



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 05:34 PM EDT

PDB ID : 3EJ8
Title : Structure of double mutant of human iNOS oxygenase domain with bound imidazole
Authors : Garcin, E.D.; Arvai, A.S.; Rosenfeld, R.J.; Kroeger, M.D.; Crane, B.R.; Andersson, G.; Andrews, G.; Hamley, P.J.; Mallinder, P.R.; Nicholls, D.J.; St-Gallay, S.A.; Tinker, A.C.; Gensmantel, N.P.; Mete, A.; Cheshire, D.R.; Connolly, S.; Stuehr, D.J.; Aberg, A.; Wallace, A.V.; Tainer, J.A.; Getzoff, E.D.
Deposited on : 2008-09-17
Resolution : 2.55 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

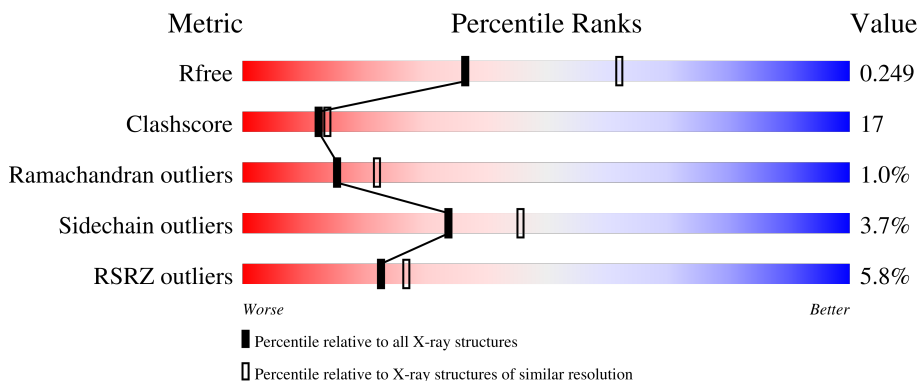
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	424	 4% (red), 64% (green), 33% (yellow), .. (grey)
1	B	424	 9% (red), 65% (green), 33% (yellow), .. (grey)
1	C	424	 5% (red), 67% (green), 30% (yellow), .. (grey)
1	D	424	 5% (red), 69% (green), 29% (yellow), .. (grey)

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
3	H4B	A	1902	X	-	-	-
3	H4B	B	2902	X	-	-	-
3	H4B	C	3902	X	-	-	-
3	H4B	D	4902	X	-	-	-
5	IMD	A	1904	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14119 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.

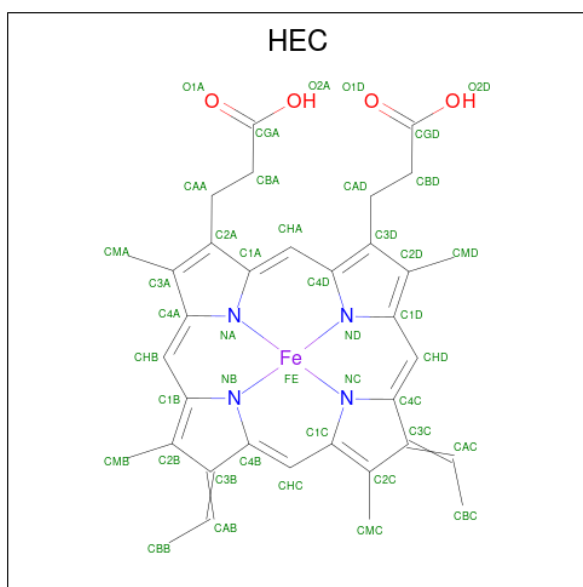
- Molecule 1 is a protein called Nitric oxide synthase, inducible.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	421	3416	2184	597	613	22	0	0	0
1	B	421	3416	2184	597	613	22	0	0	0
1	C	421	3416	2184	597	613	22	0	0	0
1	D	421	3416	2184	597	613	22	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

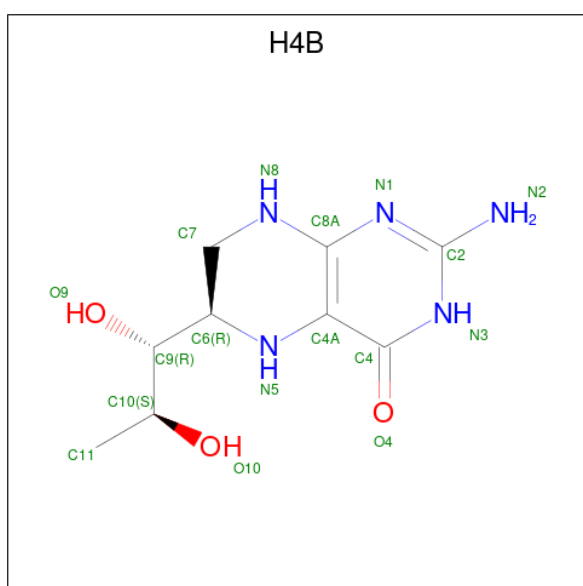
Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ILE	PHE	engineered mutation	UNP P35228
A	305	LEU	VAL	engineered mutation	UNP P35228
B	286	ILE	PHE	engineered mutation	UNP P35228
B	305	LEU	VAL	engineered mutation	UNP P35228
C	286	ILE	PHE	engineered mutation	UNP P35228
C	305	LEU	VAL	engineered mutation	UNP P35228
D	286	ILE	PHE	engineered mutation	UNP P35228
D	305	LEU	VAL	engineered mutation	UNP P35228

- Molecule 2 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).

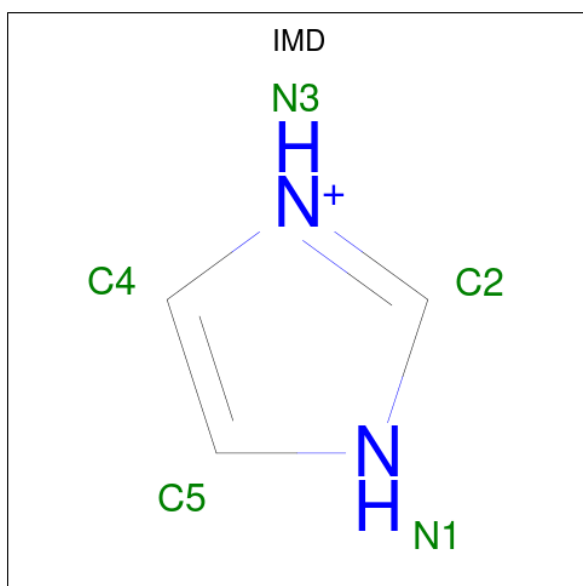


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



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

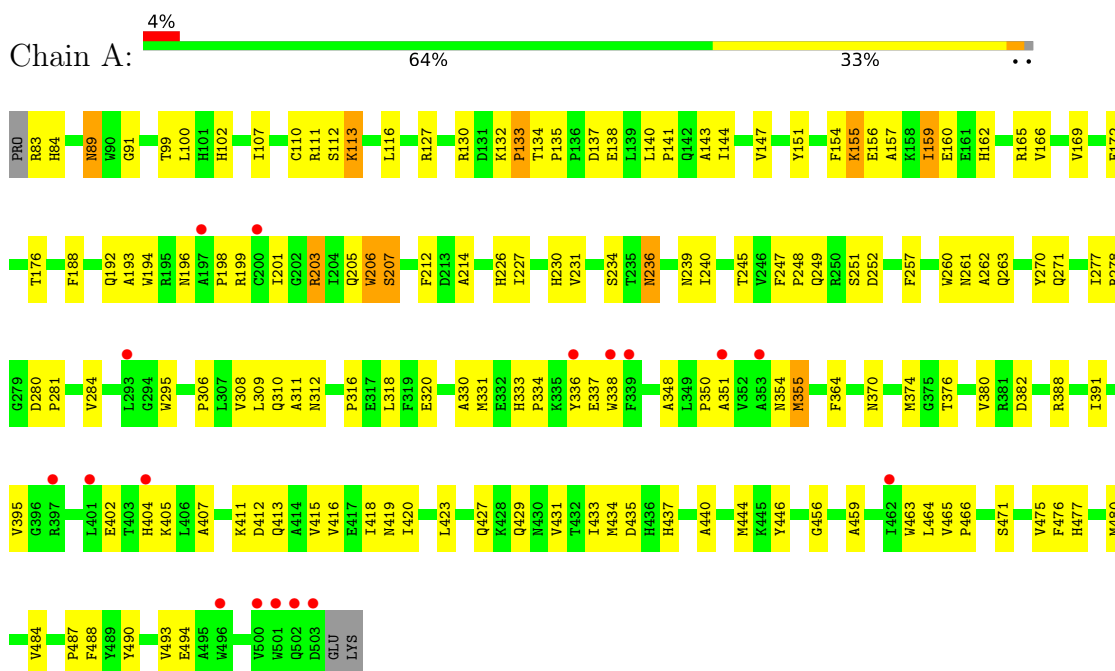
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	49	Total O 49 49	0	0
6	B	46	Total O 46 46	0	0
6	C	45	Total O 45 45	0	0
6	D	53	Total O 53 53	0	0

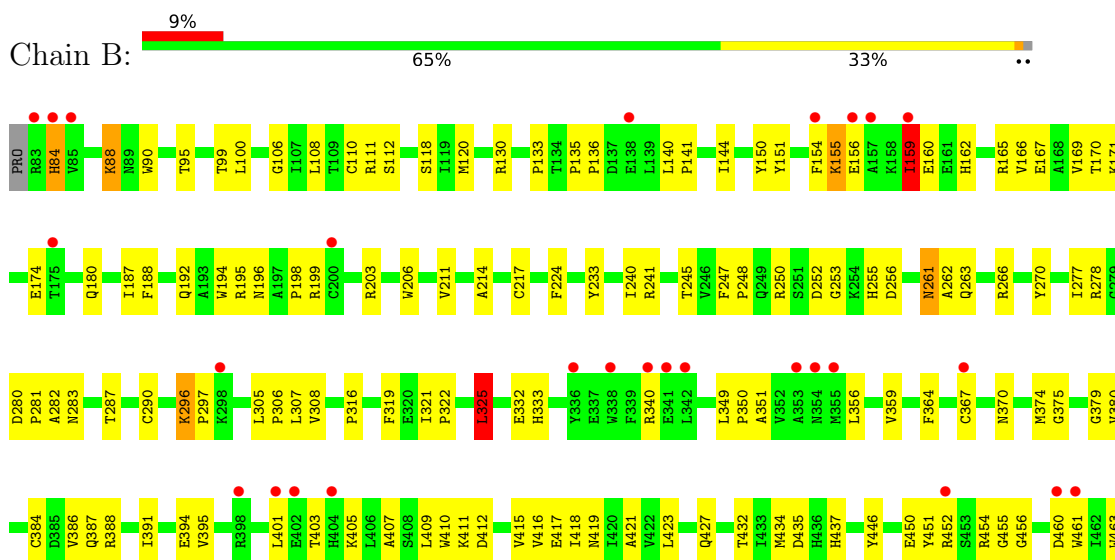
3 Residue-property plots

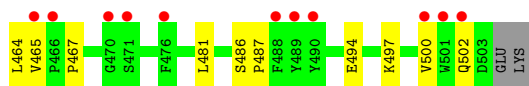
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nitric oxide synthase, inducible

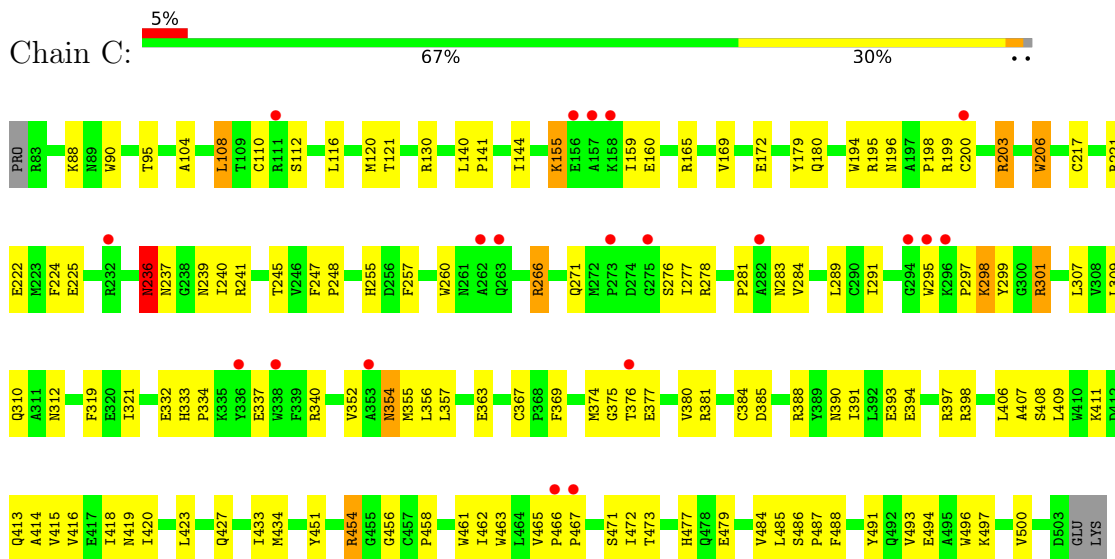


- Molecule 1: Nitric oxide synthase, inducible

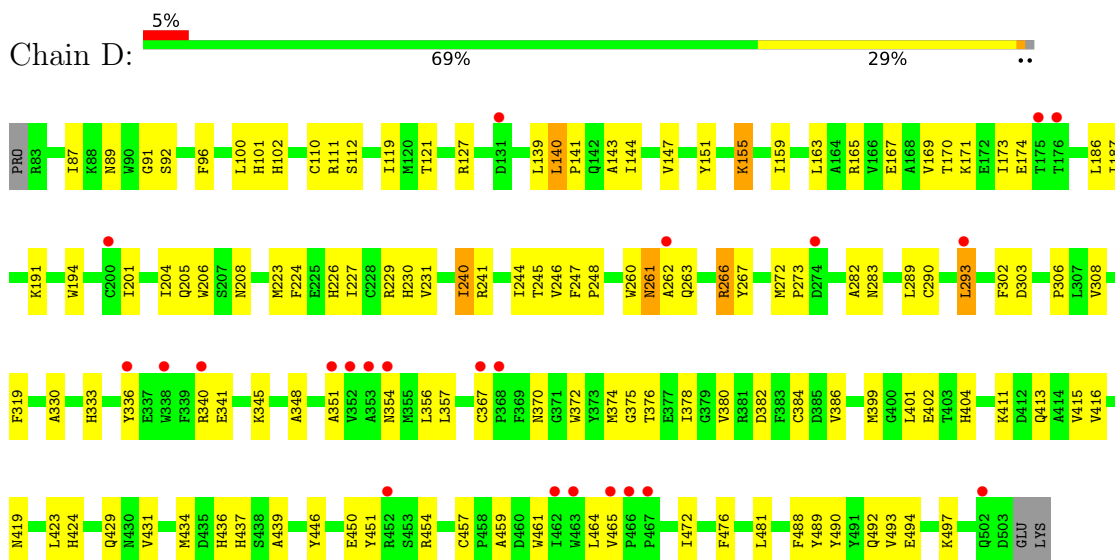




- Molecule 1: Nitric oxide synthase, inducible



- Molecule 1: Nitric oxide synthase, inducible



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.88Å 150.71Å 191.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.85 – 2.55 39.85 – 2.56	Depositor EDS
% Data completeness (in resolution range)	91.3 (39.85-2.55) 91.4 (39.85-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.54Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.232 , 0.271 0.217 , 0.249	Depositor DCC
R_{free} test set	3931 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtrriage
Anisotropy	1.099	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14119	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: H4B, ZN, HEC, IMD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/3514	0.61	0/4770
1	B	0.38	0/3514	0.61	1/4770 (0.0%)
1	C	0.37	0/3514	0.61	0/4770
1	D	0.37	0/3514	0.60	0/4770
All	All	0.37	0/14056	0.61	1/19080 (0.0%)

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	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	325	LEU	N-CA-C	-6.87	92.44	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	451	TYR	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	3416	0	3321	122	0
1	B	3416	0	3321	121	0
1	C	3416	0	3321	118	0
1	D	3416	0	3321	117	0
2	A	43	0	32	5	0
2	B	43	0	32	3	0
2	C	43	0	32	6	0
2	D	43	0	32	5	0
3	A	17	0	13	3	0
3	B	17	0	13	3	0
3	C	17	0	13	2	0
3	D	17	0	13	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	5	0	5	0	0
5	B	5	0	5	0	0
5	C	5	0	5	1	0
5	D	5	0	5	0	0
6	A	49	0	0	0	0
6	B	46	0	0	1	0
6	C	45	0	0	0	0
6	D	53	0	0	2	0
All	All	14119	0	13484	459	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 17.

All (459) 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:C:155:LYS:H	1:C:155:LYS:HD3	1.08	1.13
1:A:155:LYS:H	1:A:155:LYS:HD3	1.16	1.08
1:D:155:LYS:H	1:D:155:LYS:HD3	1.25	1.01
1:C:155:LYS:HD3	1:C:155:LYS:N	1.87	0.88
1:C:200:CYS:HB3	1:C:203:ARG:HD3	1.57	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:HIS:HE1	1:D:370:ASN:HD22	1.23	0.85
1:A:262:ALA:HA	1:A:354:ASN:ND2	1.95	0.82
1:B:261:ASN:HD22	1:B:261:ASN:N	1.79	0.81
1:D:262:ALA:HA	1:D:354:ASN:ND2	1.96	0.81
1:A:212:PHE:HB2	1:A:245:THR:HG22	1.61	0.80
1:D:230:HIS:CE1	1:D:370:ASN:HD22	2.00	0.79
1:B:261:ASN:HD22	1:B:261:ASN:H	1.30	0.78
1:B:240:ILE:HG12	1:B:432:THR:HB	1.66	0.78
1:C:155:LYS:H	1:C:155:LYS:CD	1.93	0.77
1:C:194:TRP:HB2	2:C:3901:HEC:HBC3	1.67	0.76
1:B:144:ILE:HD12	1:B:166:VAL:HG13	1.68	0.75
1:A:138:GLU:O	1:A:141:PRO:HD2	1.85	0.75
1:B:159:ILE:HD13	1:B:159:ILE:H	1.50	0.74
1:B:250:ARG:HD2	1:B:253:GLY:HA2	1.71	0.72
1:A:193:ALA:HB2	1:A:487:PRO:HB2	1.71	0.72
1:D:155:LYS:HD3	1:D:155:LYS:N	2.03	0.72
1:A:135:PRO:HB2	1:A:138:GLU:HG3	1.72	0.72
1:B:159:ILE:HD13	1:B:159:ILE:N	2.05	0.72
1:A:194:TRP:HB2	2:A:1901:HEC:HBC3	1.72	0.71
1:C:307:LEU:HB3	1:C:309:LEU:HD21	1.73	0.71
1:A:89:ASN:HD22	1:A:91:GLY:H	1.39	0.71
1:D:380:VAL:HG22	1:D:419:ASN:HD21	1.56	0.71
1:B:194:TRP:CE3	1:B:206:TRP:HA	2.27	0.70
1:D:201:ILE:HG21	1:D:374:MET:HE1	1.74	0.70
1:A:423:LEU:O	1:A:427:GLN:HG3	1.92	0.70
1:A:155:LYS:HD3	1:A:155:LYS:N	2.00	0.70
1:D:374:MET:HE2	1:D:439:ALA:HB3	1.73	0.70
1:C:380:VAL:HG22	1:C:419:ASN:HD21	1.56	0.69
1:B:391:ILE:O	1:B:395:VAL:HG13	1.91	0.69
1:A:380:VAL:HG22	1:A:419:ASN:HD21	1.57	0.69
1:D:159:ILE:HD12	1:D:159:ILE:H	1.56	0.69
1:D:194:TRP:CH2	2:D:4901:HEC:HMC3	2.28	0.69
1:C:88:LYS:HD3	1:C:90:TRP:CZ2	2.29	0.68
1:D:434:MET:HG2	1:D:439:ALA:HB2	1.75	0.68
1:C:110:CYS:HB3	1:D:110:CYS:HB3	1.74	0.68
1:C:108:LEU:HB2	1:D:112:SER:O	1.94	0.67
1:A:111:ARG:HH12	1:B:112:SER:HB3	1.57	0.67
1:D:89:ASN:HD22	1:D:92:SER:H	1.41	0.67
1:C:88:LYS:HB3	1:C:95:THR:HG22	1.77	0.67
1:D:356:LEU:HD12	1:D:492:GLN:NE2	2.10	0.67
1:B:194:TRP:CZ3	1:B:206:TRP:HA	2.29	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ILE:HG21	1:B:281:PRO:HB3	1.76	0.66
1:C:332:GLU:HG2	1:C:340:ARG:HG2	1.78	0.66
1:D:155:LYS:H	1:D:155:LYS:CD	2.00	0.66
1:C:416:VAL:O	1:C:420:ILE:HG13	1.96	0.66
1:C:414:ALA:O	1:C:418:ILE:HG13	1.95	0.66
1:C:271:GLN:HB2	1:C:284:VAL:HG11	1.78	0.65
1:A:132:LYS:HB2	1:A:132:LYS:NZ	2.10	0.65
1:D:290:CYS:SG	1:D:306:PRO:HG2	2.36	0.65
1:A:227:ILE:O	1:A:231:VAL:HG23	1.97	0.65
1:D:330:ALA:H	1:D:429:GLN:HE22	1.45	0.65
1:C:130:ARG:HD3	1:C:363:GLU:OE2	1.98	0.64
1:A:155:LYS:HG2	1:A:156:GLU:H	1.62	0.64
1:B:261:ASN:HD21	1:B:308:VAL:H	1.45	0.64
1:D:194:TRP:HB2	2:D:4901:HEC:HBC3	1.79	0.64
1:B:322:PRO:O	1:B:325:LEU:HB2	1.97	0.64
1:A:336:TYR:HB3	1:A:338:TRP:CE2	2.33	0.63
1:C:494:GLU:HG3	1:C:497:LYS:HE3	1.79	0.63
1:B:196:ASN:O	1:B:198:PRO:HD3	1.98	0.63
1:B:250:ARG:HD3	1:B:256:ASP:OD2	1.99	0.62
1:C:194:TRP:CE3	1:C:206:TRP:HA	2.35	0.62
1:A:111:ARG:NH1	1:B:112:SER:HB3	2.13	0.62
1:A:309:LEU:O	1:A:316:PRO:HA	2.00	0.62
1:B:155:LYS:H	1:B:155:LYS:HZ3	1.48	0.62
1:C:159:ILE:HG23	1:C:160:GLU:N	2.15	0.62
1:C:247:PHE:HB3	1:C:248:PRO:CD	2.30	0.62
1:D:459:ALA:HB1	1:D:464:LEU:HD11	1.83	0.61
1:A:194:TRP:CE3	1:A:206:TRP:HA	2.36	0.61
1:A:143:ALA:O	1:A:147:VAL:HG23	2.01	0.61
1:B:380:VAL:HG11	1:B:467:PRO:HB2	1.83	0.61
1:A:162:HIS:O	1:A:166:VAL:HG23	2.00	0.61
1:A:402:GLU:HB3	1:A:404:HIS:CE1	2.35	0.60
1:A:355:MET:HG3	1:A:490:TYR:O	2.00	0.60
1:C:88:LYS:HD3	1:C:90:TRP:CH2	2.36	0.60
1:D:488:PHE:HB3	1:D:490:TYR:CE1	2.37	0.60
1:C:413:GLN:HG2	1:D:416:VAL:HG11	1.82	0.60
1:B:140:LEU:HB3	1:B:141:PRO:HD3	1.84	0.60
1:B:165:ARG:O	1:B:169:VAL:HG23	2.02	0.60
1:D:159:ILE:HD12	1:D:159:ILE:N	2.17	0.60
1:A:333:HIS:ND1	1:A:334:PRO:HD2	2.17	0.60
1:C:380:VAL:CG2	1:C:419:ASN:HD21	2.14	0.60
1:D:194:TRP:CZ3	2:D:4901:HEC:HMC3	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:ARG:NH1	1:D:283:ASN:HD21	1.99	0.60
1:C:307:LEU:HD21	1:C:321:ILE:HD11	1.84	0.59
1:B:240:ILE:CG1	1:B:432:THR:HB	2.32	0.59
1:C:195:ARG:HH21	1:C:454:ARG:HG2	1.66	0.59
1:C:291:ILE:HD11	1:C:297:PRO:HG3	1.83	0.59
1:D:186:LEU:HD21	1:D:246:VAL:HG21	1.84	0.59
1:B:349:LEU:HD11	1:B:370:ASN:ND2	2.17	0.59
1:C:356:LEU:C	1:C:356:LEU:HD23	2.23	0.59
1:D:459:ALA:HB1	1:D:464:LEU:CD1	2.33	0.59
1:B:159:ILE:HG12	1:B:160:GLU:H	1.68	0.59
1:D:380:VAL:O	1:D:384:CYS:HB2	2.02	0.59
1:B:435:ASP:OD1	1:B:437:HIS:HB2	2.03	0.58
1:B:88:LYS:HB2	1:B:88:LYS:NZ	2.18	0.58
1:A:196:ASN:O	1:A:198:PRO:HD3	2.03	0.58
1:A:411:LYS:O	1:A:415:VAL:HG23	2.03	0.58
1:A:140:LEU:O	1:A:144:ILE:HG12	2.04	0.58
1:A:463:TRP:HA	3:A:1902:H4B:N1	2.17	0.58
1:B:195:ARG:NH2	1:B:454:ARG:HD2	2.18	0.58
1:C:140:LEU:HB3	1:C:141:PRO:HD3	1.86	0.58
1:C:194:TRP:CH2	2:C:3901:HEC:HMC3	2.38	0.58
1:D:230:HIS:HD2	1:D:245:THR:OG1	1.86	0.58
1:B:261:ASN:N	1:B:261:ASN:ND2	2.50	0.58
1:A:100:LEU:HB3	1:A:456:GLY:HA3	1.86	0.58
1:B:88:LYS:HD3	1:B:90:TRP:CZ2	2.39	0.58
1:B:188:PHE:CZ	1:B:192:GLN:HG3	2.39	0.58
1:B:282:ALA:C	1:B:283:ASN:HD22	2.07	0.58
1:D:266:ARG:HH11	1:D:266:ARG:HG2	1.67	0.58
1:D:450:GLU:OE1	1:D:454:ARG:HD3	2.03	0.58
1:D:374:MET:HE2	1:D:439:ALA:CB	2.33	0.57
1:D:165:ARG:O	1:D:169:VAL:HG23	2.04	0.57
1:B:412:ASP:O	1:B:416:VAL:HG23	2.04	0.57
1:C:494:GLU:HB2	1:C:497:LYS:HG3	1.86	0.57
1:B:194:TRP:CZ3	2:B:2901:HEC:HMC3	2.39	0.57
1:A:380:VAL:HG22	1:A:419:ASN:ND2	2.19	0.57
1:A:395:VAL:HG21	1:A:418:ILE:HD11	1.86	0.57
1:B:247:PHE:HB3	1:B:248:PRO:HD2	1.87	0.57
1:B:332:GLU:HG2	1:B:340:ARG:HG2	1.86	0.56
1:B:155:LYS:HG2	1:B:156:GLU:H	1.69	0.56
1:D:204:ILE:HG23	1:D:205:GLN:HG2	1.87	0.56
1:A:247:PHE:HB3	1:A:248:PRO:CD	2.35	0.56
1:B:494:GLU:HG3	1:B:497:LYS:HE3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:LEU:HD22	1:D:144:ILE:HD11	1.88	0.56
1:B:194:TRP:CH2	2:B:2901:HEC:HMC3	2.41	0.56
1:D:356:LEU:HD12	1:D:492:GLN:HE21	1.69	0.56
1:A:110:CYS:CB	1:B:110:CYS:HB3	2.36	0.55
1:B:350:PRO:O	1:B:370:ASN:HB2	2.05	0.55
1:C:301:ARG:HG3	1:C:301:ARG:HH11	1.71	0.55
1:C:247:PHE:HB3	1:C:248:PRO:HD2	1.86	0.55
1:C:165:ARG:O	1:C:169:VAL:HG23	2.07	0.55
1:C:271:GLN:HB2	1:C:284:VAL:CG1	2.36	0.55
1:A:412:ASP:O	1:A:416:VAL:HG23	2.06	0.55
1:D:230:HIS:CE1	1:D:370:ASN:ND2	2.74	0.55
1:A:230:HIS:ND1	1:A:245:THR:HG23	2.23	0.54
1:A:263:GLN:HA	1:A:351:ALA:O	2.07	0.54
1:D:169:VAL:O	1:D:173:ILE:HG13	2.07	0.54
1:C:297:PRO:HG2	1:C:299:TYR:CZ	2.43	0.54
1:D:127:ARG:NH1	6:D:5097:HOH:O	2.40	0.54
1:D:151:TYR:HE2	1:D:165:ARG:HG2	1.72	0.54
1:A:110:CYS:HB3	1:B:110:CYS:HB3	1.88	0.54
1:A:172:GLU:O	1:A:176:THR:HB	2.07	0.54
1:A:336:TYR:HB3	1:A:338:TRP:NE1	2.21	0.54
1:B:118:SER:O	3:B:2902:H4B:H111	2.08	0.54
1:A:165:ARG:O	1:A:169:VAL:HG23	2.07	0.54
1:A:199:ARG:HB3	1:A:463:TRP:CE3	2.43	0.54
1:B:195:ARG:HH21	1:B:454:ARG:HD2	1.71	0.54
1:A:459:ALA:HB1	1:A:464:LEU:CD1	2.38	0.54
1:C:195:ARG:NH2	1:C:454:ARG:HG2	2.22	0.54
1:A:435:ASP:OD1	1:A:437:HIS:HB2	2.08	0.54
1:B:100:LEU:HB3	1:B:456:GLY:HA3	1.90	0.54
1:C:295:TRP:CZ3	1:C:297:PRO:HB3	2.43	0.54
1:C:121:THR:O	1:C:121:THR:HG22	2.08	0.53
1:C:471:SER:O	1:C:477:HIS:HE1	1.90	0.53
1:D:159:ILE:O	1:D:163:LEU:HD23	2.08	0.53
1:D:170:THR:O	1:D:174:GLU:HG3	2.07	0.53
1:C:451:TYR:CE2	1:C:456:GLY:HA2	2.42	0.53
1:A:159:ILE:HD12	1:A:159:ILE:N	2.24	0.53
1:A:112:SER:HB3	1:B:111:ARG:NH2	2.23	0.53
1:A:137:ASP:O	1:A:141:PRO:HD3	2.08	0.53
1:D:194:TRP:CE3	1:D:206:TRP:HA	2.43	0.53
1:A:194:TRP:CH2	2:A:1901:HEC:HMC3	2.44	0.53
1:A:459:ALA:HB1	1:A:464:LEU:HD11	1.89	0.53
1:C:298:LYS:HD3	1:C:298:LYS:N	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4901:HEC:HMC1	2:D:4901:HEC:HBC2	1.90	0.53
1:D:244:ILE:HD11	1:D:367:CYS:HB2	1.90	0.53
1:A:477:HIS:CD2	1:B:387:GLN:HE22	2.27	0.53
1:B:159:ILE:H	1:B:159:ILE:CD1	2.20	0.53
1:D:411:LYS:O	1:D:415:VAL:HG23	2.09	0.53
1:C:217:CYS:HA	1:C:222:GLU:OE2	2.09	0.52
1:A:159:ILE:CD1	1:A:160:GLU:H	2.21	0.52
1:C:172:GLU:HG2	1:C:179:TYR:HA	1.90	0.52
1:A:444:MET:CE	1:A:475:VAL:HG22	2.39	0.52
1:C:388:ARG:HH11	1:C:388:ARG:HG3	1.73	0.52
1:D:247:PHE:HB3	1:D:248:PRO:CD	2.38	0.52
1:B:460:ASP:O	1:B:464:LEU:HG	2.09	0.52
1:C:240:ILE:HG22	1:C:241:ARG:N	2.25	0.52
1:A:155:LYS:H	1:A:155:LYS:CD	1.99	0.52
1:C:266:ARG:HG2	1:C:283:ASN:ND2	2.24	0.52
1:A:201:ILE:HD11	1:A:440:ALA:HA	1.92	0.52
1:A:247:PHE:HB3	1:A:248:PRO:HD2	1.92	0.52
1:C:221:ARG:O	1:C:225:GLU:HG3	2.10	0.52
1:C:374:MET:HA	1:C:434:MET:O	2.10	0.52
1:D:375:GLY:HA3	1:D:423:LEU:HD11	1.92	0.52
1:A:155:LYS:HG2	1:A:156:GLU:N	2.26	0.51
1:B:452:ARG:HG2	1:B:452:ARG:HH21	1.75	0.51
2:B:2901:HEC:HMC1	2:B:2901:HEC:HBC3	1.93	0.51
1:D:224:PHE:CD1	1:D:319:PHE:HB3	2.45	0.51
1:D:289:LEU:CD2	1:D:293:LEU:HD12	2.39	0.51
1:D:330:ALA:H	1:D:429:GLN:NE2	2.09	0.51
1:C:415:VAL:HG21	1:D:472:ILE:HG13	1.93	0.51
2:C:3901:HEC:HMC1	2:C:3901:HEC:HBC2	1.91	0.51
1:D:424:HIS:HD2	6:D:5162:HOH:O	1.94	0.51
1:C:381:ARG:O	1:C:385:ASP:HB2	2.11	0.51
1:D:87:ILE:HG21	1:D:481:LEU:CD1	2.40	0.51
1:D:230:HIS:HE1	1:D:370:ASN:ND2	2.00	0.51
1:A:212:PHE:CB	1:A:245:THR:HG22	2.37	0.51
1:C:297:PRO:HG2	1:C:299:TYR:CE2	2.46	0.51
1:A:440:ALA:HB1	1:A:475:VAL:HG23	1.93	0.50
1:B:84:HIS:ND1	1:B:84:HIS:C	2.64	0.50
1:A:437:HIS:NE2	1:B:412:ASP:OD1	2.39	0.50
1:A:159:ILE:HD12	1:A:160:GLU:H	1.77	0.50
1:A:374:MET:HA	1:A:434:MET:O	2.11	0.50
1:C:203:ARG:O	1:C:206:TRP:HD1	1.94	0.50
1:B:374:MET:HA	1:B:434:MET:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:HIS:HB3	1:C:312:ASN:OD1	2.11	0.50
1:B:133:PRO:HG3	1:B:252:ASP:HA	1.92	0.50
1:C:393:GLU:HG3	1:C:397:ARG:NH2	2.27	0.50
1:D:143:ALA:O	1:D:147:VAL:HG23	2.12	0.50
1:C:200:CYS:O	1:C:203:ARG:NH1	2.42	0.50
1:D:201:ILE:HG21	1:D:374:MET:CE	2.41	0.50
1:A:444:MET:HE3	1:A:475:VAL:HG22	1.94	0.50
1:C:278:ARG:HG3	1:C:278:ARG:HH11	1.76	0.50
1:D:302:PHE:HB2	1:D:345:LYS:HE2	1.93	0.50
1:C:194:TRP:CZ3	2:C:3901:HEC:HMC3	2.47	0.50
1:A:205:GLN:HG3	2:A:1901:HEC:HBB2	1.93	0.49
1:A:260:TRP:HB2	1:A:308:VAL:HB	1.94	0.49
1:B:155:LYS:NZ	1:B:155:LYS:HB3	2.27	0.49
1:B:486:SER:HA	1:B:487:PRO:C	2.32	0.49
1:C:493:VAL:O	1:C:494:GLU:C	2.50	0.49
1:B:187:ILE:HG12	1:B:211:VAL:HG21	1.93	0.49
1:A:89:ASN:ND2	1:A:91:GLY:H	2.07	0.49
2:A:1901:HEC:HMC1	2:A:1901:HEC:HBC2	1.95	0.49
1:B:88:LYS:HD3	1:B:90:TRP:CH2	2.48	0.49
1:B:333:HIS:NE2	1:B:417:GLU:OE1	2.44	0.49
1:B:247:PHE:HB3	1:B:248:PRO:CD	2.42	0.49
1:B:270:TYR:HB2	1:B:278:ARG:HB3	1.93	0.49
1:B:379:GLY:HA3	1:B:419:ASN:OD1	2.13	0.49
1:B:418:ILE:O	1:B:421:ALA:HB3	2.12	0.49
1:B:411:LYS:O	1:B:415:VAL:HG12	2.12	0.49
1:A:107:ILE:HD11	1:A:484:VAL:HG21	1.94	0.49
1:B:140:LEU:O	1:B:144:ILE:HG12	2.13	0.49
1:A:230:HIS:HD1	1:A:245:THR:HG23	1.78	0.48
1:C:194:TRP:CB	2:C:3901:HEC:HBC3	2.41	0.48
1:C:352:VAL:HB	1:C:369:PHE:CE1	2.48	0.48
1:D:376:THR:HA	1:D:380:VAL:HG23	1.93	0.48
1:A:382:ASP:OD1	1:A:388:ARG:NH1	2.45	0.48
1:A:484:VAL:HG13	1:A:488:PHE:CD1	2.48	0.48
1:D:223:MET:HG2	1:D:247:PHE:CE2	2.49	0.48
1:B:88:LYS:HB2	1:B:88:LYS:HZ2	1.77	0.48
1:B:100:LEU:CB	1:B:456:GLY:HA3	2.43	0.48
1:B:403:THR:HA	1:B:410:TRP:CD1	2.48	0.48
1:C:266:ARG:HG2	1:C:283:ASN:HD21	1.76	0.48
1:C:159:ILE:HG23	1:C:160:GLU:H	1.77	0.48
1:D:283:ASN:N	1:D:283:ASN:ND2	2.61	0.48
1:A:405:LYS:O	1:A:405:LYS:HG3	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:THR:HA	1:A:380:VAL:HG23	1.95	0.48
3:A:1902:H4B:H112	1:B:461:TRP:NE1	2.29	0.47
1:B:170:THR:O	1:B:174:GLU:HB2	2.14	0.47
1:D:494:GLU:OE1	1:D:497:LYS:HE3	2.14	0.47
3:A:1902:H4B:H112	1:B:461:TRP:HE1	1.79	0.47
1:D:140:LEU:CB	1:D:141:PRO:HD3	2.44	0.47
1:D:240:ILE:HG22	1:D:241:ARG:N	2.28	0.47
1:A:277:ILE:HG21	1:A:281:PRO:HA	1.95	0.47
1:B:388:ARG:HG3	1:B:388:ARG:HH11	1.79	0.47
1:C:236:ASN:HB3	1:C:239:ASN:O	2.14	0.47
1:C:257:PHE:HA	1:C:310:GLN:O	2.14	0.47
1:A:484:VAL:HG13	1:A:488:PHE:CE1	2.49	0.47
1:B:120:MET:CE	3:B:2902:H4B:HN5	2.28	0.47
1:B:84:HIS:HB3	1:B:99:THR:HG22	1.95	0.47
1:A:214:ALA:HB2	1:A:226:HIS:CD2	2.50	0.47
1:D:348:ALA:HB1	1:D:431:VAL:HG11	1.97	0.47
1:A:100:LEU:CB	1:A:456:GLY:HA3	2.44	0.47
1:C:277:ILE:HG21	1:C:281:PRO:HB3	1.96	0.47
1:D:481:LEU:N	1:D:481:LEU:HD12	2.30	0.47
1:B:224:PHE:CD1	1:B:319:PHE:HB3	2.50	0.47
1:A:433:ILE:HG12	1:A:434:MET:N	2.30	0.47
1:A:336:TYR:CD1	1:A:338:TRP:CZ2	3.03	0.46
1:C:196:ASN:O	1:C:198:PRO:HD3	2.15	0.46
1:C:224:PHE:CD1	1:C:319:PHE:HB3	2.50	0.46
1:D:247:PHE:HB3	1:D:248:PRO:HD2	1.96	0.46
1:D:450:GLU:HB3	1:D:457:CYS:HB2	1.96	0.46
1:C:236:ASN:O	1:C:237:ASN:HB2	2.16	0.46
1:C:423:LEU:HD23	1:C:433:ILE:HD13	1.97	0.46
1:A:230:HIS:NE2	1:A:370:ASN:ND2	2.63	0.46
1:B:151:TYR:HA	1:B:154:PHE:CE2	2.50	0.46
1:C:462:ILE:HG23	1:D:461:TRP:CZ3	2.50	0.46
1:B:423:LEU:O	1:B:427:GLN:HG3	2.16	0.46
1:D:283:ASN:N	1:D:283:ASN:HD22	2.14	0.46
1:A:84:HIS:HB3	1:A:99:THR:HG22	1.97	0.46
1:C:110:CYS:CB	1:D:110:CYS:HB3	2.45	0.46
1:C:333:HIS:CG	1:C:334:PRO:HD2	2.51	0.46
1:C:423:LEU:O	1:C:427:GLN:HG3	2.16	0.46
1:A:188:PHE:CZ	1:A:192:GLN:HG3	2.51	0.46
1:A:270:TYR:HB2	1:A:278:ARG:HB3	1.98	0.46
1:C:380:VAL:HG11	1:C:467:PRO:HB2	1.98	0.46
1:D:260:TRP:HB2	1:D:308:VAL:HB	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LYS:HB2	1:A:132:LYS:HZ3	1.81	0.46
1:A:205:GLN:HG3	2:A:1901:HEC:CBB	2.46	0.46
1:B:446:TYR:CZ	1:B:450:GLU:HG3	2.51	0.46
1:C:112:SER:HB3	1:D:111:ARG:HH21	1.80	0.46
1:C:260:TRP:CE3	1:C:289:LEU:HD21	2.51	0.46
1:D:159:ILE:H	1:D:159:ILE:CD1	2.23	0.46
1:A:205:GLN:O	1:A:207:SER:N	2.49	0.45
1:B:287:THR:OG1	1:B:305:LEU:HD21	2.17	0.45
1:C:277:ILE:HD13	1:C:281:PRO:HB3	1.99	0.45
1:D:372:TRP:H	2:D:4901:HEC:HAB	1.81	0.45
1:A:194:TRP:CZ3	1:A:206:TRP:HA	2.51	0.45
1:C:352:VAL:CG1	1:C:355:MET:HG3	2.46	0.45
1:B:88:LYS:HB3	1:B:95:THR:HG22	1.97	0.45
1:D:376:THR:HG22	1:D:380:VAL:HG21	1.98	0.45
1:A:471:SER:O	1:A:477:HIS:HE1	2.00	0.45
1:A:151:TYR:HA	1:A:154:PHE:CE2	2.51	0.45
1:B:405:LYS:HE2	1:B:407:ALA:HB3	1.98	0.45
1:C:380:VAL:HG22	1:C:419:ASN:ND2	2.28	0.45
1:A:113:LYS:HE3	1:A:113:LYS:H	1.81	0.45
1:A:280:ASP:OD2	1:A:388:ARG:NH2	2.48	0.45
1:A:391:ILE:O	1:A:395:VAL:HG23	2.17	0.45
1:B:452:ARG:HG2	1:B:452:ARG:NH2	2.32	0.45
1:C:116:LEU:N	1:C:116:LEU:HD12	2.32	0.45
1:A:330:ALA:H	1:A:429:GLN:NE2	2.14	0.45
1:A:433:ILE:HG12	1:A:434:MET:H	1.82	0.45
1:B:165:ARG:O	1:B:165:ARG:HD2	2.16	0.45
1:C:88:LYS:CB	1:C:95:THR:HG22	2.45	0.45
1:C:413:GLN:CG	1:D:416:VAL:HG11	2.47	0.45
1:A:257:PHE:CD2	1:A:311:ALA:HA	2.51	0.45
1:B:461:TRP:CZ2	1:B:465:VAL:HG21	2.52	0.45
1:D:266:ARG:NH1	1:D:266:ARG:HG2	2.30	0.45
1:B:308:VAL:HG13	1:B:316:PRO:HB2	1.98	0.44
1:C:463:TRP:HA	3:C:3902:H4B:N1	2.32	0.44
1:C:494:GLU:HB3	1:C:496:TRP:CE2	2.52	0.44
1:A:133:PRO:HG3	1:A:252:ASP:HA	1.99	0.44
1:A:476:PHE:O	1:A:476:PHE:CD1	2.70	0.44
1:C:203:ARG:NH2	1:C:458:PRO:O	2.49	0.44
1:C:381:ARG:HH12	3:C:3902:H4B:C4	2.31	0.44
1:C:411:LYS:O	1:C:415:VAL:HG23	2.17	0.44
1:B:203:ARG:O	1:B:206:TRP:HD1	2.01	0.44
1:B:263:GLN:HA	1:B:351:ALA:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:LEU:O	1:B:403:THR:HG23	2.17	0.44
1:C:461:TRP:CZ2	1:C:465:VAL:HG21	2.53	0.44
1:D:348:ALA:CB	1:D:431:VAL:HG11	2.48	0.44
1:A:257:PHE:HA	1:A:310:GLN:O	2.17	0.44
1:A:488:PHE:HB3	1:A:490:TYR:CE1	2.53	0.44
1:C:380:VAL:O	1:C:384:CYS:HB2	2.18	0.44
1:B:252:ASP:OD2	1:B:255:HIS:HD2	2.01	0.44
1:C:159:ILE:CG2	1:C:160:GLU:N	2.80	0.44
1:A:132:LYS:HB2	1:A:132:LYS:HZ2	1.83	0.44
1:D:89:ASN:HD22	1:D:91:GLY:H	1.66	0.44
1:A:234:SER:O	1:A:240:ILE:HA	2.18	0.44
1:A:444:MET:HE3	1:A:475:VAL:HA	2.00	0.44
1:D:140:LEU:HD22	1:D:144:ILE:CD1	2.47	0.44
1:C:199:ARG:NH1	1:C:491:TYR:OH	2.51	0.44
1:C:278:ARG:HG3	1:C:278:ARG:NH1	2.31	0.44
1:D:87:ILE:HG13	1:D:96:PHE:HB2	2.00	0.44
1:D:89:ASN:ND2	1:D:91:GLY:H	2.16	0.44
1:A:306:PRO:HB3	1:A:320:GLU:HG2	1.99	0.43
1:A:336:TYR:N	1:A:336:TYR:CD2	2.85	0.43
1:B:120:MET:HE2	3:B:2902:H4B:HN5	1.82	0.43
1:B:502:GLN:HE21	1:B:502:GLN:HB2	1.66	0.43
1:D:140:LEU:HB3	1:D:141:PRO:HD3	1.98	0.43
1:A:230:HIS:HB2	1:A:245:THR:HG21	2.00	0.43
1:B:140:LEU:HD11	1:B:170:THR:HG23	2.01	0.43
1:C:217:CYS:SG	1:C:222:GLU:HB3	2.59	0.43
1:D:340:ARG:HG3	1:D:341:GLU:N	2.33	0.43
1:A:113:LYS:HE3	1:A:113:LYS:N	2.34	0.43
1:C:391:ILE:HD11	1:C:418:ILE:HD13	1.99	0.43
1:A:348:ALA:HB1	1:A:431:VAL:HG11	2.01	0.43
1:B:325:LEU:HD23	1:B:325:LEU:HA	1.78	0.43
1:C:245:THR:O	1:C:367:CYS:HA	2.18	0.43
1:C:394:GLU:O	1:C:398:ARG:HG3	2.19	0.43
1:D:226:HIS:CD2	1:D:229:ARG:HH12	2.35	0.43
1:B:214:ALA:O	1:B:217:CYS:HB2	2.19	0.43
1:C:200:CYS:HB3	1:C:203:ARG:CD	2.40	0.43
1:D:194:TRP:CZ3	1:D:206:TRP:HA	2.53	0.43
1:D:378:ILE:HA	1:D:382:ASP:OD2	2.19	0.43
1:C:260:TRP:CZ3	1:C:289:LEU:HD21	2.54	0.43
1:C:484:VAL:HG13	1:C:488:PHE:CE1	2.54	0.43
1:D:333:HIS:HB3	1:D:336:TYR:O	2.19	0.43
1:D:402:GLU:C	1:D:404:HIS:H	2.22	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:ILE:CD1	1:D:415:VAL:HG21	2.49	0.43
1:B:266:ARG:HG3	1:B:283:ASN:OD1	2.18	0.43
1:D:100:LEU:O	1:D:102:HIS:N	2.52	0.43
1:D:263:GLN:HA	1:D:351:ALA:O	2.19	0.43
1:D:267:TYR:CE2	1:D:302:PHE:HD1	2.36	0.43
1:D:434:MET:CG	1:D:439:ALA:HB2	2.48	0.43
1:B:110:CYS:O	1:B:111:ARG:HD2	2.19	0.42
1:D:204:ILE:HG23	1:D:205:GLN:N	2.34	0.42
1:A:83:ARG:O	1:A:102:HIS:HE1	2.02	0.42
1:B:384:CYS:SG	1:B:418:ILE:HD12	2.59	0.42
1:A:89:ASN:HD22	1:A:89:ASN:C	2.22	0.42
1:A:116:LEU:HG	1:B:481:LEU:HD22	2.00	0.42
1:B:108:LEU:O	1:B:111:ARG:NH2	2.52	0.42
1:B:356:LEU:C	1:B:356:LEU:HD23	2.40	0.42
1:C:104:ALA:HA	1:C:485:LEU:HD23	2.01	0.42
1:A:130:ARG:NH1	1:A:134:THR:OG1	2.52	0.42
1:B:364:PHE:N	1:B:364:PHE:CD1	2.88	0.42
1:C:140:LEU:O	1:C:144:ILE:HG12	2.20	0.42
1:D:272:MET:HB3	1:D:273:PRO:HD2	2.01	0.42
1:B:150:TYR:HD2	1:B:188:PHE:CG	2.37	0.42
1:C:194:TRP:CG	2:C:3901:HEC:HBC3	2.54	0.42
1:D:227:ILE:O	1:D:231:VAL:HG23	2.19	0.42
1:A:130:ARG:NH2	1:A:251:SER:O	2.53	0.42
1:B:261:ASN:H	1:B:261:ASN:ND2	2.06	0.42
1:B:296:LYS:HA	1:B:297:PRO:HD2	1.93	0.42
1:B:307:LEU:HD11	1:B:321:ILE:HG12	2.01	0.42
1:C:406:LEU:HD22	1:D:437:HIS:HB3	2.02	0.42
1:B:199:ARG:HD3	1:B:463:TRP:CD2	2.54	0.42
1:C:112:SER:HB3	1:D:111:ARG:NH2	2.33	0.42
1:C:388:ARG:HG3	1:C:388:ARG:NH1	2.34	0.42
1:A:127:ARG:HA	1:A:127:ARG:HD3	1.88	0.42
1:C:484:VAL:HG13	1:C:488:PHE:CD1	2.55	0.42
1:C:479:GLU:HG2	1:D:119:ILE:HA	2.02	0.41
1:A:203:ARG:HD2	1:A:446:TYR:OH	2.21	0.41
1:D:187:ILE:O	1:D:191:LYS:HG3	2.21	0.41
1:A:249:GLN:HB3	1:A:364:PHE:CE2	2.55	0.41
1:B:155:LYS:HG2	1:B:156:GLU:N	2.35	0.41
1:B:388:ARG:HG3	1:B:388:ARG:NH1	2.35	0.41
1:A:151:TYR:HA	1:A:154:PHE:CD2	2.56	0.41
1:A:212:PHE:CD1	1:A:245:THR:HG22	2.55	0.41
1:A:295:TRP:HB2	1:A:318:LEU:HD13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:VAL:HA	1:A:466:PRO:HD3	1.94	0.41
1:B:135:PRO:HA	1:B:136:PRO:HD3	1.87	0.41
1:B:280:ASP:OD1	1:B:282:ALA:HB3	2.21	0.41
1:D:374:MET:HA	1:D:434:MET:O	2.20	0.41
1:D:493:VAL:O	1:D:494:GLU:C	2.59	0.41
1:D:261:ASN:OD1	1:D:261:ASN:N	2.54	0.41
1:D:476:PHE:CD1	1:D:476:PHE:C	2.94	0.41
1:B:245:THR:O	1:B:367:CYS:HA	2.20	0.41
1:C:486:SER:HA	1:C:487:PRO:C	2.40	0.41
1:D:267:TYR:HA	1:D:303:ASP:O	2.21	0.41
1:D:402:GLU:HB3	1:D:404:HIS:CE1	2.56	0.41
1:A:476:PHE:CD1	1:A:476:PHE:C	2.94	0.41
1:B:290:CYS:SG	1:B:306:PRO:HG2	2.61	0.41
1:B:380:VAL:O	1:B:384:CYS:HB2	2.21	0.41
1:C:354:ASN:C	1:C:354:ASN:HD22	2.23	0.41
1:C:376:THR:HA	1:C:380:VAL:HG23	2.01	0.41
1:C:406:LEU:C	1:C:408:SER:H	2.23	0.41
1:C:494:GLU:CG	1:C:497:LYS:HE3	2.47	0.41
1:D:282:ALA:C	1:D:283:ASN:HD22	2.25	0.41
1:A:194:TRP:CH2	1:A:205:GLN:HB2	2.57	0.41
1:A:420:ILE:HG13	1:B:409:LEU:HD12	2.02	0.41
1:B:266:ARG:NE	6:B:5143:HOH:O	2.53	0.41
1:C:466:PRO:HG2	1:C:473:THR:HG21	2.03	0.41
1:D:167:GLU:O	1:D:171:LYS:HG3	2.21	0.41
1:D:262:ALA:HA	1:D:354:ASN:HD22	1.78	0.41
1:A:112:SER:O	1:B:106:GLY:HA2	2.20	0.40
1:B:195:ARG:HG2	1:B:454:ARG:NH1	2.35	0.40
1:C:409:LEU:HD22	1:D:436:HIS:CE1	2.56	0.40
1:A:281:PRO:O	1:A:284:VAL:HG23	2.21	0.40
1:B:233:TYR:CD1	1:B:241:ARG:NH2	2.88	0.40
1:B:451:TYR:O	1:B:455:GLY:HA2	2.22	0.40
1:C:291:ILE:CD1	1:C:297:PRO:HG3	2.51	0.40
1:D:357:LEU:HD13	1:D:489:TYR:CE1	2.57	0.40
1:D:399:MET:HE2	1:D:401:LEU:HD11	2.02	0.40
1:D:446:TYR:CZ	1:D:450:GLU:HG3	2.56	0.40
1:D:450:GLU:CB	1:D:457:CYS:HB2	2.51	0.40
1:A:493:VAL:O	1:A:494:GLU:C	2.60	0.40
1:B:262:ALA:HB3	1:B:266:ARG:HH12	1.87	0.40
1:D:461:TRP:CE2	1:D:465:VAL:HG21	2.56	0.40
1:B:155:LYS:HB3	1:B:155:LYS:HZ2	1.85	0.40
1:B:167:GLU:O	1:B:171:LYS:HG2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:LYS:N	1:C:298:LYS:CD	2.85	0.40
1:C:377:GLU:OE2	5:C:3904:IMD:H5	2.22	0.40
1:D:374:MET:CE	1:D:439:ALA:CB	2.99	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	419/424 (99%)	384 (92%)	28 (7%)	7 (2%)	9 11
1	B	419/424 (99%)	382 (91%)	35 (8%)	2 (0%)	29 40
1	C	419/424 (99%)	378 (90%)	36 (9%)	5 (1%)	13 17
1	D	419/424 (99%)	383 (91%)	34 (8%)	2 (0%)	29 40
All	All	1676/1696 (99%)	1527 (91%)	133 (8%)	16 (1%)	15 22

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	TRP
1	C	276	SER
1	A	203	ARG
1	B	159	ILE
1	C	407	ALA
1	D	101	HIS
1	A	157	ALA
1	A	407	ALA
1	C	206	TRP
1	A	133	PRO
1	A	236	ASN
1	B	375	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	236	ASN
1	C	375	GLY
1	A	350	PRO
1	D	240	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	365/370 (99%)	350 (96%)	15 (4%)	30	41
1	B	365/370 (99%)	351 (96%)	14 (4%)	33	45
1	C	365/370 (99%)	350 (96%)	15 (4%)	30	41
1	D	365/370 (99%)	355 (97%)	10 (3%)	44	59
All	All	1460/1480 (99%)	1406 (96%)	54 (4%)	34	46

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	113	LYS
1	A	155	LYS
1	A	159	ILE
1	A	207	SER
1	A	236	ASN
1	A	239	ASN
1	A	261	ASN
1	A	271	GLN
1	A	312	ASN
1	A	331	MET
1	A	337	GLU
1	A	355	MET
1	A	413	GLN
1	A	480	MET
1	B	84	HIS
1	B	88	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	130	ARG
1	B	155	LYS
1	B	159	ILE
1	B	162	HIS
1	B	180	GLN
1	B	261	ASN
1	B	296	LYS
1	B	325	LEU
1	B	359	VAL
1	B	386	VAL
1	B	394	GLU
1	B	500	VAL
1	C	108	LEU
1	C	120	MET
1	C	155	LYS
1	C	180	GLN
1	C	203	ARG
1	C	236	ASN
1	C	266	ARG
1	C	298	LYS
1	C	301	ARG
1	C	337	GLU
1	C	354	ASN
1	C	357	LEU
1	C	390	ASN
1	C	454	ARG
1	C	500	VAL
1	D	121	THR
1	D	139	LEU
1	D	140	LEU
1	D	155	LYS
1	D	208	ASN
1	D	261	ASN
1	D	266	ARG
1	D	293	LEU
1	D	386	VAL
1	D	413	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	102	HIS
1	A	148	ASN
1	A	236	ASN
1	A	239	ASN
1	A	255	HIS
1	A	263	GLN
1	A	271	GLN
1	A	312	ASN
1	A	370	ASN
1	A	404	HIS
1	A	413	GLN
1	A	419	ASN
1	A	427	GLN
1	A	429	GLN
1	A	477	HIS
1	A	492	GLN
1	A	499	HIS
1	B	148	ASN
1	B	149	GLN
1	B	180	GLN
1	B	192	GLN
1	B	210	GLN
1	B	237	ASN
1	B	255	HIS
1	B	261	ASN
1	B	263	GLN
1	B	429	GLN
1	B	449	ASN
1	B	502	GLN
1	C	148	ASN
1	C	149	GLN
1	C	180	GLN
1	C	192	GLN
1	C	236	ASN
1	C	354	ASN
1	C	390	ASN
1	C	419	ASN
1	C	427	GLN
1	C	429	GLN
1	C	448	GLN
1	C	449	ASN
1	C	477	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	89	ASN
1	D	97	GLN
1	D	102	HIS
1	D	226	HIS
1	D	230	HIS
1	D	283	ASN
1	D	370	ASN
1	D	413	GLN
1	D	419	ASN
1	D	427	GLN
1	D	429	GLN
1	D	448	GLN
1	D	477	HIS
1	D	478	GLN
1	D	492	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 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
5	IMD	A	1904	-	3,5,5	0.67	0	4,5,5	0.45	0
2	HEC	A	1901	1	26,50,50	1.66	3 (11%)	18,82,82	1.91	6 (33%)
3	H4B	B	2902	-	16,18,18	2.63	5 (31%)	11,26,26	2.41	5 (45%)
5	IMD	C	3904	-	3,5,5	0.59	0	4,5,5	0.43	0
3	H4B	C	3902	-	16,18,18	2.90	6 (37%)	11,26,26	2.37	5 (45%)
2	HEC	C	3901	1	26,50,50	1.59	3 (11%)	18,82,82	1.90	4 (22%)
3	H4B	A	1902	-	16,18,18	3.02	8 (50%)	11,26,26	2.35	5 (45%)
3	H4B	D	4902	-	16,18,18	3.06	6 (37%)	11,26,26	2.40	5 (45%)
5	IMD	B	2904	-	3,5,5	0.70	0	4,5,5	0.40	0
5	IMD	D	4904	-	3,5,5	0.72	0	4,5,5	0.56	0
2	HEC	B	2901	1	26,50,50	1.67	5 (19%)	18,82,82	1.90	6 (33%)
2	HEC	D	4901	1	26,50,50	1.63	6 (23%)	18,82,82	1.55	3 (16%)

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
5	IMD	A	1904	-	-	-	0/1/1/1
2	HEC	A	1901	1	-	0/6/54/54	-
3	H4B	B	2902	-	3/3/3/5	4/8/17/17	0/2/2/2
5	IMD	C	3904	-	-	-	0/1/1/1
3	H4B	C	3902	-	3/3/3/5	7/8/17/17	0/2/2/2
2	HEC	C	3901	1	-	0/6/54/54	-
3	H4B	A	1902	-	3/3/3/5	7/8/17/17	0/2/2/2
3	H4B	D	4902	-	3/3/3/5	7/8/17/17	0/2/2/2
5	IMD	B	2904	-	-	-	0/1/1/1
5	IMD	D	4904	-	-	-	0/1/1/1
2	HEC	B	2901	1	-	3/6/54/54	-
2	HEC	D	4901	1	-	3/6/54/54	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1902	H4B	C4-N3	8.37	1.47	1.33
3	D	4902	H4B	C4-N3	7.91	1.46	1.33
3	C	3902	H4B	C4-N3	7.86	1.46	1.33
3	B	2902	H4B	C4-N3	7.73	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1901	HEC	C3B-C2B	-5.41	1.35	1.40
2	B	2901	HEC	C3B-C2B	-4.75	1.35	1.40
3	D	4902	H4B	C8A-N1	4.69	1.43	1.34
3	D	4902	H4B	C2-N3	4.52	1.43	1.35
2	C	3901	HEC	C3B-C2B	-4.49	1.36	1.40
3	A	1902	H4B	C8A-N1	4.49	1.43	1.34
3	C	3902	H4B	C2-N3	4.48	1.43	1.35
2	D	4901	HEC	C3B-C2B	-4.42	1.36	1.40
3	B	2902	H4B	C2-N3	4.33	1.43	1.35
3	A	1902	H4B	C2-N3	4.24	1.42	1.35
3	D	4902	H4B	C4-C4A	4.18	1.47	1.41
3	C	3902	H4B	C8A-N1	4.10	1.42	1.34
2	C	3901	HEC	C3C-C2C	-3.86	1.36	1.40
3	B	2902	H4B	C8A-N1	3.83	1.41	1.34
2	D	4901	HEC	C3C-C2C	-3.76	1.36	1.40
2	B	2901	HEC	C3C-C2C	-3.34	1.37	1.40
3	C	3902	H4B	C4A-C8A	3.24	1.47	1.41
2	A	1901	HEC	C3C-C2C	-3.01	1.37	1.40
3	A	1902	H4B	C9-C6	-2.95	1.48	1.53
3	D	4902	H4B	C4A-C8A	2.86	1.46	1.41
3	A	1902	H4B	C4-C4A	2.79	1.45	1.41
3	C	3902	H4B	C4-C4A	2.55	1.45	1.41
2	B	2901	HEC	C1D-ND	2.54	1.41	1.36
2	B	2901	HEC	C1A-C2A	2.52	1.48	1.42
2	C	3901	HEC	C1D-ND	2.45	1.41	1.36
3	A	1902	H4B	C2-N1	2.41	1.39	1.35
3	B	2902	H4B	C2-N2	2.40	1.38	1.33
3	D	4902	H4B	C2-N2	2.37	1.38	1.33
2	D	4901	HEC	C1A-C2A	2.32	1.47	1.42
2	D	4901	HEC	C1C-NC	2.29	1.40	1.36
3	A	1902	H4B	C4A-C8A	2.29	1.45	1.41
2	A	1901	HEC	C1D-ND	2.27	1.40	1.36
3	C	3902	H4B	C9-C6	-2.13	1.49	1.53
2	B	2901	HEC	C3C-C4C	2.08	1.46	1.43
3	A	1902	H4B	C2-N2	2.08	1.38	1.33
2	D	4901	HEC	C3C-C4C	2.07	1.46	1.43
2	D	4901	HEC	C1D-ND	2.06	1.40	1.36
3	B	2902	H4B	C4A-C8A	2.03	1.45	1.41

All (39) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1902	H4B	C4-C4A-C8A	4.74	118.78	114.57
3	C	3902	H4B	C4-C4A-C8A	4.61	118.66	114.57
2	C	3901	HEC	CBD-CAD-C3D	-4.41	104.36	112.49
3	B	2902	H4B	C4-C4A-C8A	4.34	118.43	114.57
3	D	4902	H4B	C4-N3-C2	4.15	122.52	115.93
2	B	2901	HEC	CBD-CAD-C3D	-4.09	104.94	112.49
2	A	1901	HEC	C1D-C2D-C3D	-4.00	104.21	107.00
2	C	3901	HEC	C1D-C2D-C3D	-3.96	104.24	107.00
3	C	3902	H4B	C4-N3-C2	3.95	122.20	115.93
3	D	4902	H4B	C4-C4A-C8A	3.83	117.97	114.57
3	B	2902	H4B	C4-N3-C2	3.74	121.87	115.93
2	B	2901	HEC	C1D-C2D-C3D	-3.67	104.44	107.00
3	D	4902	H4B	O9-C9-C6	3.66	117.74	108.98
2	D	4901	HEC	C1D-C2D-C3D	-3.63	104.47	107.00
3	A	1902	H4B	C4-N3-C2	3.63	121.69	115.93
2	A	1901	HEC	CBD-CAD-C3D	-3.52	106.00	112.49
3	B	2902	H4B	O9-C9-C6	3.44	117.21	108.98
2	B	2901	HEC	CAA-CBA-CGA	3.01	117.72	112.67
2	A	1901	HEC	CAA-CBA-CGA	3.01	117.72	112.67
2	D	4901	HEC	CBD-CAD-C3D	-2.77	107.37	112.49
3	C	3902	H4B	C4A-C4-N3	-2.73	116.24	124.01
3	D	4902	H4B	C4A-C4-N3	-2.71	116.30	124.01
3	B	2902	H4B	C4A-C4-N3	-2.68	116.38	124.01
3	A	1902	H4B	C4A-C4-N3	-2.59	116.66	124.01
3	C	3902	H4B	O9-C9-C6	2.50	114.96	108.98
2	C	3901	HEC	CAA-CBA-CGA	2.49	116.84	112.67
2	D	4901	HEC	CAA-CBA-CGA	2.46	116.80	112.67
2	A	1901	HEC	CBA-CAA-C2A	-2.31	108.22	112.48
2	B	2901	HEC	CMB-C2B-C3B	2.30	128.53	125.82
2	B	2901	HEC	CMC-C2C-C3C	2.29	128.51	125.82
3	A	1902	H4B	N3-C2-N1	-2.28	121.84	125.42
3	D	4902	H4B	N3-C2-N1	-2.28	121.85	125.42
2	A	1901	HEC	CAD-CBD-CGD	2.24	116.43	112.67
3	B	2902	H4B	N3-C2-N1	-2.19	121.98	125.42
3	A	1902	H4B	O9-C9-C6	2.17	114.16	108.98
2	C	3901	HEC	CMB-C2B-C3B	2.15	128.35	125.82
2	A	1901	HEC	CMC-C2C-C3C	2.13	128.33	125.82
3	C	3902	H4B	N3-C2-N1	-2.10	122.13	125.42
2	B	2901	HEC	CAD-CBD-CGD	2.07	116.15	112.67

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1902	H4B	C9
3	A	1902	H4B	C6
3	A	1902	H4B	C10
3	B	2902	H4B	C9
3	B	2902	H4B	C6
3	B	2902	H4B	C10
3	C	3902	H4B	C9
3	C	3902	H4B	C6
3	C	3902	H4B	C10
3	D	4902	H4B	C9
3	D	4902	H4B	C6
3	D	4902	H4B	C10

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2901	HEC	C1A-C2A-CAA-CBA
2	D	4901	HEC	C2A-CAA-CBA-CGA
3	A	1902	H4B	N5-C6-C9-O9
3	A	1902	H4B	C7-C6-C9-C10
3	A	1902	H4B	C11-C10-C9-C6
3	A	1902	H4B	O10-C10-C9-C6
3	A	1902	H4B	O10-C10-C9-O9
3	B	2902	H4B	N5-C6-C9-O9
3	B	2902	H4B	C7-C6-C9-C10
3	C	3902	H4B	N5-C6-C9-O9
3	C	3902	H4B	C7-C6-C9-C10
3	C	3902	H4B	C11-C10-C9-C6
3	C	3902	H4B	O10-C10-C9-C6
3	C	3902	H4B	O10-C10-C9-O9
3	D	4902	H4B	N5-C6-C9-O9
3	D	4902	H4B	C7-C6-C9-C10
3	D	4902	H4B	C11-C10-C9-C6
3	D	4902	H4B	O10-C10-C9-C6
3	D	4902	H4B	O10-C10-C9-O9
3	C	3902	H4B	C11-C10-C9-O9
3	A	1902	H4B	C11-C10-C9-O9
3	B	2902	H4B	C11-C10-C9-O9
3	D	4902	H4B	C11-C10-C9-O9
2	B	2901	HEC	C2A-CAA-CBA-CGA
3	B	2902	H4B	O10-C10-C9-O9
3	A	1902	H4B	N5-C6-C9-C10
3	C	3902	H4B	N5-C6-C9-C10

Continued on next page...

Continued from previous page...

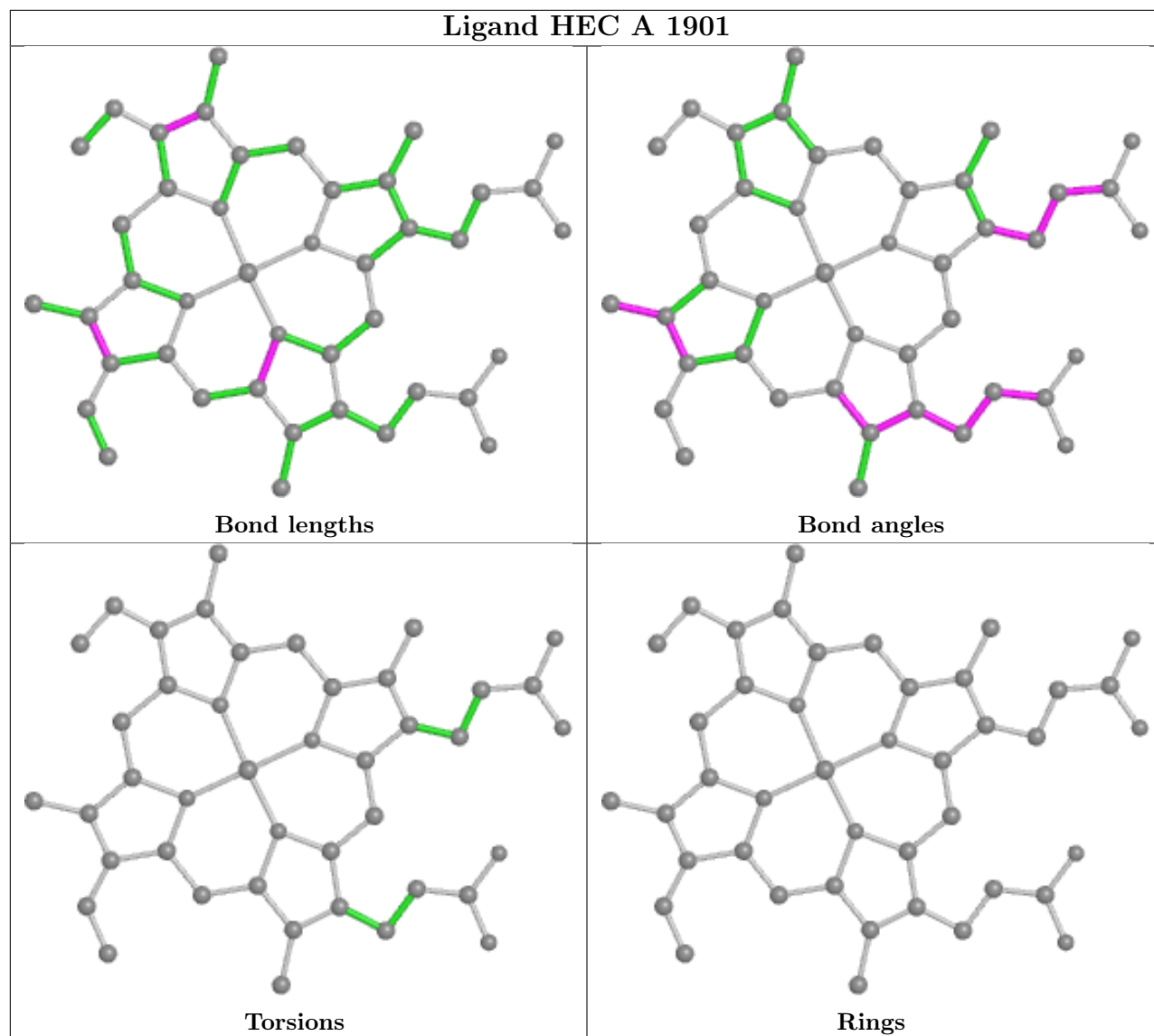
Mol	Chain	Res	Type	Atoms
2	B	2901	HEC	C3A-C2A-CAA-CBA
2	D	4901	HEC	C1A-C2A-CAA-CBA
2	D	4901	HEC	C3A-C2A-CAA-CBA
3	D	4902	H4B	N5-C6-C9-C10

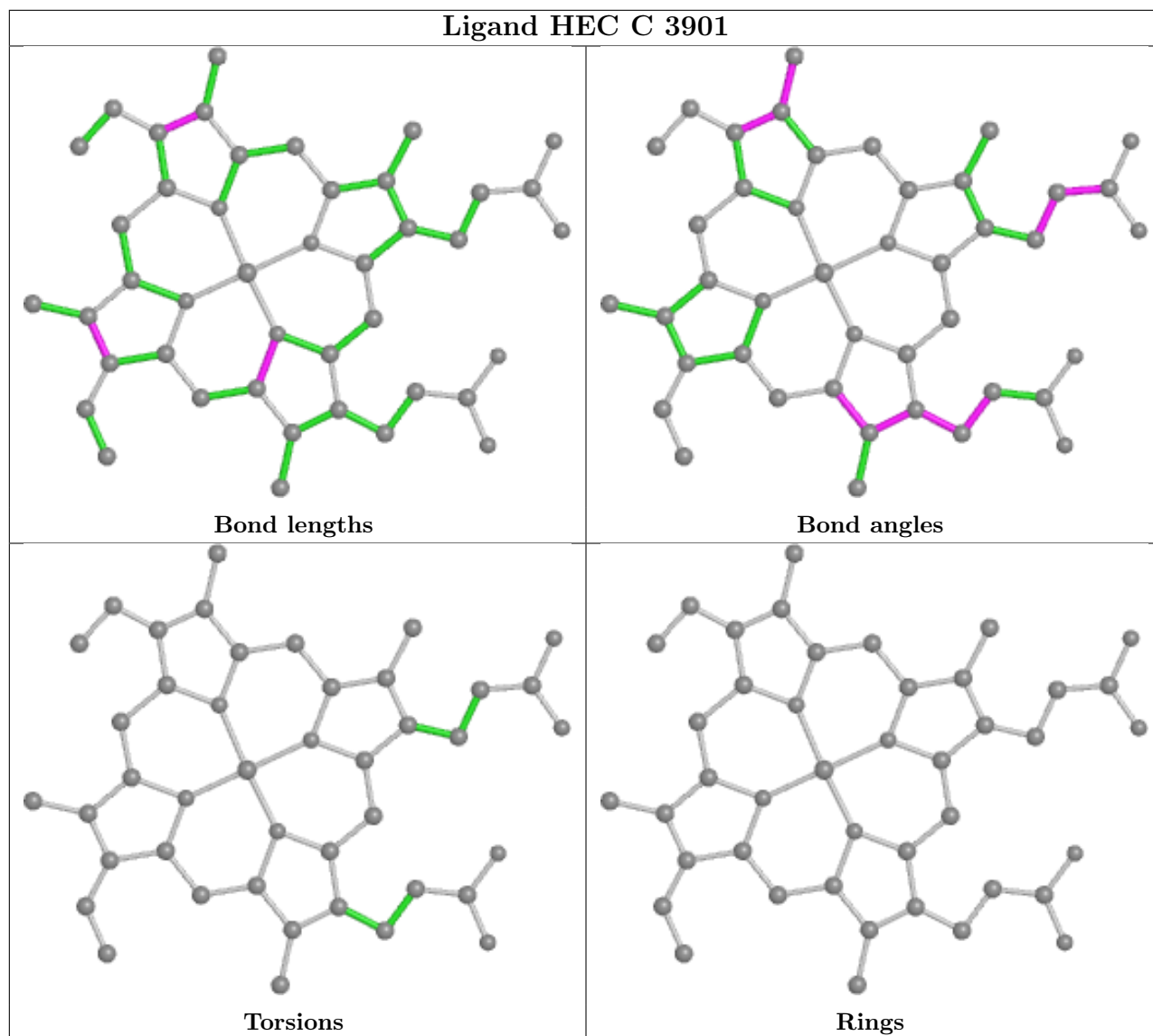
There are no ring outliers.

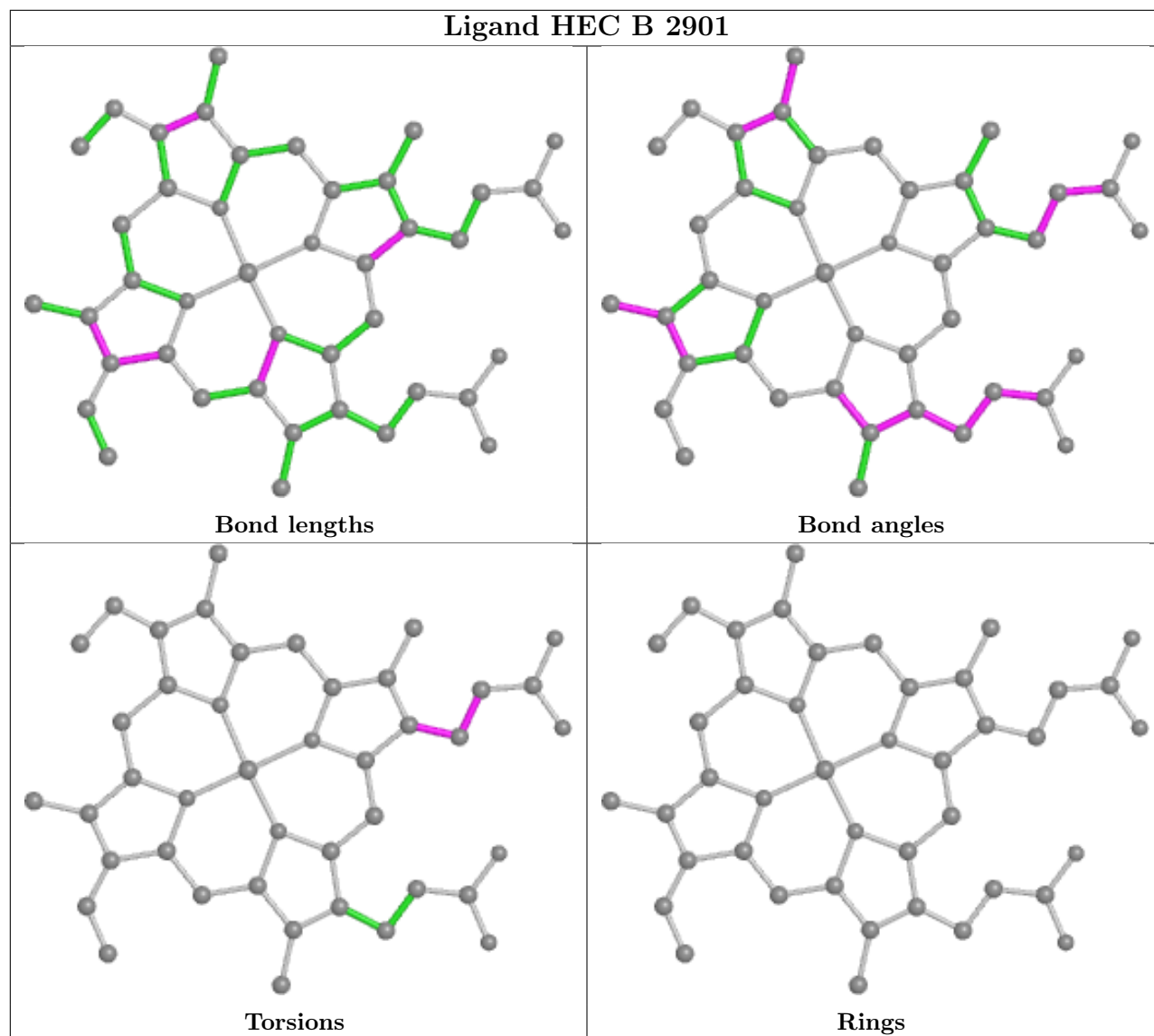
8 monomers are involved in 28 short contacts:

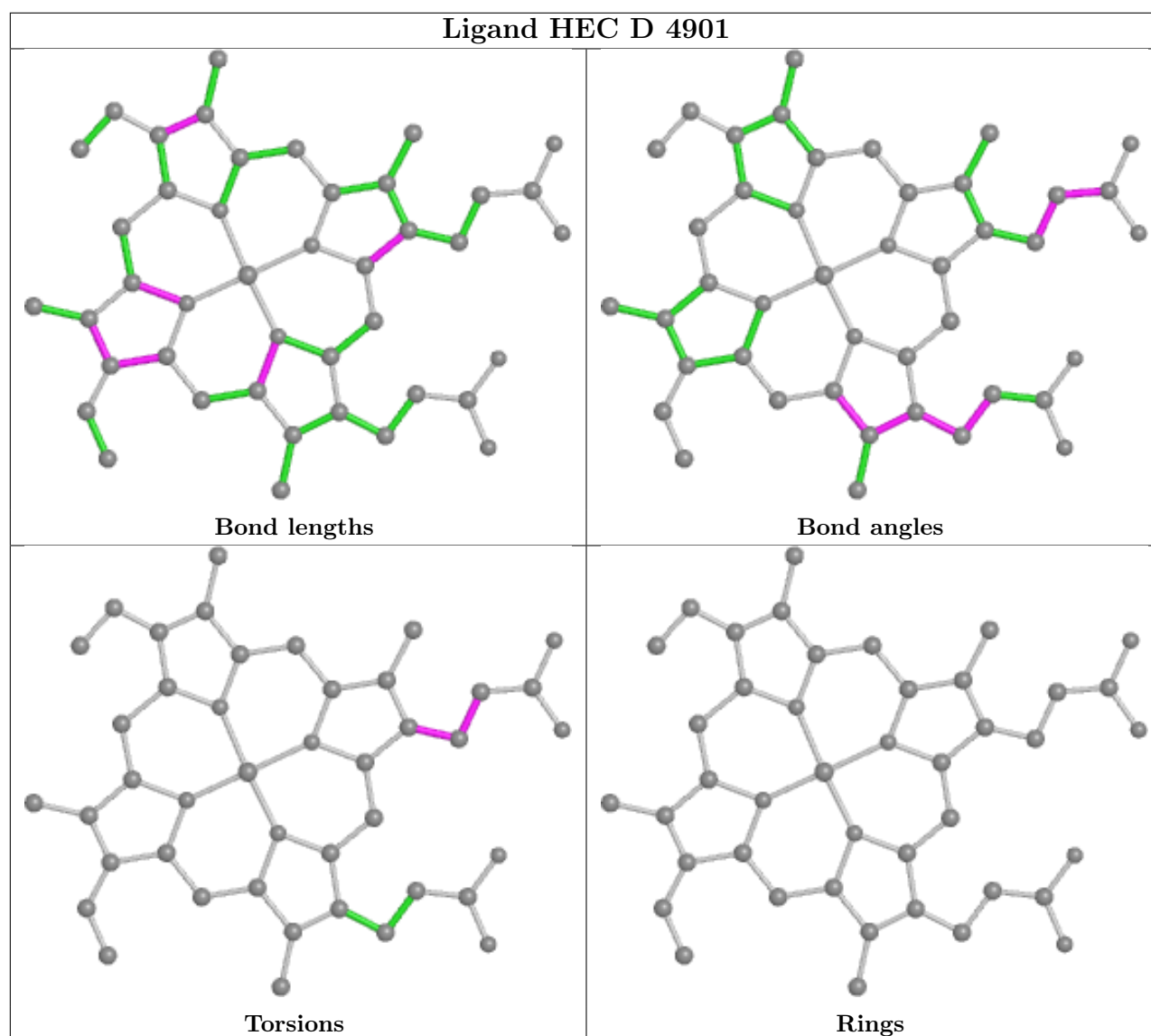
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1901	HEC	5	0
3	B	2902	H4B	3	0
5	C	3904	IMD	1	0
3	C	3902	H4B	2	0
2	C	3901	HEC	6	0
3	A	1902	H4B	3	0
2	B	2901	HEC	3	0
2	D	4901	HEC	5	0

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









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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	421/424 (99%)	0.29	17 (4%) 38 45	46, 68, 93, 117	0
1	B	421/424 (99%)	0.50	38 (9%) 9 11	35, 70, 98, 119	0
1	C	421/424 (99%)	0.26	20 (4%) 30 37	47, 67, 95, 136	0
1	D	421/424 (99%)	0.34	23 (5%) 25 30	49, 67, 91, 125	0
All	All	1684/1696 (99%)	0.35	98 (5%) 23 27	35, 68, 95, 136	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	273	PRO	5.9
1	B	401	LEU	3.9
1	C	338	TRP	3.9
1	B	502	GLN	3.8
1	D	353	ALA	3.8
1	D	336	TYR	3.7
1	D	293	LEU	3.7
1	A	338	TRP	3.6
1	B	154	PHE	3.5
1	D	463	TRP	3.5
1	D	352	VAL	3.4
1	A	501	TRP	3.3
1	B	342	LEU	3.3
1	C	296	LYS	3.3
1	B	355	MET	3.2
1	D	176	THR	3.1
1	B	200	CYS	3.1
1	D	502	GLN	3.1
1	D	367	CYS	3.0
1	B	338	TRP	3.0
1	C	353	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	404	HIS	2.9
1	A	503	ASP	2.9
1	B	465	VAL	2.9
1	B	157	ALA	2.9
1	B	156	GLU	2.9
1	B	500	VAL	2.8
1	B	452	ARG	2.8
1	D	351	ALA	2.8
1	C	262	ALA	2.8
1	A	502	GLN	2.7
1	B	340	ARG	2.7
1	A	500	VAL	2.6
1	B	461	TRP	2.6
1	B	84	HIS	2.6
1	D	465	VAL	2.6
1	A	200	CYS	2.6
1	C	156	GLU	2.6
1	A	401	LEU	2.5
1	D	452	ARG	2.5
1	C	111	ARG	2.5
1	A	293	LEU	2.5
1	B	353	ALA	2.5
1	D	466	PRO	2.5
1	B	471	SER	2.4
1	B	398	ARG	2.4
1	B	367	CYS	2.4
1	A	351	ALA	2.4
1	A	353	ALA	2.4
1	D	262	ALA	2.4
1	B	490	TYR	2.4
1	D	340	ARG	2.4
1	A	336	TYR	2.4
1	B	83	ARG	2.4
1	C	200	CYS	2.4
1	B	466	PRO	2.3
1	C	294	GLY	2.3
1	A	339	PHE	2.3
1	B	85	VAL	2.3
1	B	460	ASP	2.3
1	C	263	GLN	2.3
1	B	354	ASN	2.3
1	C	466	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	131	ASP	2.2
1	C	376	THR	2.2
1	B	489	TYR	2.2
1	C	336	TYR	2.2
1	A	197	ALA	2.2
1	C	232	ARG	2.2
1	D	338	TRP	2.2
1	C	157	ALA	2.2
1	C	275	GLY	2.2
1	C	467	PRO	2.2
1	C	158	LYS	2.1
1	C	295	TRP	2.1
1	B	404	HIS	2.1
1	A	496	TRP	2.1
1	D	354	ASN	2.1
1	D	368	PRO	2.1
1	D	462	ILE	2.1
1	B	402	GLU	2.1
1	B	336	TYR	2.1
1	A	462	ILE	2.1
1	B	488	PHE	2.1
1	B	501	TRP	2.1
1	B	470	GLY	2.1
1	D	175	THR	2.1
1	D	200	CYS	2.1
1	D	274	ASP	2.0
1	B	138	GLU	2.0
1	B	159	ILE	2.0
1	B	298	LYS	2.0
1	A	397	ARG	2.0
1	B	175	THR	2.0
1	B	341	GLU	2.0
1	B	476	PHE	2.0
1	D	467	PRO	2.0
1	C	282	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

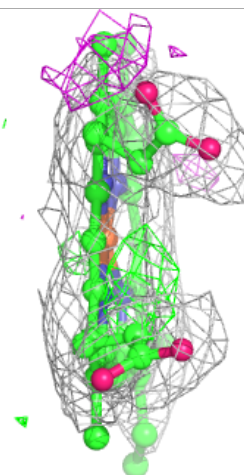
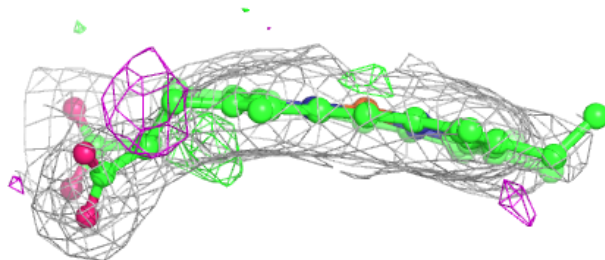
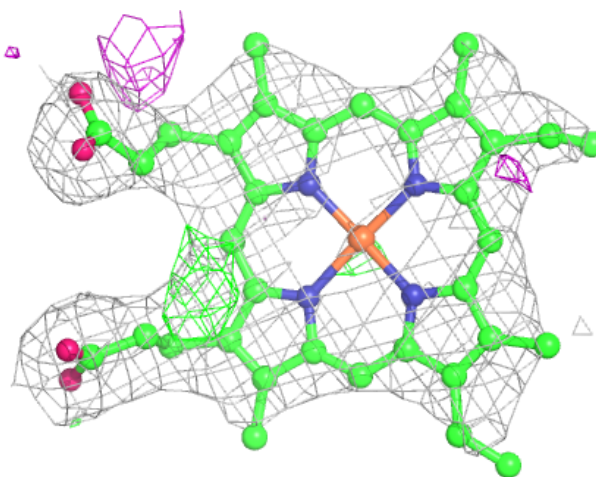
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	IMD	A	1904	5/5	0.80	0.66	87,87,96,97	0
5	IMD	C	3904	5/5	0.88	0.65	69,75,81,85	0
5	IMD	D	4904	5/5	0.88	0.60	81,84,87,90	0
5	IMD	B	2904	5/5	0.91	0.51	67,69,77,81	0
3	H4B	D	4902	17/17	0.92	0.34	49,62,72,90	0
3	H4B	C	3902	17/17	0.94	0.32	51,62,72,87	0
2	HEC	D	4901	43/43	0.94	0.29	54,64,69,79	0
3	H4B	A	1902	17/17	0.94	0.32	50,61,67,80	0
2	HEC	C	3901	43/43	0.95	0.25	55,63,73,86	0
3	H4B	B	2902	17/17	0.95	0.26	33,47,69,83	0
2	HEC	B	2901	43/43	0.97	0.29	58,65,71,75	0
4	ZN	C	3903	1/1	0.97	0.15	72,72,72,72	0
2	HEC	A	1901	43/43	0.97	0.30	52,61,67,73	0
4	ZN	A	1903	1/1	0.99	0.13	70,70,70,70	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.

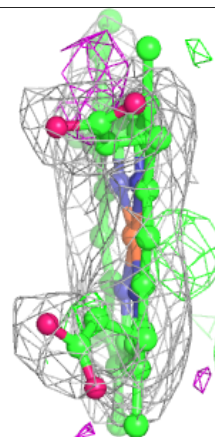
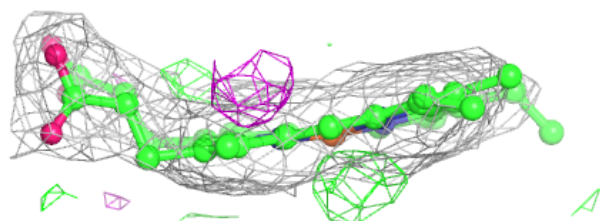
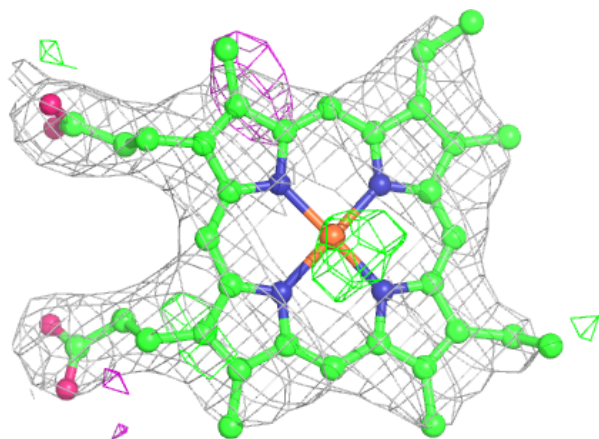
Electron density around HEC D 4901:

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



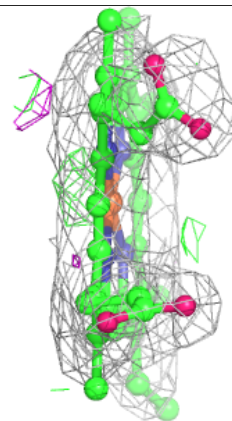
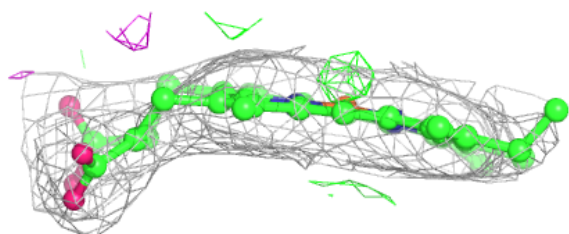
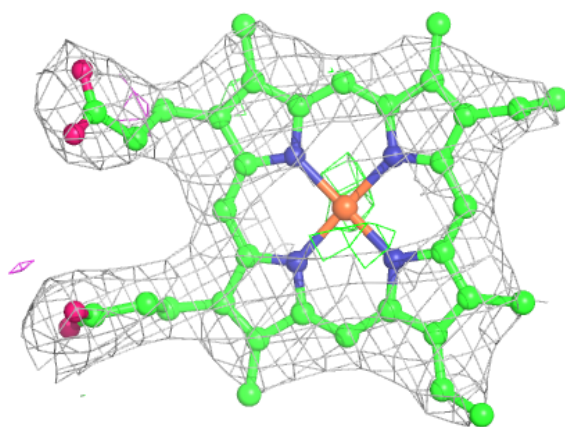
Electron density around HEC C 3901:

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

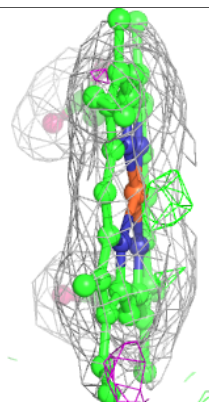
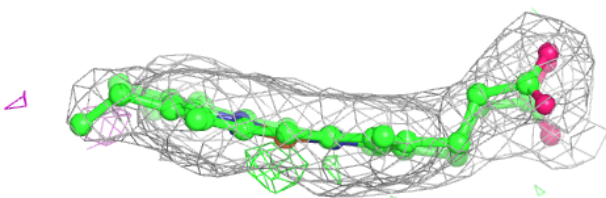
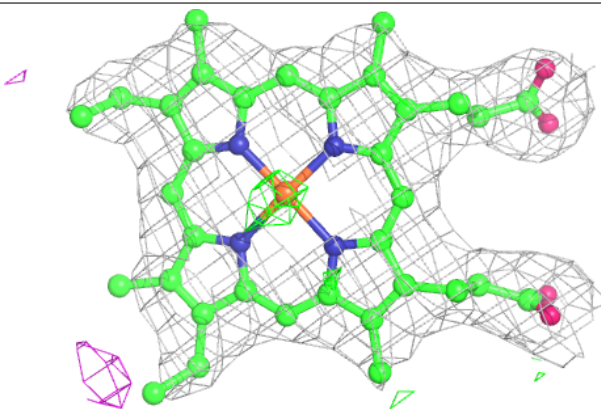


Electron density around HEC B 2901:

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

**Electron density around HEC A 1901:**

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



6.5 Other polymers

There are no such residues in this entry.