Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 11:15 AM EDT

PDB ID	:	3E7S / pdb_00003e7s
Title	:	Structure of bovine eNOS oxygenase domain with inhibitor AR-C95791
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	:	2008-08-18
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

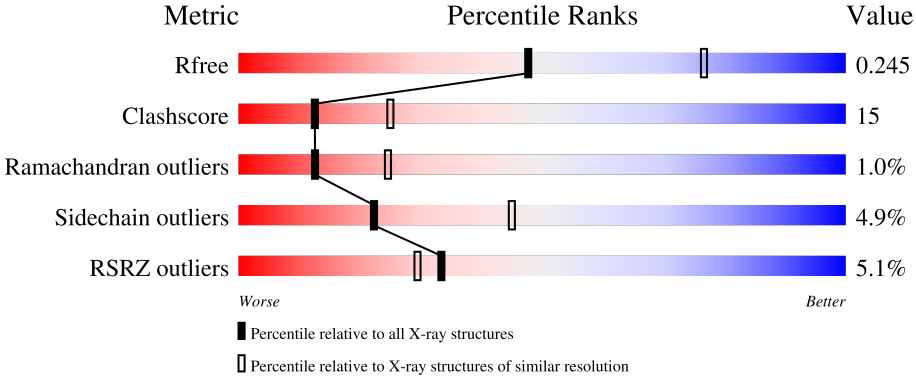
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	431	6% 65% 24% • 6%
2	B	431	3% 64% 26% • 5%

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
4	HEC	A	901	X	-	-	-
4	HEC	B	902	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6703 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, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	403	3168	2019	559	574	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ARG	CYS	SEE REMARK 999	UNP P29473

- Molecule 2 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	As	C	N	O	S			
2	B	409	3205	1	2041	565	582	16	0	0	0

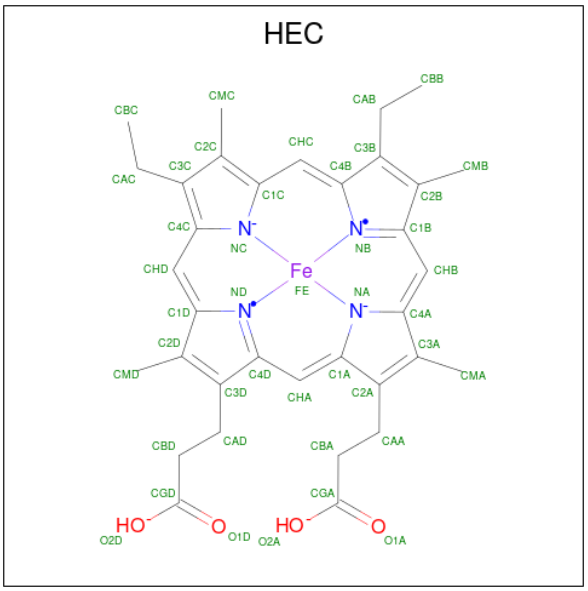
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	97	ARG	CYS	SEE REMARK 999	UNP P29473

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

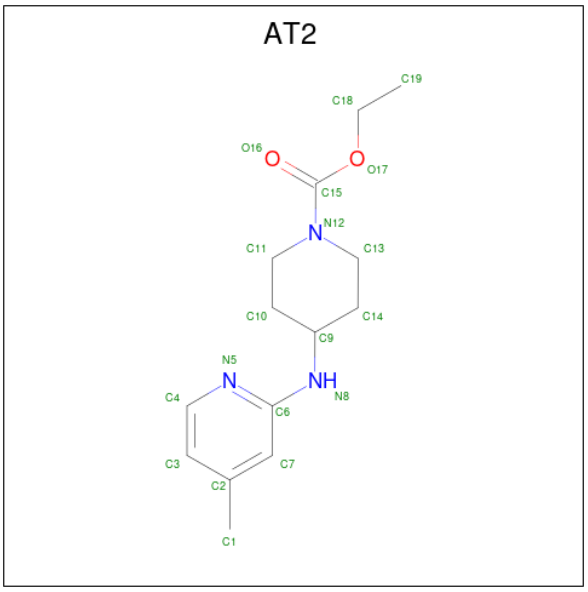
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

- Molecule 4 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 5 is ETHYL 4-[(4-METHYLPYRIDIN-2-YL)AMINO]PIPERIDINE-1-CARBOXYLATE (CCD ID: AT2) (formula: $C_{14}H_{21}N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	19	14	3	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	19	14	3	2	0	0
5	B	1	19	14	3	2	0	0
5	B	1	19	14	3	2	0	0

- Molecule 6 is water.

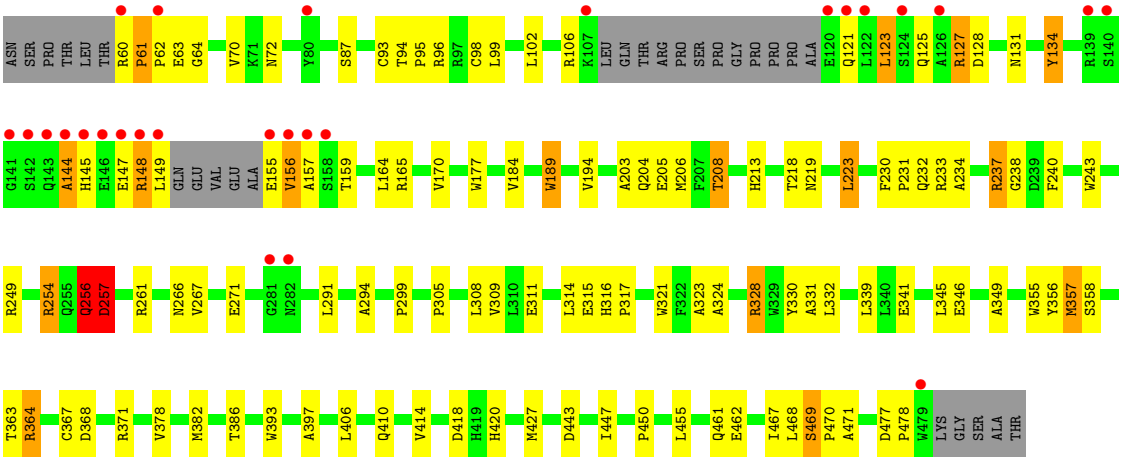
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	74	74	74	0	0
6	B	93	93	93	0	0

3 Residue-property plots (i)

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

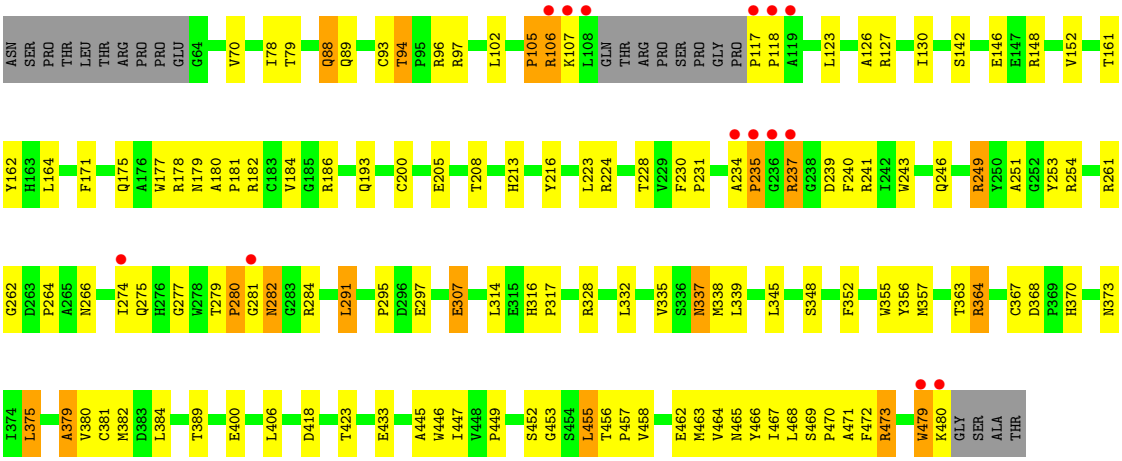
- Molecule 1: Nitric oxide synthase, endothelial

Chain A:



- Molecule 2: Nitric oxide synthase, endothelial

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.93Å 104.37Å 156.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	86.1 (30.00-2.50) 86.0 (30.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.57 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.254 0.203 , 0.245	Depositor DCC
R_{free} test set	1453 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	26.2	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6703	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, ZN, CAS, AT2

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	0.57	0/3258	1.34	31/4444 (0.7%)
2	B	0.57	0/3285	0.99	17/4482 (0.4%)
All	All	0.57	0/6543	1.18	48/8926 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	ARG	CA-C-N	34.68	156.10	120.38
1	A	60	ARG	C-N-CA	34.68	156.10	120.38
1	A	61	PRO	CA-N-CD	-17.80	87.08	112.00
1	A	61	PRO	N-CA-CB	13.18	115.86	103.08
1	A	61	PRO	N-CD-CG	11.27	120.10	103.20
1	A	256	GLN	OE1-CD-NE2	-10.26	112.34	122.60
1	A	60	ARG	C-N-CD	-9.43	86.33	125.00
1	A	127	ARG	N-CA-C	-8.97	102.92	114.04
2	B	107	LYS	N-CA-C	7.95	117.63	108.49
1	A	61	PRO	N-CA-C	7.27	119.58	110.70
2	B	279	THR	CA-C-N	7.21	128.85	119.84
2	B	279	THR	C-N-CA	7.21	128.85	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	256	GLN	CG-CD-NE2	7.11	127.06	116.40
1	A	128	ASP	N-CA-C	-7.10	103.47	111.14
2	B	357	MET	N-CA-C	-7.07	97.21	108.73
2	B	332	LEU	N-CA-C	7.04	121.07	108.47
1	A	64	GLY	CA-C-N	6.95	126.66	119.64
1	A	64	GLY	C-N-CA	6.95	126.66	119.64
1	A	63	GLU	N-CA-C	-6.54	99.80	109.81
1	A	294	ALA	N-CA-C	-6.37	101.82	110.36
2	B	117	PRO	CA-C-N	6.29	127.70	119.84
2	B	117	PRO	C-N-CA	6.29	127.70	119.84
1	A	332	LEU	N-CA-C	6.25	118.55	109.04
1	A	189	TRP	N-CA-C	6.24	119.74	111.75
2	B	449	PRO	CA-C-N	6.15	125.85	119.82
2	B	449	PRO	C-N-CA	6.15	125.85	119.82
2	B	117	PRO	N-CA-CB	6.14	109.76	103.00
1	A	223	LEU	N-CA-C	6.11	118.85	110.24
1	A	356	TYR	N-CA-C	5.93	118.86	110.50
1	A	309	VAL	N-CA-C	5.80	115.60	107.37
1	A	62	PRO	CB-CA-C	5.80	118.65	111.23
2	B	356	TYR	N-CA-C	5.75	118.17	110.35
1	A	156	VAL	N-CA-C	-5.74	103.88	111.05
2	B	455	LEU	N-CA-C	-5.72	106.28	113.20
1	A	254	ARG	N-CA-C	-5.67	102.89	110.55
1	A	257	ASP	N-CA-C	-5.67	98.72	110.80
1	A	165	ARG	N-CA-C	-5.65	102.92	110.55
1	A	477	ASP	CA-C-N	5.53	125.24	119.82
1	A	477	ASP	C-N-CA	5.53	125.24	119.82
2	B	379	ALA	N-CA-C	-5.49	105.40	111.71
2	B	180	ALA	CA-C-N	5.48	125.30	119.28
2	B	180	ALA	C-N-CA	5.48	125.30	119.28
2	B	186	ARG	N-CA-C	5.34	119.28	112.87
1	A	455	LEU	N-CA-C	-5.30	106.59	113.16
1	A	467	ILE	N-CA-C	5.14	115.71	108.36
1	A	256	GLN	CA-C-N	5.01	131.11	121.54
1	A	256	GLN	C-N-CA	5.01	131.11	121.54
2	B	467	ILE	N-CA-C	5.00	115.05	107.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	380	VAL	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3168	0	3048	99	0
2	B	3205	0	3073	104	0
3	A	1	0	0	0	0
4	A	43	0	32	3	0
4	B	43	0	32	1	0
5	A	38	0	42	1	0
5	B	38	0	42	3	0
6	A	74	0	0	2	0
6	B	93	0	0	4	0
All	All	6703	0	6269	196	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 15.

All (196) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:THR:HG22	1:A:96:ARG:H	1.23	1.00
2:B:94:THR:HG23	2:B:96:ARG:H	1.35	0.90
2:B:175:GLN:HE22	2:B:178:ARG:HH11	1.17	0.87
1:A:378:VAL:HG12	1:A:382:MET:CE	2.06	0.85
2:B:123:LEU:HD13	2:B:127:ARG:HH21	1.42	0.84
1:A:131:ASN:HA	1:A:145:HIS:HE1	1.42	0.83
1:A:131:ASN:HA	1:A:145:HIS:CE1	2.13	0.82
1:A:328:ARG:HH11	1:A:328:ARG:HG2	1.47	0.80
2:B:142:SER:O	2:B:146:GLU:HG2	1.82	0.80
2:B:282:ASN:O	2:B:282:ASN:OD1	2.01	0.79
1:A:127:ARG:HG3	1:A:127:ARG:HH11	1.49	0.78
2:B:123:LEU:HD13	2:B:127:ARG:NH2	1.99	0.78
1:A:177:TRP:HB2	4:A:901:HEC:HBC3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:HH11	1:A:328:ARG:CG	1.97	0.77
2:B:94:THR:HG22	2:B:97:ARG:H	1.51	0.76
1:A:134:TYR:CG	1:A:145:HIS:HB2	2.22	0.75
1:A:378:VAL:HG12	1:A:382:MET:HE3	1.69	0.74
1:A:127:ARG:HG3	1:A:127:ARG:NH1	2.01	0.73
1:A:378:VAL:HG12	1:A:382:MET:HE2	1.71	0.72
1:A:131:ASN:OD1	1:A:145:HIS:CE1	2.43	0.72
2:B:105:PRO:O	2:B:106:ARG:CB	2.39	0.71
2:B:456:THR:CG2	2:B:458:VAL:HG22	2.20	0.71
1:A:406:LEU:O	1:A:410:GLN:HG3	1.91	0.70
2:B:205:GLU:O	2:B:208:THR:HG22	1.92	0.69
2:B:261:ARG:NE	2:B:282:ASN:OD1	2.26	0.68
2:B:452:SER:HB3	2:B:455:LEU:HD12	1.75	0.68
2:B:200:CYS:SG	2:B:205:GLU:HB3	2.34	0.67
1:A:328:ARG:HG2	1:A:328:ARG:NH1	2.06	0.67
2:B:423:THR:HG21	2:B:456:THR:HG21	1.76	0.67
2:B:88:GLN:HE21	2:B:88:GLN:HA	1.61	0.66
1:A:234:ALA:HB3	1:A:237:ARG:CD	2.26	0.65
2:B:123:LEU:CD1	2:B:127:ARG:HH21	2.08	0.65
2:B:479:TRP:CD1	2:B:480:LYS:N	2.64	0.65
2:B:249:ARG:HG3	2:B:266:ASN:ND2	2.12	0.64
2:B:314:LEU:HG	2:B:328:ARG:HA	1.81	0.62
1:A:256:GLN:O	1:A:256:GLN:HG3	1.99	0.62
2:B:274:ILE:CD1	2:B:280:PRO:HG3	2.29	0.62
1:A:427:MET:HE1	1:A:461:GLN:HE21	1.65	0.62
1:A:311:GLU:OE1	1:A:328:ARG:HD2	2.02	0.60
2:B:246:GLN:HB2	2:B:249:ARG:CD	2.32	0.60
2:B:123:LEU:HB3	2:B:127:ARG:HH21	1.65	0.60
2:B:246:GLN:HB2	2:B:249:ARG:HD2	1.84	0.59
1:A:364:ARG:CZ	5:A:905:AT2:H101	2.32	0.59
1:A:121:GLN:O	1:A:125:GLN:HG3	2.03	0.59
2:B:274:ILE:HD11	2:B:280:PRO:HG3	1.84	0.58
1:A:386:THR:HA	1:A:393:TRP:CD1	2.38	0.58
2:B:456:THR:HG21	2:B:458:VAL:HG22	1.83	0.58
2:B:94:THR:CG2	2:B:96:ARG:H	2.12	0.58
2:B:447:ILE:HG21	2:B:463:MET:HE1	1.85	0.58
1:A:378:VAL:CG1	1:A:382:MET:HE2	2.33	0.57
1:A:230:PHE:HB3	1:A:231:PRO:CD	2.34	0.57
1:A:123:LEU:HD23	1:A:156:VAL:HG11	1.86	0.57
1:A:93:CYS:HB3	2:B:93:CYS:HB3	1.85	0.57
1:A:382:MET:HE1	1:A:397:ALA:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:VAL:HG11	1:A:357:MET:HE3	1.87	0.56
1:A:363:THR:O	1:A:367:CYS:HB2	2.06	0.56
2:B:253:TYR:CE2	2:B:281:GLY:O	2.59	0.56
1:A:328:ARG:HH11	1:A:328:ARG:CB	2.19	0.56
2:B:253:TYR:CZ	2:B:281:GLY:O	2.59	0.56
2:B:307:GLU:H	2:B:307:GLU:CD	2.12	0.55
2:B:456:THR:HG22	2:B:458:VAL:HG22	1.88	0.55
2:B:274:ILE:HG12	2:B:280:PRO:HG3	1.88	0.55
1:A:134:TYR:CD2	1:A:145:HIS:HB2	2.41	0.55
1:A:314:LEU:HG	1:A:328:ARG:HA	1.89	0.55
2:B:295:PRO:O	2:B:297:GLU:HG3	2.07	0.55
1:A:144:ALA:O	1:A:147:GLU:N	2.40	0.54
2:B:453:GLY:O	2:B:456:THR:HB	2.07	0.54
2:B:456:THR:HG22	2:B:458:VAL:H	1.73	0.54
2:B:249:ARG:HG3	2:B:266:ASN:HD21	1.70	0.54
2:B:237:ARG:HH21	2:B:240:PHE:HE1	1.56	0.54
1:A:315:GLU:HB3	1:A:323:ALA:HB2	1.91	0.53
1:A:328:ARG:HH11	1:A:328:ARG:HB3	1.73	0.53
1:A:170:VAL:HG22	1:A:194:VAL:HB	1.90	0.53
1:A:94:THR:HG23	1:A:95:PRO:HD2	1.92	0.52
1:A:468:LEU:O	1:A:471:ALA:HB2	2.09	0.52
1:A:249:ARG:HG3	6:A:969:HOH:O	2.09	0.52
2:B:123:LEU:O	2:B:127:ARG:HG3	2.10	0.52
1:A:230:PHE:HB3	1:A:231:PRO:HD2	1.92	0.52
1:A:469:SER:HA	1:A:470:PRO:C	2.35	0.52
2:B:363:THR:O	2:B:367:CYS:HB2	2.10	0.51
2:B:364:ARG:HH11	2:B:364:ARG:HB3	1.74	0.51
2:B:379:ALA:HA	2:B:384:LEU:HD12	1.93	0.51
2:B:282:ASN:O	2:B:282:ASN:CG	2.54	0.50
2:B:213:HIS:HD2	2:B:228:THR:OG1	1.95	0.50
2:B:274:ILE:CG1	2:B:280:PRO:HG3	2.42	0.50
1:A:72:ASN:HD22	1:A:461:GLN:NE2	2.10	0.50
1:A:233:ARG:HG3	1:A:346:GLU:O	2.10	0.50
1:A:102:LEU:HD22	2:B:462:GLU:OE2	2.11	0.50
1:A:131:ASN:OD1	1:A:145:HIS:HE1	1.95	0.49
1:A:243:TRP:HB2	1:A:291:LEU:HB3	1.94	0.49
1:A:243:TRP:CD1	1:A:478:PRO:HG3	2.47	0.49
1:A:331:ALA:HB1	1:A:414:VAL:HG11	1.94	0.49
2:B:406:LEU:HD21	2:B:418:ASP:HB3	1.95	0.49
2:B:423:THR:HG21	2:B:456:THR:CG2	2.41	0.49
1:A:316:HIS:CG	1:A:317:PRO:HD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ALA:HB3	1:A:237:ARG:HD3	1.94	0.48
1:A:131:ASN:CA	1:A:145:HIS:HE1	2.20	0.48
2:B:335:VAL:HB	2:B:352:PHE:CE1	2.48	0.48
2:B:382:MET:HE3	2:B:400:GLU:HG3	1.95	0.48
1:A:99:LEU:CD2	2:B:464:VAL:HG22	2.43	0.48
2:B:464:VAL:HG12	2:B:466:TYR:CD1	2.49	0.48
1:A:177:TRP:CE3	1:A:189:TRP:HA	2.48	0.48
1:A:123:LEU:HD13	1:A:123:LEU:O	2.14	0.48
2:B:230:PHE:HB3	2:B:231:PRO:CD	2.43	0.48
1:A:144:ALA:O	1:A:145:HIS:C	2.57	0.47
2:B:241:ARG:HD3	2:B:348:SER:HB2	1.96	0.47
1:A:177:TRP:CZ3	1:A:189:TRP:HA	2.49	0.47
2:B:367:CYS:SG	2:B:375:LEU:HD13	2.54	0.47
1:A:231:PRO:HB2	1:A:240:PHE:CE1	2.49	0.47
2:B:182:ARG:HD3	2:B:446:TRP:CD2	2.49	0.47
1:A:378:VAL:CG1	1:A:382:MET:CE	2.87	0.47
2:B:175:GLN:HE22	2:B:178:ARG:NH1	1.98	0.47
2:B:177:TRP:HB2	4:B:902:HEC:HBC3	1.97	0.47
1:A:230:PHE:HB2	1:A:349:ALA:O	2.14	0.46
1:A:218:THR:HA	1:A:223:LEU:HD22	1.95	0.46
1:A:420:HIS:HB2	2:B:389:THR:HB	1.96	0.46
1:A:237:ARG:HG2	1:A:238:GLY:N	2.30	0.46
2:B:184:VAL:HG22	2:B:184:VAL:O	2.15	0.46
1:A:164:LEU:HG	1:A:345:LEU:HD12	1.98	0.46
2:B:445:ALA:O	5:B:907:AT2:H3	2.16	0.46
1:A:123:LEU:CD1	1:A:127:ARG:HH11	2.29	0.46
1:A:131:ASN:OD1	1:A:145:HIS:NE2	2.49	0.46
2:B:223:LEU:HD12	2:B:355:TRP:HB3	1.97	0.46
1:A:155:GLU:O	1:A:159:THR:OG1	2.31	0.45
2:B:70:VAL:HG23	6:B:936:HOH:O	2.16	0.45
1:A:378:VAL:O	1:A:382:MET:HG3	2.16	0.45
2:B:243:TRP:HB2	2:B:291:LEU:HB3	1.99	0.45
2:B:469:SER:HA	2:B:470:PRO:C	2.40	0.45
1:A:134:TYR:HB2	1:A:145:HIS:ND1	2.32	0.45
1:A:418:ASP:OD1	1:A:420:HIS:HB2	2.16	0.45
2:B:364:ARG:HH22	5:B:907:AT2:H102	1.82	0.45
1:A:291:LEU:HG	1:A:299:PRO:HB2	2.00	0.44
2:B:94:THR:HG22	2:B:97:ARG:N	2.27	0.44
1:A:177:TRP:CB	4:A:901:HEC:HBC3	2.44	0.44
2:B:423:THR:CB	2:B:456:THR:HG23	2.47	0.44
1:A:256:GLN:O	1:A:257:ASP:OD1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:TRP:H	4:A:901:HEC:HAB	1.82	0.44
1:A:249:ARG:HG3	1:A:266:ASN:HD21	1.83	0.44
1:A:123:LEU:CD1	1:A:127:ARG:NH1	2.81	0.44
1:A:148:ARG:O	1:A:149:LEU:C	2.60	0.43
1:A:339:LEU:HD23	1:A:339:LEU:C	2.44	0.43
2:B:464:VAL:HG12	2:B:466:TYR:HD1	1.83	0.43
1:A:341:GLU:OE1	1:A:469:SER:OG	2.37	0.43
1:A:368:ASP:HB3	1:A:371:ARG:HG2	2.00	0.43
1:A:386:THR:HG22	1:A:393:TRP:CD2	2.54	0.43
1:A:443:ASP:O	1:A:447:ILE:HG12	2.19	0.43
1:A:321:TRP:O	1:A:324:ALA:HB3	2.18	0.43
2:B:213:HIS:CD2	2:B:228:THR:OG1	2.71	0.43
1:A:311:GLU:HA	1:A:330:TYR:HA	2.01	0.43
1:A:462:GLU:HB3	2:B:102:LEU:HD23	1.99	0.43
2:B:161:THR:HG23	2:B:162:TYR:N	2.32	0.43
1:A:218:THR:O	1:A:219:ASN:C	2.60	0.43
1:A:98:CYS:HB2	2:B:93:CYS:SG	2.58	0.43
1:A:213:HIS:CD2	1:A:213:HIS:C	2.97	0.43
1:A:123:LEU:HD12	1:A:127:ARG:NH1	2.34	0.42
2:B:223:LEU:HD12	2:B:355:TRP:CB	2.49	0.42
2:B:456:THR:HG23	2:B:457:PRO:HD2	2.01	0.42
2:B:479:TRP:CD1	2:B:480:LYS:H	2.36	0.42
1:A:87:SER:O	2:B:96:ARG:NH2	2.52	0.42
2:B:70:VAL:HG23	2:B:70:VAL:O	2.19	0.42
1:A:203:ALA:HA	1:A:206:MET:CE	2.49	0.42
2:B:373:ASN:HA	6:B:948:HOH:O	2.18	0.42
2:B:433:GLU:HA	2:B:433:GLU:OE1	2.20	0.42
2:B:179:ASN:O	2:B:181:PRO:HD3	2.19	0.42
2:B:193:GLN:HG2	2:B:216:TYR:CZ	2.55	0.42
1:A:267:VAL:O	1:A:271:GLU:HG3	2.20	0.42
2:B:126:ALA:O	2:B:130:ILE:HG12	2.19	0.42
2:B:472:PHE:C	2:B:473:ARG:HG3	2.45	0.42
1:A:256:GLN:O	1:A:257:ASP:CG	2.62	0.42
2:B:171:PHE:CZ	2:B:175:GLN:HG3	2.55	0.42
2:B:316:HIS:CG	2:B:317:PRO:HD2	2.55	0.42
1:A:106:ARG:HD3	6:B:960:HOH:O	2.19	0.42
1:A:450:PRO:HD3	6:A:914:HOH:O	2.19	0.42
2:B:251:ALA:O	2:B:262:GLY:HA3	2.20	0.42
2:B:364:ARG:HA	2:B:368:ASP:OD1	2.20	0.42
1:A:231:PRO:HB2	1:A:240:PHE:CD1	2.55	0.41
2:B:275:GLN:C	2:B:277:GLY:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:GLN:HB2	2:B:249:ARG:HD3	2.01	0.41
2:B:261:ARG:HA	6:B:950:HOH:O	2.19	0.41
1:A:204:GLN:O	1:A:208:THR:HG22	2.20	0.41
2:B:96:ARG:HB3	2:B:96:ARG:NH1	2.35	0.41
2:B:337:ASN:HD22	2:B:338:MET:N	2.17	0.41
1:A:357:MET:O	1:A:358:SER:C	2.63	0.41
2:B:264:PRO:HB2	2:B:370:HIS:O	2.20	0.41
2:B:261:ARG:NH1	2:B:284:ARG:HG3	2.35	0.41
2:B:337:ASN:HD22	2:B:337:ASN:C	2.28	0.41
2:B:164:LEU:HG	2:B:345:LEU:HD12	2.02	0.41
2:B:241:ARG:HA	2:B:241:ARG:HD2	1.87	0.41
2:B:468:LEU:O	2:B:471:ALA:HB2	2.21	0.41
2:B:78:ILE:HG22	2:B:79:THR:N	2.34	0.41
1:A:305:PRO:HD2	1:A:308:LEU:HD12	2.04	0.40
2:B:364:ARG:HH22	5:B:907:AT2:C10	2.34	0.40
2:B:339:LEU:C	2:B:339:LEU:HD23	2.46	0.40
1:A:205:GLU:O	1:A:208:THR:HG23	2.21	0.40
2:B:148:ARG:O	2:B:152:VAL:HG23	2.22	0.40
2:B:234:ALA:O	2:B:235:PRO:C	2.63	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	397/431 (92%)	363 (91%)	29 (7%)	5 (1%)	9 18
2	B	404/431 (94%)	370 (92%)	31 (8%)	3 (1%)	18 34
All	All	801/862 (93%)	733 (92%)	60 (8%)	8 (1%)	12 24

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	PRO
1	A	256	GLN
1	A	257	ASP
2	B	106	ARG
2	B	280	PRO
2	B	479	TRP
1	A	144	ALA
1	A	157	ALA

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	333/367 (91%)	319 (96%)	14 (4%)	26	52
2	B	334/366 (91%)	315 (94%)	19 (6%)	18	39
All	All	667/733 (91%)	634 (95%)	33 (5%)	22	45

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	VAL
1	A	123	LEU
1	A	148	ARG
1	A	208	THR
1	A	232	GLN
1	A	237	ARG
1	A	254	ARG
1	A	256	GLN
1	A	257	ASP
1	A	261	ARG
1	A	328	ARG
1	A	357	MET
1	A	364	ARG
1	A	469	SER
2	B	88	GLN
2	B	89	GLN

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Mol	Chain	Res	Type
2	B	94	THR
2	B	105	PRO
2	B	118	PRO
2	B	224	ARG
2	B	235	PRO
2	B	237	ARG
2	B	239	ASP
2	B	249	ARG
2	B	254	ARG
2	B	282	ASN
2	B	291	LEU
2	B	307	GLU
2	B	337	ASN
2	B	364	ARG
2	B	375	LEU
2	B	465	ASN
2	B	473	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	GLN
1	A	293	GLN
1	A	434	GLN
1	A	461	GLN
1	A	465	ASN
2	B	86	GLN
2	B	88	GLN
2	B	125	GLN
2	B	175	GLN
2	B	193	GLN
2	B	204	GLN
2	B	213	HIS
2	B	232	GLN
2	B	337	ASN
2	B	402	ASN
2	B	461	GLN
2	B	465	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CAS	B	381	-	5,8,9	1.92	1 (20%)	1,9,11	0.47	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
2	CAS	B	381	-	-	0/0/7/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	381	CAS	O-C	3.88	1.34	1.20

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	AT2	A	905	-	20,20,20	3.59	11 (55%)	25,26,26	3.16	13 (52%)
5	AT2	B	907	-	20,20,20	3.47	11 (55%)	25,26,26	3.12	15 (60%)
5	AT2	A	904	-	20,20,20	2.98	10 (50%)	25,26,26	3.16	14 (56%)
4	HEC	B	902	2	50,50,50	2.09	13 (26%)	68,82,82	1.46	9 (13%)
5	AT2	B	906	-	20,20,20	3.01	8 (40%)	25,26,26	2.69	14 (56%)
4	HEC	A	901	1	50,50,50	1.91	14 (28%)	68,82,82	1.41	7 (10%)

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	AT2	A	905	-	-	1/11/21/21	0/2/2/2
5	AT2	B	907	-	-	1/11/21/21	0/2/2/2
5	AT2	A	904	-	-	0/11/21/21	0/2/2/2
4	HEC	B	902	2	1/1/3/7	8/14/54/54	-
5	AT2	B	906	-	-	0/11/21/21	0/2/2/2
4	HEC	A	901	1	1/1/3/7	8/14/54/54	-

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	905	AT2	C4-N5	7.80	1.50	1.34
5	B	907	AT2	C11-N12	6.28	1.58	1.47
5	B	907	AT2	C13-N12	6.18	1.58	1.47
5	A	904	AT2	C3-C4	6.15	1.50	1.38
5	B	906	AT2	O16-C15	5.82	1.29	1.21
5	B	906	AT2	C3-C4	5.80	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	905	AT2	C6-N5	5.79	1.44	1.34
5	A	905	AT2	O16-C15	5.76	1.29	1.21
5	B	907	AT2	C3-C4	5.57	1.49	1.38
5	B	907	AT2	C6-N5	5.53	1.44	1.34
5	A	905	AT2	C11-N12	5.52	1.56	1.47
5	A	904	AT2	C4-N5	5.51	1.46	1.34
5	A	905	AT2	C3-C4	5.33	1.48	1.38
5	B	907	AT2	O16-C15	5.25	1.28	1.21
5	B	906	AT2	C4-N5	5.22	1.45	1.34
5	B	907	AT2	C4-N5	5.21	1.45	1.34
5	A	904	AT2	C6-N5	5.14	1.43	1.34
4	B	902	HEC	CMA-C3A	5.11	1.61	1.50
4	B	902	HEC	CMC-C2C	4.85	1.60	1.50
4	A	901	HEC	CMA-C3A	4.81	1.60	1.50
4	B	902	HEC	CMB-C2B	4.77	1.60	1.50
4	A	901	HEC	FE-ND	4.57	2.09	1.94
5	A	904	AT2	C13-N12	4.37	1.54	1.47
5	B	906	AT2	C10-C9	4.36	1.62	1.52
5	A	905	AT2	C7-C6	4.23	1.50	1.39
5	B	906	AT2	C6-N5	4.22	1.41	1.34
4	B	902	HEC	FE-ND	4.20	2.07	1.94
4	A	901	HEC	CAB-C3B	4.13	1.61	1.51
5	B	906	AT2	C7-C6	4.12	1.50	1.39
5	B	907	AT2	C7-C6	3.86	1.49	1.39
4	B	902	HEC	CMD-C2D	3.85	1.58	1.50
4	B	902	HEC	FE-NA	3.74	2.07	1.95
5	A	905	AT2	C10-C9	3.60	1.60	1.52
5	A	904	AT2	C10-C11	3.54	1.62	1.52
4	B	902	HEC	C1A-C2A	3.51	1.51	1.45
5	A	905	AT2	C10-C11	3.50	1.61	1.52
5	B	906	AT2	C13-N12	3.48	1.53	1.47
5	A	904	AT2	O16-C15	3.43	1.26	1.21
5	A	904	AT2	C11-N12	3.34	1.53	1.47
4	A	901	HEC	CMB-C2B	3.32	1.57	1.50
4	A	901	HEC	FE-NC	3.16	2.05	1.95
4	A	901	HEC	CMC-C2C	3.11	1.57	1.50
5	B	906	AT2	C11-N12	3.09	1.52	1.47
5	A	905	AT2	C14-C9	3.07	1.59	1.52
5	A	904	AT2	C7-C6	3.01	1.47	1.39
4	B	902	HEC	CAB-C3B	3.00	1.58	1.51
4	B	902	HEC	C1C-NC	-2.91	1.34	1.39
4	A	901	HEC	C1A-C2A	2.79	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	907	AT2	C3-C2	2.77	1.45	1.38
5	A	904	AT2	C10-C9	2.77	1.58	1.52
4	B	902	HEC	CHA-C4D	2.66	1.45	1.39
5	A	905	AT2	C14-C13	-2.66	1.45	1.52
4	B	902	HEC	C1C-C2C	2.61	1.49	1.43
5	B	907	AT2	C14-C9	2.61	1.58	1.52
4	A	901	HEC	CHA-C4D	2.44	1.44	1.39
4	A	901	HEC	CAC-C3C	2.43	1.57	1.51
5	B	907	AT2	C10-C9	2.36	1.57	1.52
5	B	907	AT2	C10-C11	2.33	1.58	1.52
4	A	901	HEC	C4C-C3C	2.26	1.49	1.44
4	A	901	HEC	CHB-C1B	2.24	1.44	1.39
4	A	901	HEC	CMD-C2D	2.19	1.55	1.50
4	A	901	HEC	C4D-C3D	2.19	1.48	1.45
4	B	902	HEC	C1B-C2B	-2.05	1.40	1.44
4	A	901	HEC	CAD-C3D	2.04	1.56	1.51
5	A	904	AT2	C14-C9	2.02	1.56	1.52
5	A	905	AT2	C3-C2	2.01	1.43	1.38
4	B	902	HEC	O2A-CGA	-2.00	1.24	1.30

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	907	AT2	C10-C9-N8	7.21	122.39	110.77
5	A	904	AT2	C3-C4-N5	-6.37	116.17	123.97
5	B	907	AT2	C3-C4-N5	-6.19	116.39	123.97
5	A	905	AT2	C3-C4-N5	-6.06	116.55	123.97
5	A	904	AT2	C11-C10-C9	-6.02	101.16	110.67
5	A	905	AT2	C7-C6-N5	-5.99	115.07	122.92
5	A	905	AT2	C7-C6-N8	5.36	133.67	122.07
4	A	901	HEC	CBC-CAC-C3C	5.16	126.42	112.42
5	A	904	AT2	C10-C9-N8	-5.06	102.62	110.77
5	B	907	AT2	C11-C10-C9	-4.99	102.80	110.67
4	B	902	HEC	CBC-CAC-C3C	4.96	125.86	112.42
5	B	906	AT2	C7-C6-N5	-4.92	116.46	122.92
5	B	906	AT2	C3-C4-N5	-4.83	118.05	123.97
5	A	905	AT2	C4-N5-C6	4.81	124.08	117.21
5	A	905	AT2	C14-C9-N8	4.70	118.35	110.77
5	A	904	AT2	C4-N5-C6	4.66	123.87	117.21
5	B	906	AT2	C4-N5-C6	4.56	123.73	117.21
5	A	905	AT2	C18-O17-C15	4.50	123.96	115.66
5	A	904	AT2	C1-C2-C7	-4.36	115.02	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	905	AT2	C3-C2-C7	4.24	124.22	117.96
5	B	907	AT2	C13-N12-C11	4.19	121.24	112.68
5	B	906	AT2	C14-C9-C10	4.16	117.99	110.80
5	A	904	AT2	C7-C6-N5	-4.15	117.47	122.92
4	B	902	HEC	CBB-CAB-C3B	3.97	123.18	112.42
4	A	901	HEC	CBB-CAB-C3B	3.96	123.17	112.42
5	B	907	AT2	C4-N5-C6	3.91	122.80	117.21
5	A	905	AT2	C1-C2-C7	-3.87	115.68	120.92
5	A	904	AT2	C7-C6-N8	3.66	129.97	122.07
5	B	906	AT2	C18-O17-C15	3.65	122.38	115.66
5	B	906	AT2	C1-C2-C7	-3.60	116.05	120.92
5	B	907	AT2	C1-C2-C7	-3.56	116.11	120.92
5	A	904	AT2	C3-C2-C7	3.54	123.19	117.96
5	A	904	AT2	C14-C9-N8	3.53	116.46	110.77
5	A	905	AT2	N8-C6-N5	-3.48	111.20	116.85
4	B	902	HEC	CMD-C2D-C1D	3.45	130.42	125.03
5	A	905	AT2	C2-C7-C6	3.39	121.67	119.14
5	B	906	AT2	C14-C9-N8	3.33	116.14	110.77
5	B	907	AT2	C7-C6-N5	-3.30	118.59	122.92
5	A	904	AT2	O16-C15-N12	-3.26	118.28	124.30
5	B	907	AT2	O16-C15-N12	-3.17	118.43	124.30
5	A	904	AT2	O17-C15-N12	3.17	117.30	111.77
5	B	907	AT2	O17-C15-N12	3.11	117.19	111.77
4	A	901	HEC	C2B-C1B-NB	3.08	113.47	109.90
4	B	902	HEC	C2B-C1B-NB	3.05	113.43	109.90
4	B	902	HEC	C1D-C2D-C3D	-3.01	103.81	106.98
5	B	907	AT2	C3-C2-C7	2.95	122.31	117.96
5	B	906	AT2	C3-C2-C7	2.94	122.30	117.96
5	B	907	AT2	C7-C6-N8	2.93	128.40	122.07
5	B	907	AT2	C14-C9-C10	-2.92	105.75	110.80
5	A	904	AT2	C18-O17-C15	2.81	120.84	115.66
5	A	905	AT2	O17-C15-N12	2.78	116.63	111.77
5	A	904	AT2	N8-C6-N5	-2.66	112.54	116.85
5	B	906	AT2	C13-C14-C9	2.65	114.86	110.67
4	A	901	HEC	CMD-C2D-C1D	2.57	129.05	125.03
5	A	905	AT2	O16-C15-N12	-2.56	119.57	124.30
4	A	901	HEC	C2D-C1D-ND	2.53	112.75	109.84
5	B	906	AT2	C10-C9-N8	-2.51	106.74	110.77
5	A	904	AT2	C13-C14-C9	-2.49	106.75	110.67
5	B	906	AT2	O16-C15-N12	-2.47	119.72	124.30
5	B	906	AT2	C2-C7-C6	2.46	120.98	119.14
4	A	901	HEC	C1D-C2D-C3D	-2.42	104.43	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	907	AT2	N8-C6-N5	-2.37	113.00	116.85
5	B	906	AT2	C7-C6-N8	2.37	127.19	122.07
5	B	907	AT2	C10-C11-N12	2.37	115.30	110.66
4	B	902	HEC	C2D-C1D-ND	2.35	112.54	109.84
5	B	906	AT2	C10-C11-N12	-2.34	106.08	110.66
5	B	907	AT2	C18-O17-C15	2.24	119.80	115.66
4	B	902	HEC	O2D-CGD-CBD	2.24	121.06	114.00
5	A	905	AT2	C13-C14-C9	2.15	114.06	110.67
4	B	902	HEC	CHB-C1B-C2B	-2.11	121.69	125.03
4	A	901	HEC	O2D-CGD-CBD	2.10	120.65	114.00
4	B	902	HEC	O1D-CGD-CBD	-2.07	116.51	123.09

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	901	HEC	NA
4	B	902	HEC	NA

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	HEC	C2C-C3C-CAC-CBC
5	A	905	AT2	C14-C9-N8-C6
5	B	907	AT2	C14-C9-N8-C6
4	B	902	HEC	C2C-C3C-CAC-CBC
4	A	901	HEC	C4C-C3C-CAC-CBC
4	B	902	HEC	C4C-C3C-CAC-CBC
4	B	902	HEC	C2B-C3B-CAB-CBB
4	A	901	HEC	C2B-C3B-CAB-CBB
4	B	902	HEC	C4B-C3B-CAB-CBB
4	A	901	HEC	C4B-C3B-CAB-CBB
4	A	901	HEC	CAD-CBD-CGD-O1D
4	A	901	HEC	CAD-CBD-CGD-O2D
4	B	902	HEC	CAD-CBD-CGD-O2D
4	A	901	HEC	CAA-CBA-CGA-O1A
4	B	902	HEC	CAD-CBD-CGD-O1D
4	B	902	HEC	CAA-CBA-CGA-O1A
4	B	902	HEC	CAA-CBA-CGA-O2A
4	A	901	HEC	CAA-CBA-CGA-O2A

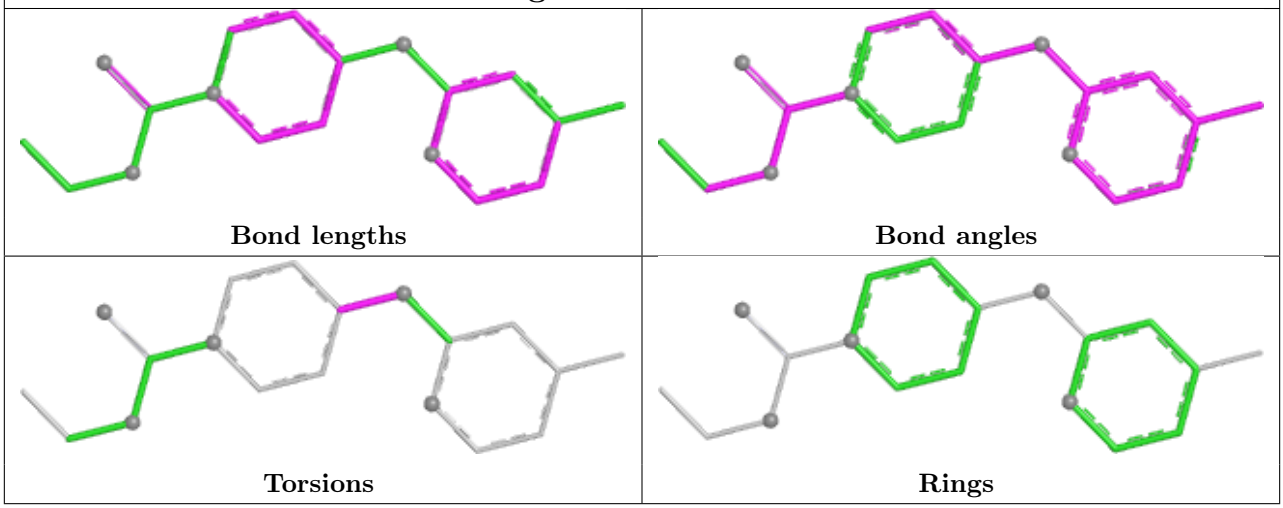
There are no ring outliers.

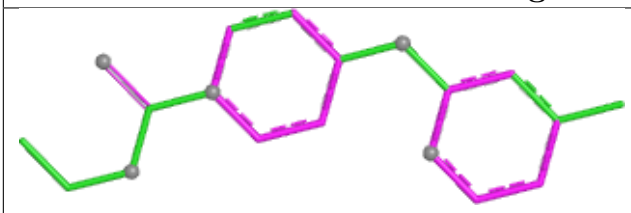
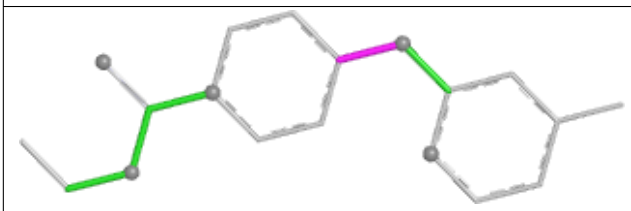
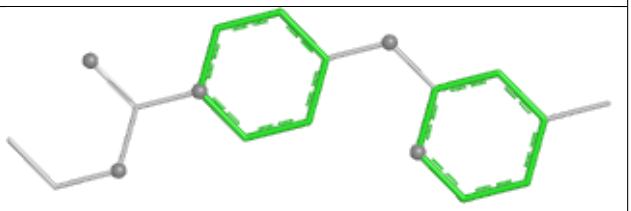
4 monomers are involved in 8 short contacts:

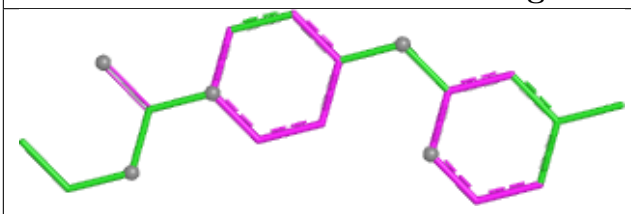
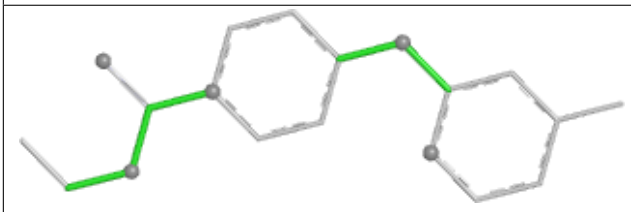
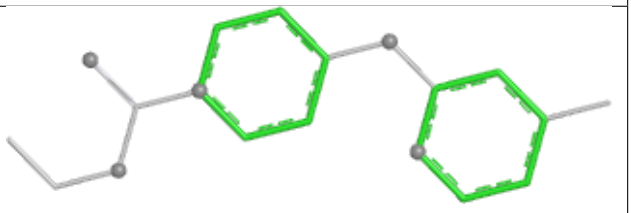
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	905	AT2	1	0
5	B	907	AT2	3	0
4	B	902	HEC	1	0
4	A	901	HEC	3	0

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

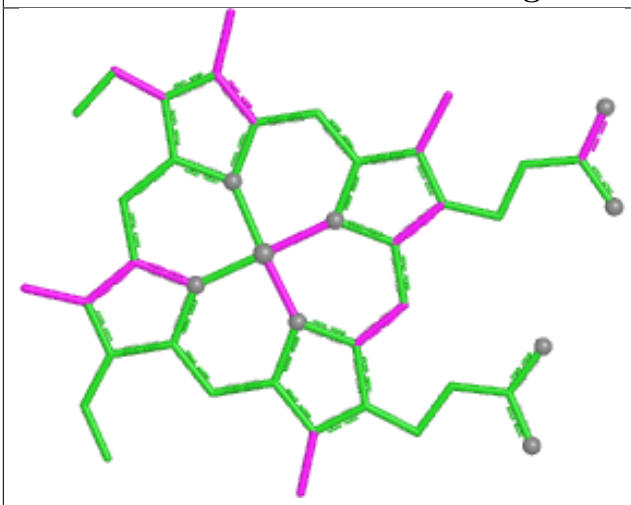
Ligand AT2 A 905



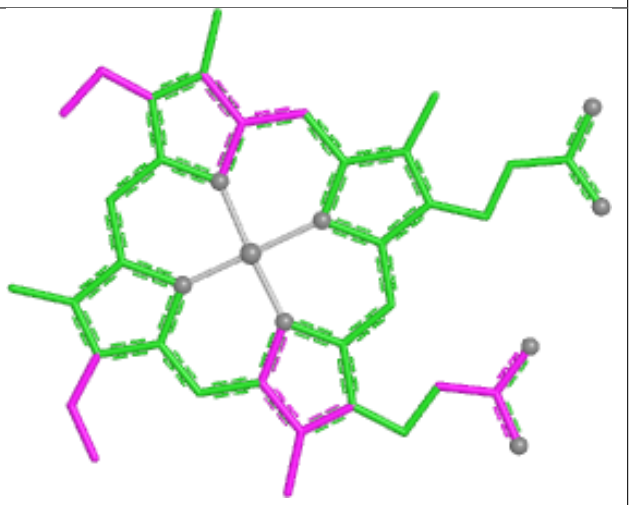
Ligand AT2 B 907	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand AT2 A 904	
 Bond lengths	Bond angles
 Torsions	 Rings

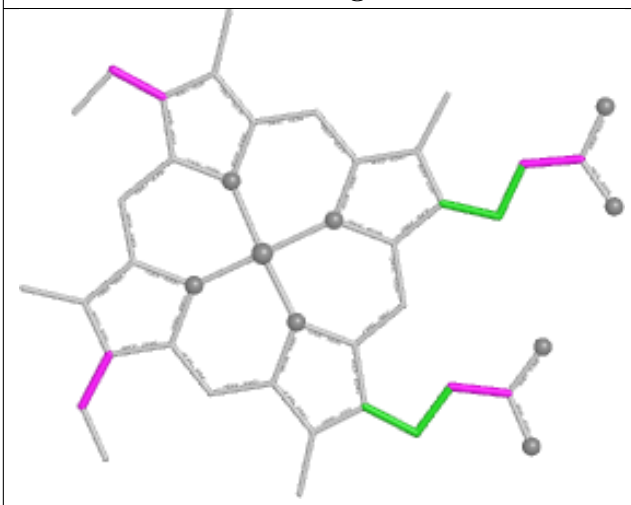
Ligand HEC B 902



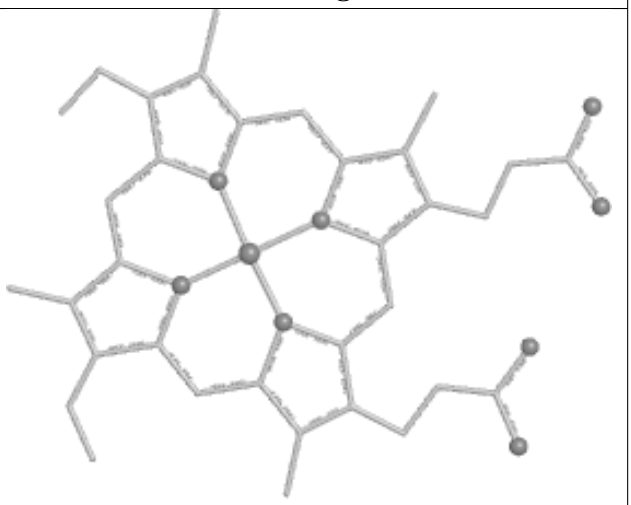
Bond lengths



Bond angles

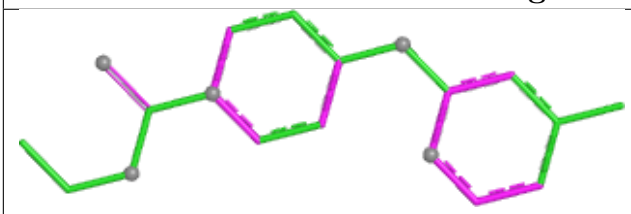


Torsions



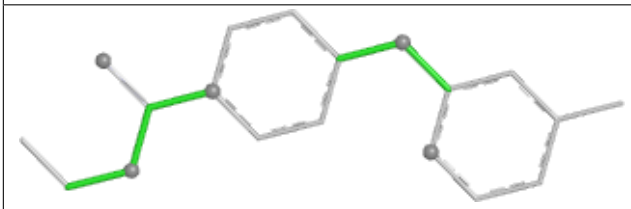
Rings

Ligand AT2 B 906

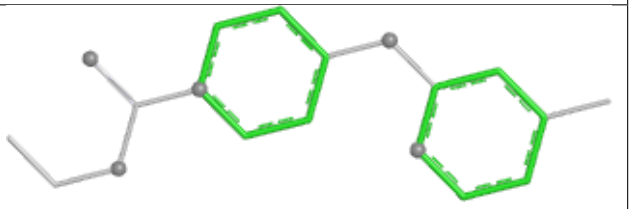


Bond lengths

Bond angles

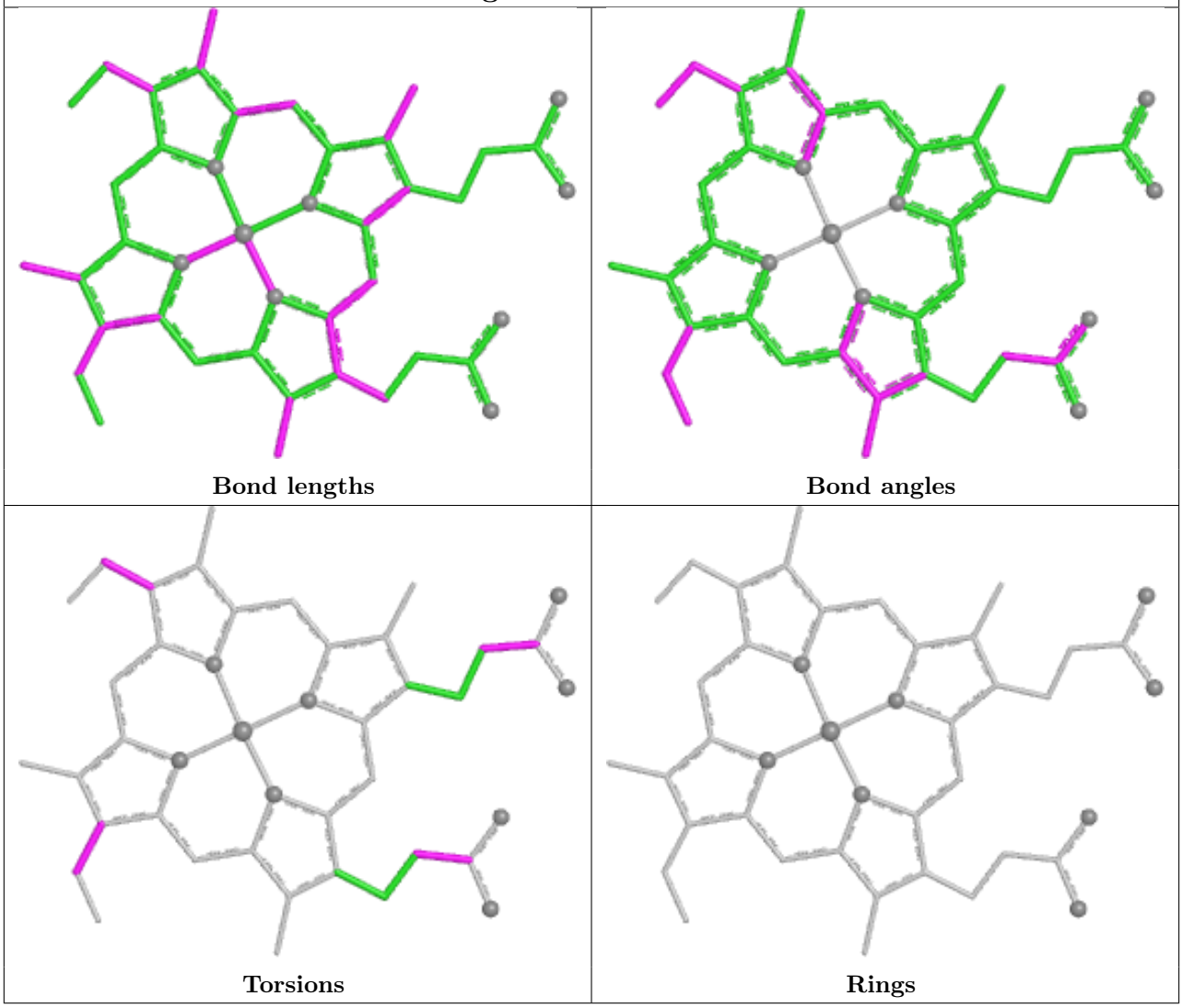


Torsions



Rings

Ligand HEC A 901



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	380:VAL	C	381:CAS	N	1.11
1	B	381:CAS	C	382:MET	N	0.91

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	403/431 (93%)	0.06	27 (6%)	24	21	9, 26, 61, 78	0
2	B	408/431 (94%)	-0.03	14 (3%)	48	43	11, 24, 51, 83	0
All	All	811/862 (94%)	0.02	41 (5%)	33	29	9, 25, 57, 83	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	118	PRO	6.0
1	A	126	ALA	5.0
1	A	149	LEU	4.7
2	B	108	LEU	4.5
2	B	119	ALA	4.3
2	B	117	PRO	4.2
1	A	120	GLU	4.0
2	B	480	LYS	3.9
1	A	144	ALA	3.9
2	B	281	GLY	3.8
1	A	147	GLU	3.7
2	B	235	PRO	3.7
1	A	156	VAL	3.3
1	A	146	GLU	3.2
1	A	141	GLY	3.2
1	A	155	GLU	3.1
1	A	148	ARG	3.0
1	A	60	ARG	2.9
1	A	145	HIS	2.9
1	A	143	GLN	2.9
2	B	236	GLY	2.9
2	B	106	ARG	2.8
1	A	139	ARG	2.8
1	A	121	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	282	ASN	2.6
1	A	62	PRO	2.5
1	A	124	SER	2.5
1	A	142	SER	2.5
2	B	107	LYS	2.4
1	A	122	LEU	2.4
2	B	234	ALA	2.4
1	A	140	SER	2.3
1	A	157	ALA	2.3
1	A	80	TYR	2.3
1	A	281	GLY	2.2
1	A	158	SER	2.2
2	B	274	ILE	2.2
1	A	107	LYS	2.2
2	B	237	ARG	2.2
1	A	479	TRP	2.1
2	B	479	TRP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CAS	B	381	9/10	0.91	0.15	28,30,42,46	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

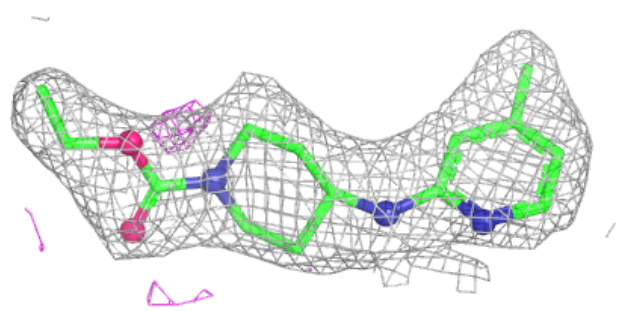
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

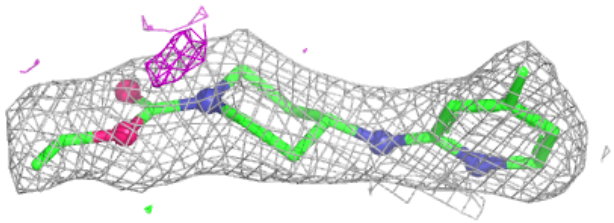
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	AT2	A	904	19/19	0.92	0.09	16,21,26,26	0
5	AT2	B	906	19/19	0.92	0.12	15,28,40,42	0
5	AT2	A	905	19/19	0.93	0.09	15,28,36,36	0
5	AT2	B	907	19/19	0.93	0.12	23,34,40,42	0
4	HEC	A	901	43/43	0.97	0.07	13,17,30,32	0
4	HEC	B	902	43/43	0.97	0.07	9,16,31,37	0
3	ZN	A	903	1/1	1.00	0.02	18,18,18,18	0

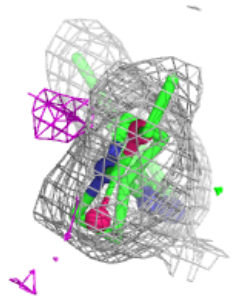
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AT2 A 904:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

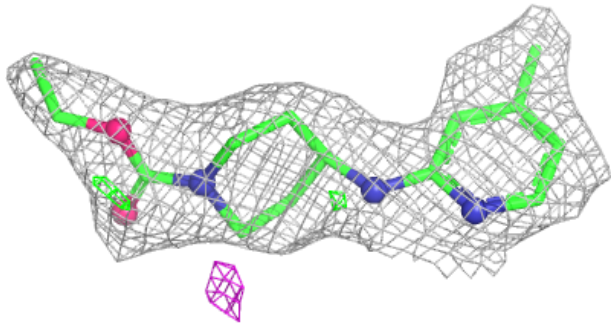


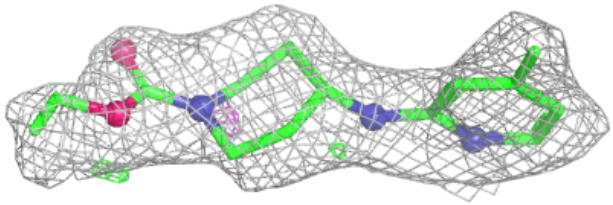


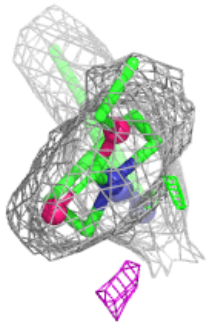


Electron density around AT2 B 906:

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

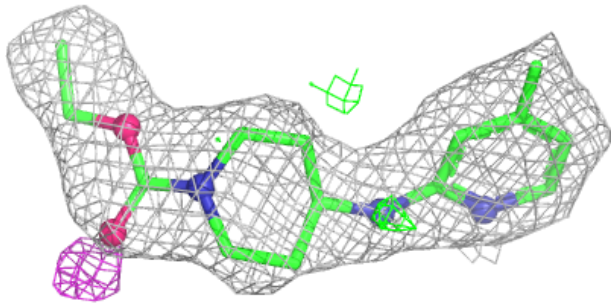


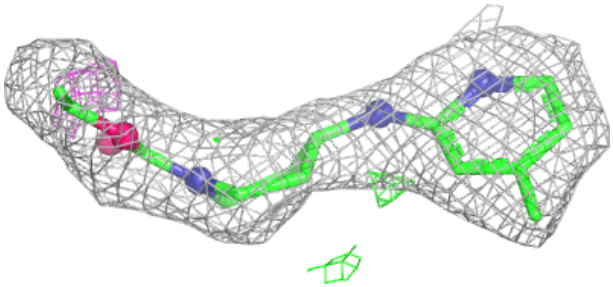


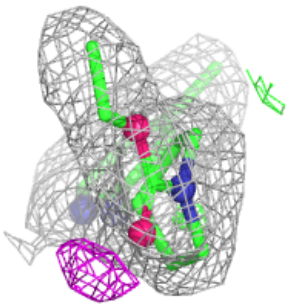


Electron density around AT2 A 905:

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

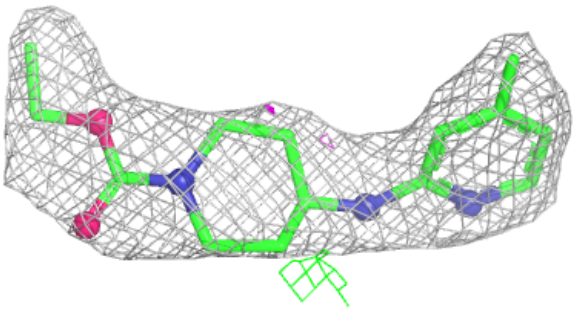


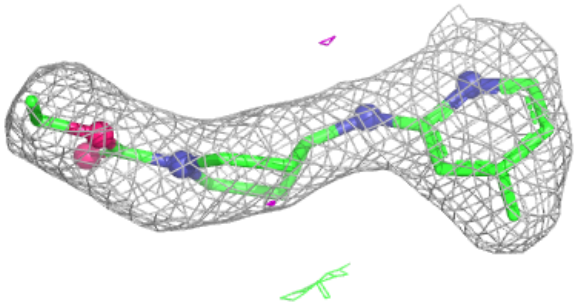


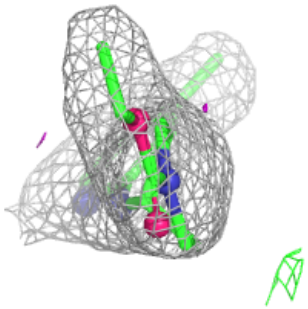


Electron density around AT2 B 907:

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

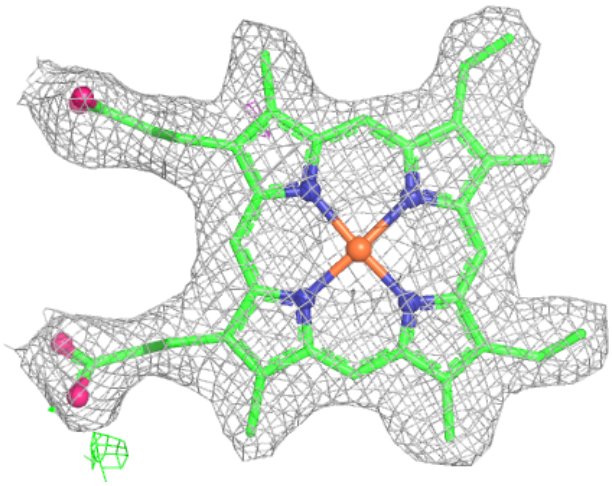


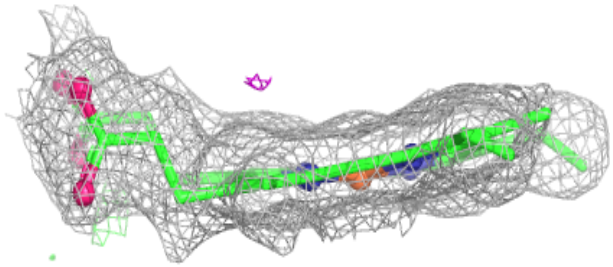


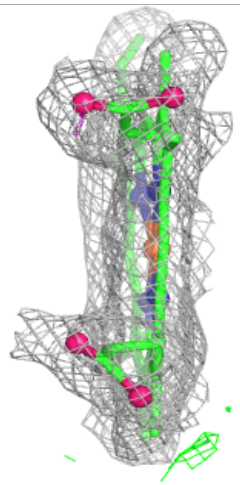


Electron density around HEC A 901:

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

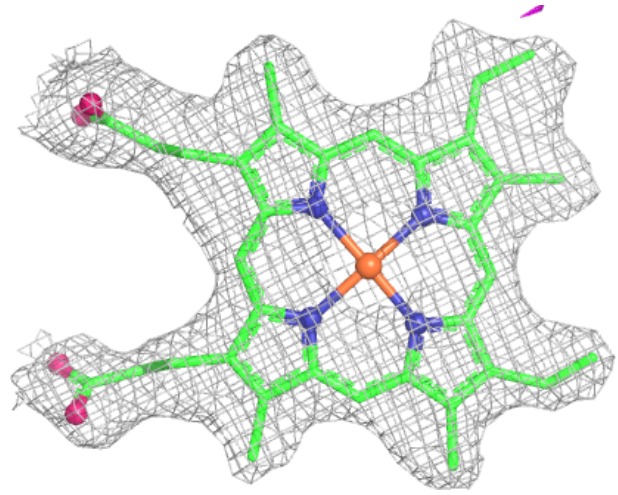


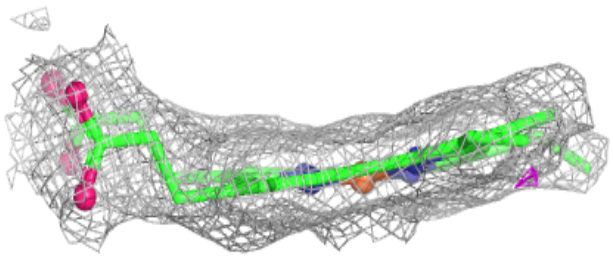


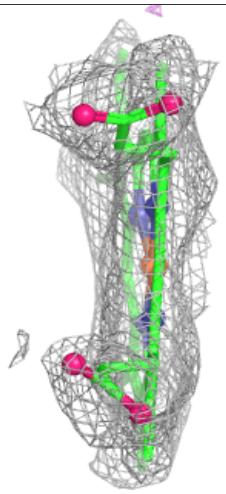


Electron density around HEC B 902:

$2mF_o$-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.