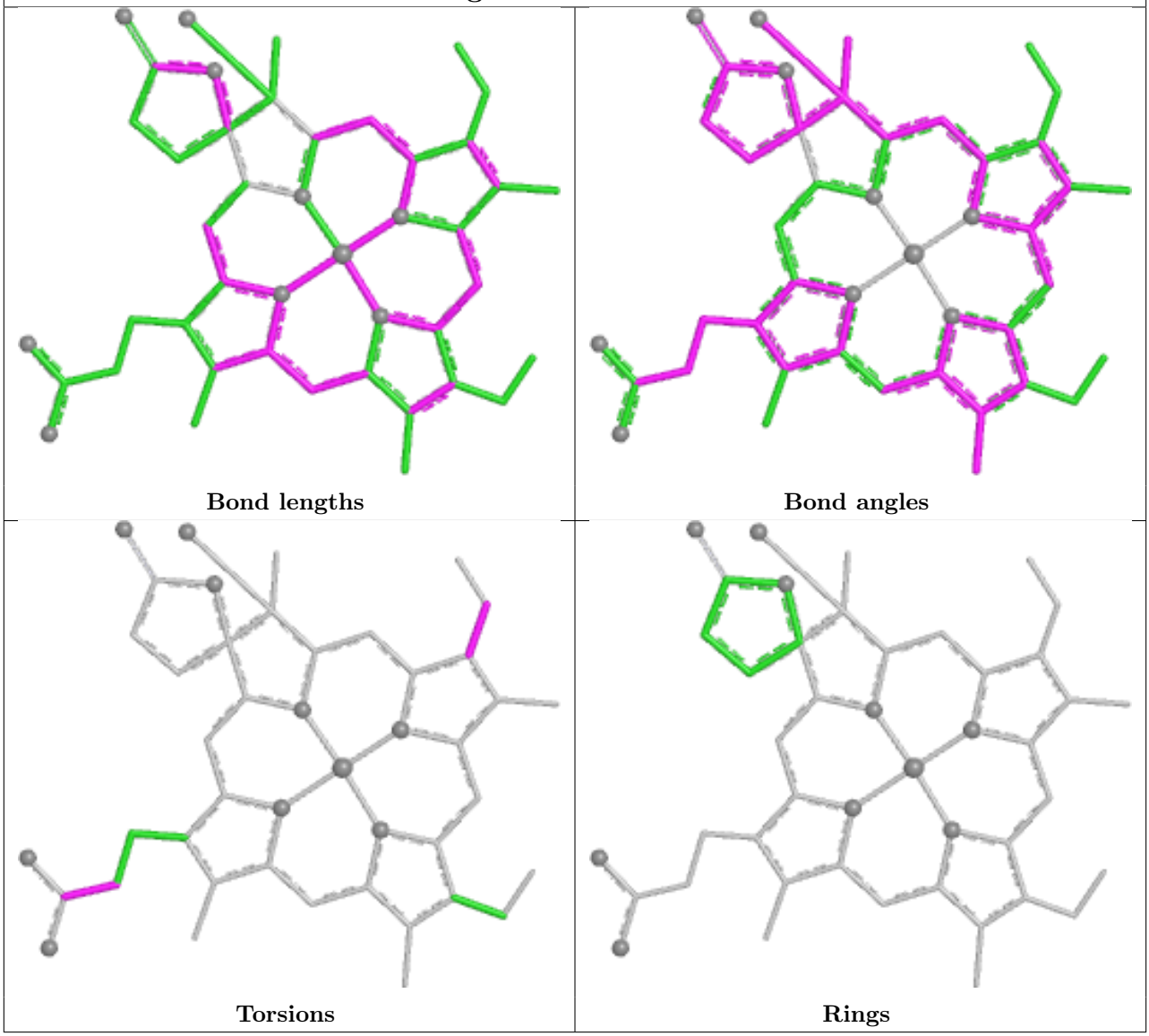
Ligand HDD A 801



Ligand HDD C 801



Ligand HDD B 801



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	724/753 (96%)	-0.61	10 (1%)	73	76	4, 10, 31, 76	4 (0%)
1	B	724/753 (96%)	-0.27	40 (5%)	30	32	3, 13, 58, 76	4 (0%)
1	C	724/753 (96%)	-0.39	16 (2%)	62	66	5, 12, 46, 70	4 (0%)
1	D	724/753 (96%)	-0.61	3 (0%)	88	90	3, 11, 28, 64	3 (0%)
All	All	2896/3012 (96%)	-0.47	69 (2%)	59	63	3, 11, 45, 76	15 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	676	ALA	5.1
1	A	29	LEU	4.8
1	B	675	ILE	3.7
1	B	672	ILE	3.4
1	B	751	ILE	3.3
1	C	721	ALA	3.3
1	B	711	ALA	3.2
1	B	673	ALA	3.2
1	A	710	ILE	3.0
1	C	675	ILE	3.0
1	C	726	GLY	3.0
1	B	707	THR	3.0
1	B	611	VAL	3.0
1	C	616	LEU	2.9
1	B	704	PHE	2.9
1	B	701	ALA	2.9
1	B	670	GLY	2.8
1	B	726	GLY	2.8
1	C	719	VAL	2.8
1	A	35	SER	2.8
1	C	676	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	711	ALA	2.8
1	B	674	ASP	2.8
1	D	751	ILE	2.8
1	A	38	PRO	2.8
1	B	753	ALA	2.7
1	A	711	ALA	2.7
1	B	714	GLY	2.6
1	B	700	ASP	2.6
1	B	608	ASN	2.5
1	C	706	ALA	2.5
1	C	749	ASP	2.5
1	C	698	ALA	2.5
1	B	609	ASP	2.5
1	C	750	LYS	2.5
1	B	637	MET	2.4
1	A	39	ALA	2.4
1	B	671	ASN	2.4
1	C	703	LYS	2.4
1	B	568	ASP	2.4
1	B	719	VAL	2.4
1	B	698	ALA	2.4
1	C	701	ALA	2.4
1	B	723	SER	2.4
1	C	753	ALA	2.3
1	B	752	PRO	2.3
1	B	37	ARG	2.3
1	A	36	HIS	2.3
1	B	717	GLY	2.3
1	B	595	ASP	2.3
1	A	750	LYS	2.3
1	B	706	ALA	2.3
1	D	29	LEU	2.3
1	B	643	ASP	2.2
1	B	668	PRO	2.2
1	B	721	ALA	2.2
1	B	614	ALA	2.2
1	D	750	LYS	2.2
1	A	751	ILE	2.1
1	B	677	ASP	2.1
1	B	667	VAL	2.1
1	B	750	LYS	2.1
1	B	612	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	667	VAL	2.1
1	B	642	ALA	2.1
1	C	725	ASP	2.1
1	B	606	LEU	2.1
1	B	727	SER	2.0
1	A	37	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	OCS	B	669	9/10	0.76	0.17	56,66,70,72	0
1	OCS	C	669	9/10	0.81	0.15	54,59,66,73	0
1	OCS	A	669	9/10	0.91	0.10	18,21,35,36	0
1	OCS	D	669	9/10	0.93	0.09	22,24,32,38	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

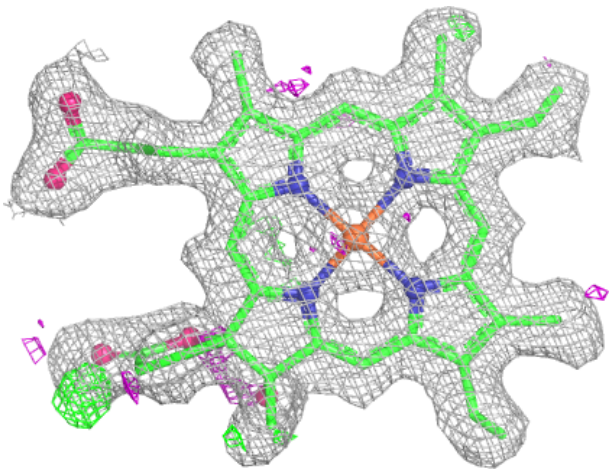
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

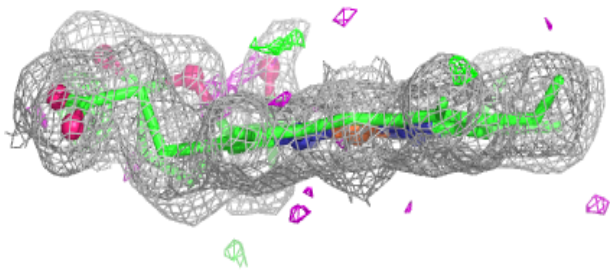
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HDD	B	801	44/44	0.97	0.06	7,9,14,17	0
2	HDD	C	801	44/44	0.97	0.06	6,10,14,16	0
2	HDD	A	801	44/44	0.98	0.06	5,8,12,16	0
2	HDD	D	801	44/44	0.98	0.05	5,7,10,12	0

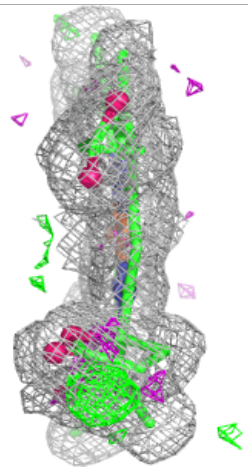
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HDD B 801:

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

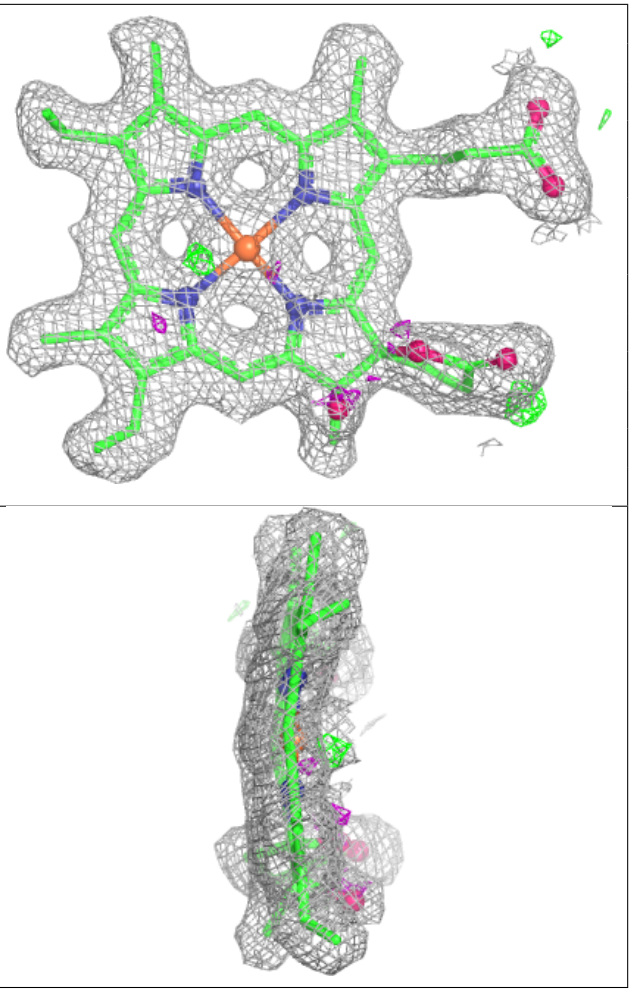






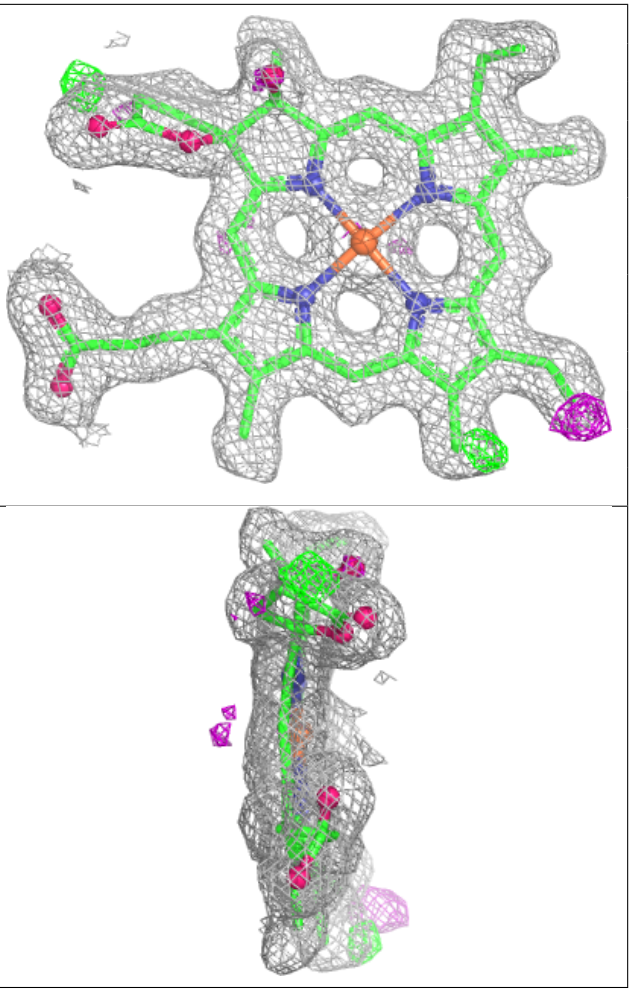
Electron density around HDD C 801:

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



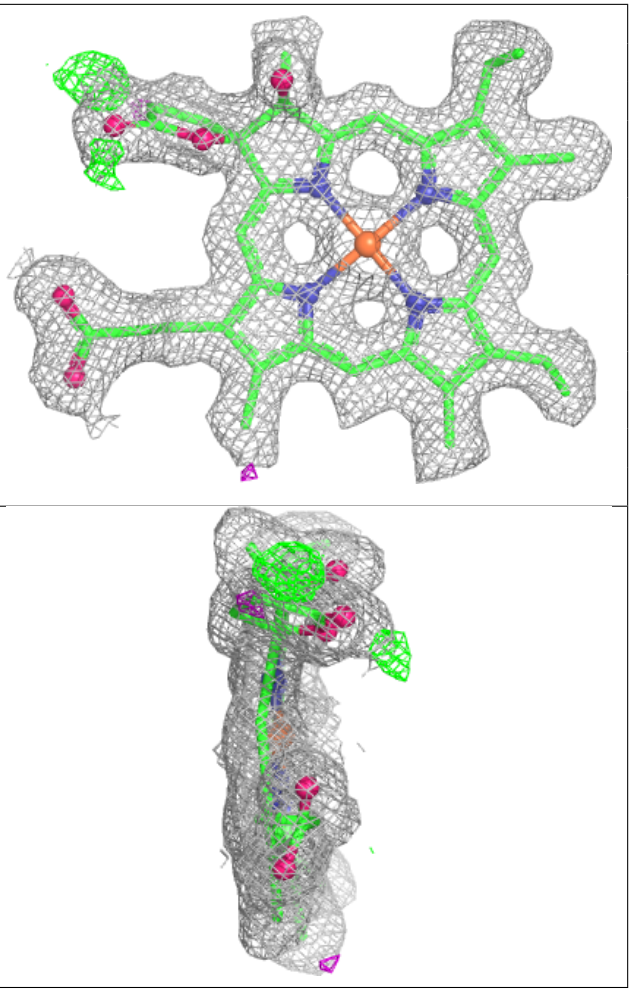
Electron density around HDD A 801:

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



Electron density around HDD D 801:

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



6.5 Other polymers (i)

There are no such residues in this entry.