



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 07:09 PM EDT

PDB ID : 3EJ8 / pdb_00003ej8
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 types of validation reports are described at

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

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

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

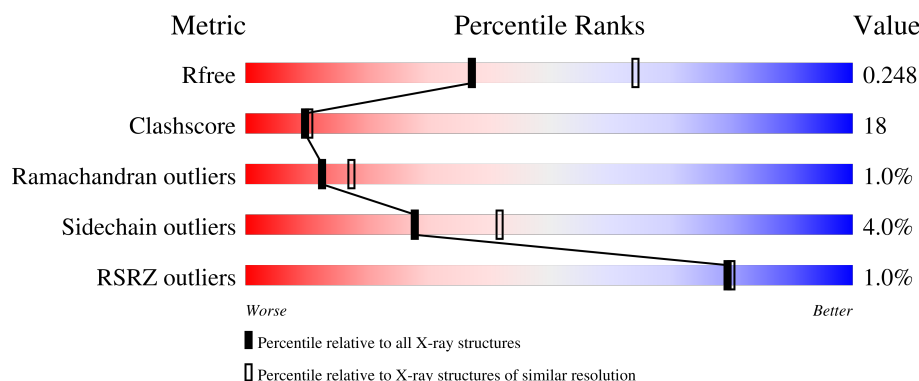
1 Overall quality at a glance

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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	
1	B	424	
1	C	424	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
1	D	424	 % 67% 30%

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	HEC	A	1901	X	-	-	-
2	HEC	B	2901	X	-	-	-
2	HEC	C	3901	X	-	-	-
2	HEC	D	4901	X	-	-	-
3	H4B	A	1902	X	-	-	-
3	H4B	B	2902	X	-	-	-
3	H4B	C	3902	X	-	-	-
3	H4B	D	4902	X	-	-	-

2 Entry composition

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.

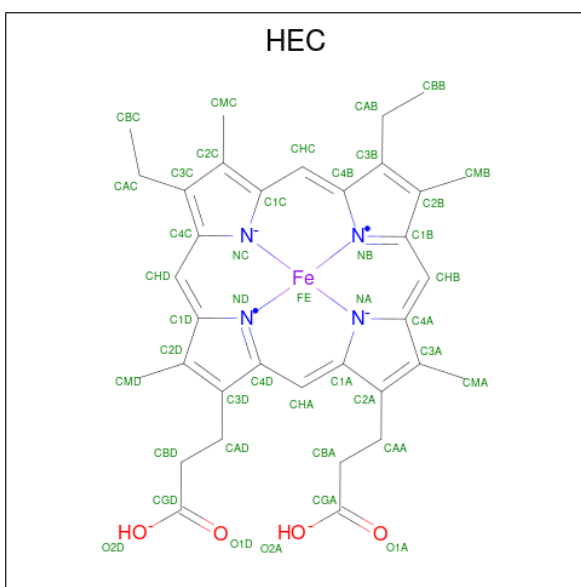
- Molecule 1 is a protein called Nitric oxide synthase, inducible.

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

There are 8 discrepancies between the modelled and reference sequences:

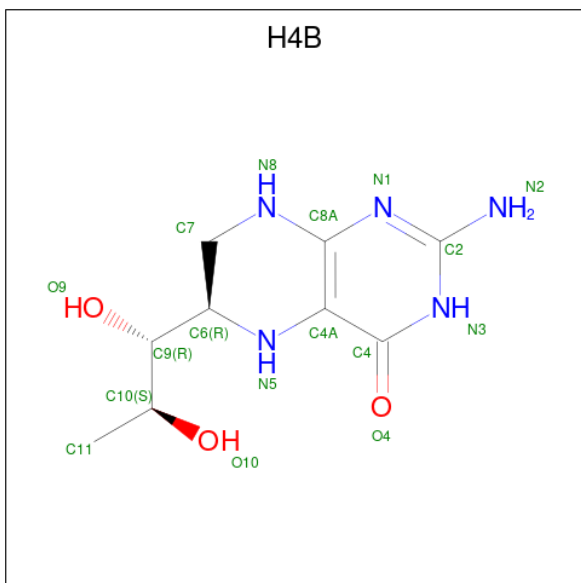
Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ILE	PHE	engineered mutation	UNP P35228
A	305	LEU	VAL	engineered mutation	UNP P35228
B	286	ILE	PHE	engineered mutation	UNP P35228
B	305	LEU	VAL	engineered mutation	UNP P35228
C	286	ILE	PHE	engineered mutation	UNP P35228
C	305	LEU	VAL	engineered mutation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

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

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

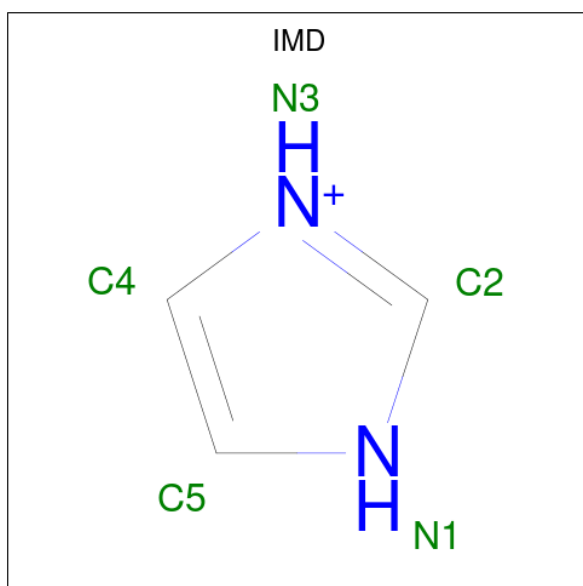


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is ZINC ION (CCD ID: 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 (CCD ID: 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		

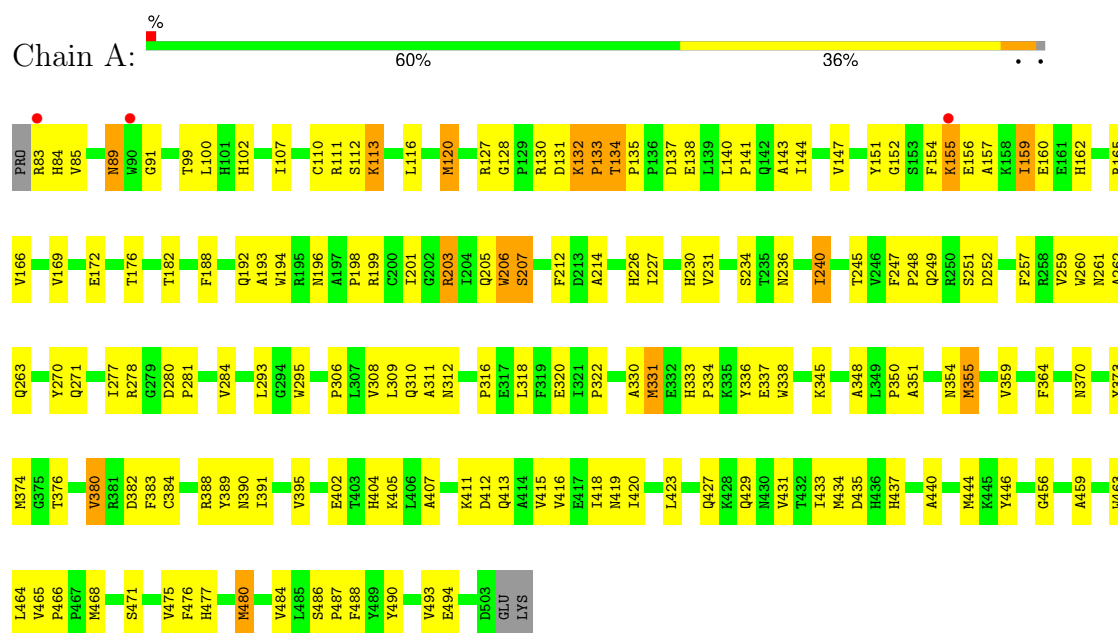
- Molecule 6 is water.

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

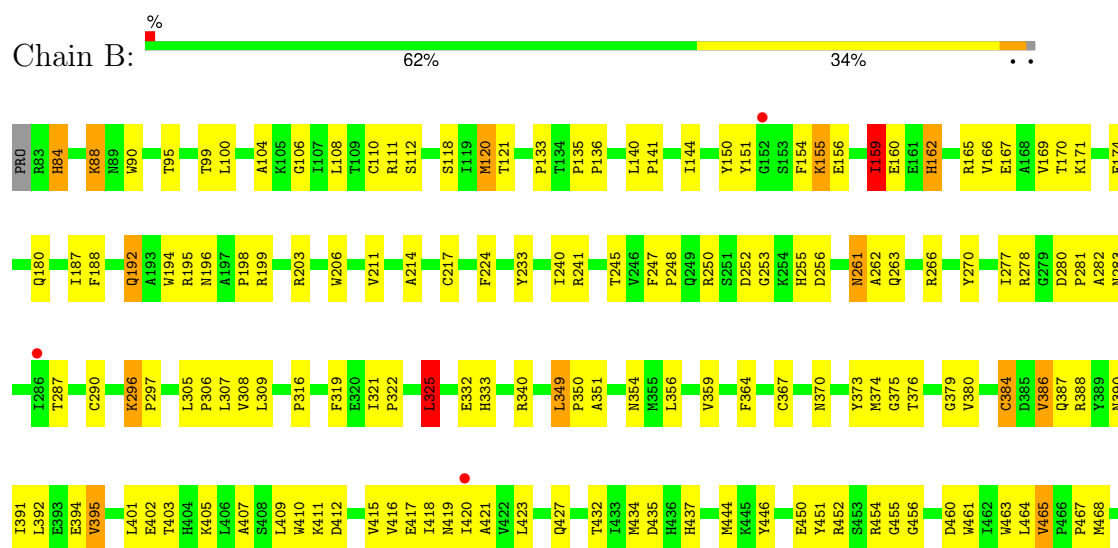
3 Residue-property plots

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

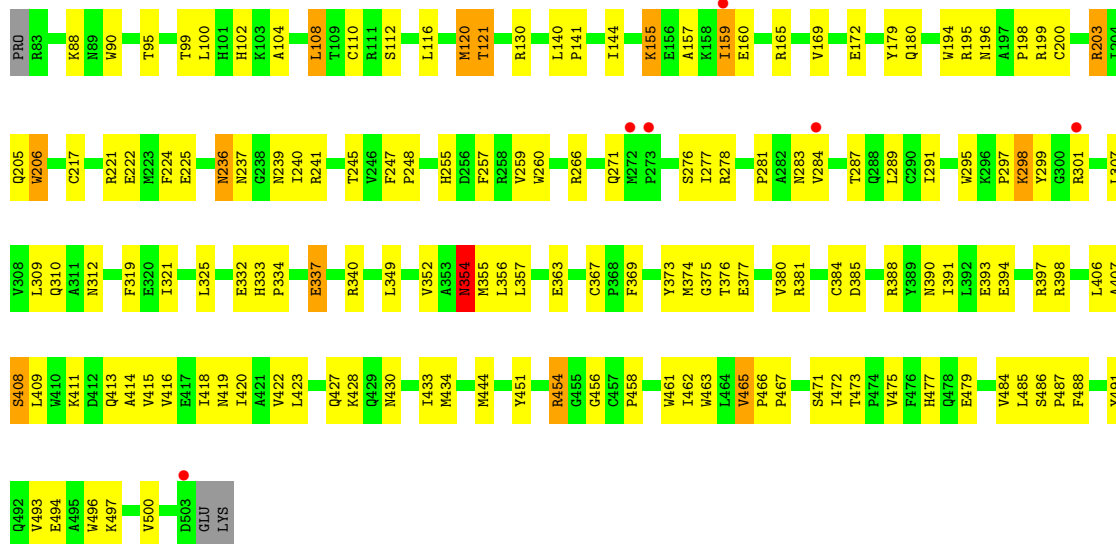


- Molecule 1: Nitric oxide synthase, inducible

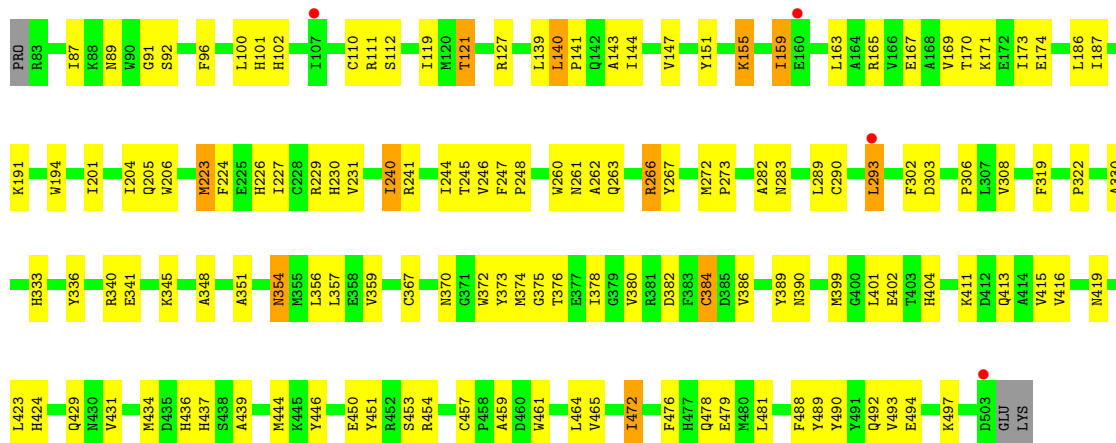




- Molecule 1: Nitric oxide synthase, inducible



- 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)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.232 , 0.271 0.214 , 0.248	Depositor DCC
R_{free} test set	3931 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	1.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

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

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	0.44	0/3514	0.94	12/4770 (0.3%)
1	B	0.44	0/3514	0.98	14/4770 (0.3%)
1	C	0.45	0/3514	0.97	15/4770 (0.3%)
1	D	0.44	0/3514	0.94	12/4770 (0.3%)
All	All	0.44	0/14056	0.96	53/19080 (0.3%)

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 (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	325	LEU	N-CA-C	-14.54	92.44	112.94
1	D	121	THR	CA-C-N	8.98	128.92	119.85
1	D	121	THR	C-N-CA	8.98	128.92	119.85
1	B	120	MET	N-CA-C	8.65	120.40	110.97
1	C	159	ILE	N-CA-C	8.28	118.84	110.23
1	C	120	MET	N-CA-C	7.60	119.25	110.97
1	B	420	ILE	N-CA-C	-7.53	103.20	110.42
1	A	240	ILE	N-CA-C	7.28	119.93	109.51
1	C	465	VAL	CA-C-N	7.15	124.88	119.66
1	C	465	VAL	C-N-CA	7.15	124.88	119.66
1	D	453	SER	N-CA-C	6.72	118.49	111.03
1	A	373	TYR	N-CA-C	6.60	119.24	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	384	CYS	N-CA-C	6.55	121.44	113.38
1	C	259	VAL	N-CA-C	-6.52	98.35	107.80
1	C	325	LEU	N-CA-C	-6.50	105.65	113.97
1	B	384	CYS	N-CA-C	6.44	121.22	113.23
1	C	354	ASN	N-CA-C	6.29	120.56	112.26
1	B	121	THR	CA-C-N	6.21	126.18	120.03
1	B	121	THR	C-N-CA	6.21	126.18	120.03
1	A	384	CYS	N-CA-C	6.14	120.93	113.38
1	A	322	PRO	CA-C-N	5.72	125.84	119.32
1	A	322	PRO	C-N-CA	5.72	125.84	119.32
1	B	354	ASN	N-CA-C	5.62	118.93	112.97
1	C	99	THR	N-CA-C	-5.61	106.11	114.64
1	C	121	THR	CA-C-N	5.60	125.50	119.85
1	C	121	THR	C-N-CA	5.60	125.50	119.85
1	A	380	VAL	CB-CA-C	-5.58	106.14	111.44
1	B	392	LEU	N-CA-C	5.49	116.95	111.07
1	C	408	SER	N-CA-C	-5.45	106.67	113.38
1	B	104	ALA	N-CA-C	5.44	117.71	110.53
1	B	373	TYR	N-CA-C	5.41	117.71	110.35
1	A	259	VAL	N-CA-C	-5.41	100.63	108.36
1	B	309	LEU	N-CA-C	5.37	117.27	108.52
1	B	465	VAL	CA-C-N	5.36	123.58	119.66
1	B	465	VAL	C-N-CA	5.36	123.58	119.66
1	D	479	GLU	N-CA-C	-5.36	102.94	110.50
1	C	422	VAL	N-CA-C	5.35	115.80	110.23
1	C	373	TYR	N-CA-C	5.35	117.44	110.43
1	D	223	MET	N-CA-C	-5.34	105.15	110.97
1	D	373	TYR	N-CA-C	5.30	117.53	110.53
1	A	383	PHE	N-CA-C	5.27	118.17	111.69
1	C	157	ALA	N-CA-C	5.27	117.95	110.10
1	C	349	LEU	N-CA-C	5.22	118.08	108.69
1	B	349	LEU	N-CA-C	5.22	118.08	108.69
1	A	182	THR	N-CA-C	-5.18	104.03	110.41
1	D	159	ILE	N-CA-C	5.18	115.33	110.30
1	D	354	ASN	N-CA-C	5.14	119.04	112.26
1	A	152	GLY	N-CA-C	-5.09	109.08	114.67
1	A	120	MET	N-CA-C	5.08	116.67	111.03
1	D	322	PRO	CA-C-N	5.07	126.18	119.84
1	D	322	PRO	C-N-CA	5.07	126.18	119.84
1	D	472	ILE	N-CA-C	-5.07	106.98	112.80
1	A	128	GLY	N-CA-C	5.02	118.03	112.00

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	131	0
1	B	3416	0	3321	128	0
1	C	3416	0	3321	124	0
1	D	3416	0	3321	122	0
2	A	43	0	32	3	0
2	B	43	0	32	0	0
2	C	43	0	32	5	0
2	D	43	0	32	4	0
3	A	17	0	13	3	0
3	B	17	0	13	2	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	481	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 18.

All (481) 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:A:444:MET:HE3	1:A:475:VAL:HG22	1.55	0.89
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
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:C:444:MET:HE3	1:C:475:VAL:HG12	1.63	0.81
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:120:MET:HE3	3:B:2902:H4B:HN5	1.51	0.75
1:D:444:MET:HE1	1:D:478:GLN:HE21	1.51	0.75
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:D:374:MET:HE2	1:D:439:ALA:HB3	1.70	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:374:MET:HE2	1:D:439:ALA:CB	2.27	0.64
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:C:356:LEU:C	1:C:356:LEU:HD23	2.23	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:B:282:ALA:C	1:B:283:ASN:HD22	2.07	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:155:LYS:H	1:B:155:LYS:HZ3	1.50	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: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: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:C:444:MET:HE2	1:C:444:MET:HA	1.84	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:D:201:ILE:HG21	1:D:374:MET:HE1	1.85	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:372:TRP:HE1	1:D:434:MET:HE2	1.70	0.56
1:D:140:LEU:HD22	1:D:144:ILE:HD11	1.88	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:B:84:HIS:ND1	1:B:84:HIS:C	2.64	0.55
1:A:468:MET:HE2	1:B:412:ASP:OD2	2.06	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:C:493:VAL:O	1:C:494:GLU:C	2.50	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:486:SER:HA	1:B:487:PRO:C	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
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
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:194:TRP:CH2	2:D:4901:HEC:HMC3	2.46	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:444:MET:HE1	1:B:478:GLN:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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
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:B:155:LYS:HB3	1:B:155:LYS:HZ2	1.77	0.48
1:B:374:MET:HE3	1:B:376:THR:OG1	2.14	0.48
1:C:159:ILE:HG23	1:C:160:GLU:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:376:THR:HA	1:A:380:VAL:HG23	1.95	0.48
1:D:187:ILE:HG22	1:D:191:LYS:HZ2	1.78	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:84:HIS:HB3	1:B:99:THR:HG22	1.95	0.47
1:B:356:LEU:C	1:B:356:LEU:HD23	2.40	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:D:402:GLU:C	1:D:404:HIS:H	2.22	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:89:ASN:HD22	1:A:89:ASN:C	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:493:VAL:O	1:D:494:GLU:C	2.59	0.46
1:A:331:MET:HE2	1:A:345:LYS:HA	1.97	0.46
1:D:476:PHE:CD1	1:D:476:PHE:C	2.94	0.46
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:C:486:SER:HA	1:C:487:PRO:C	2.40	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:A:476:PHE:CD1	1:A:476:PHE:C	2.94	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:D:282:ALA:C	1:D:283:ASN:HD22	2.25	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:C:406:LEU:C	1:C:408:SER:H	2.23	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:C:354:ASN:C	1:C:354:ASN:HD22	2.23	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:A:493:VAL:O	1:A:494:GLU:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD1	1:A:476:PHE:O	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
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:100:LEU:C	1:C:102:HIS:H	2.25	0.44
1:C:380:VAL:O	1:C:384:CYS:HB2	2.18	0.44
1:D:100:LEU:C	1:D:102:HIS:H	2.26	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:B:162:HIS:ND1	1:B:162:HIS:C	2.75	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: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:C:203:ARG:C	1:C:205:GLN:N	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:ARG:HG3	1:D:341:GLU:N	2.33	0.43
1:B:282:ALA:C	1:B:283:ASN:ND2	2.76	0.43
1:C:205:GLN:O	1:C:206:TRP:C	2.61	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:194:TRP:CH2	2:C:3901:HEC:HMC3	2.53	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:A:412:ASP:OD2	1:B:468:MET:HE2	2.18	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:A:111:ARG:C	1:A:113:LYS:N	2.76	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
2:C:3901:HEC:HMC1	2:C:3901:HEC:HBC2	2.01	0.43
1:D:333:HIS:HB3	1:D:336:TYR:O	2.19	0.43
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:D:389:TYR:O	1:D:390:ASN:C	2.62	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:370:ASN:OD1	1:A:370:ASN:C	2.61	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:A:120:MET:HE2	1:B:90:TRP:CE2	2.55	0.42
1:B:386:VAL:HA	1:B:390:ASN:CG	2.44	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:A:131:ASP:OD2	1:A:131:ASP:C	2.63	0.41
1:C:479:GLU:HG2	1:D:119:ILE:HA	2.02	0.41
1:D:399:MET:HE2	1:D:401:LEU:HD11	2.01	0.41
1:A:389:TYR:O	1:A:390:ASN:C	2.63	0.41
1:A:444:MET:CE	1:A:475:VAL:HG22	2.39	0.41
1:A:486:SER:HA	1:A:487:PRO:C	2.44	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:C:100:LEU:C	1:C:102:HIS:N	2.78	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:D:356:LEU:HB2	1:D:492:GLN:CD	2.46	0.41
1:A:295:TRP:HB2	1:A:318:LEU:HD13	2.03	0.41
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:B:493:VAL:O	1:B:494:GLU:C	2.63	0.41
1:D:374:MET:HA	1:D:434:MET:O	2.20	0.41
1:D:261:ASN:OD1	1:D:261:ASN:N	2.54	0.41
1:A:475:VAL:CG1	1:A:480:MET:HE1	2.51	0.41
1:B:245:THR:O	1:B:367:CYS:HA	2.20	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:B:290:CYS:SG	1:B:306:PRO:HG2	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:VAL:O	1:B:384:CYS:HB2	2.21	0.41
1:C:376:THR:HA	1:C:380:VAL:HG23	2.01	0.41
1:C:494:GLU:CG	1:C:497:LYS:HE3	2.47	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
2:D:4901:HEC:HMC1	2:D:4901:HEC:HBC2	2.03	0.41
1:A:112:SER:O	1:B:106:GLY:HA2	2.20	0.40
1:B:194:TRP:CD1	1:B:194:TRP:C	2.99	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:C:337:GLU:CD	1:C:337:GLU:H	2.29	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: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: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:A:111:ARG:C	1:A:113:LYS:H	2.28	0.40
1:B:167:GLU:O	1:B:171:LYS:HG2	2.22	0.40
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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/424 (99%)	384 (92%)	28 (7%)	7 (2%)	7	8
1	B	419/424 (99%)	382 (91%)	35 (8%)	2 (0%)	24	34
1	C	419/424 (99%)	378 (90%)	36 (9%)	5 (1%)	10	13
1	D	419/424 (99%)	383 (91%)	34 (8%)	2 (0%)	24	34
All	All	1676/1696 (99%)	1527 (91%)	133 (8%)	16 (1%)	12	17

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
1	C	236	ASN
1	C	375	GLY
1	A	350	PRO
1	D	240	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/370 (99%)	347 (95%)	18 (5%)	22	34
1	B	365/370 (99%)	348 (95%)	17 (5%)	23	36
1	C	365/370 (99%)	350 (96%)	15 (4%)	27	41
1	D	365/370 (99%)	356 (98%)	9 (2%)	42	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1460/1480 (99%)	1401 (96%)	59 (4%)	28	42

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	VAL
1	A	89	ASN
1	A	113	LYS
1	A	132	LYS
1	A	134	THR
1	A	155	LYS
1	A	159	ILE
1	A	207	SER
1	A	261	ASN
1	A	271	GLN
1	A	293	LEU
1	A	312	ASN
1	A	331	MET
1	A	337	GLU
1	A	355	MET
1	A	359	VAL
1	A	413	GLN
1	A	480	MET
1	B	84	HIS
1	B	88	LYS
1	B	155	LYS
1	B	159	ILE
1	B	162	HIS
1	B	180	GLN
1	B	192	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	395	VAL
1	B	402	GLU
1	B	494	GLU
1	B	500	VAL
1	C	108	LEU
1	C	120	MET

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Mol	Chain	Res	Type
1	C	155	LYS
1	C	180	GLN
1	C	203	ARG
1	C	287	THR
1	C	298	LYS
1	C	337	GLU
1	C	354	ASN
1	C	357	LEU
1	C	390	ASN
1	C	428	LYS
1	C	430	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	266	ARG
1	D	293	LEU
1	D	359	VAL
1	D	386	VAL
1	D	413	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	102	HIS
1	A	142	GLN
1	A	148	ASN
1	A	226	HIS
1	A	236	ASN
1	A	239	ASN
1	A	271	GLN
1	A	312	ASN
1	A	370	ASN
1	A	413	GLN
1	A	427	GLN
1	A	429	GLN
1	A	477	HIS
1	A	492	GLN
1	A	499	HIS

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Mol	Chain	Res	Type
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	249	GLN
1	B	255	HIS
1	B	261	ASN
1	B	263	GLN
1	B	424	HIS
1	B	449	ASN
1	B	477	HIS
1	B	502	GLN
1	C	102	HIS
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	427	GLN
1	C	429	GLN
1	C	448	GLN
1	C	449	ASN
1	C	477	HIS
1	D	89	ASN
1	D	97	GLN
1	D	102	HIS
1	D	208	ASN
1	D	226	HIS
1	D	230	HIS
1	D	236	ASN
1	D	283	ASN
1	D	288	GLN
1	D	370	ASN
1	D	404	HIS
1	D	413	GLN
1	D	419	ASN
1	D	427	GLN
1	D	429	GLN
1	D	448	GLN

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Mol	Chain	Res	Type
1	D	477	HIS
1	D	478	GLN
1	D	492	GLN
1	D	502	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	-	5,5,5	1.06	0	5,5,5	0.18	0
2	HEC	A	1901	1	50,50,50	1.25	3 (6%)	68,82,82	1.28	7 (10%)
2	HEC	B	2901	1	50,50,50	1.06	2 (4%)	68,82,82	1.28	8 (11%)
3	H4B	D	4902	-	17,18,18	2.34	5 (29%)	14,26,26	2.25	3 (21%)
3	H4B	A	1902	-	17,18,18	2.34	6 (35%)	14,26,26	2.29	4 (28%)
3	H4B	B	2902	-	17,18,18	1.97	4 (23%)	14,26,26	2.88	4 (28%)
3	H4B	C	3902	-	17,18,18	2.27	7 (41%)	14,26,26	2.00	3 (21%)
2	HEC	D	4901	1	50,50,50	1.16	3 (6%)	68,82,82	1.21	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	IMD	D	4904	-	5,5,5	1.03	0	5,5,5	0.29	0
5	IMD	C	3904	-	5,5,5	0.96	0	5,5,5	0.15	0
2	HEC	C	3901	1	50,50,50	1.04	3 (6%)	68,82,82	1.28	7 (10%)
5	IMD	B	2904	-	5,5,5	1.07	1 (20%)	5,5,5	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IMD	A	1904	-	-	-	0/1/1/1
2	HEC	A	1901	1	1/1/3/7	5/14/54/54	-
2	HEC	B	2901	1	1/1/3/7	9/14/54/54	-
3	H4B	D	4902	-	3/3/3/5	7/8/17/17	0/2/2/2
3	H4B	A	1902	-	3/3/3/5	7/8/17/17	0/2/2/2
3	H4B	B	2902	-	3/3/3/5	4/8/17/17	0/2/2/2
3	H4B	C	3902	-	3/3/3/5	7/8/17/17	0/2/2/2
2	HEC	D	4901	1	1/1/3/7	7/14/54/54	-
5	IMD	D	4904	-	-	-	0/1/1/1
5	IMD	C	3904	-	-	-	0/1/1/1
2	HEC	C	3901	1	1/1/3/7	5/14/54/54	-
5	IMD	B	2904	-	-	-	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3902	H4B	C4A-C8A	5.22	1.47	1.38
3	D	4902	H4B	C4A-C8A	4.79	1.46	1.38
3	A	1902	H4B	C4-N3	4.68	1.47	1.38
3	D	4902	H4B	C8A-N1	4.67	1.43	1.36
2	A	1901	HEC	FE-ND	4.61	2.09	1.94
3	A	1902	H4B	C8A-N1	4.42	1.43	1.36
3	D	4902	H4B	C4-N3	4.25	1.46	1.38
3	C	3902	H4B	C4-N3	4.21	1.46	1.38
3	A	1902	H4B	C4A-C8A	4.16	1.45	1.38
3	B	2902	H4B	C4-N3	4.08	1.46	1.38
3	C	3902	H4B	C8A-N1	3.96	1.42	1.36
3	B	2902	H4B	C4A-C8A	3.87	1.45	1.38
3	B	2902	H4B	C8A-N1	3.63	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4901	HEC	FE-ND	3.31	2.05	1.94
3	A	1902	H4B	C9-C6	-3.12	1.48	1.53
3	A	1902	H4B	C2-N1	2.69	1.39	1.33
2	A	1901	HEC	CMC-C2C	2.45	1.55	1.50
2	D	4901	HEC	FE-NC	2.42	2.03	1.95
2	C	3901	HEC	FE-NA	2.41	2.03	1.95
3	D	4902	H4B	C2-N3	2.39	1.43	1.37
3	D	4902	H4B	C2-N1	2.38	1.38	1.33
3	C	3902	H4B	C2-N1	2.37	1.38	1.33
3	C	3902	H4B	C2-N3	2.36	1.43	1.37
2	B	2901	HEC	CMC-C2C	2.36	1.55	1.50
2	A	1901	HEC	CMD-C2D	2.32	1.55	1.50
2	C	3901	HEC	CMB-C2B	2.27	1.55	1.50
3	B	2902	H4B	C2-N3	2.25	1.43	1.37
3	C	3902	H4B	C9-C6	-2.25	1.49	1.53
2	D	4901	HEC	CMB-C2B	2.21	1.55	1.50
3	A	1902	H4B	C2-N3	2.19	1.42	1.37
2	B	2901	HEC	CMB-C2B	2.17	1.55	1.50
2	C	3901	HEC	CMC-C2C	2.05	1.55	1.50
5	B	2904	IMD	C5-N1	2.02	1.42	1.35
3	C	3902	H4B	C7-C6	2.00	1.54	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2902	H4B	O10-C10-C9	8.34	123.58	109.77
3	A	1902	H4B	O10-C10-C9	6.55	120.62	109.77
3	D	4902	H4B	O10-C10-C9	6.24	120.11	109.77
3	C	3902	H4B	O10-C10-C9	5.36	118.64	109.77
2	A	1901	HEC	CBC-CAC-C3C	4.48	124.57	112.42
2	D	4901	HEC	CBC-CAC-C3C	4.43	124.43	112.42
2	B	2901	HEC	CBC-CAC-C3C	4.40	124.35	112.42
2	C	3901	HEC	CBC-CAC-C3C	4.21	123.83	112.42
3	B	2902	H4B	C11-C10-C9	-3.84	107.41	112.11
3	D	4902	H4B	O9-C9-C6	3.53	117.74	109.28
3	B	2902	H4B	O9-C9-C6	3.31	117.21	109.28
2	C	3901	HEC	CBD-CAD-C3D	-2.96	104.36	112.53
2	A	1901	HEC	CBB-CAB-C3B	2.86	120.18	112.42
2	B	2901	HEC	CBD-CAD-C3D	-2.75	104.94	112.53
2	A	1901	HEC	C1D-C2D-C3D	-2.63	104.21	106.98
2	D	4901	HEC	CBB-CAB-C3B	2.63	119.55	112.42
2	C	3901	HEC	C1D-C2D-C3D	-2.60	104.24	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1901	HEC	C2D-C1D-ND	2.58	112.81	109.84
3	A	1902	H4B	C2-N1-C8A	2.50	117.76	113.36
2	A	1901	HEC	C2B-C1B-NB	2.46	112.74	109.90
2	B	2901	HEC	CBB-CAB-C3B	2.46	119.08	112.42
2	B	2901	HEC	C1D-C2D-C3D	-2.41	104.44	106.98
3	D	4902	H4B	C2-N1-C8A	2.41	117.61	113.36
2	B	2901	HEC	C2D-C1D-ND	2.40	112.60	109.84
2	C	3901	HEC	CMD-C2D-C1D	2.39	128.76	125.03
2	D	4901	HEC	C1D-C2D-C3D	-2.39	104.47	106.98
2	D	4901	HEC	C2D-C1D-ND	2.37	112.57	109.84
2	D	4901	HEC	C2B-C1B-NB	2.37	112.64	109.90
3	C	3902	H4B	O9-C9-C6	2.37	114.96	109.28
2	C	3901	HEC	C2D-C1D-ND	2.36	112.56	109.84
2	C	3901	HEC	C2B-C1B-NB	2.36	112.64	109.90
2	A	1901	HEC	CBD-CAD-C3D	-2.36	106.00	112.53
3	C	3902	H4B	C2-N1-C8A	2.29	117.39	113.36
2	D	4901	HEC	CMD-C2D-C1D	2.25	128.55	125.03
2	C	3901	HEC	CBB-CAB-C3B	2.24	118.48	112.42
3	B	2902	H4B	C2-N1-C8A	2.23	117.30	113.36
2	B	2901	HEC	C2B-C1B-NB	2.22	112.47	109.90
3	A	1902	H4B	O9-C9-C10	2.20	113.33	109.14
2	B	2901	HEC	O2A-CGA-CBA	2.07	120.55	114.00
2	A	1901	HEC	CMD-C2D-C1D	2.04	128.23	125.03
3	A	1902	H4B	O9-C9-C6	2.04	114.16	109.28
2	B	2901	HEC	CMD-C2D-C1D	2.03	128.20	125.03

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1901	HEC	NA
2	B	2901	HEC	NA
2	C	3901	HEC	NA
2	D	4901	HEC	NA
3	A	1902	H4B	C9
3	A	1902	H4B	C10
3	A	1902	H4B	C6
3	B	2902	H4B	C9
3	B	2902	H4B	C10
3	B	2902	H4B	C6
3	C	3902	H4B	C9
3	C	3902	H4B	C10
3	C	3902	H4B	C6

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Mol	Chain	Res	Type	Atom
3	D	4902	H4B	C9
3	D	4902	H4B	C10
3	D	4902	H4B	C6

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3901	HEC	C2C-C3C-CAC-CBC
2	D	4901	HEC	C2C-C3C-CAC-CBC
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
2	A	1901	HEC	C2C-C3C-CAC-CBC
2	B	2901	HEC	C2C-C3C-CAC-CBC
2	A	1901	HEC	C4C-C3C-CAC-CBC
2	B	2901	HEC	C4C-C3C-CAC-CBC
2	C	3901	HEC	C4C-C3C-CAC-CBC
2	D	4901	HEC	C4C-C3C-CAC-CBC
3	C	3902	H4B	C11-C10-C9-O9
2	B	2901	HEC	C2A-CAA-CBA-CGA
2	D	4901	HEC	C2A-CAA-CBA-CGA
3	A	1902	H4B	C11-C10-C9-O9
3	B	2902	H4B	C11-C10-C9-O9
3	D	4902	H4B	C11-C10-C9-O9
3	B	2902	H4B	O10-C10-C9-O9
3	A	1902	H4B	N5-C6-C9-C10
3	C	3902	H4B	N5-C6-C9-C10
2	B	2901	HEC	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
3	D	4902	H4B	N5-C6-C9-C10
2	D	4901	HEC	C1A-C2A-CAA-CBA
2	A	1901	HEC	C2B-C3B-CAB-CBB
2	B	2901	HEC	C3A-C2A-CAA-CBA
2	C	3901	HEC	C2A-CAA-CBA-CGA
2	A	1901	HEC	CAD-CBD-CGD-O2D
2	B	2901	HEC	CAD-CBD-CGD-O2D
2	C	3901	HEC	CAD-CBD-CGD-O2D
2	D	4901	HEC	CAD-CBD-CGD-O2D
2	A	1901	HEC	CAD-CBD-CGD-O1D
2	B	2901	HEC	CAD-CBD-CGD-O1D
2	D	4901	HEC	CAD-CBD-CGD-O1D
2	C	3901	HEC	CAD-CBD-CGD-O1D
2	B	2901	HEC	CAA-CBA-CGA-O2A
2	D	4901	HEC	C3A-C2A-CAA-CBA
2	B	2901	HEC	CAA-CBA-CGA-O1A

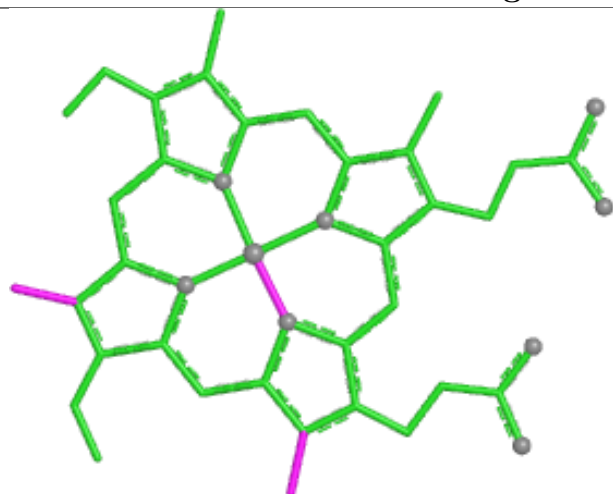
There are no ring outliers.

7 monomers are involved in 20 short contacts:

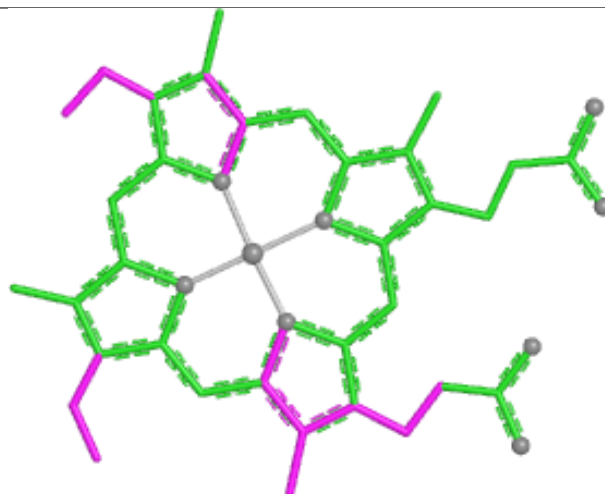
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1901	HEC	3	0
3	A	1902	H4B	3	0
3	B	2902	H4B	2	0
3	C	3902	H4B	2	0
2	D	4901	HEC	4	0
5	C	3904	IMD	1	0
2	C	3901	HEC	5	0

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.

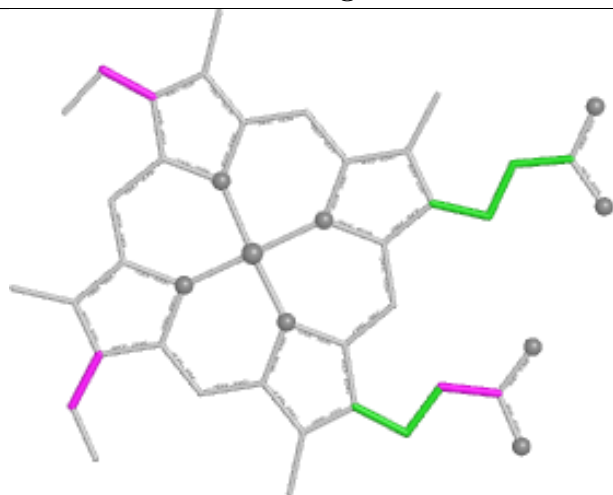
Ligand HEC A 1901



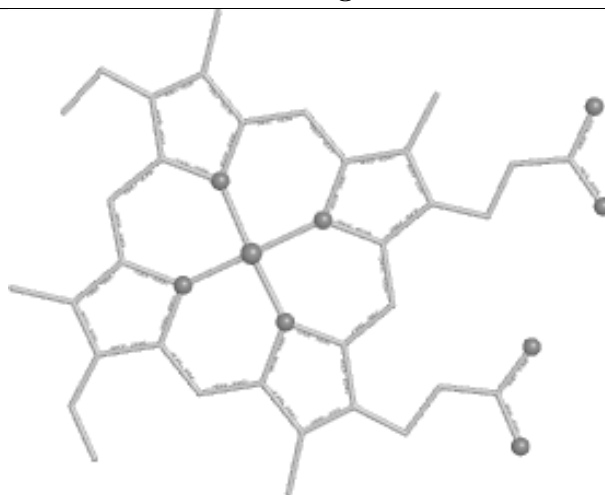
Bond lengths



Bond angles

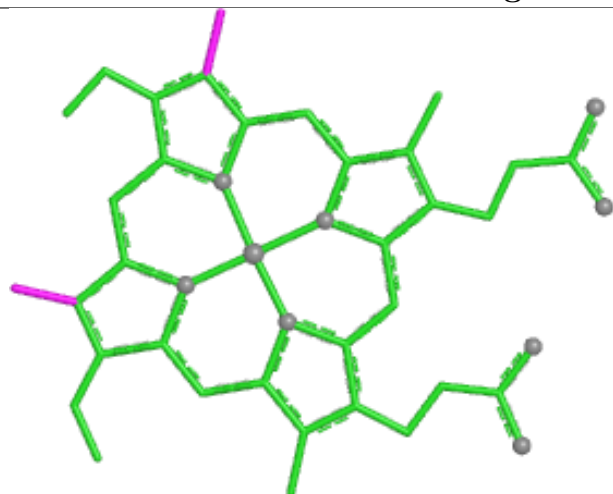


Torsions

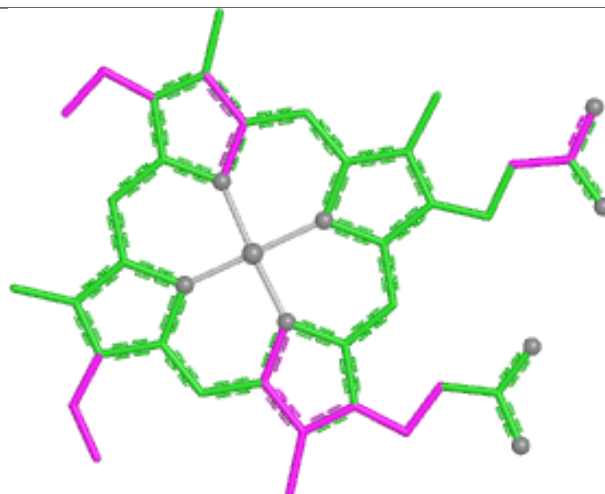


Rings

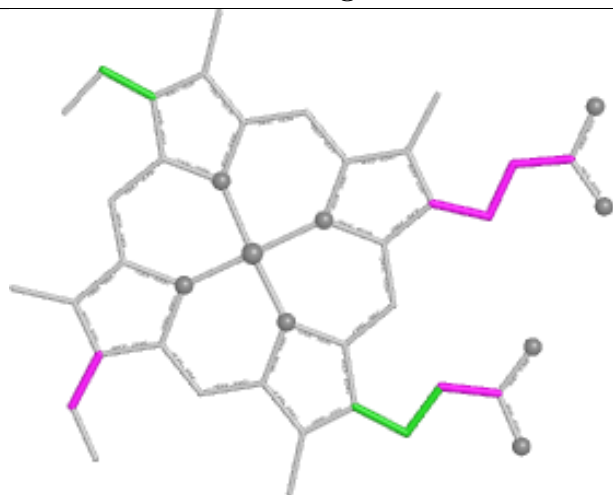
Ligand HEC B 2901



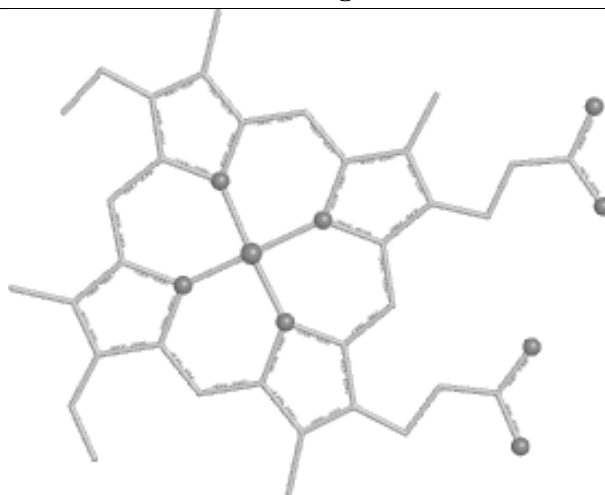
Bond lengths



Bond angles

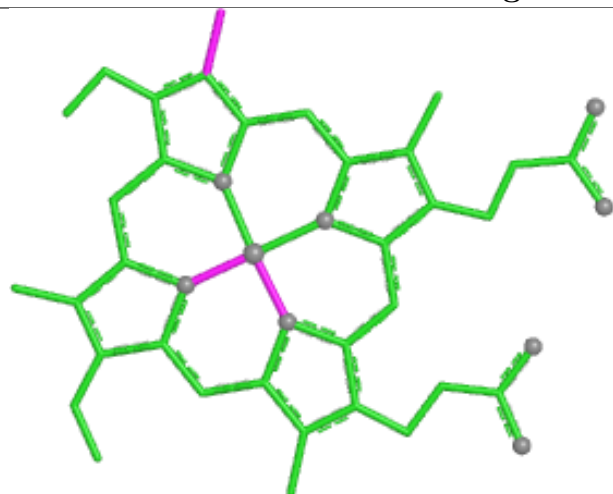


Torsions

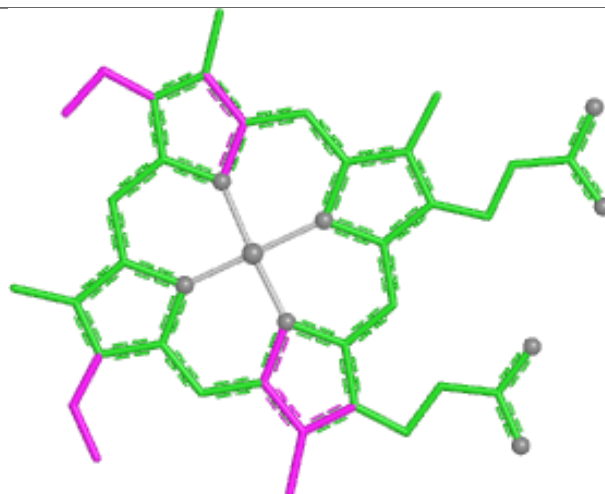


Rings

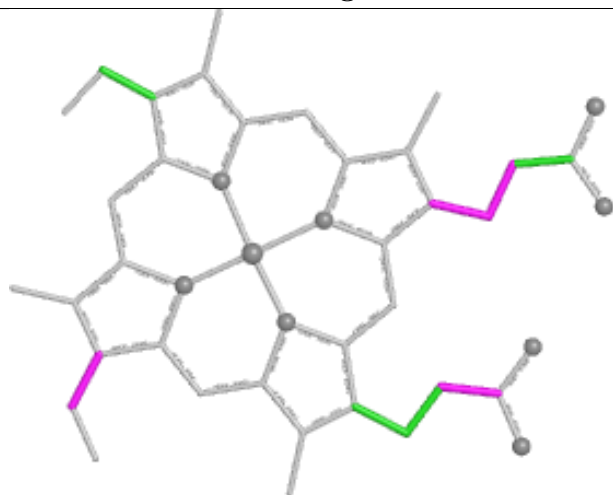
Ligand HEC D 4901



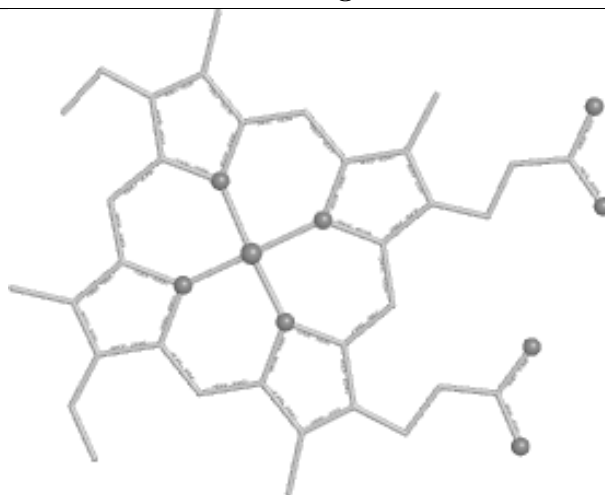
Bond lengths



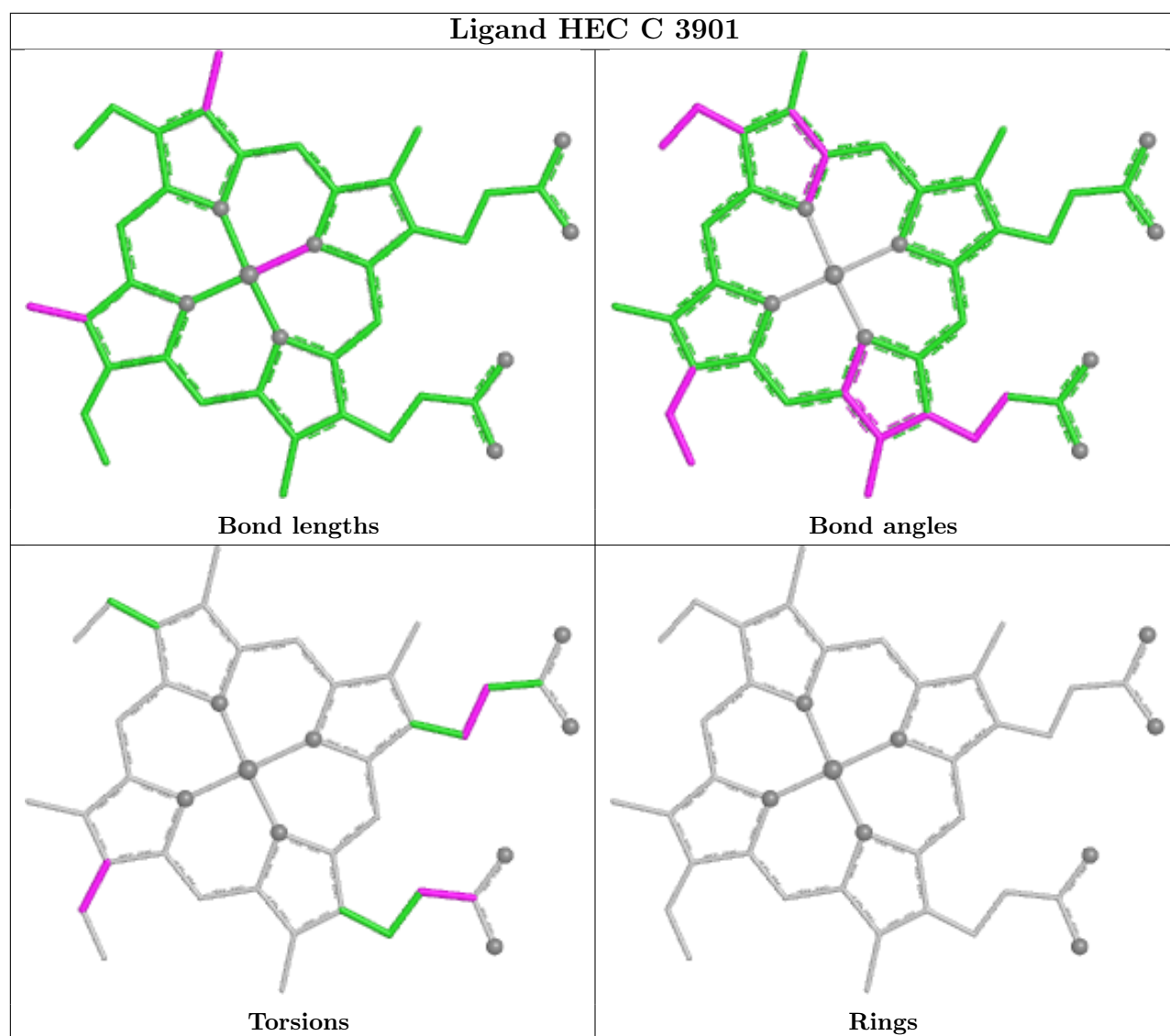
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	421/424 (99%)	0.18	3 (0%) 84 86	46, 68, 93, 117	0
1	B	421/424 (99%)	0.28	4 (0%) 79 80	35, 70, 98, 119	0
1	C	421/424 (99%)	0.22	6 (1%) 73 74	47, 67, 95, 136	0
1	D	421/424 (99%)	0.13	4 (0%) 79 80	49, 67, 91, 125	0
All	All	1684/1696 (99%)	0.20	17 (1%) 79 80	35, 68, 95, 136	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	272	MET	4.6
1	C	503	ASP	4.5
1	B	503	ASP	4.2
1	D	503	ASP	4.2
1	D	293	LEU	3.7
1	C	273	PRO	3.7
1	B	152	GLY	3.6
1	C	284	VAL	3.6
1	C	159	ILE	2.8
1	D	160	GLU	2.5
1	B	286	ILE	2.4
1	C	301	ARG	2.3
1	A	83	ARG	2.2
1	A	155	LYS	2.2
1	A	90	TRP	2.1
1	B	420	ILE	2.0
1	D	107	ILE	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

There are no oligosaccharides in this entry.

6.4 Ligands

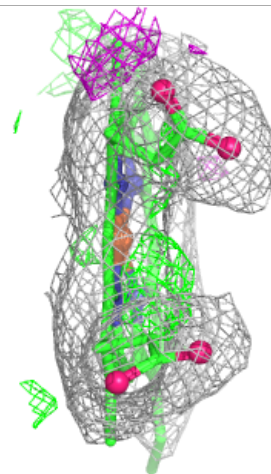
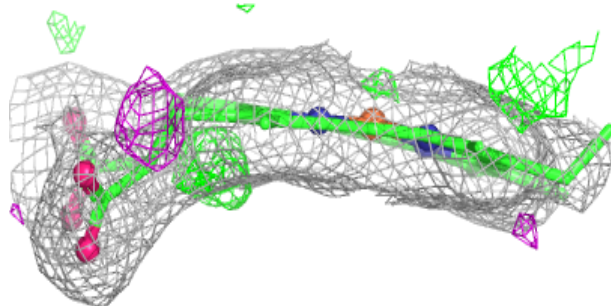
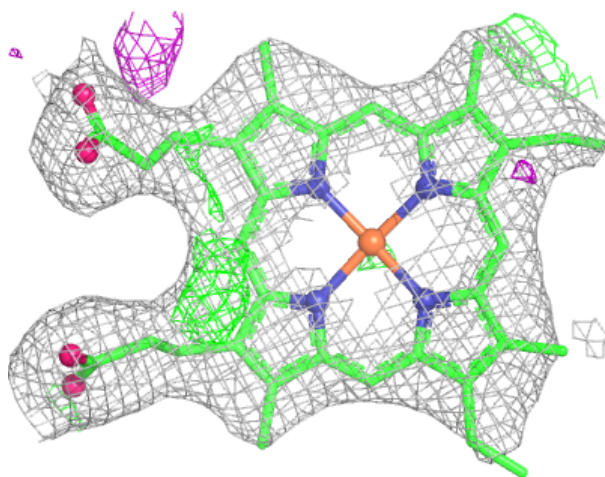
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	IMD	A	1904	5/5	0.68	0.34	87,87,96,97	0
5	IMD	C	3904	5/5	0.69	0.29	69,75,81,85	0
5	IMD	D	4904	5/5	0.82	0.24	81,84,87,90	0
5	IMD	B	2904	5/5	0.85	0.20	67,69,77,81	0
3	H4B	A	1902	17/17	0.90	0.12	50,61,67,80	0
3	H4B	C	3902	17/17	0.92	0.12	51,62,72,87	0
3	H4B	B	2902	17/17	0.93	0.11	33,47,69,83	0
3	H4B	D	4902	17/17	0.94	0.12	49,62,72,90	0
2	HEC	D	4901	43/43	0.96	0.10	54,64,69,79	0
2	HEC	A	1901	43/43	0.97	0.09	52,61,67,73	0
2	HEC	B	2901	43/43	0.97	0.09	58,65,71,75	0
2	HEC	C	3901	43/43	0.97	0.10	55,63,73,86	0
4	ZN	A	1903	1/1	1.00	0.03	70,70,70,70	0
4	ZN	C	3903	1/1	1.00	0.03	72,72,72,72	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.

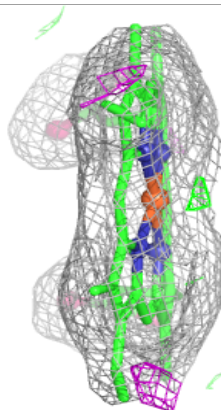
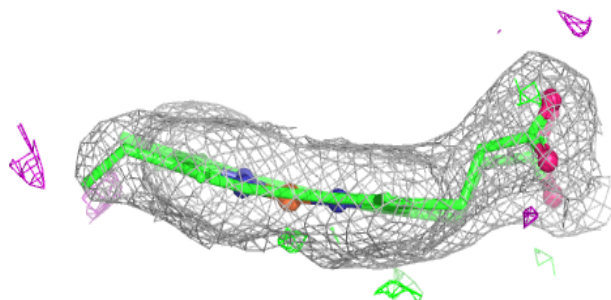
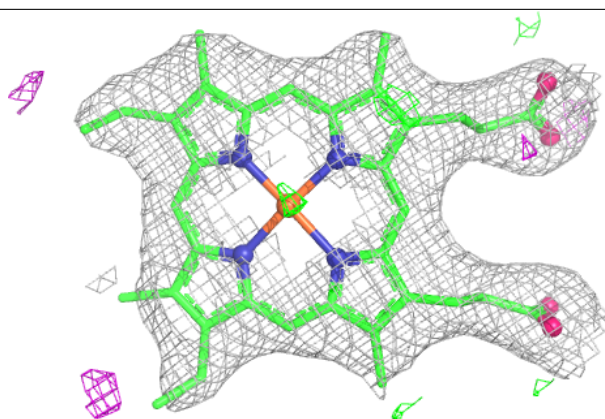
Electron density around HEC D 4901:

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

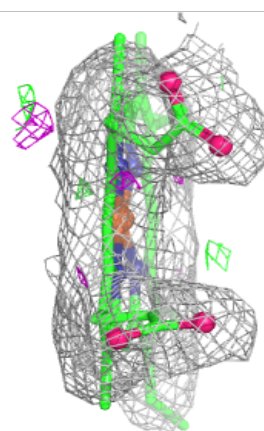
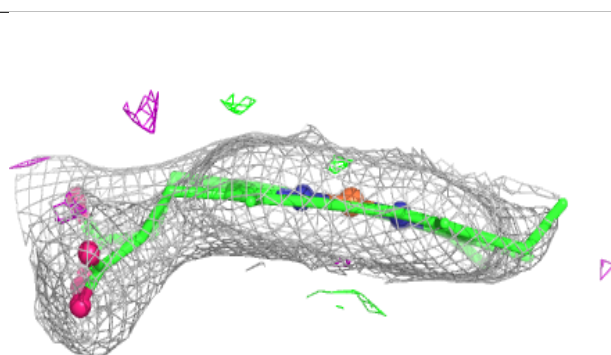
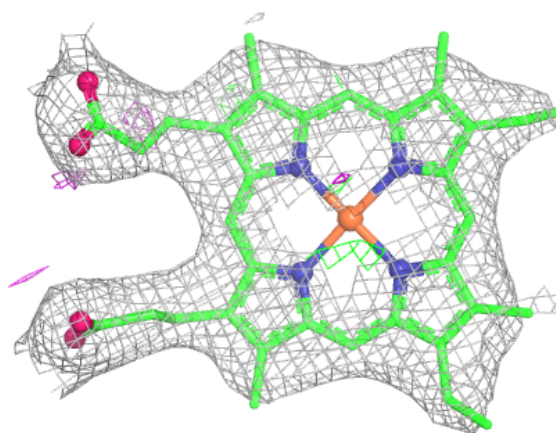


Electron density around HEC A 1901:

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

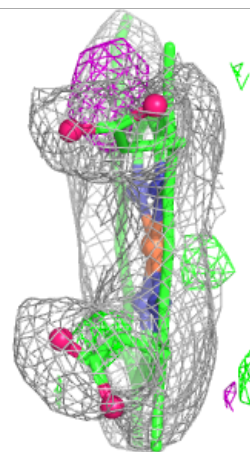
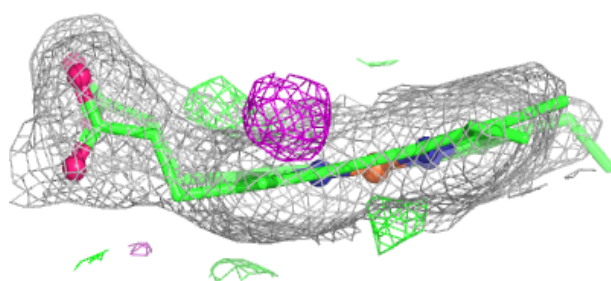
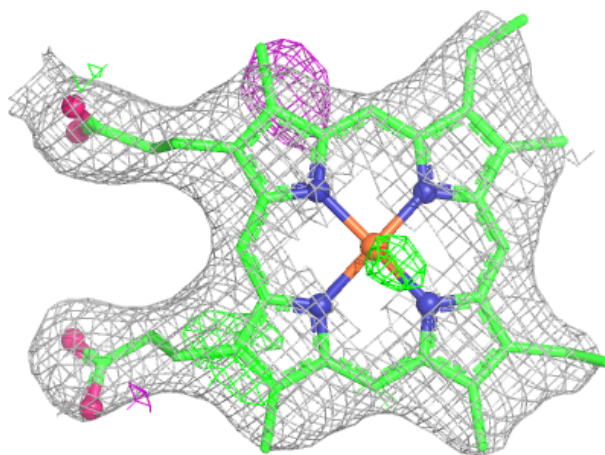
**Electron density around HEC B 2901:**

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



Electron density around HEC 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.