



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:03 AM EDT

PDB ID : 1NIR / pdb_00001nir
Title : OXYDIZED NITRITE REDUCTASE FROM PSEUDOMONAS AERUGINOSA
Authors : Nurizzo, D.; Tegoni, M.; Cambillau, C.
Deposited on : 1997-06-17
Resolution : 2.15 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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

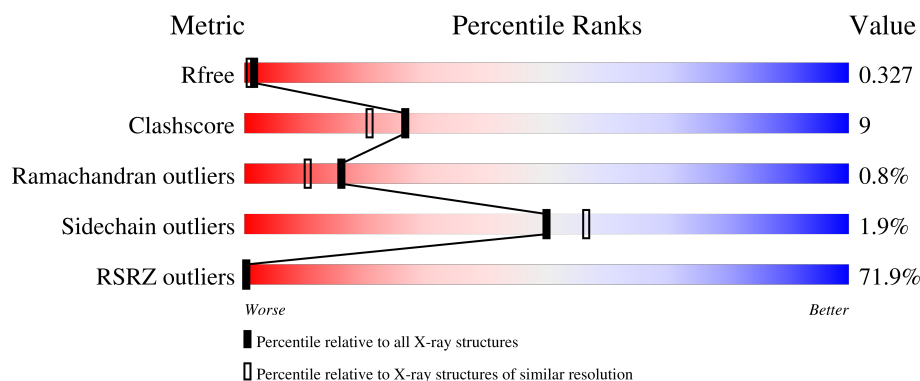
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	543	
1	B	543	

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	PO4	A	604	-	X	-	-
2	PO4	B	604	-	X	-	-
5	HEC	A	601	X	-	-	-
5	HEC	B	601	X	-	-	-
6	DHE	A	602	X	-	-	-
6	DHE	B	602	X	-	-	-

2 Entry composition [i](#)

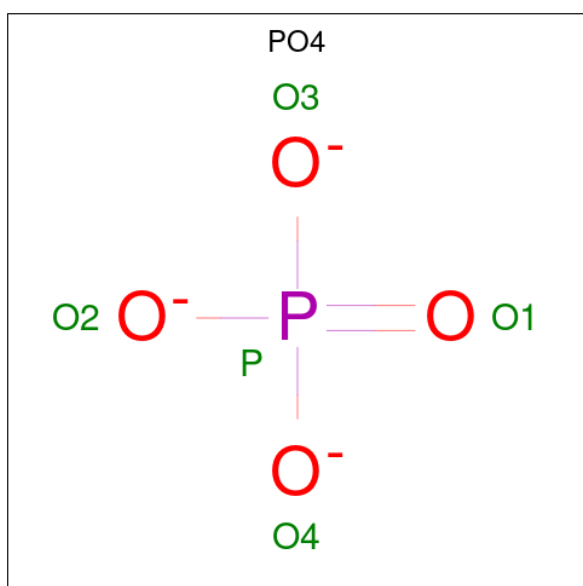
There are 7 unique types of molecules in this entry. The entry contains 9483 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4203	2665	733	793	12			
1	B	539	Total	C	N	O	S	0	0	0
			4212	2671	735	794	12			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

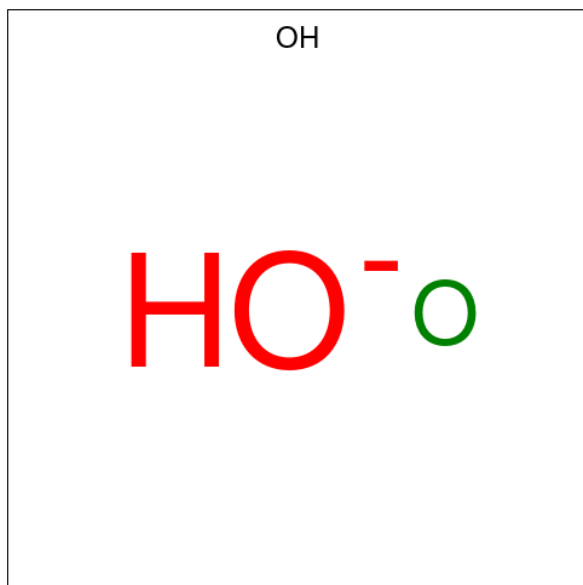


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

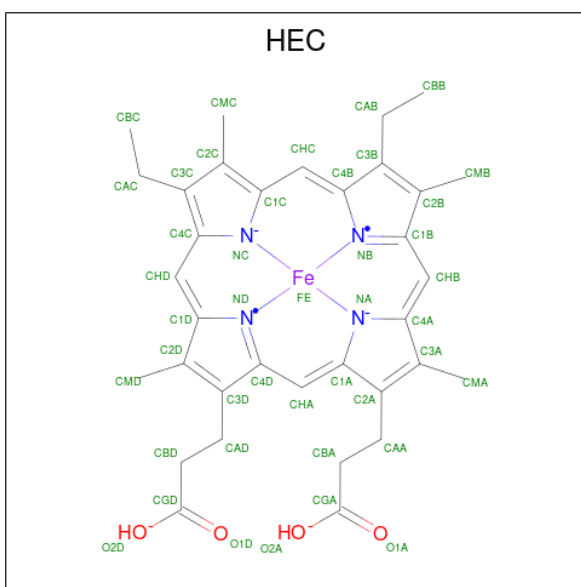
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



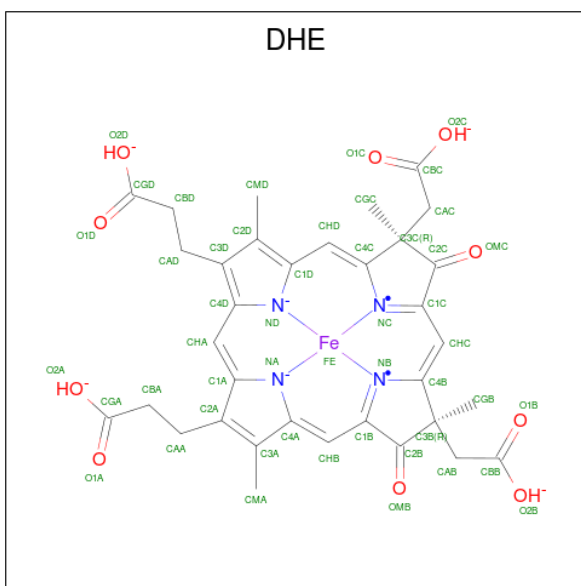
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		

- Molecule 5 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



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

- Molecule 6 is HEME D (CCD ID: DHE) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_{10}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 49	C 34	Fe 1	N 4	O 10	0	0
6	B	1	Total 49	C 34	Fe 1	N 4	O 10	0	0

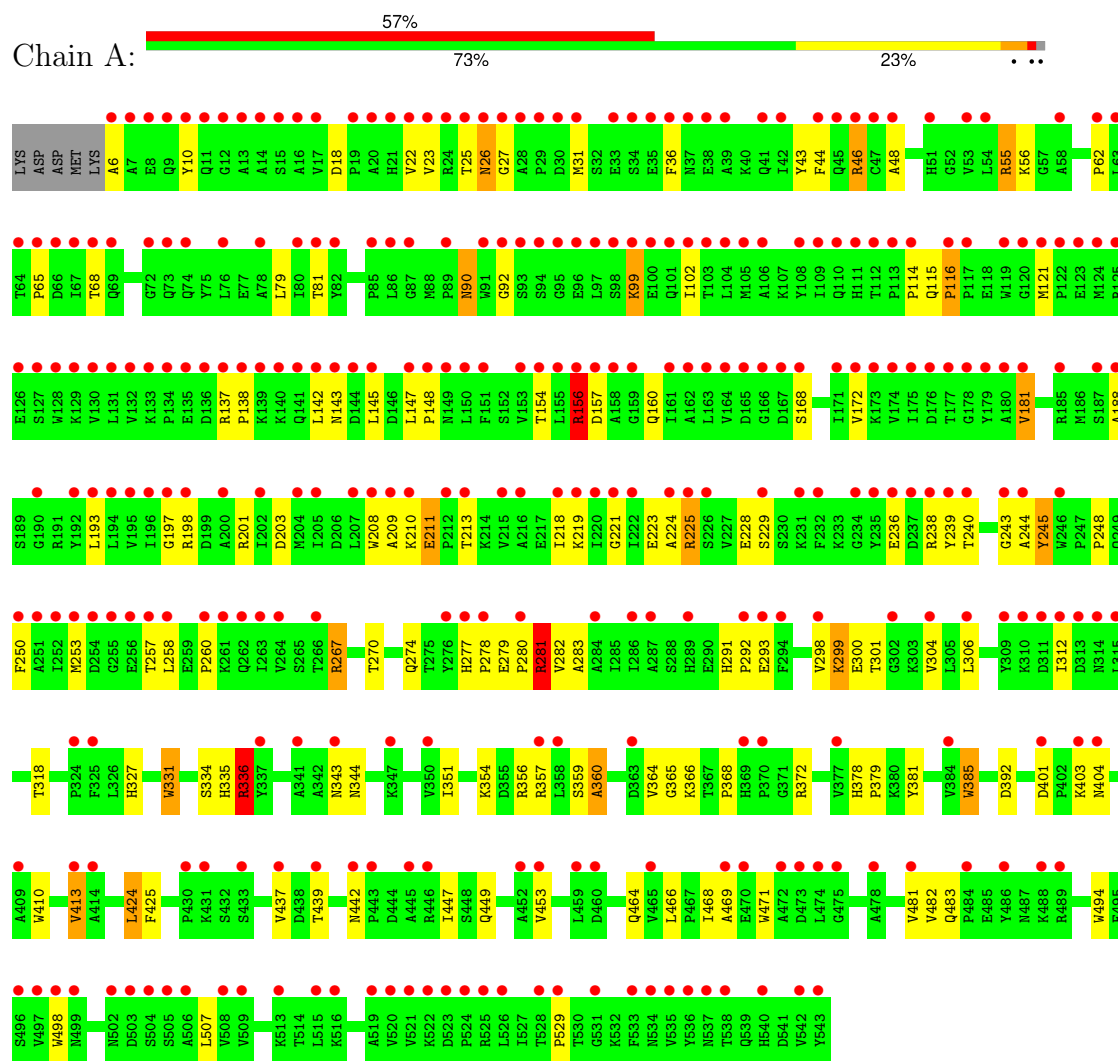
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	449	Total 449	O 449	0	0
7	B	421	Total 421	O 421	0	0

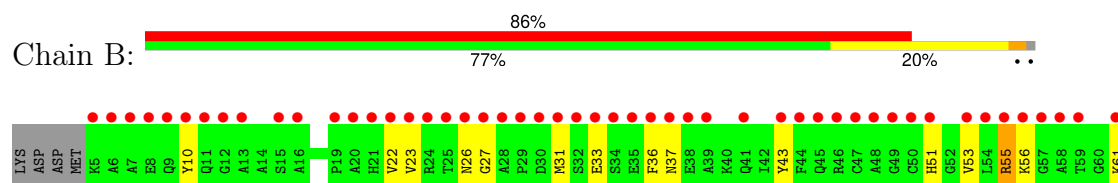
3 Residue-property plots

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: NITRITE REDUCTASE



• Molecule 1: NITRITE REDUCTASE



G500	K501	N502	D503	S504	S505	A506	L507	V508	V509	V510	D511	D512	K513	T514	L515	K516	L517	K518	A519	V520	V521	K522	D523	P524	R525	L526	L527	T528	P529	T530	G531	K532	F533	N534	V535	V536	N537	T538	Q539	H540	D541	V542	Y543																	
T440	F441	N442	P443	D444	A445	R446	T447	S448	Q449	S450	V451	A452	V453	F454	D455	L456	K457	N458	L459	D460	A461	K462	V463	Q464	V465	L466	P467	L468	A469	E470	W471	A472	D473	L474	E475	E476	G477	A478	K479	R480	V481	V482	Q483	P484	E485	Y486	N487	K488	R489	G490	D491	E492	V493	W494	F495	S496	V497	N498	N499	
K380	Y381	G382	P383	V384	W385	S386	T387	S388	H389	L390	G391	D392	G393	S394	T395	S396	L397	T398	G399	T400	D401	P402	K403	N404	H405	P406	Q407	Y408	A409	W410	K411	K412	V413	A414	E415	L416	Q417	G418	Q419	R420	G421	G422	S423	L424	F425	I426	K427	T428	H429	P430	K431	S432	S433	H434	L435	Y436	V437	D438	T439	
S319	A320	A321	M322	D323	G324	E325	T326	H327	D328	G329	G330	W331	D332	S333	S334	H335	R336	Y337	F338	K339	T340	A341	A342	T343	N344	S345	K346	K347	V348	A349	V350	L351	D352	S353	K354	D355	R356	R357	L358	S359	A360	L361	V362	D363	V364	G365	K366	T367	P368	H369	G370	G371	R372	G373	A374	N375	F376	V377	H378	P379
F250	A251	M252	D253	G254	W255	E256	T257	L258	E259	P260	T261	V262	S263	T264	S265	T266	R267	G268	M269	T270	D271	D272	T273	Q274	T275	Y276	H277	P278	E279	A280	R281	V282	A283	A284	I285	I286	A287	S288	H289	F294	I295	T296	V297	K298	K299	E300	T301	L305	L306	V307	N308	Y309	K310	D311	I312	D313	N314	L315		
S184	R185	M186	D187	A188	S189	G190	V191	Y192	L193	K194	V195	I196	G197	R198	D199	A200	R201	L202	D203	M204	L205	D206	L207	W208	T209	A209	K210	E211	P212	V213	T214	A215	E217	I218	K219	I220	G221	L222	E223	A224	R225	S226	V227	S230	K231	F232	I235	E236	D237	L241	A244	Y245	W246	P247	N248	Q249				
H124	R125	E126	S127	W128	K129	V130	L131	V132	K133	P134	E135	I136	R137	P138	K139	A140	Q141	L142	N143	D144	L145	D146	L147	P148	N149	L150	F151	S152	V153	T154	L155	R156	D157	A158	G159	Q160	T161	A162	L163	V164	D165	G166	D167	S168	K169	I170	I171	V172	K173	V174	D175	T176	T177	G178	Y179	A180	H181	W182	I183	
P62	L63	T64	P65	D66	L67	T68	Q69	Q70	R71	G72	Q73	Q74	Y75	E77	A78	L79	T80	T81	T82	G83	T84	P85	L86	G87	M88	P89	N90	G92	S93	S94	G95	E96	L97	S98	K99	E100	Q101	I102	T103	L104	M105	A106	K107	Y108	I109	Q110	H111	T112	P113	P114	Q115	P116	W119	G120	M121					

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	163.07Å 90.07Å 111.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.15 30.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	89.0 (30.00-2.15) 89.5 (30.00-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.31 (at 2.14Å)	Xtrriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.209 , 0.242 0.318 , 0.327	Depositor DCC
R_{free} test set	3270 reflections (3.57%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9483	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9823e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DHE, HEC, CL, OH, PO4

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	0.93	9/4308 (0.2%)	1.20	34/5854 (0.6%)
1	B	0.82	8/4317 (0.2%)	1.14	22/5865 (0.4%)
All	All	0.88	17/8625 (0.2%)	1.17	56/11719 (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
1	B	0	2
All	All	0	3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	248	PRO	C-N	-11.17	1.19	1.33
1	A	244	ALA	C-N	-8.90	1.22	1.33
1	B	244	ALA	C-N	-8.02	1.22	1.33
1	B	483	GLN	C-N	6.17	1.41	1.33
1	B	331	TRP	NE1-CE2	-5.73	1.31	1.37
1	A	331	TRP	NE1-CE2	-5.55	1.31	1.37
1	A	385	TRP	NE1-CE2	-5.54	1.31	1.37
1	B	410	TRP	NE1-CE2	-5.45	1.31	1.37
1	A	208	TRP	NE1-CE2	-5.40	1.31	1.37
1	B	494	TRP	NE1-CE2	-5.37	1.31	1.37
1	A	494	TRP	NE1-CE2	-5.24	1.31	1.37
1	A	471	TRP	NE1-CE2	-5.24	1.31	1.37
1	B	498	TRP	NE1-CE2	-5.17	1.31	1.37
1	A	248	PRO	C-N	-5.15	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	498	TRP	NE1-CE2	-5.04	1.31	1.37
1	B	208	TRP	NE1-CE2	-5.02	1.31	1.37
1	A	410	TRP	NE1-CE2	-5.01	1.31	1.37

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	VAL	N-CA-C	8.54	120.58	108.36
1	A	27	GLY	N-CA-C	-8.23	103.37	115.63
1	B	244	ALA	O-C-N	-7.70	113.46	123.16
1	B	23	VAL	N-CA-C	7.64	119.61	108.53
1	B	309	TYR	O-C-N	-7.45	113.10	122.26
1	B	226	SER	N-CA-C	7.32	121.07	109.50
1	B	483	GLN	O-C-N	-7.12	113.13	121.32
1	A	116	PRO	N-CA-C	-6.78	102.43	110.70
1	B	245	TYR	N-CA-C	-6.42	103.79	111.69
1	B	244	ALA	CA-C-N	6.30	131.36	120.58
1	B	244	ALA	C-N-CA	6.30	131.36	120.58
1	B	116	PRO	N-CA-C	-6.02	103.36	110.70
1	A	283	ALA	CB-CA-C	-5.98	108.46	117.07
1	A	482	VAL	O-C-N	5.88	129.47	123.00
1	B	115	GLN	N-CA-C	5.79	116.96	109.72
1	A	360	ALA	CA-C-N	5.53	131.15	123.07
1	A	360	ALA	C-N-CA	5.53	131.15	123.07
1	A	281	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	B	489	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	B	427	LYS	N-CA-C	5.39	117.28	108.76
1	A	156	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	A	267	ARG	NE-CZ-NH2	5.38	124.05	119.20
1	A	283	ALA	O-C-N	5.38	125.51	121.47
1	A	238	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	B	156	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	B	468	ILE	N-CA-C	5.36	115.50	110.30
1	A	201	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	B	220	ILE	N-CA-C	5.34	118.12	112.83
1	B	480	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	B	336	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	B	27	GLY	N-CA-C	-5.30	107.71	115.72
1	A	203	ASP	CA-C-N	5.30	129.82	122.77
1	A	203	ASP	C-N-CA	5.30	129.82	122.77
1	B	372	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	372	ARG	NE-CZ-NH2	5.28	123.95	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	A	55	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	283	ALA	CA-C-O	5.21	120.96	117.94
1	A	507	LEU	O-C-N	-5.21	117.13	123.27
1	A	46	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	A	181	VAL	CA-C-N	-5.16	112.63	122.53
1	A	181	VAL	C-N-CA	-5.16	112.63	122.53
1	A	168	SER	O-C-N	-5.14	115.37	122.46
1	A	336	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	A	356	ARG	NE-CZ-NH2	5.12	123.80	119.20
1	A	137	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	245	TYR	N-CA-C	-5.11	103.74	111.56
1	A	464	GLN	CA-C-N	-5.11	116.48	123.12
1	A	464	GLN	C-N-CA	-5.11	116.48	123.12
1	A	385	TRP	O-C-N	-5.11	117.30	123.27
1	A	357	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	B	474	LEU	N-CA-C	5.08	120.47	113.97
1	A	18	ASP	CA-C-N	5.07	125.35	119.47
1	A	18	ASP	C-N-CA	5.07	125.35	119.47
1	B	55	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	B	476	GLU	N-CA-C	5.04	117.03	110.53

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	TRP	Mainchain
1	B	309	TYR	Mainchain
1	B	483	GLN	Mainchain

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	4203	0	4158	87	0
1	B	4212	0	4171	78	2
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	43	0	30	0	0
5	B	43	0	30	2	0
6	A	49	0	24	3	0
6	B	49	0	24	3	0
7	A	449	0	0	5	1
7	B	421	0	0	7	2
All	All	9483	0	8437	158	5

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 9.

All (158) 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:B:488:LYS:HB3	7:B:1008:HOH:O	1.62	0.98
1:A:277:HIS:O	1:A:280:PRO:HD3	1.84	0.78
1:A:114:PRO:HB2	1:B:22:VAL:HG12	1.64	0.78
1:B:211:GLU:O	1:B:213:THR:HG23	1.87	0.75
1:B:489:ARG:HG2	7:B:1008:HOH:O	1.88	0.73
1:A:257:THR:O	1:A:258:LEU:HB2	1.88	0.72
1:A:364:VAL:CG2	1:A:368:PRO:HG3	2.21	0.70
1:A:22:VAL:HG12	1:B:114:PRO:HB2	1.75	0.68
1:A:278:PRO:HG3	7:A:947:HOH:O	1.93	0.67
1:A:219:LYS:HE3	1:A:221:GLY:O	1.95	0.67
1:A:147:LEU:HB2	1:A:148:PRO:HD3	1.77	0.66
1:A:43:TYR:OH	1:A:55:ARG:HG2	1.96	0.66
1:B:364:VAL:CG2	1:B:368:PRO:HG3	2.26	0.65
1:A:10:TYR:OH	1:B:327:HIS:HE1	1.81	0.63
1:B:487:ASN:HD21	1:B:489:ARG:HG3	1.63	0.63
1:B:401:ASP:HB3	1:B:405:HIS:HB2	1.81	0.63
1:B:257:THR:O	1:B:258:LEU:HB2	1.99	0.62
1:A:228:GLU:HG3	1:A:229:SER:N	2.15	0.60
1:B:343:ASN:HA	1:B:368:PRO:HD2	1.82	0.60
1:B:489:ARG:HD2	7:B:815:HOH:O	2.00	0.60
1:B:395:ILE:HB	1:B:416:LEU:HB2	1.82	0.60
1:B:484:PRO:HB3	1:B:495:PHE:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ARG:NH2	7:A:789:HOH:O	2.29	0.59
1:A:364:VAL:HG21	1:A:368:PRO:HG3	1.84	0.59
1:A:36:PHE:HZ	1:A:114:PRO:HG3	1.67	0.59
1:A:90:ASN:H	1:A:90:ASN:HD22	1.50	0.59
1:B:53:VAL:HG11	1:B:116:PRO:HG2	1.85	0.58
1:A:304:VAL:HG11	1:A:351:ILE:HG12	1.86	0.57
1:B:99:LYS:HD3	1:B:99:LYS:O	2.04	0.57
1:A:25:THR:O	1:A:26:ASN:HB2	2.03	0.57
1:B:507:LEU:HB2	1:B:521:VAL:HB	1.86	0.57
1:A:364:VAL:HG23	1:A:368:PRO:HG3	1.86	0.56
1:A:279:GLU:O	1:A:279:GLU:HG2	2.04	0.56
1:A:291:HIS:O	1:A:293:GLU:N	2.38	0.56
1:A:327:HIS:HE1	1:B:10:TYR:OH	1.88	0.56
1:B:250:PHE:CD1	1:B:250:PHE:C	2.83	0.56
1:A:211:GLU:O	1:A:213:THR:HG23	2.06	0.55
1:B:55:ARG:NH2	7:B:693:HOH:O	2.27	0.55
1:B:61:LYS:HD2	1:B:71:ARG:NH2	2.22	0.55
1:A:366:LYS:HE3	1:A:392:ASP:OD2	2.08	0.54
1:B:453:VAL:HG21	1:B:466:LEU:HD22	1.90	0.53
1:A:90:ASN:H	1:A:90:ASN:ND2	2.07	0.53
1:B:364:VAL:HG21	1:B:368:PRO:HG3	1.91	0.53
1:A:209:ALA:O	1:A:210:LYS:C	2.51	0.53
1:A:381:TYR:CD1	1:A:413:VAL:HG22	2.43	0.53
1:B:198:ARG:HH22	6:B:602:DHE:CBB	2.21	0.53
1:B:381:TYR:CD1	1:B:413:VAL:HG22	2.44	0.53
1:B:299:LYS:NZ	1:B:327:HIS:HD2	2.06	0.52
1:B:72:GLY:O	1:B:76:LEU:HG	2.10	0.52
1:B:36:PHE:HZ	1:B:114:PRO:HG3	1.75	0.51
1:B:378:HIS:CG	1:B:379:PRO:HD2	2.46	0.51
1:B:51:HIS:O	1:B:55:ARG:HA	2.11	0.51
1:A:181:VAL:HA	1:A:197:GLY:HA2	1.91	0.51
1:B:366:LYS:HD2	1:B:392:ASP:OD2	2.10	0.51
1:B:426:ILE:HG13	1:B:437:VAL:HG22	1.93	0.51
1:B:56:LYS:HE2	7:B:1003:HOH:O	2.10	0.51
1:A:250:PHE:C	1:A:250:PHE:CD1	2.89	0.51
1:B:405:HIS:N	1:B:406:PRO:HD3	2.26	0.50
1:A:439:THR:OG1	1:A:442:ASN:HB2	2.11	0.50
1:A:6:ALA:HB1	1:B:422:GLY:HA2	1.94	0.50
1:A:270:THR:O	1:A:274:GLN:HA	2.11	0.50
1:A:306:LEU:HB2	1:A:318:THR:HB	1.94	0.50
1:B:148:PRO:HB2	1:B:488:LYS:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LEU:HB2	1:B:148:PRO:HD3	1.95	0.49
1:A:381:TYR:CD2	1:A:413:VAL:HG13	2.48	0.49
1:A:114:PRO:HB2	1:B:22:VAL:CG1	2.39	0.48
1:A:267:ARG:NH1	7:A:1040:HOH:O	2.44	0.48
1:B:55:ARG:HB3	1:B:63:LEU:HB2	1.94	0.48
1:B:386:SER:HB3	1:B:397:LEU:HD23	1.95	0.48
1:A:298:VAL:HG12	1:A:301:THR:OG1	2.14	0.48
1:A:188:ALA:HB3	1:A:236:GLU:HG2	1.95	0.48
1:B:334:SER:O	1:B:335:HIS:HB2	2.13	0.48
1:A:10:TYR:OH	1:B:327:HIS:CE1	2.64	0.48
1:B:299:LYS:HZ1	1:B:327:HIS:HD2	1.62	0.47
1:B:436:TYR:CE1	1:B:493:VAL:HG21	2.49	0.47
1:B:250:PHE:CD1	1:B:250:PHE:O	2.68	0.47
1:B:181:VAL:HA	1:B:197:GLY:HA2	1.95	0.47
1:A:343:ASN:OD1	1:A:344:ASN:N	2.43	0.47
1:A:378:HIS:CG	1:A:379:PRO:HD2	2.49	0.47
1:A:424:LEU:HB3	1:A:425:PHE:CD2	2.49	0.47
1:B:370:PRO:HB3	1:B:387:THR:HB	1.97	0.47
1:A:145:LEU:HD11	1:A:172:VAL:HG11	1.97	0.47
1:A:439:THR:HG23	1:A:447:ILE:O	2.15	0.47
1:B:79:LEU:HD13	5:B:601:HEC:HAA1	1.97	0.47
1:B:381:TYR:CD1	1:B:413:VAL:CG2	2.99	0.46
1:B:279:GLU:N	1:B:280:PRO:HD3	2.30	0.46
1:A:198:ARG:NH2	6:A:602:DHE:O2B	2.47	0.46
1:A:219:LYS:HE2	7:A:857:HOH:O	2.16	0.46
1:A:160:GLN:NE2	7:A:1031:HOH:O	2.49	0.46
1:B:378:HIS:ND1	1:B:379:PRO:HD2	2.30	0.46
1:A:223:GLU:HG2	1:A:245:TYR:HB2	1.97	0.46
1:B:267:ARG:NH1	7:B:787:HOH:O	2.46	0.46
1:A:154:THR:O	1:A:529:PRO:HA	2.16	0.46
1:B:31:MET:HE2	1:B:36:PHE:HA	1.99	0.45
1:A:10:TYR:CZ	6:B:602:DHE:HGB2	2.51	0.45
1:A:331:TRP:HB3	1:A:335:HIS:HA	1.99	0.45
1:B:331:TRP:HB3	1:B:335:HIS:HA	1.98	0.45
1:B:364:VAL:HG23	1:B:368:PRO:HG3	1.97	0.45
1:A:218:ILE:HD11	1:A:260:PRO:HG3	1.98	0.45
1:A:449:GLN:HB3	1:A:469:ALA:HB3	1.99	0.45
1:A:299:LYS:NZ	1:A:327:HIS:HD2	2.14	0.45
1:A:138:PRO:HB3	1:A:142:LEU:HD11	1.99	0.44
1:A:401:ASP:OD2	1:A:404:ASN:HB2	2.18	0.44
1:B:198:ARG:NH2	6:B:602:DHE:O2B	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LYS:HB3	1:A:300:GLU:OE1	2.18	0.44
1:A:468:ILE:HB	1:A:481:VAL:HG21	1.99	0.44
1:A:31:MET:HE2	1:A:36:PHE:HA	1.98	0.44
1:A:239:TYR:CE1	1:A:312:ILE:HD12	2.52	0.44
6:A:602:DHE:C2C	6:A:602:DHE:O2C	2.65	0.44
1:B:43:TYR:OH	1:B:55:ARG:HG2	2.18	0.44
1:A:44:PHE:HA	1:A:48:ALA:HB2	1.99	0.44
1:A:359:SER:O	1:A:360:ALA:HB2	2.17	0.44
1:B:113:PRO:HA	1:B:114:PRO:HD3	1.90	0.44
1:B:218:ILE:HD11	1:B:260:PRO:HG3	1.99	0.44
1:B:299:LYS:HB3	1:B:300:GLU:OE1	2.18	0.44
1:A:243:GLY:HA3	1:A:282:VAL:HG11	1.99	0.43
1:A:453:VAL:HG21	1:A:466:LEU:HD22	2.00	0.43
1:A:281:ARG:HD2	1:A:300:GLU:OE2	2.19	0.43
1:A:99:LYS:HE2	1:A:102:ILE:HD12	2.00	0.43
1:A:156:ARG:HB3	1:A:157:ASP:H	1.62	0.43
1:A:381:TYR:HB3	1:A:413:VAL:HG21	2.01	0.43
1:A:279:GLU:N	1:A:280:PRO:HD3	2.32	0.43
1:B:33:GLU:HG2	1:B:37:ASN:ND2	2.34	0.43
1:B:436:TYR:CZ	1:B:493:VAL:HG21	2.54	0.43
1:A:279:GLU:N	1:A:280:PRO:CD	2.82	0.42
1:A:334:SER:O	1:A:335:HIS:HB2	2.18	0.42
1:A:336:ARG:NH1	1:A:354:LYS:HB3	2.34	0.42
1:B:115:GLN:HA	1:B:116:PRO:HD3	1.90	0.42
1:A:81:THR:HG23	1:A:92:GLY:HA3	2.00	0.42
1:B:90:ASN:HD22	1:B:93:SER:HB2	1.84	0.42
1:B:403:LYS:HG3	7:B:822:HOH:O	2.19	0.42
1:A:240:THR:O	1:A:253:MET:HE3	2.19	0.42
1:A:280:PRO:HB3	1:A:301:THR:HG23	2.01	0.42
1:B:79:LEU:HD13	5:B:601:HEC:CAA	2.50	0.42
1:B:149:ASN:HB2	1:B:488:LYS:HE3	2.01	0.42
1:B:405:HIS:N	1:B:406:PRO:CD	2.82	0.42
1:A:115:GLN:HA	1:A:116:PRO:HD3	1.90	0.42
1:A:143:ASN:OD1	1:A:145:LEU:HB2	2.20	0.42
1:B:154:THR:O	1:B:529:PRO:HA	2.19	0.42
1:A:56:LYS:HG2	1:A:62:PRO:HB3	2.01	0.41
1:B:338:PHE:HB3	1:B:351:ILE:HB	2.01	0.41
1:B:487:ASN:HD21	1:B:489:ARG:CG	2.31	0.41
1:A:188:ALA:CB	1:A:236:GLU:HG2	2.50	0.41
1:B:381:TYR:CG	1:B:413:VAL:HG21	2.55	0.41
1:A:336:ARG:HH11	1:A:354:LYS:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HH22	6:A:602:DHE:CBB	2.34	0.41
1:A:327:HIS:CE1	1:B:10:TYR:OH	2.70	0.41
1:A:403:LYS:HB2	1:A:403:LYS:NZ	2.35	0.41
1:A:224:ALA:C	1:A:225:ARG:HG2	2.46	0.41
1:B:121:MET:SD	1:B:260:PRO:HB2	2.61	0.41
1:A:65:PRO:HA	1:A:68:THR:OG1	2.21	0.41
1:A:121:MET:SD	1:A:260:PRO:HB2	2.61	0.41
1:B:247:PRO:O	1:B:249:GLN:HG2	2.21	0.41
1:B:156:ARG:HB3	1:B:157:ASP:H	1.79	0.41
1:B:211:GLU:O	1:B:212:PRO:C	2.64	0.41
1:A:228:GLU:CG	1:A:229:SER:N	2.83	0.40
1:A:364:VAL:HB	1:A:365:GLY:H	1.69	0.40
1:B:481:VAL:HA	1:B:496:SER:O	2.22	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLN:NE2	1:B:473:ASP:O[3_556]	1.93	0.27
7:A:616:HOH:O	7:A:772:HOH:O[3_545]	2.01	0.19
7:B:706:HOH:O	7:B:874:HOH:O[3_546]	2.07	0.13
1:B:74:GLN:OE1	1:B:169:LYS:O[3_556]	2.08	0.12
7:B:768:HOH:O	7:B:898:HOH:O[3_556]	2.18	0.02

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	536/543 (99%)	496 (92%)	35 (6%)	5 (1%)	14	9
1	B	537/543 (99%)	502 (94%)	31 (6%)	4 (1%)	18	13
All	All	1073/1086 (99%)	998 (93%)	66 (6%)	9 (1%)	16	10

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	156	ARG
1	A	299	LYS
1	B	156	ARG
1	B	299	LYS
1	B	26	ASN
1	B	483	GLN
1	A	292	PRO
1	A	483	GLN

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	453/458 (99%)	442 (98%)	11 (2%)	43	47
1	B	454/458 (99%)	448 (99%)	6 (1%)	61	68
All	All	907/916 (99%)	890 (98%)	17 (2%)	50	56

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	79	LEU
1	A	90	ASN
1	A	99	LYS
1	A	193	LEU
1	A	211	GLU
1	A	281	ARG
1	A	336	ARG
1	A	413	VAL
1	A	424	LEU
1	A	437	VAL
1	B	198	ARG
1	B	281	ARG
1	B	407	GLN

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Mol	Chain	Res	Type
1	B	413	VAL
1	B	424	LEU
1	B	439	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	45	GLN
1	A	90	ASN
1	A	110	GLN
1	A	111	HIS
1	A	115	GLN
1	A	327	HIS
1	A	344	ASN
1	A	540	HIS
1	B	21	HIS
1	B	45	GLN
1	B	90	ASN
1	B	115	GLN
1	B	289	HIS
1	B	327	HIS
1	B	344	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are monoatomic and 2 are modelled with single atom - 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	HEC	A	601	1	50,50,50	0.88	0	68,82,82	1.11	4 (5%)
6	DHE	B	602	4,1	52,56,56	1.88	8 (15%)	68,94,94	1.73	14 (20%)
5	HEC	B	601	1	50,50,50	0.84	0	68,82,82	1.16	4 (5%)
2	PO4	B	604	-	4,4,4	3.35	4 (100%)	6,6,6	1.23	1 (16%)
6	DHE	A	602	4,1	52,56,56	1.90	8 (15%)	68,94,94	1.71	10 (14%)
2	PO4	A	604	-	4,4,4	3.39	4 (100%)	6,6,6	0.58	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	HEC	A	601	1	1/1/3/7	6/14/54/54	-
6	DHE	A	602	4,1	1/1/15/19	6/20/108/108	-
5	HEC	B	601	1	1/1/3/7	6/14/54/54	-
6	DHE	B	602	4,1	1/1/15/19	8/20/108/108	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	602	DHE	CBD-CAD	-6.52	1.29	1.51
6	B	602	DHE	CBD-CAD	-6.44	1.29	1.51
2	A	604	PO4	P-O1	5.15	1.62	1.50
2	B	604	PO4	P-O1	4.69	1.61	1.50
6	A	602	DHE	FE-NC	4.55	2.08	1.94
6	B	602	DHE	FE-NC	4.32	2.08	1.94
6	B	602	DHE	CGC-C3C	4.22	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	602	DHE	FE-ND	4.15	2.08	1.95
6	A	602	DHE	CGB-C3B	4.12	1.61	1.54
6	B	602	DHE	FE-NB	4.00	2.07	1.94
6	A	602	DHE	CGC-C3C	3.86	1.61	1.54
6	B	602	DHE	CGB-C3B	3.80	1.61	1.54
6	B	602	DHE	FE-ND	3.76	2.07	1.95
6	A	602	DHE	FE-NA	3.76	2.07	1.95
6	A	602	DHE	FE-NB	3.70	2.06	1.94
6	B	602	DHE	FE-NA	3.66	2.07	1.95
2	B	604	PO4	P-O3	2.89	1.63	1.54
2	B	604	PO4	P-O2	2.87	1.63	1.54
2	A	604	PO4	P-O4	2.79	1.62	1.54
2	B	604	PO4	P-O4	2.52	1.62	1.54
2	A	604	PO4	P-O3	2.51	1.62	1.54
2	A	604	PO4	P-O2	2.31	1.61	1.54
6	B	602	DHE	CAB-C3B	-2.18	1.48	1.54
6	A	602	DHE	CAB-C3B	-2.13	1.48	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	602	DHE	CBD-CAD-C3D	5.25	127.06	112.53
6	A	602	DHE	CAD-CBD-CGD	5.05	127.07	113.67
6	B	602	DHE	C1C-NC-C4C	4.87	110.98	105.21
6	A	602	DHE	C1C-NC-C4C	4.82	110.91	105.21
6	A	602	DHE	CBD-CAD-C3D	4.72	125.58	112.53
6	A	602	DHE	C4B-NB-C1B	4.63	110.69	105.21
6	B	602	DHE	CAD-CBD-CGD	4.63	125.93	113.67
6	B	602	DHE	C4B-NB-C1B	4.50	110.53	105.21
5	B	601	HEC	CBB-CAB-C3B	4.02	123.33	112.42
5	B	601	HEC	CBC-CAC-C3C	3.65	122.32	112.42
6	A	602	DHE	C3B-C4B-CHC	3.51	125.56	122.44
6	B	602	DHE	C3B-C4B-CHC	3.49	125.54	122.44
6	A	602	DHE	CHB-C1B-NB	3.05	127.71	124.42
5	A	601	HEC	CBC-CAC-C3C	2.77	119.92	112.42
6	B	602	DHE	C3C-C4C-CHD	2.60	124.75	122.44
6	B	602	DHE	C3D-C4D-ND	-2.51	107.36	110.15
6	A	602	DHE	C3C-C4C-CHD	2.45	124.62	122.44
6	A	602	DHE	C3D-C4D-ND	-2.39	107.50	110.15
6	A	602	DHE	CHC-C1C-NC	2.36	126.97	124.42
6	B	602	DHE	CHB-C1B-NB	2.31	126.91	124.42
5	B	601	HEC	CMA-C3A-C4A	2.29	128.75	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	602	DHE	C1C-CHC-C4B	2.27	128.83	125.23
6	B	602	DHE	CHC-C1C-NC	2.26	126.86	124.42
5	A	601	HEC	CBB-CAB-C3B	2.26	118.55	112.42
6	B	602	DHE	C2A-C1A-NA	-2.20	108.20	110.32
6	B	602	DHE	C4D-ND-C1D	2.17	109.36	105.82
5	A	601	HEC	C2D-C1D-ND	2.17	112.33	109.84
6	A	602	DHE	C1C-CHC-C4B	2.17	128.67	125.23
5	A	601	HEC	CBD-CAD-C3D	-2.11	106.70	112.53
6	B	602	DHE	CHA-C1A-C2A	2.07	128.14	124.86
2	B	604	PO4	O4-P-O1	-2.06	103.66	110.95
5	B	601	HEC	CAA-C2A-C3A	-2.04	124.04	127.87
6	B	602	DHE	C4A-NA-C1A	2.03	109.13	105.82

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	601	HEC	NA
5	B	601	HEC	NA
6	A	602	DHE	NA
6	B	602	DHE	NA

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	DHE	C2D-C3D-CAD-CBD
6	A	602	DHE	C4D-C3D-CAD-CBD
6	B	602	DHE	C2D-C3D-CAD-CBD
6	B	602	DHE	C4D-C3D-CAD-CBD
5	B	601	HEC	C4B-C3B-CAB-CBB
5	B	601	HEC	C2B-C3B-CAB-CBB
5	A	601	HEC	C4B-C3B-CAB-CBB
5	B	601	HEC	C4C-C3C-CAC-CBC
5	A	601	HEC	C4C-C3C-CAC-CBC
5	B	601	HEC	C2C-C3C-CAC-CBC
5	A	601	HEC	C2C-C3C-CAC-CBC
5	A	601	HEC	C2B-C3B-CAB-CBB
6	A	602	DHE	C3C-CAC-CBC-O1C
6	B	602	DHE	C3C-CAC-CBC-O1C
6	B	602	DHE	C3C-CAC-CBC-O2C
6	A	602	DHE	C3B-CAB-CBB-O1B
6	B	602	DHE	C3B-CAB-CBB-O1B
6	A	602	DHE	C3B-CAB-CBB-O2B

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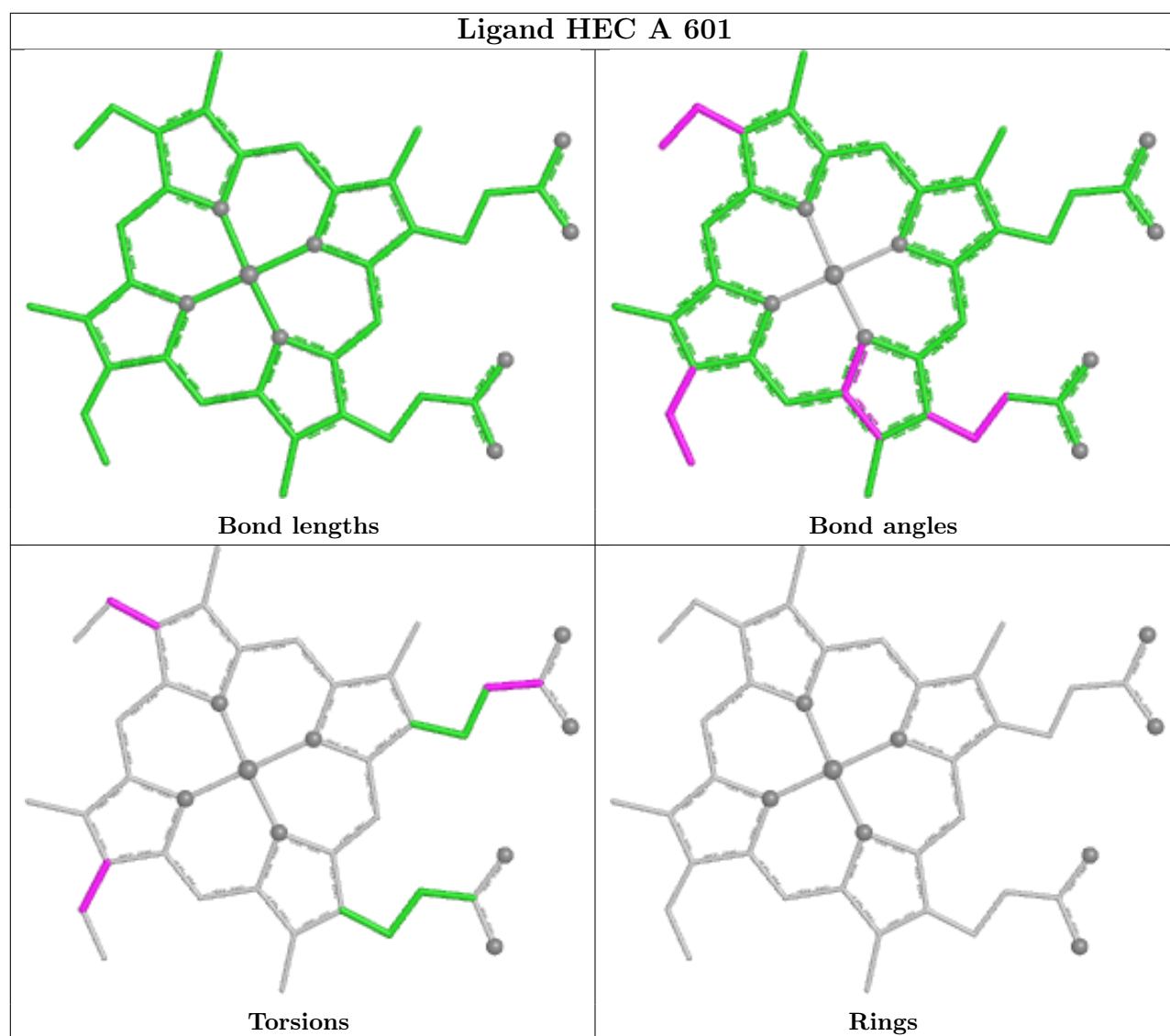
Mol	Chain	Res	Type	Atoms
6	A	602	DHE	C3C-CAC-CBC-O2C
6	B	602	DHE	C3B-CAB-CBB-O2B
5	B	601	HEC	CAA-CBA-CGA-O1A
5	B	601	HEC	CAA-CBA-CGA-O2A
6	B	602	DHE	CAA-CBA-CGA-O2A
5	A	601	HEC	CAA-CBA-CGA-O2A
5	A	601	HEC	CAA-CBA-CGA-O1A
6	B	602	DHE	CAA-CBA-CGA-O1A

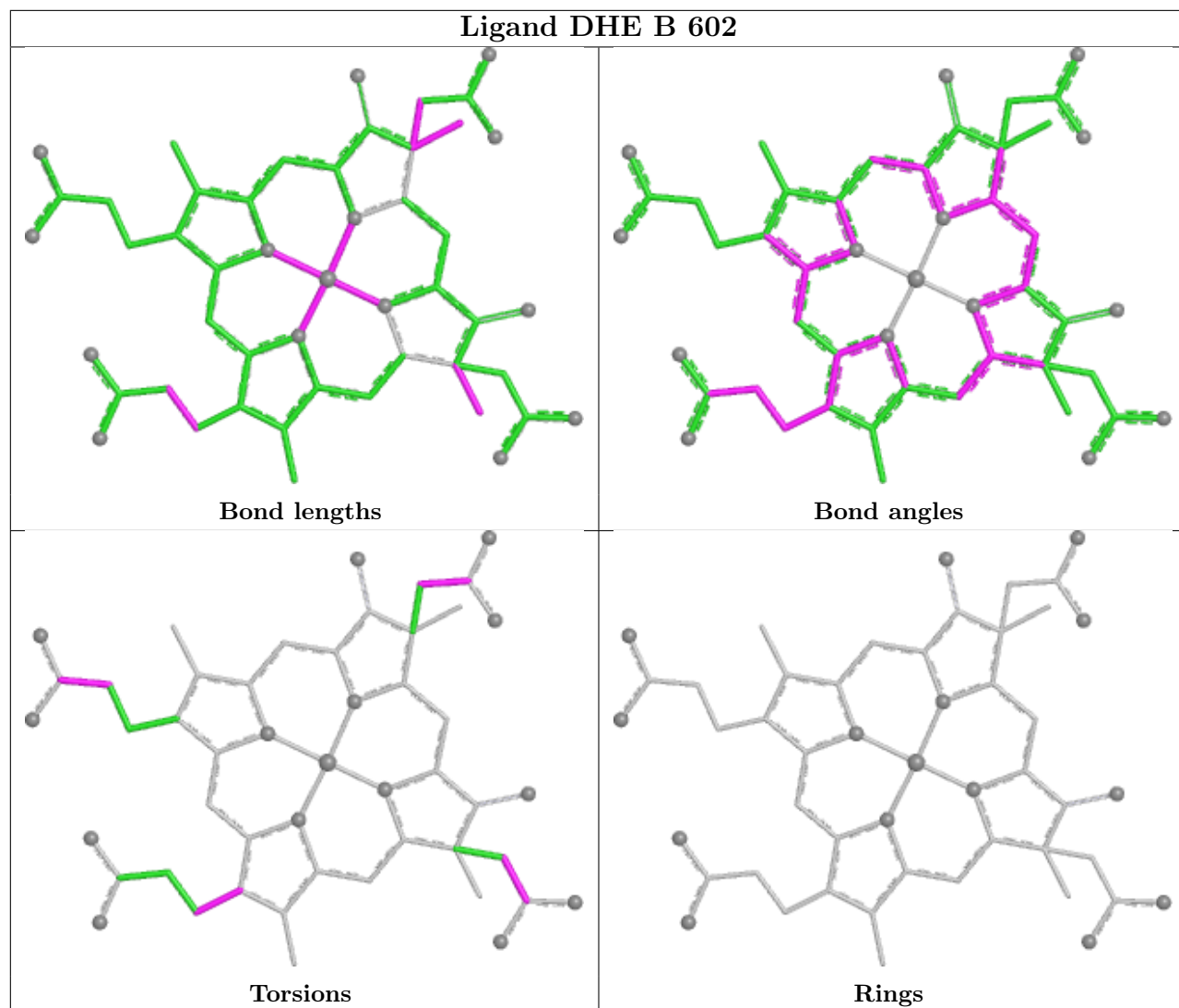
There are no ring outliers.

3 monomers are involved in 8 short contacts:

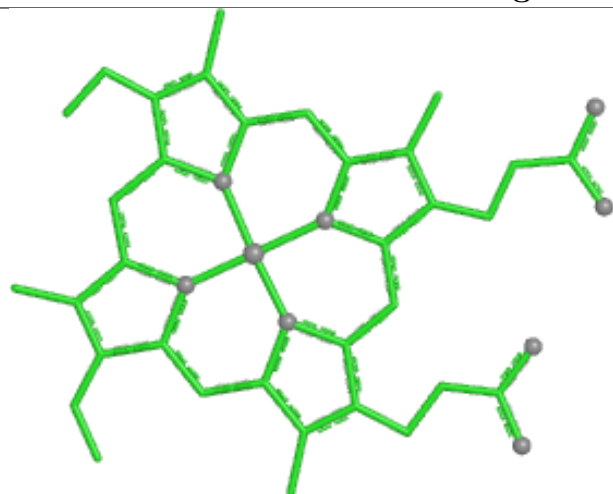
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	602	DHE	3	0
5	B	601	HEC	2	0
6	A	602	DHE	3	0

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 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.

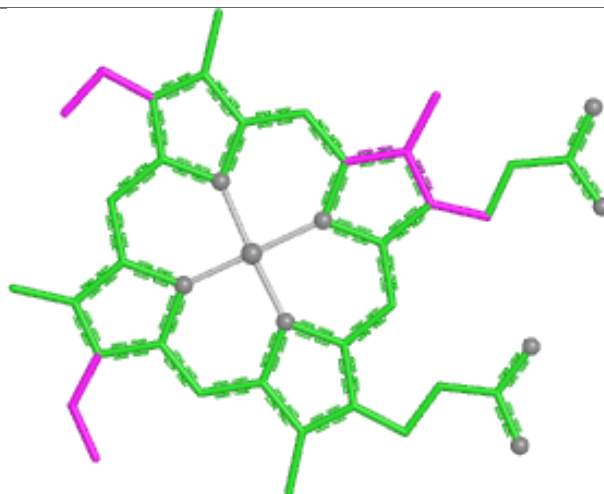




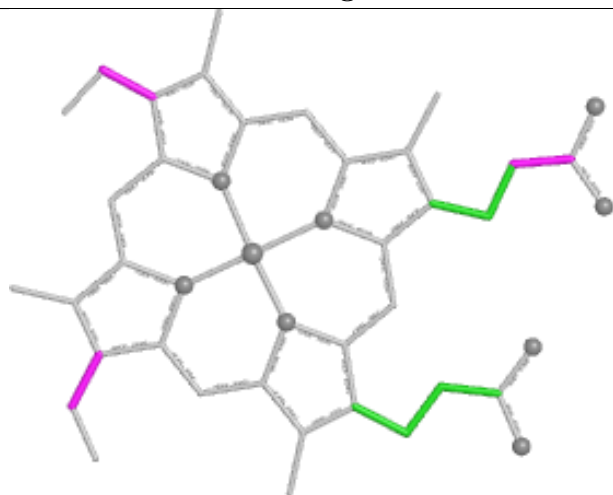
Ligand HEC B 601



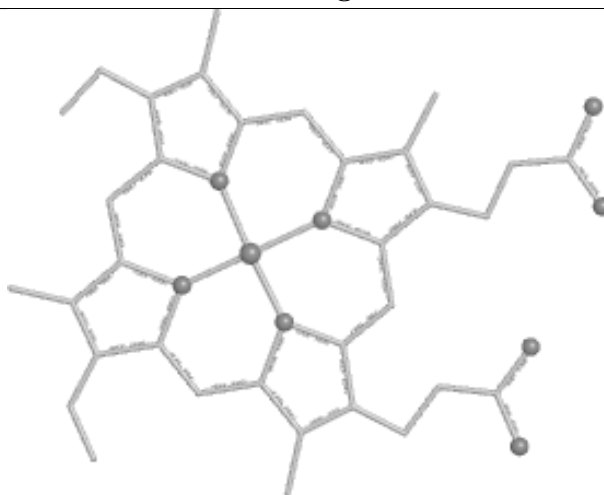
Bond lengths



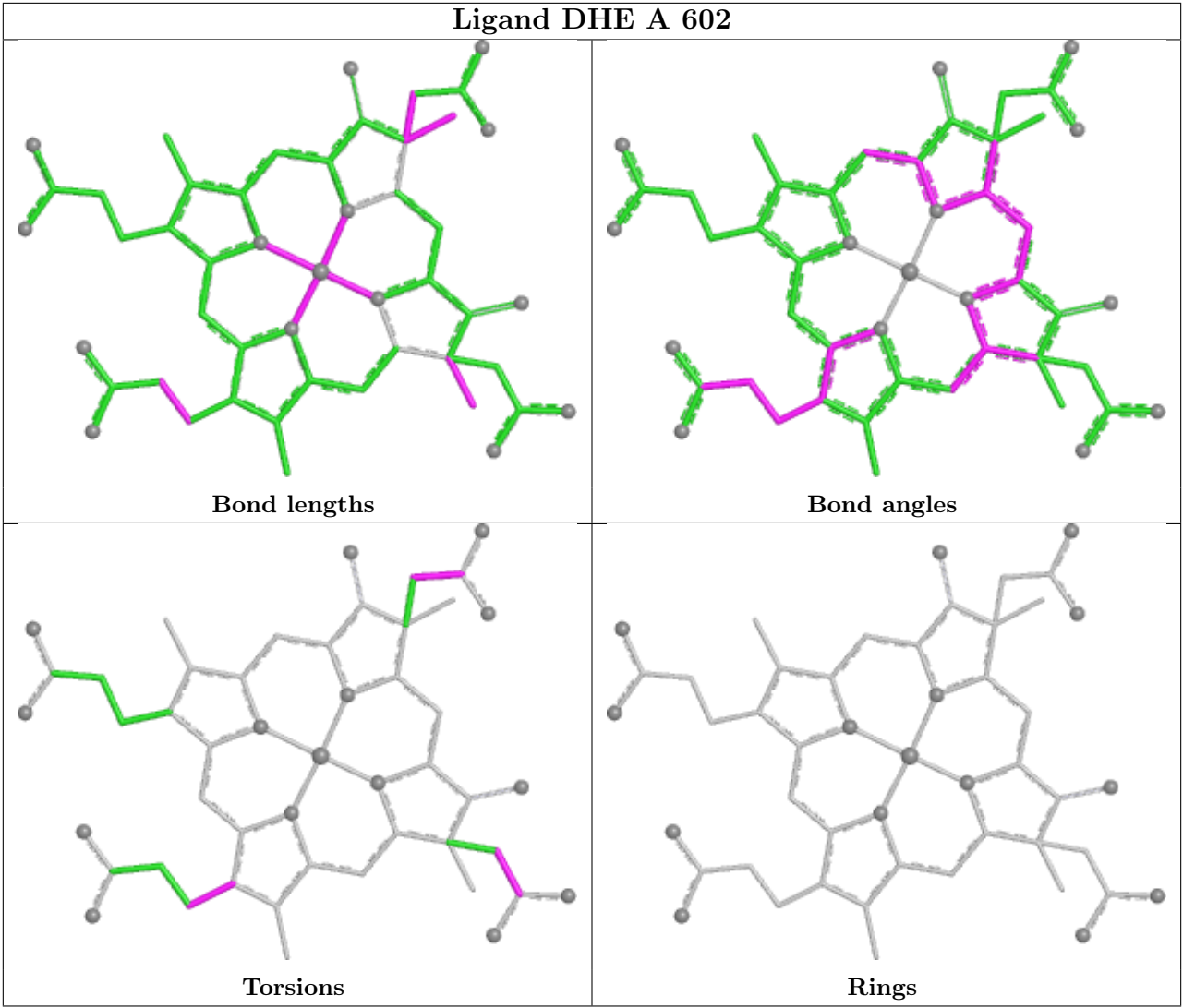
Bond angles



Torsions



Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	248:PRO	C	249:GLN	N	1.19

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	538/543 (99%)	2.35	307 (57%) 0 0	22, 36, 54, 71	0
1	B	539/543 (99%)	3.32	467 (86%) 0 0	23, 37, 56, 72	0
All	All	1077/1086 (99%)	2.83	774 (71%) 0 0	22, 36, 55, 72	0

All (774) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	312	ILE	7.6
1	B	454	PHE	7.3
1	A	99	LYS	7.2
1	B	475	GLY	7.1
1	B	370	PRO	6.9
1	B	5	LYS	6.9
1	B	453	VAL	6.7
1	B	498	TRP	6.7
1	B	389	HIS	6.6
1	B	74	GLN	6.6
1	B	486	TYR	6.5
1	A	104	LEU	6.5
1	B	99	LYS	6.3
1	B	494	TRP	6.3
1	B	436	TYR	6.2
1	B	102	ILE	6.1
1	B	463	TYR	6.1
1	B	467	PRO	6.0
1	A	142	LEU	6.0
1	B	484	PRO	5.9
1	A	27	GLY	5.9
1	B	131	LEU	5.9
1	B	466	LEU	5.8
1	B	497	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	506	ALA	5.8
1	B	505	SER	5.8
1	B	385	TRP	5.7
1	B	510	VAL	5.7
1	B	384	VAL	5.6
1	B	465	VAL	5.6
1	B	78	ALA	5.6
1	B	28	ALA	5.5
1	B	75	TYR	5.5
1	B	25	THR	5.4
1	B	87	GLY	5.4
1	B	504	SER	5.4
1	B	391	GLY	5.3
1	B	155	LEU	5.3
1	B	393	GLY	5.3
1	B	408	TYR	5.3
1	B	524	PRO	5.3
1	A	205	ILE	5.2
1	B	421	GLY	5.2
1	B	526	LEU	5.2
1	A	128	TRP	5.2
1	B	26	ASN	5.2
1	B	478	ALA	5.2
1	A	278	PRO	5.2
1	B	423	SER	5.2
1	A	216	ALA	5.2
1	B	72	GLY	5.2
1	B	283	ALA	5.2
1	A	8	GLU	5.1
1	B	98	SER	5.1
1	A	6	ALA	5.1
1	B	148	PRO	5.1
1	B	495	PHE	5.1
1	B	144	ASP	5.1
1	B	523	ASP	5.1
1	B	377	VAL	5.1
1	B	519	ALA	5.1
1	B	298	VAL	5.0
1	B	329	GLY	5.0
1	B	527	ILE	5.0
1	B	429	HIS	5.0
1	B	27	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	515	LEU	5.0
1	B	83	GLY	4.9
1	B	180	ALA	4.9
1	B	536	TYR	4.9
1	B	443	PRO	4.9
1	B	452	ALA	4.9
1	A	171	ILE	4.9
1	B	435	LEU	4.9
1	B	82	TYR	4.9
1	A	140	LYS	4.9
1	B	451	VAL	4.9
1	B	409	ALA	4.9
1	A	221	GLY	4.9
1	B	418	GLY	4.9
1	B	477	GLY	4.9
1	A	22	VAL	4.9
1	A	65	PRO	4.8
1	B	162	ALA	4.8
1	B	67	ILE	4.8
1	A	178	GLY	4.8
1	A	7	ALA	4.8
1	A	459	LEU	4.7
1	B	543	TYR	4.7
1	A	445	ALA	4.7
1	B	106	ALA	4.7
1	A	212	PRO	4.7
1	A	210	LYS	4.7
1	B	394	SER	4.7
1	B	509	VAL	4.7
1	B	158	ALA	4.7
1	A	163	LEU	4.7
1	B	63	LEU	4.7
1	B	533	PHE	4.6
1	B	70	GLN	4.6
1	B	472	ALA	4.6
1	A	23	VAL	4.6
1	B	29	PRO	4.6
1	B	459	LEU	4.6
1	B	103	THR	4.6
1	B	80	ILE	4.6
1	B	344	ASN	4.6
1	B	172	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	208	TRP	4.5
1	B	169	LYS	4.5
1	A	28	ALA	4.5
1	A	10	TYR	4.5
1	B	395	ILE	4.5
1	B	84	THR	4.5
1	B	181	VAL	4.5
1	B	134	PRO	4.5
1	B	390	LEU	4.5
1	A	127	SER	4.5
1	B	514	THR	4.5
1	A	86	LEU	4.5
1	B	91	TRP	4.4
1	A	102	ILE	4.4
1	B	513	LYS	4.4
1	B	207	LEU	4.4
1	B	416	LEU	4.4
1	B	517	LEU	4.4
1	B	471	TRP	4.4
1	A	232	PHE	4.4
1	A	130	VAL	4.4
1	A	153	VAL	4.4
1	B	364	VAL	4.4
1	B	142	LEU	4.4
1	B	450	SER	4.4
1	B	398	ILE	4.4
1	B	46	ARG	4.4
1	B	473	ASP	4.4
1	B	32	SER	4.3
1	B	468	ILE	4.3
1	B	41	GLN	4.3
1	A	131	LEU	4.3
1	B	512	ASP	4.3
1	B	23	VAL	4.3
1	B	76	LEU	4.3
1	B	456	LEU	4.3
1	A	312	ILE	4.3
1	B	171	ILE	4.3
1	A	13	ALA	4.2
1	B	109	ILE	4.2
1	A	97	LEU	4.2
1	A	145	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	397	LEU	4.2
1	A	12	GLY	4.2
1	A	236	GLU	4.2
1	B	387	THR	4.2
1	B	447	ILE	4.2
1	B	73	GLN	4.2
1	B	68	THR	4.2
1	B	167	ASP	4.2
1	B	369	HIS	4.2
1	B	507	LEU	4.2
1	B	535	VAL	4.2
1	B	457	LYS	4.1
1	B	469	ALA	4.1
1	B	86	LEU	4.1
1	A	465	VAL	4.1
1	A	520	VAL	4.1
1	B	428	THR	4.1
1	A	513	LYS	4.1
1	B	464	GLN	4.1
1	A	37	ASN	4.1
1	A	39	ALA	4.1
1	A	108	TYR	4.1
1	B	413	VAL	4.1
1	B	81	THR	4.1
1	B	202	ILE	4.1
1	B	518	LYS	4.1
1	A	78	ALA	4.1
1	B	424	LEU	4.1
1	B	482	VAL	4.1
1	B	426	ILE	4.1
1	A	95	GLY	4.0
1	A	150	LEU	4.0
1	B	104	LEU	4.0
1	A	403	LYS	4.0
1	B	437	VAL	4.0
1	B	493	VAL	4.0
1	B	345	SER	4.0
1	B	406	PRO	4.0
1	B	430	PRO	4.0
1	A	161	ILE	4.0
1	B	95	GLY	4.0
1	A	526	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	34	SER	4.0
1	B	65	PRO	4.0
1	A	164	VAL	4.0
1	B	434	HIS	4.0
1	B	446	ARG	4.0
1	B	461	ALA	3.9
1	B	151	PHE	3.9
1	B	376	PHE	3.9
1	B	212	PRO	3.9
1	A	11	GLN	3.9
1	A	218	ILE	3.9
1	B	445	ALA	3.9
1	A	119	TRP	3.9
1	B	346	ASN	3.9
1	B	375	ASN	3.9
1	B	113	PRO	3.9
1	B	422	GLY	3.9
1	B	529	PRO	3.9
1	A	179	TYR	3.9
1	B	10	TYR	3.9
1	A	144	ASP	3.9
1	B	268	GLY	3.9
1	B	417	GLN	3.9
1	B	419	GLN	3.9
1	A	215	VAL	3.8
1	B	153	VAL	3.8
1	B	108	TYR	3.8
1	B	500	GLY	3.8
1	B	516	LYS	3.8
1	B	6	ALA	3.8
1	B	379	PRO	3.8
1	B	441	PHE	3.8
1	B	373	GLY	3.8
1	A	168	SER	3.8
1	A	143	ASN	3.8
1	B	39	ALA	3.8
1	B	88	MET	3.8
1	B	114	PRO	3.8
1	B	402	PRO	3.8
1	B	178	GLY	3.8
1	A	74	GLN	3.8
1	B	351	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	93	SER	3.8
1	B	209	ALA	3.8
1	B	150	LEU	3.8
1	B	157	ASP	3.8
1	B	520	VAL	3.8
1	A	26	ASN	3.7
1	B	342	ALA	3.7
1	A	473	ASP	3.7
1	A	134	PRO	3.7
1	A	73	GLN	3.7
1	B	127	SER	3.7
1	B	189	SER	3.7
1	B	343	ASN	3.7
1	B	396	SER	3.7
1	B	487	ASN	3.7
1	B	287	ALA	3.7
1	A	157	ASP	3.7
1	B	380	LYS	3.7
1	B	492	GLU	3.7
1	A	292	PRO	3.7
1	B	186	MET	3.7
1	B	53	VAL	3.7
1	B	386	SER	3.7
1	B	433	SER	3.7
1	B	476	GLU	3.7
1	B	97	LEU	3.7
1	B	92	GLY	3.7
1	B	37	ASN	3.7
1	B	168	SER	3.7
1	B	30	ASP	3.7
1	A	103	THR	3.7
1	B	244	ALA	3.7
1	B	79	LEU	3.6
1	A	17	VAL	3.6
1	A	174	VAL	3.6
1	A	139	LYS	3.6
1	B	411	LYS	3.6
1	A	254	ASP	3.6
1	B	165	ASP	3.6
1	B	20	ALA	3.6
1	B	31	MET	3.6
1	B	474	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	120	GLY	3.6
1	A	534	ASN	3.6
1	B	330	GLY	3.6
1	B	485	GLU	3.6
1	A	172	VAL	3.6
1	B	154	THR	3.6
1	A	148	PRO	3.6
1	B	145	LEU	3.6
1	A	431	LYS	3.6
1	A	446	ARG	3.6
1	B	137	ARG	3.6
1	A	25	THR	3.6
1	B	112	THR	3.6
1	B	341	ALA	3.6
1	A	280	PRO	3.6
1	A	474	LEU	3.6
1	B	198	ARG	3.6
1	A	34	SER	3.6
1	B	388	SER	3.6
1	B	22	VAL	3.5
1	B	521	VAL	3.5
1	A	196	ILE	3.5
1	B	161	ILE	3.5
1	A	497	VAL	3.5
1	B	537	ASN	3.5
1	A	114	PRO	3.5
1	B	365	GLY	3.5
1	B	382	GLY	3.5
1	B	192	TYR	3.5
1	A	126	GLU	3.5
1	B	286	ILE	3.5
1	A	207	LEU	3.5
1	A	531	GLY	3.5
1	B	448	SER	3.5
1	B	105	MET	3.5
1	B	50	CYS	3.5
1	A	235	TYR	3.5
1	B	55	ARG	3.5
1	A	542	VAL	3.5
1	B	85	PRO	3.4
1	B	49	GLY	3.4
1	B	425	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	438	ASP	3.4
1	B	470	GLU	3.4
1	B	366	LYS	3.4
1	A	9	GLN	3.4
1	B	270	THR	3.4
1	A	29	PRO	3.4
1	B	197	GLY	3.4
1	A	66	ASP	3.4
1	A	151	PHE	3.4
1	B	66	ASP	3.4
1	B	45	GLN	3.4
1	B	449	GLN	3.4
1	B	177	THR	3.4
1	A	302	GLY	3.4
1	B	236	GLU	3.4
1	A	543	TYR	3.4
1	B	337	TYR	3.4
1	B	271	VAL	3.4
1	B	460	ASP	3.4
1	B	511	ASP	3.4
1	B	399	GLY	3.4
1	A	202	ILE	3.4
1	A	506	ALA	3.4
1	B	58	ALA	3.4
1	B	285	ILE	3.4
1	A	41	GLN	3.4
1	B	110	GLN	3.4
1	B	294	PHE	3.4
1	B	213	THR	3.3
1	B	136	ASP	3.3
1	A	98	SER	3.3
1	B	350	VAL	3.3
1	A	45	GLN	3.3
1	A	48	ALA	3.3
1	B	374	ALA	3.3
1	A	147	LEU	3.3
1	A	258	LEU	3.3
1	A	46	ARG	3.3
1	B	170	LYS	3.3
1	B	501	LYS	3.3
1	A	240	THR	3.3
1	B	248	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	195	VAL	3.3
1	B	540	HIS	3.3
1	A	155	LEU	3.3
1	B	246	TRP	3.3
1	A	30	ASP	3.3
1	B	313	ASP	3.3
1	B	187	SER	3.3
1	A	337	TYR	3.3
1	A	536	TYR	3.3
1	A	306	LEU	3.3
1	B	499	ASN	3.3
1	B	410	TRP	3.2
1	A	15	SER	3.2
1	B	439	THR	3.2
1	B	538	THR	3.2
1	B	19	PRO	3.2
1	B	480	ARG	3.2
1	B	481	VAL	3.2
1	A	251	ALA	3.2
1	B	35	GLU	3.2
1	B	135	GLU	3.2
1	B	188	ALA	3.2
1	B	257	THR	3.2
1	A	138	PRO	3.2
1	B	525	ARG	3.2
1	A	502	ASN	3.2
1	B	534	ASN	3.2
1	A	109	ILE	3.2
1	B	381	TYR	3.2
1	B	101	GLN	3.2
1	A	136	ASP	3.2
1	B	325	PHE	3.2
1	A	21	HIS	3.2
1	A	94	SER	3.2
1	A	528	THR	3.2
1	B	201	ARG	3.2
1	A	234	GLY	3.2
1	B	256	GLU	3.2
1	B	488	LYS	3.2
1	A	404	ASN	3.2
1	B	404	ASN	3.2
1	B	276	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	489	ARG	3.2
1	B	338	PHE	3.2
1	A	112	THR	3.2
1	B	420	GLY	3.2
1	B	116	PRO	3.2
1	B	138	PRO	3.2
1	A	91	TRP	3.1
1	A	222	ILE	3.1
1	B	326	LEU	3.1
1	B	64	THR	3.1
1	B	124	MET	3.1
1	B	47	CYS	3.1
1	B	392	ASP	3.1
1	A	208	TRP	3.1
1	B	431	LYS	3.1
1	A	110	GLN	3.1
1	B	62	PRO	3.1
1	B	260	PRO	3.1
1	A	35	GLU	3.1
1	A	96	GLU	3.1
1	A	106	ALA	3.1
1	B	360	ALA	3.1
1	A	54	LEU	3.1
1	B	21	HIS	3.1
1	A	213	THR	3.1
1	B	489	ARG	3.1
1	B	38	GLU	3.1
1	B	455	ASP	3.1
1	B	51	HIS	3.1
1	B	129	LYS	3.1
1	B	69	GLN	3.1
1	B	531	GLY	3.0
1	A	257	THR	3.0
1	B	442	ASN	3.0
1	B	24	ARG	3.0
1	A	176	ASP	3.0
1	B	327	HIS	3.0
1	B	378	HIS	3.0
1	A	129	LYS	3.0
1	A	133	LYS	3.0
1	A	16	ALA	3.0
1	A	298	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	147	LEU	3.0
1	B	174	VAL	3.0
1	B	220	ILE	3.0
1	B	230	SER	3.0
1	B	156	ARG	3.0
1	B	490	GLY	3.0
1	A	68	THR	3.0
1	A	117	PRO	3.0
1	B	324	PRO	3.0
1	A	523	ASP	3.0
1	B	405	HIS	3.0
1	A	58	ALA	3.0
1	A	200	ALA	3.0
1	A	209	ALA	3.0
1	A	244	ALA	3.0
1	B	9	GLN	3.0
1	B	160	GLN	3.0
1	B	54	LEU	3.0
1	B	59	THR	3.0
1	B	301	THR	3.0
1	A	401	ASP	3.0
1	B	254	ASP	3.0
1	A	516	LYS	3.0
1	A	44	PHE	3.0
1	A	469	ALA	3.0
1	B	71	ARG	3.0
1	A	453	VAL	3.0
1	A	521	VAL	3.0
1	B	542	VAL	3.0
1	A	72	GLY	3.0
1	B	340	THR	3.0
1	B	401	ASP	3.0
1	B	359	SER	2.9
1	A	190	GLY	2.9
1	B	166	GLY	2.9
1	B	462	LYS	2.9
1	A	538	THR	2.9
1	B	528	THR	2.9
1	B	182	HIS	2.9
1	B	289	HIS	2.9
1	A	19	PRO	2.9
1	A	430	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	105	MET	2.9
1	B	128	TRP	2.9
1	A	100	GLU	2.9
1	A	261	LYS	2.9
1	A	154	THR	2.9
1	A	239	TYR	2.9
1	B	232	PHE	2.9
1	A	93	SER	2.9
1	A	537	ASN	2.9
1	B	143	ASN	2.9
1	B	479	LYS	2.9
1	B	48	ALA	2.9
1	A	255	GLY	2.9
1	A	509	VAL	2.9
1	A	535	VAL	2.9
1	B	311	ASP	2.9
1	A	263	ILE	2.9
1	B	295	ILE	2.9
1	B	77	GLU	2.9
1	B	427	LYS	2.9
1	A	246	TRP	2.9
1	A	237	ASP	2.8
1	B	163	LEU	2.8
1	B	503	ASP	2.8
1	A	31	MET	2.8
1	A	125	ARG	2.8
1	A	53	VAL	2.8
1	B	164	VAL	2.8
1	A	69	GLN	2.8
1	A	92	GLY	2.8
1	A	519	ALA	2.8
1	B	444	ASP	2.8
1	B	258	LEU	2.8
1	A	256	GLU	2.8
1	B	348	VAL	2.8
1	B	332	ASP	2.8
1	A	87	GLY	2.8
1	A	20	ALA	2.8
1	A	38	GLU	2.8
1	A	89	PRO	2.8
1	A	116	PRO	2.8
1	A	132	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	132	VAL	2.8
1	B	56	LYS	2.8
1	B	183	ILE	2.8
1	B	275	THR	2.8
1	B	400	THR	2.8
1	B	403	LYS	2.8
1	A	122	PRO	2.8
1	A	47	CYS	2.8
1	B	252	ILE	2.8
1	A	498	TRP	2.8
1	A	226	SER	2.7
1	B	15	SER	2.7
1	B	415	GLU	2.7
1	B	530	THR	2.7
1	B	383	PRO	2.7
1	A	413	VAL	2.7
1	A	124	MET	2.7
1	A	504	SER	2.7
1	B	328	ASP	2.7
1	A	36	PHE	2.7
1	B	224	ALA	2.7
1	A	149	ASN	2.7
1	B	149	ASN	2.7
1	B	100	GLU	2.7
1	B	222	ILE	2.7
1	B	355	ASP	2.7
1	B	185	ARG	2.7
1	A	266	THR	2.7
1	A	358	LEU	2.7
1	B	121	MET	2.7
1	A	175	ILE	2.7
1	B	440	THR	2.6
1	A	289	HIS	2.6
1	B	352	ASP	2.6
1	A	173	LYS	2.6
1	B	508	VAL	2.6
1	B	407	GLN	2.6
1	A	470	GLU	2.6
1	A	224	ALA	2.6
1	B	216	ALA	2.6
1	A	76	LEU	2.6
1	A	294	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	139	LYS	2.6
1	B	432	SER	2.6
1	B	191	ARG	2.6
1	B	356	ARG	2.6
1	B	539	GLN	2.6
1	A	253	MET	2.6
1	A	162	ALA	2.6
1	A	443	PRO	2.6
1	B	107	LYS	2.6
1	B	140	LYS	2.6
1	B	173	LYS	2.6
1	A	460	ASP	2.6
1	B	361	LEU	2.6
1	A	137	ARG	2.6
1	A	187	SER	2.6
1	A	525	ARG	2.6
1	B	353	SER	2.6
1	A	350	VAL	2.6
1	B	282	VAL	2.6
1	A	166	GLY	2.6
1	A	310	LYS	2.6
1	A	64	THR	2.6
1	A	180	ALA	2.6
1	B	16	ALA	2.6
1	B	251	ALA	2.6
1	B	541	ASP	2.6
1	B	152	SER	2.6
1	A	508	VAL	2.5
1	B	196	ILE	2.5
1	B	227	VAL	2.5
1	B	264	VAL	2.5
1	A	159	GLY	2.5
1	A	499	ASN	2.5
1	B	267	ARG	2.5
1	A	505	SER	2.5
1	B	496	SER	2.5
1	B	204	MET	2.5
1	A	264	VAL	2.5
1	B	205	ILE	2.5
1	B	218	ILE	2.5
1	B	61	LYS	2.5
1	B	336	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	177	THR	2.5
1	B	33	GLU	2.5
1	B	322	ALA	2.5
1	B	339	MET	2.5
1	B	371	GLY	2.5
1	B	125	ARG	2.5
1	B	263	ILE	2.5
1	B	458	ASN	2.5
1	A	81	THR	2.5
1	A	287	ALA	2.5
1	A	409	ALA	2.5
1	A	472	ALA	2.5
1	B	306	LEU	2.5
1	B	210	LYS	2.5
1	B	372	ARG	2.5
1	B	57	GLY	2.5
1	B	331	TRP	2.5
1	A	67	ILE	2.5
1	A	384	VAL	2.4
1	A	33	GLU	2.4
1	B	94	SER	2.4
1	B	414	ALA	2.4
1	B	231	LYS	2.4
1	B	12	GLY	2.4
1	A	343	ASN	2.4
1	A	220	ILE	2.4
1	A	304	VAL	2.4
1	B	241	ILE	2.4
1	A	433	SER	2.4
1	B	184	SER	2.4
1	B	235	TYR	2.4
1	B	253	MET	2.4
1	A	341	ALA	2.4
1	A	478	ALA	2.4
1	A	488	LYS	2.4
1	B	349	ALA	2.4
1	B	522	LYS	2.4
1	A	475	GLY	2.4
1	B	44	PHE	2.4
1	A	165	ASP	2.4
1	A	313	ASP	2.4
1	B	206	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	237	ASP	2.4
1	A	252	ILE	2.4
1	B	362	VAL	2.4
1	A	192	TYR	2.4
1	A	260	PRO	2.4
1	B	111	HIS	2.4
1	A	414	ALA	2.4
1	B	159	GLY	2.4
1	A	250	PHE	2.4
1	A	121	MET	2.4
1	B	130	VAL	2.4
1	B	307	VAL	2.4
1	A	219	LYS	2.4
1	B	119	TRP	2.4
1	B	277	HIS	2.4
1	B	96	GLU	2.3
1	A	156	ARG	2.3
1	A	325	PHE	2.3
1	B	36	PHE	2.3
1	A	540	HIS	2.3
1	B	335	HIS	2.3
1	A	123	GLU	2.3
1	B	89	PRO	2.3
1	B	367	THR	2.3
1	B	211	GLU	2.3
1	A	188	ALA	2.3
1	B	179	TYR	2.3
1	B	255	GLY	2.3
1	A	204	MET	2.3
1	A	522	LYS	2.3
1	A	195	VAL	2.3
1	A	82	TYR	2.3
1	A	193	LEU	2.3
1	A	486	TYR	2.3
1	A	503	ASP	2.3
1	B	193	LEU	2.3
1	A	111	HIS	2.3
1	B	8	GLU	2.3
1	B	250	PHE	2.3
1	A	80	ILE	2.3
1	A	181	VAL	2.3
1	A	377	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	324	PRO	2.3
1	A	529	PRO	2.3
1	A	363	ASP	2.3
1	B	133	LYS	2.3
1	B	272	ASP	2.3
1	B	347	LYS	2.3
1	A	315	LEU	2.3
1	A	370	PRO	2.2
1	B	412	LYS	2.2
1	B	199	ASP	2.2
1	A	243	GLY	2.2
1	A	286	ILE	2.2
1	A	314	ASN	2.2
1	A	524	PRO	2.2
1	B	278	PRO	2.2
1	B	221	GLY	2.2
1	B	13	ALA	2.2
1	A	194	LEU	2.2
1	A	141	GLN	2.2
1	A	309	TYR	2.2
1	A	231	LYS	2.2
1	A	347	LYS	2.2
1	A	113	PRO	2.2
1	A	484	PRO	2.2
1	A	481	VAL	2.2
1	A	293	GLU	2.2
1	A	101	GLN	2.2
1	A	158	ALA	2.2
1	A	515	LEU	2.2
1	B	269	MET	2.2
1	A	85	PRO	2.1
1	A	167	ASP	2.2
1	B	273	THR	2.2
1	A	42	ILE	2.1
1	B	126	GLU	2.1
1	A	185	ARG	2.1
1	A	198	ARG	2.1
1	A	225	ARG	2.1
1	B	305	LEU	2.1
1	B	358	LEU	2.1
1	A	496	SER	2.1
1	B	319	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	276	TYR	2.1
1	B	203	ASP	2.1
1	A	439	THR	2.1
1	B	266	THR	2.1
1	B	274	GLN	2.1
1	A	533	PHE	2.1
1	A	277	HIS	2.1
1	A	63	LEU	2.1
1	A	135	GLU	2.1
1	B	502	ASN	2.1
1	B	43	TYR	2.1
1	B	368	PRO	2.1
1	A	24	ARG	2.1
1	A	284	ALA	2.1
1	B	176	ASP	2.1
1	B	491	ASP	2.1
1	A	262	GLN	2.1
1	A	357	ARG	2.1
1	B	357	ARG	2.1
1	A	197	GLY	2.1
1	B	190	GLY	2.1
1	A	14	ALA	2.1
1	A	229	SER	2.1
1	A	452	ALA	2.1
1	B	7	ALA	2.1
1	A	442	ASN	2.0
1	A	51	HIS	2.0
1	A	62	PRO	2.0
1	B	310	LYS	2.0
1	A	437	VAL	2.0
1	B	11	GLN	2.0
1	B	115	GLN	2.0
1	B	315	LEU	2.0
1	A	311	ASP	2.0
1	A	238	ARG	2.0
1	A	369	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

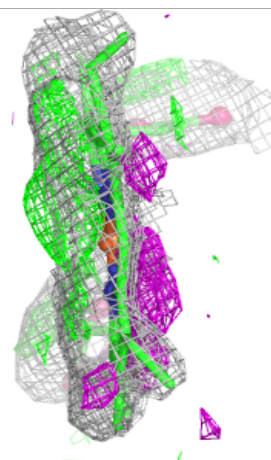
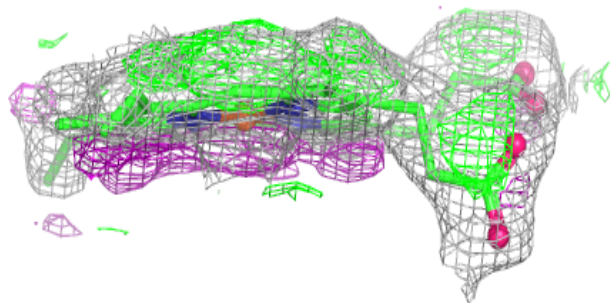
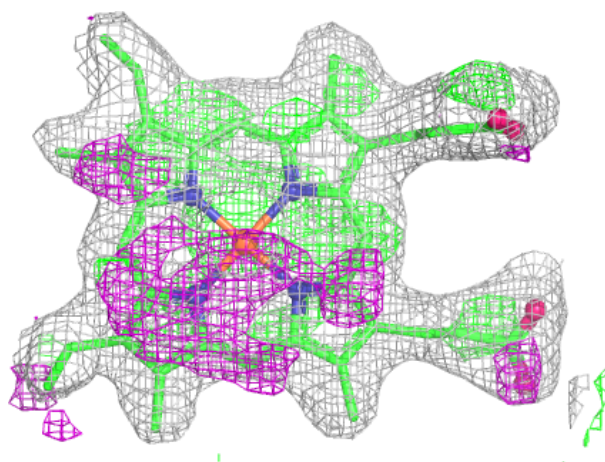
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	OH	B	603	1/1	0.44	0.40	39,39,39,39	0
2	PO4	A	604	5/5	0.73	0.19	75,75,78,78	0
5	HEC	B	601	43/43	0.77	0.24	24,31,34,41	0
2	PO4	B	604	5/5	0.83	0.15	82,82,84,85	0
3	CL	A	605	1/1	0.83	0.13	28,28,28,28	0
6	DHE	B	602	49/49	0.84	0.18	25,30,39,50	0
5	HEC	A	601	43/43	0.89	0.16	24,29,38,42	0
6	DHE	A	602	49/49	0.90	0.14	22,29,36,47	0
4	OH	A	603	1/1	0.93	0.28	36,36,36,36	0
3	CL	B	605	1/1	0.93	0.08	27,27,27,27	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.

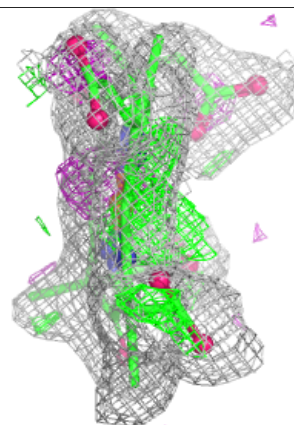
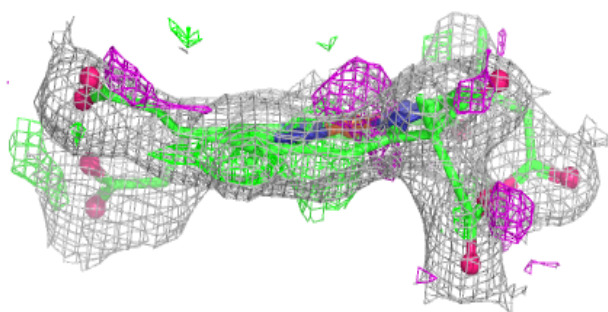
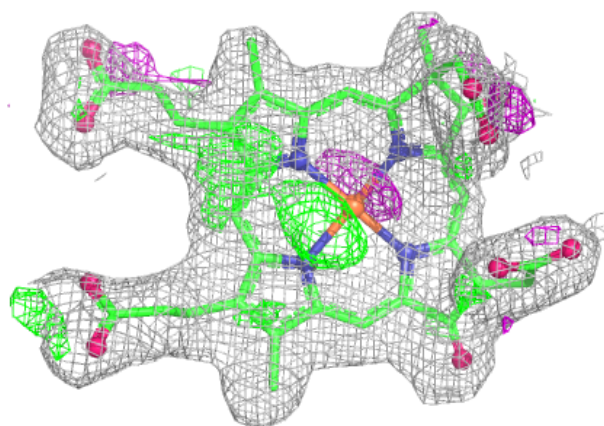
Electron density around HEC B 601:

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



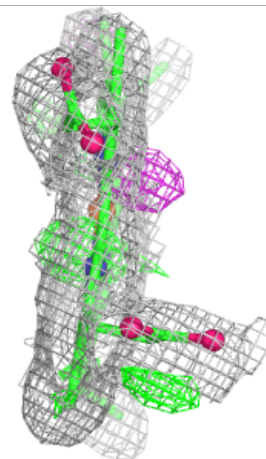
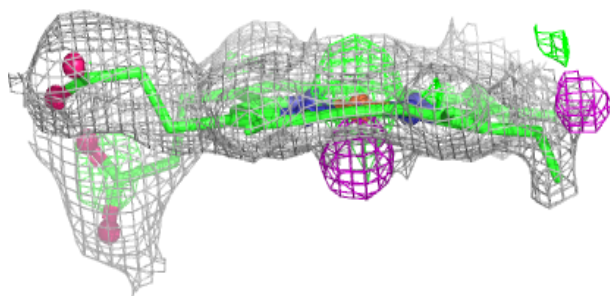
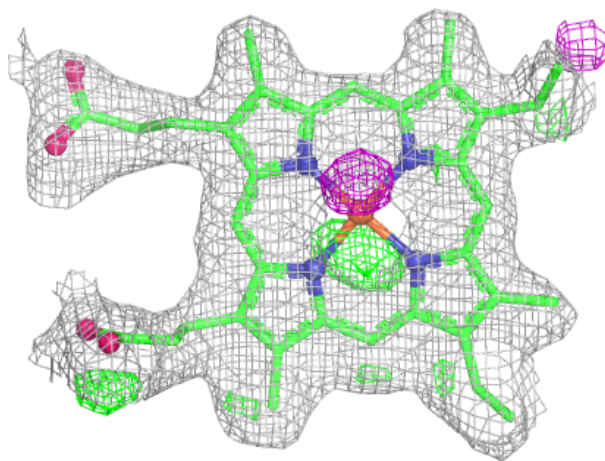
Electron density around DHE B 602:

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



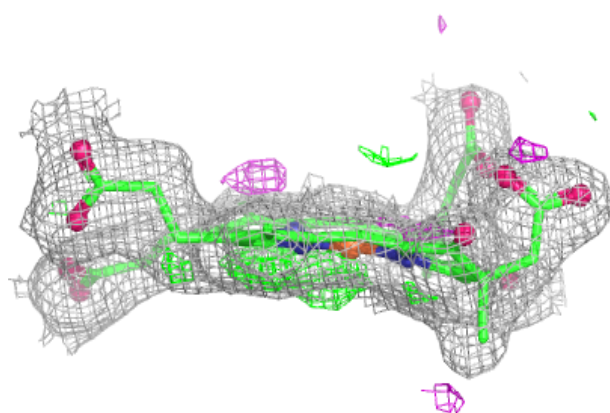
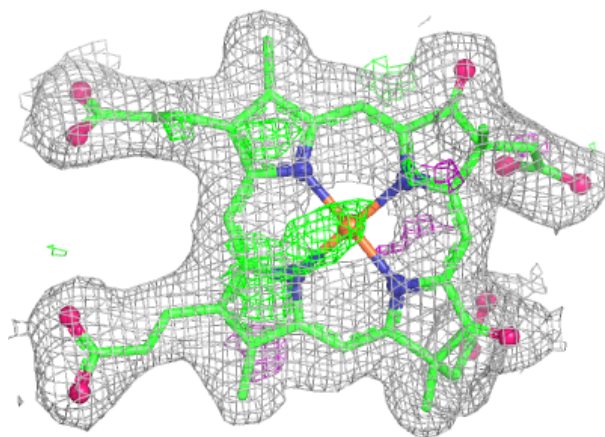
Electron density around HEC A 601:

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



Electron density around DHE A 602:

$2mF_o-DF_c$ (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.