



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 11:55 PM EDT

PDB ID : 1N5U / pdb_00001n5u
Title : X-RAY STUDY OF HUMAN SERUM ALBUMIN COMPLEXED WITH
HEME
Authors : Wardell, M.; Wang, Z.; Ho, J.X.; Robert, J.; Ruker, F.; Ruble, J.; Carter,
D.C.
Deposited on : 2002-11-07
Resolution : 1.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

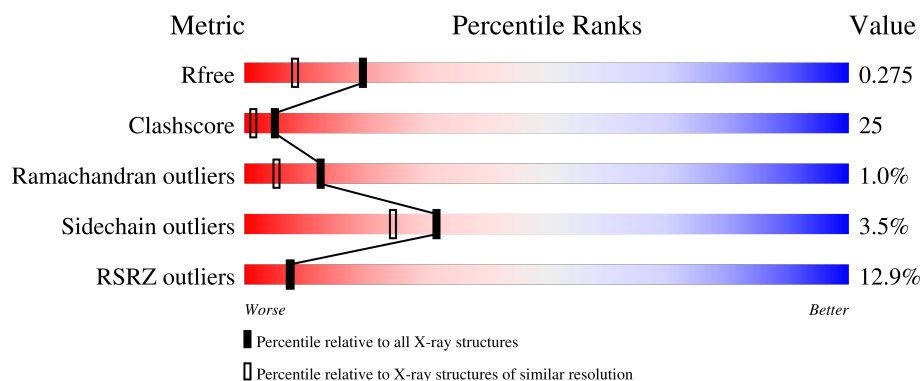
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	585	13% 59% 37% .

2 Entry composition [i](#)

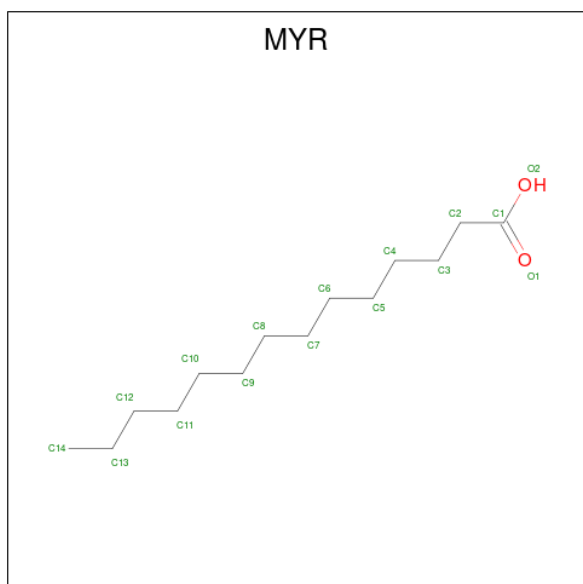
There are 4 unique types of molecules in this entry. The entry contains 5186 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERUM ALBUMIN.

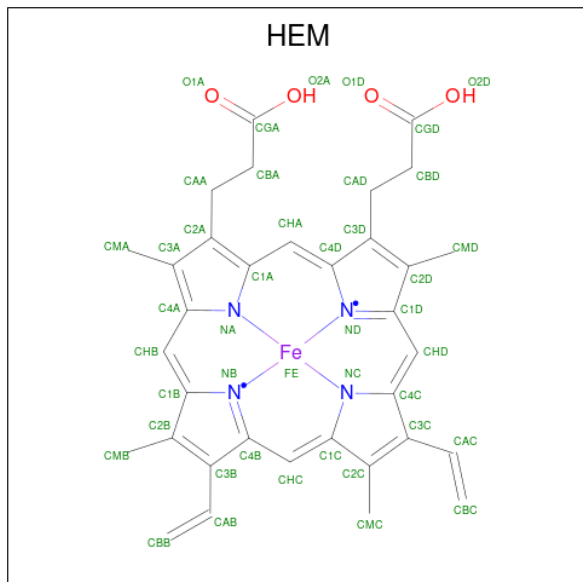
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	0	0
			4635	2926	784	884	41			

- Molecule 2 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

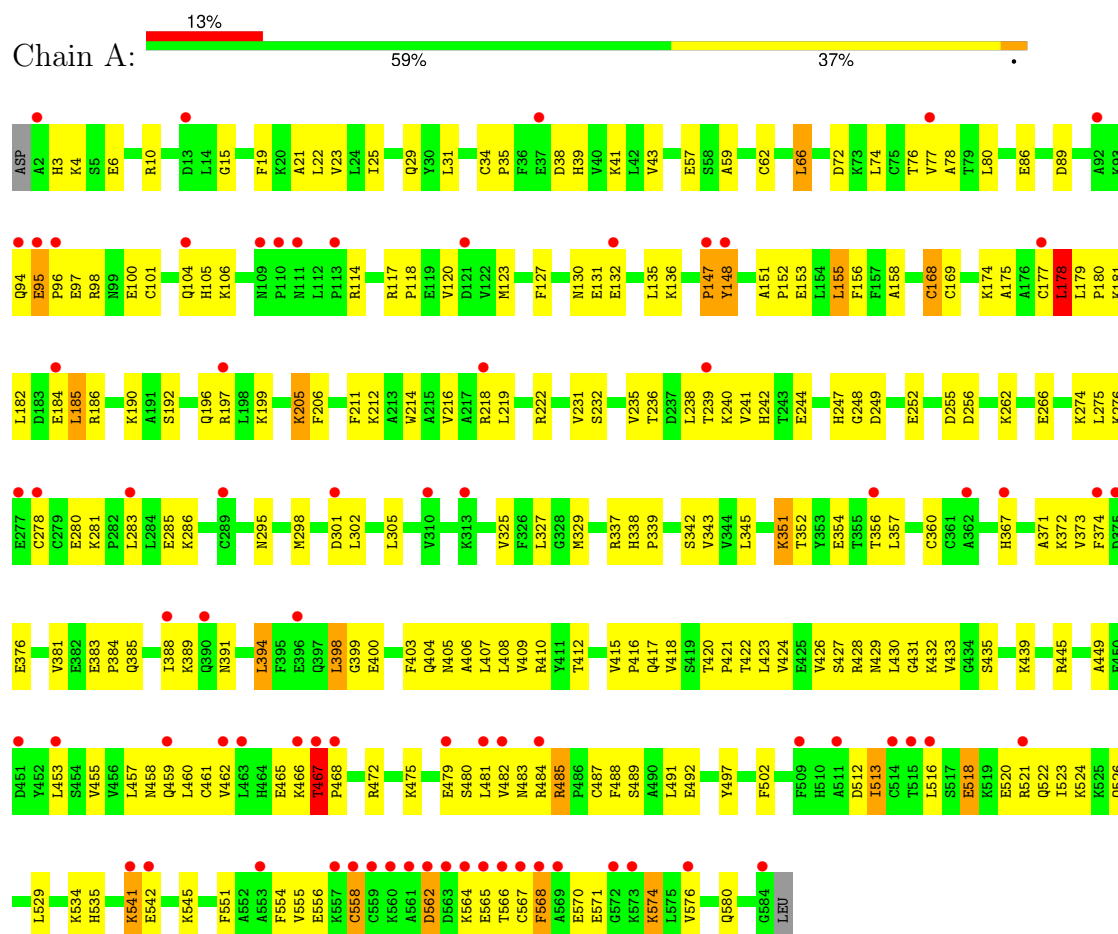
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	428	Total O 428 428	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: SERUM ALBUMIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.12Å 37.91Å 94.83Å 90.00° 105.04° 90.00°	Depositor
Resolution (Å)	45.81 – 1.90 45.81 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.0 (45.81-1.90) 88.1 (45.81-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 1.89Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, R_{free}	0.235 , 0.280 0.230 , 0.275	Depositor DCC
R_{free} test set	2282 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5186	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.38	0/4725	0.90	16/6373 (0.3%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	GLU	N-CA-C	-8.52	100.93	112.94
1	A	248	GLY	N-CA-C	7.42	124.56	114.92
1	A	360	CYS	N-CA-C	7.17	119.09	111.28
1	A	178	LEU	N-CA-C	6.93	118.72	111.03
1	A	147	PRO	N-CA-C	-6.83	100.47	111.19
1	A	15	GLY	N-CA-C	-6.56	104.55	112.48
1	A	342	SER	N-CA-C	-6.23	102.13	110.55
1	A	399	GLY	N-CA-C	-5.83	105.76	112.29
1	A	78	ALA	N-CA-C	5.83	118.10	111.11
1	A	168	CYS	N-CA-C	5.80	118.54	111.82
1	A	205	LYS	N-CA-C	5.76	117.64	111.36
1	A	338	HIS	N-CA-C	5.69	118.96	108.94
1	A	339	PRO	N-CA-C	-5.64	107.09	114.03
1	A	445	ARG	N-CA-C	5.47	117.32	111.36
1	A	568	PHE	N-CA-C	-5.41	106.81	113.41
1	A	286	LYS	N-CA-C	5.34	117.54	111.02

There are no chirality outliers.

There are no planarity outliers.

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	4635	0	4557	236	0
2	A	80	0	135	17	0
3	A	43	0	30	4	0
4	A	428	0	0	14	0
All	All	5186	0	4722	236	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 25.

All (236) 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:466:LYS:H	1:A:466:LYS:HE2	1.38	0.86
1:A:418:VAL:HG11	2:A:1004:MYR:H141	1.56	0.86
1:A:516:LEU:HD12	1:A:520:GLU:HB3	1.57	0.84
1:A:96:PRO:HG2	1:A:97:GLU:OE2	1.78	0.84
1:A:236:THR:O	1:A:239:THR:HG22	1.78	0.83
1:A:567:CYS:O	1:A:571:GLU:HB2	1.77	0.83
1:A:467:THR:H	1:A:468:PRO:CD	1.92	0.83
1:A:222:ARG:HD3	1:A:295:ASN:HD22	1.41	0.83
1:A:428:ARG:HH21	1:A:526:GLN:HE22	1.26	0.81
1:A:467:THR:H	1:A:468:PRO:HD3	1.45	0.80
1:A:232:SER:O	1:A:235:VAL:HG22	1.81	0.80
1:A:429:ASN:HD22	1:A:432:LYS:NZ	1.79	0.80
1:A:466:LYS:HE2	1:A:466:LYS:N	1.97	0.80
1:A:403:PHE:O	1:A:407:LEU:HD13	1.84	0.77
1:A:488:PHE:HA	1:A:491:LEU:HD23	1.67	0.76
1:A:430:LEU:O	1:A:433:VAL:HG12	1.87	0.75
1:A:467:THR:N	1:A:468:PRO:CD	2.48	0.75
1:A:385:GLN:O	1:A:388:ILE:HG13	1.86	0.75
1:A:562:ASP:HB2	1:A:564:LYS:HZ2	1.51	0.74
1:A:488:PHE:HA	1:A:491:LEU:CD2	2.18	0.74
1:A:77:VAL:HG21	1:A:80:LEU:HD13	1.70	0.73
1:A:23:VAL:HG22	2:A:1002:MYR:H122	1.70	0.73
1:A:77:VAL:HG23	1:A:80:LEU:HB2	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ASP:O	1:A:516:LEU:HD23	1.91	0.70
1:A:405:ASN:HD21	1:A:526:GLN:HG2	1.58	0.69
1:A:562:ASP:HB2	1:A:564:LYS:NZ	2.07	0.69
1:A:472:ARG:HH21	1:A:472:ARG:HG3	1.57	0.68
1:A:400:GLU:O	1:A:404:GLN:HG3	1.95	0.67
1:A:100:GLU:OE2	1:A:247:HIS:HE1	1.77	0.67
1:A:455:VAL:O	1:A:459:GLN:HG2	1.95	0.67
1:A:429:ASN:HA	1:A:432:LYS:HZ3	1.58	0.66
1:A:147:PRO:O	1:A:148:TYR:HB2	1.94	0.66
1:A:158:ALA:HA	3:A:605:HEM:HAB	1.77	0.66
1:A:488:PHE:HB3	2:A:1004:MYR:H61	1.76	0.65
1:A:101:CYS:O	1:A:105:HIS:HD2	1.78	0.65
1:A:571:GLU:O	1:A:574:LYS:HG2	1.96	0.65
1:A:298:MET:HE3	1:A:302:LEU:HD12	1.78	0.65
1:A:405:ASN:ND2	1:A:526:GLN:HG2	2.11	0.65
1:A:117:ARG:HH21	1:A:179:LEU:HD12	1.60	0.64
1:A:526:GLN:HB2	4:A:1381:HOH:O	1.97	0.64
1:A:86:GLU:OE1	1:A:105:HIS:HE1	1.81	0.63
1:A:394:LEU:CD2	1:A:398:LEU:HD22	2.29	0.63
1:A:275:LEU:HG	4:A:1279:HOH:O	1.99	0.63
1:A:429:ASN:HA	1:A:432:LYS:NZ	2.14	0.62
1:A:475:LYS:O	1:A:479:GLU:HG2	1.99	0.62
1:A:394:LEU:HD22	1:A:398:LEU:HD22	1.80	0.62
1:A:415:VAL:HG23	1:A:415:VAL:O	1.99	0.62
1:A:381:VAL:O	1:A:384:PRO:HD2	2.00	0.62
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.82	0.62
1:A:576:VAL:O	1:A:580:GLN:HG3	2.00	0.62
1:A:238:LEU:O	1:A:241:VAL:HG22	2.00	0.61
1:A:199:LYS:HB3	1:A:242:HIS:HE1	1.64	0.61
1:A:429:ASN:ND2	1:A:432:LYS:NZ	2.47	0.61
1:A:513:ILE:CD1	1:A:521:ARG:HG3	2.31	0.60
1:A:576:VAL:HG12	1:A:580:GLN:NE2	2.17	0.60
1:A:35:PRO:HD2	1:A:38:ASP:OD1	2.01	0.60
1:A:175:ALA:O	1:A:179:LEU:HD23	2.02	0.60
1:A:433:VAL:HG21	1:A:453:LEU:CD2	2.32	0.60
1:A:77:VAL:CG2	1:A:80:LEU:HD13	2.32	0.59
1:A:480:SER:OG	1:A:482:VAL:HG22	2.02	0.59
1:A:6:GLU:HB3	1:A:66:LEU:HD23	1.83	0.59
1:A:460:LEU:HG	4:A:1233:HOH:O	2.02	0.59
1:A:278:CYS:SG	1:A:281:LYS:HD2	2.41	0.59
1:A:352:THR:O	1:A:356:THR:HG23	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:HD22	1:A:182:LEU:HG	1.85	0.59
1:A:554:PHE:O	1:A:558:CYS:HB3	2.02	0.59
1:A:199:LYS:HB3	1:A:242:HIS:CE1	2.36	0.59
1:A:383:GLU:OE1	1:A:485:ARG:NH1	2.36	0.59
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.85	0.58
1:A:22:LEU:HD13	2:A:1002:MYR:H72	1.85	0.58
1:A:147:PRO:O	1:A:148:TYR:CB	2.51	0.58
1:A:576:VAL:HG12	1:A:580:GLN:HE21	1.68	0.58
1:A:416:PRO:HD2	1:A:417:GLN:HE22	1.68	0.58
1:A:262:LYS:O	1:A:266:GLU:HG3	2.03	0.58
1:A:77:VAL:CG2	1:A:80:LEU:HB2	2.33	0.58
1:A:429:ASN:ND2	1:A:432:LYS:HZ1	2.01	0.58
1:A:235:VAL:HG21	2:A:1006:MYR:H143	1.86	0.58
1:A:186:ARG:O	1:A:190:LYS:HG3	2.03	0.57
1:A:541:LYS:O	1:A:545:LYS:HG3	2.04	0.57
1:A:502:PHE:HB2	1:A:535:HIS:CE1	2.39	0.57
1:A:298:MET:HE2	4:A:1162:HOH:O	2.04	0.57
1:A:428:ARG:HH22	1:A:522:GLN:HE21	1.53	0.57
1:A:388:ILE:HG22	2:A:1003:MYR:H92	1.85	0.56
1:A:240:LYS:O	1:A:244:GLU:HG3	2.05	0.56
1:A:95:GLU:O	1:A:96:PRO:C	2.46	0.56
1:A:566:THR:O	1:A:570:GLU:HG2	2.05	0.56
1:A:337:ARG:HH21	1:A:337:ARG:HG3	1.71	0.55
1:A:244:GLU:OE1	1:A:256:ASP:OD1	2.24	0.55
1:A:74:LEU:O	1:A:77:VAL:HG22	2.06	0.55
1:A:72:ASP:O	1:A:76:THR:HG23	2.07	0.55
1:A:77:VAL:HG23	1:A:77:VAL:O	2.06	0.55
1:A:325:VAL:O	1:A:329:MET:HG3	2.07	0.55
1:A:430:LEU:O	1:A:433:VAL:CG1	2.55	0.55
1:A:238:LEU:O	1:A:238:LEU:HD23	2.07	0.55
1:A:404:GLN:HG2	1:A:431:GLY:HA3	1.89	0.55
1:A:100:GLU:O	1:A:104:GLN:HG3	2.07	0.55
1:A:372:LYS:HB3	1:A:372:LYS:NZ	2.22	0.54
1:A:351:LYS:HD3	1:A:351:LYS:C	2.31	0.54
1:A:95:GLU:O	1:A:95:GLU:OE1	2.25	0.54
1:A:97:GLU:H	1:A:97:GLU:CD	2.15	0.54
1:A:423:LEU:HD23	2:A:1004:MYR:H142	1.88	0.54
1:A:179:LEU:HD22	1:A:179:LEU:H	1.72	0.54
1:A:211:PHE:HZ	1:A:238:LEU:HD22	1.72	0.54
1:A:298:MET:CE	1:A:302:LEU:HD12	2.37	0.54
1:A:376:GLU:HB3	4:A:1175:HOH:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ASN:HD22	1:A:432:LYS:HZ1	1.54	0.54
1:A:485:ARG:HD2	2:A:1003:MYR:C4	2.38	0.54
1:A:219:LEU:HD12	1:A:235:VAL:HG12	1.89	0.53
1:A:222:ARG:HD3	1:A:295:ASN:ND2	2.18	0.53
1:A:458:ASN:HA	1:A:484:ARG:HH11	1.73	0.53
1:A:467:THR:N	1:A:468:PRO:HD3	2.14	0.53
1:A:19:PHE:O	1:A:23:VAL:HG23	2.08	0.53
1:A:118:PRO:O	1:A:123:MET:HE2	2.09	0.52
1:A:513:ILE:HD13	1:A:513:ILE:O	2.09	0.52
1:A:127:PHE:CE1	1:A:131:GLU:HG2	2.45	0.52
1:A:130:ASN:HD22	1:A:130:ASN:C	2.18	0.51
1:A:274:LYS:HB2	4:A:1279:HOH:O	2.09	0.51
1:A:95:GLU:OE1	1:A:95:GLU:C	2.53	0.50
1:A:96:PRO:HG2	1:A:97:GLU:CD	2.34	0.50
1:A:417:GLN:CD	1:A:417:GLN:H	2.18	0.50
1:A:541:LYS:HD3	1:A:542:GLU:H	1.76	0.50
1:A:179:LEU:HD22	1:A:179:LEU:N	2.26	0.50
1:A:461:CYS:HA	4:A:1233:HOH:O	2.12	0.50
1:A:120:VAL:HA	1:A:123:MET:HE3	1.94	0.50
1:A:351:LYS:HD3	1:A:351:LYS:O	2.12	0.50
1:A:66:LEU:HD13	4:A:1412:HOH:O	2.11	0.50
1:A:518:GLU:O	1:A:522:GLN:HG3	2.11	0.50
1:A:117:ARG:NH2	1:A:179:LEU:HD12	2.27	0.50
1:A:415:VAL:HG21	2:A:1004:MYR:H132	1.94	0.50
1:A:276:LYS:O	1:A:280:GLU:HG3	2.10	0.49
1:A:485:ARG:HD3	2:A:1003:MYR:O1	2.12	0.49
1:A:211:PHE:CZ	1:A:238:LEU:HD22	2.47	0.49
1:A:433:VAL:HG21	1:A:453:LEU:HD22	1.93	0.49
1:A:10:ARG:HH22	1:A:255:ASP:CG	2.21	0.49
1:A:356:THR:HG21	1:A:373:VAL:HG23	1.95	0.49
1:A:555:VAL:HG23	1:A:556:GLU:N	2.27	0.49
1:A:31:LEU:HB2	1:A:39:HIS:HE1	1.78	0.49
1:A:218:ARG:NH1	1:A:238:LEU:HD11	2.28	0.49
1:A:212:LYS:O	1:A:216:VAL:HG23	2.13	0.48
1:A:416:PRO:HD2	1:A:417:GLN:NE2	2.28	0.48
1:A:231:VAL:O	1:A:235:VAL:HG13	2.13	0.48
1:A:205:LYS:HE3	1:A:206:PHE:CZ	2.49	0.48
1:A:430:LEU:HB3	2:A:1003:MYR:C14	2.44	0.48
1:A:426:VAL:HG23	1:A:427:SER:N	2.29	0.47
1:A:462:VAL:O	1:A:465:GLU:HB3	2.15	0.47
1:A:485:ARG:HD2	2:A:1003:MYR:H41	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ILE:HD11	1:A:521:ARG:HG3	1.95	0.47
1:A:488:PHE:O	1:A:491:LEU:HD23	2.13	0.47
1:A:449:ALA:O	1:A:453:LEU:HD23	2.15	0.47
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.50	0.47
1:A:181:LYS:O	1:A:185:LEU:HD22	2.15	0.47
1:A:241:VAL:HG23	1:A:242:HIS:N	2.28	0.47
1:A:412:THR:O	1:A:416:PRO:HG3	2.13	0.47
1:A:31:LEU:HB2	1:A:39:HIS:CE1	2.50	0.47
1:A:428:ARG:HD2	1:A:523:ILE:HD13	1.96	0.47
1:A:232:SER:O	1:A:235:VAL:CG2	2.57	0.47
1:A:238:LEU:HA	1:A:241:VAL:HG22	1.97	0.47
1:A:120:VAL:CG2	1:A:179:LEU:HD21	2.45	0.46
1:A:488:PHE:CA	1:A:491:LEU:HD23	2.40	0.46
1:A:41:LYS:HE3	4:A:1322:HOH:O	2.14	0.46
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.97	0.46
1:A:391:ASN:ND2	4:A:1286:HOH:O	2.49	0.46
1:A:435:SER:O	1:A:439:LYS:HG2	2.16	0.46
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.80	0.46
1:A:241:VAL:HG12	1:A:256:ASP:HB3	1.98	0.46
1:A:466:LYS:HE2	1:A:466:LYS:CA	2.46	0.46
1:A:95:GLU:HA	1:A:98:ARG:HB3	1.98	0.46
1:A:409:VAL:HG23	1:A:410:ARG:N	2.30	0.46
1:A:416:PRO:O	1:A:534:LYS:HE2	2.17	0.45
1:A:428:ARG:HH21	1:A:526:GLN:NE2	2.05	0.45
1:A:466:LYS:C	1:A:467:THR:OG1	2.59	0.45
1:A:481:LEU:C	1:A:481:LEU:HD23	2.41	0.45
1:A:114:ARG:HG2	3:A:605:HEM:O1D	2.17	0.45
1:A:232:SER:C	1:A:235:VAL:HG22	2.41	0.45
1:A:239:THR:HG23	4:A:1044:HOH:O	2.16	0.45
1:A:416:PRO:HB2	1:A:497:TYR:CD2	2.51	0.45
1:A:132:GLU:O	1:A:136:LYS:HG2	2.17	0.44
1:A:367:HIS:O	1:A:371:ALA:HB2	2.18	0.44
1:A:39:HIS:O	1:A:43:VAL:HG23	2.17	0.44
1:A:513:ILE:HG12	1:A:524:LYS:HD3	1.99	0.44
1:A:566:THR:C	1:A:568:PHE:H	2.26	0.44
1:A:186:ARG:HD2	1:A:190:LYS:HD2	1.99	0.44
1:A:95:GLU:O	1:A:98:ARG:N	2.50	0.44
1:A:405:ASN:HD21	1:A:526:GLN:CG	2.30	0.44
1:A:457:LEU:HD21	2:A:1004:MYR:H51	2.00	0.44
1:A:420:THR:HB	1:A:421:PRO:HD3	2.00	0.44
1:A:21:ALA:HB1	1:A:155:LEU:HD11	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:HG21	1:A:179:LEU:HD21	1.99	0.44
1:A:480:SER:HB3	1:A:483:ASN:HD22	1.82	0.43
1:A:487:CYS:O	1:A:491:LEU:HD22	2.18	0.43
1:A:100:GLU:OE2	1:A:247:HIS:CE1	2.63	0.43
1:A:472:ARG:HG3	1:A:472:ARG:NH2	2.28	0.43
1:A:249:ASP:OD1	1:A:252:GLU:OE1	2.36	0.43
1:A:156:PHE:HZ	1:A:285:GLU:HA	1.84	0.43
1:A:551:PHE:O	1:A:554:PHE:HB3	2.18	0.43
1:A:86:GLU:O	1:A:89:ASP:HB2	2.18	0.43
1:A:422:THR:O	1:A:426:VAL:HG22	2.19	0.43
1:A:25:ILE:O	1:A:29:GLN:HG3	2.18	0.43
1:A:305:LEU:HD11	1:A:337:ARG:HD2	2.00	0.43
1:A:34:CYS:HA	1:A:35:PRO:HD3	1.87	0.43
1:A:190:LYS:HA	3:A:605:HEM:O2A	2.19	0.42
1:A:430:LEU:C	1:A:433:VAL:HG12	2.43	0.42
1:A:169:CYS:O	1:A:174:LYS:HE2	2.19	0.42
1:A:485:ARG:HD2	2:A:1003:MYR:H42	1.99	0.42
1:A:168:CYS:SG	1:A:177:CYS:C	3.02	0.42
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.60	0.42
1:A:388:ILE:CG2	2:A:1003:MYR:H72	2.49	0.42
1:A:424:VAL:HG11	4:A:1381:HOH:O	2.20	0.42
1:A:327:LEU:HD11	1:A:354:GLU:HG3	2.02	0.42
1:A:180:PRO:O	1:A:184:GLU:HG3	2.20	0.42
1:A:325:VAL:HG23	4:A:1046:HOH:O	2.20	0.42
1:A:408:LEU:HD23	1:A:529:LEU:HD23	2.00	0.42
1:A:492:GLU:HA	1:A:492:GLU:OE1	2.20	0.42
1:A:337:ARG:HG3	1:A:337:ARG:NH2	2.36	0.41
1:A:516:LEU:O	1:A:521:ARG:NH1	2.53	0.41
1:A:394:LEU:HD21	1:A:398:LEU:HD22	2.03	0.41
1:A:94:GLN:O	1:A:95:GLU:C	2.63	0.41
1:A:418:VAL:HG11	2:A:1004:MYR:C14	2.37	0.41
1:A:430:LEU:HB3	2:A:1003:MYR:H142	2.02	0.41
1:A:4:LYS:HB2	1:A:57:GLU:OE1	2.20	0.41
1:A:192:SER:O	1:A:196:GLN:HG3	2.21	0.41
1:A:385:GLN:O	1:A:389:LYS:HG3	2.20	0.41
1:A:415:VAL:HA	1:A:417:GLN:NE2	2.36	0.41
1:A:97:GLU:CD	1:A:97:GLU:N	2.79	0.41
1:A:222:ARG:HA	1:A:295:ASN:HD22	1.86	0.41
1:A:430:LEU:HA	1:A:433:VAL:HG12	2.02	0.41
1:A:485:ARG:HH11	1:A:489:SER:CB	2.34	0.41
1:A:283:LEU:C	1:A:283:LEU:HD23	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ALA:O	1:A:409:VAL:HG22	2.21	0.41
1:A:432:LYS:HD3	4:A:1406:HOH:O	2.20	0.41
1:A:541:LYS:NZ	1:A:542:GLU:HG2	2.36	0.40
1:A:153:GLU:HA	1:A:156:PHE:HD2	1.87	0.40
1:A:415:VAL:HA	1:A:417:GLN:HE21	1.86	0.40
1:A:118:PRO:HD2	3:A:605:HEM:HBC1	2.03	0.40
1:A:372:LYS:HZ2	1:A:372:LYS:CB	2.35	0.40
1:A:574:LYS:NZ	1:A:574:LYS:CB	2.85	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	581/585 (99%)	557 (96%)	18 (3%)	6 (1%)	12 5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	THR
1	A	3	HIS
1	A	562	ASP
1	A	148	TYR
1	A	301	ASP
1	A	558	CYS

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	509/511 (100%)	491 (96%)	18 (4%)	32	24

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	95	GLU
1	A	135	LEU
1	A	155	LEU
1	A	178	LEU
1	A	185	LEU
1	A	197	ARG
1	A	345	LEU
1	A	351	LYS
1	A	357	LEU
1	A	394	LEU
1	A	398	LEU
1	A	467	THR
1	A	485	ARG
1	A	513	ILE
1	A	518	GLU
1	A	541	LYS
1	A	574	LYS

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	18	ASN
1	A	33	GLN
1	A	39	HIS
1	A	44	ASN
1	A	94	GLN
1	A	105	HIS
1	A	130	ASN
1	A	247	HIS
1	A	268	GLN
1	A	295	ASN
1	A	405	ASN
1	A	417	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	429	ASN
1	A	483	ASN
1	A	510	HIS
1	A	522	GLN
1	A	526	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MYR	A	1002	-	15,15,15	0.70	0	15,15,15	0.74	0
2	MYR	A	1006	-	15,15,15	0.68	0	15,15,15	0.71	0
3	HEM	A	605	1	50,50,50	1.22	5 (10%)	67,82,82	1.04	2 (2%)
2	MYR	A	1003	-	15,15,15	0.64	0	15,15,15	0.68	0
2	MYR	A	1004	-	15,15,15	0.64	0	15,15,15	0.65	0
2	MYR	A	1005	-	15,15,15	0.65	0	15,15,15	0.69	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	MYR	A	1002	-	-	5/13/13/13	-
2	MYR	A	1006	-	-	6/13/13/13	-
3	HEM	A	605	1	-	5/14/54/54	-
2	MYR	A	1003	-	-	4/13/13/13	-
2	MYR	A	1004	-	-	10/13/13/13	-
2	MYR	A	1005	-	-	5/13/13/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	HEM	C2A-C3A	4.01	1.49	1.38
3	A	605	HEM	FE-ND	2.61	2.02	1.94
3	A	605	HEM	C4C-NC	-2.40	1.35	1.39
3	A	605	HEM	FE-NA	2.19	2.02	1.95
3	A	605	HEM	FE-NC	2.10	2.02	1.95

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	605	HEM	C3B-C4B-NB	4.67	112.82	109.47
3	A	605	HEM	C1A-C2A-C3A	-2.07	103.67	106.87

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	605	HEM	C2B-C3B-CAB-CBB
3	A	605	HEM	C4B-C3B-CAB-CBB
2	A	1002	MYR	C7-C8-C9-C10
2	A	1006	MYR	C4-C5-C6-C7
2	A	1002	MYR	C9-C10-C11-C12
2	A	1004	MYR	C5-C6-C7-C8
2	A	1002	MYR	C11-C10-C9-C8
2	A	1003	MYR	C11-C10-C9-C8
2	A	1006	MYR	C11-C10-C9-C8
2	A	1005	MYR	C1-C2-C3-C4
2	A	1004	MYR	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1006	MYR	C3-C4-C5-C6
2	A	1005	MYR	C6-C7-C8-C9
2	A	1002	MYR	C3-C4-C5-C6
2	A	1004	MYR	C9-C10-C11-C12
2	A	1004	MYR	C3-C4-C5-C6
2	A	1004	MYR	C7-C8-C9-C10
2	A	1005	MYR	C3-C4-C5-C6
2	A	1006	MYR	C7-C8-C9-C10
2	A	1003	MYR	C5-C6-C7-C8
2	A	1005	MYR	C9-C10-C11-C12
2	A	1004	MYR	C4-C5-C6-C7
2	A	1004	MYR	C1-C2-C3-C4
2	A	1002	MYR	C6-C7-C8-C9
2	A	1004	MYR	C6-C7-C8-C9
2	A	1003	MYR	O2-C1-C2-C3
2	A	1004	MYR	O1-C1-C2-C3
2	A	1005	MYR	C5-C6-C7-C8
2	A	1003	MYR	O1-C1-C2-C3
2	A	1004	MYR	O2-C1-C2-C3
3	A	605	HEM	CAA-CBA-CGA-O1A
3	A	605	HEM	CAA-CBA-CGA-O2A
2	A	1006	MYR	O1-C1-C2-C3
2	A	1006	MYR	O2-C1-C2-C3
3	A	605	HEM	C2C-C3C-CAC-CBC

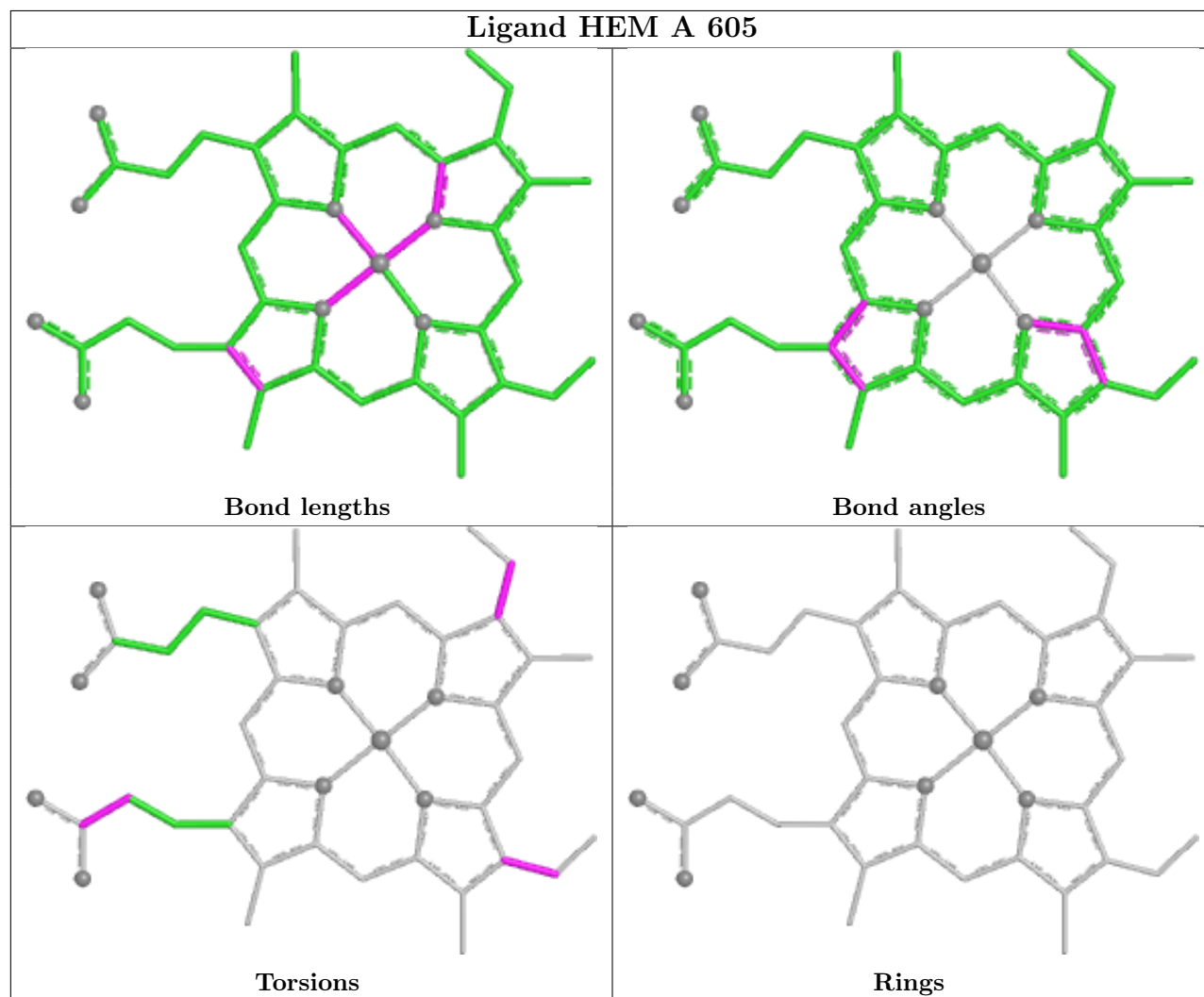
There are no ring outliers.

5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	MYR	2	0
2	A	1006	MYR	1	0
3	A	605	HEM	4	0
2	A	1003	MYR	8	0
2	A	1004	MYR	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	583/585 (99%)	0.80	75 (12%) 7 7	13, 26, 43, 79	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	567	CYS	6.6
1	A	558	CYS	6.1
1	A	564	LYS	5.9
1	A	278	CYS	5.6
1	A	561	ALA	5.5
1	A	568	PHE	4.8
1	A	557	LYS	4.7
1	A	2	ALA	4.3
1	A	562	ASP	4.2
1	A	514	CYS	4.1
1	A	95	GLU	4.1
1	A	466	LYS	4.1
1	A	566	THR	4.0
1	A	559	CYS	3.7
1	A	301	ASP	3.7
1	A	565	GLU	3.6
1	A	560	LYS	3.6
1	A	541	LYS	3.5
1	A	467	THR	3.4
1	A	563	ASP	3.4
1	A	111	ASN	3.3
1	A	96	PRO	3.2
1	A	390	GLN	3.1
1	A	584	GLY	3.1
1	A	147	PRO	3.1
1	A	388	ILE	3.0
1	A	572	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	283	LEU	2.9
1	A	374	PHE	2.8
1	A	481	LEU	2.8
1	A	197	ARG	2.8
1	A	468	PRO	2.8
1	A	451	ASP	2.7
1	A	109	ASN	2.7
1	A	148	TYR	2.7
1	A	396	GLU	2.7
1	A	479	GLU	2.6
1	A	511	ALA	2.6
1	A	104	GLN	2.6
1	A	218	ARG	2.5
1	A	13	ASP	2.5
1	A	453	LEU	2.5
1	A	553	ALA	2.5
1	A	462	VAL	2.5
1	A	184	GLU	2.4
1	A	77	VAL	2.4
1	A	310	VAL	2.4
1	A	289	CYS	2.4
1	A	542	GLU	2.3
1	A	110	PRO	2.3
1	A	94	GLN	2.3
1	A	121	ASP	2.3
1	A	515	THR	2.3
1	A	484	ARG	2.2
1	A	132	GLU	2.2
1	A	375	ASP	2.2
1	A	459	GLN	2.2
1	A	362	ALA	2.2
1	A	569	ALA	2.2
1	A	367	HIS	2.2
1	A	356	THR	2.2
1	A	177	CYS	2.2
1	A	509	PHE	2.1
1	A	239	THR	2.1
1	A	37	GLU	2.1
1	A	516	LEU	2.1
1	A	521	ARG	2.1
1	A	482	VAL	2.1
1	A	113	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	463	LEU	2.1
1	A	277	GLU	2.0
1	A	313	LYS	2.0
1	A	92	ALA	2.0
1	A	573	LYS	2.0
1	A	576	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

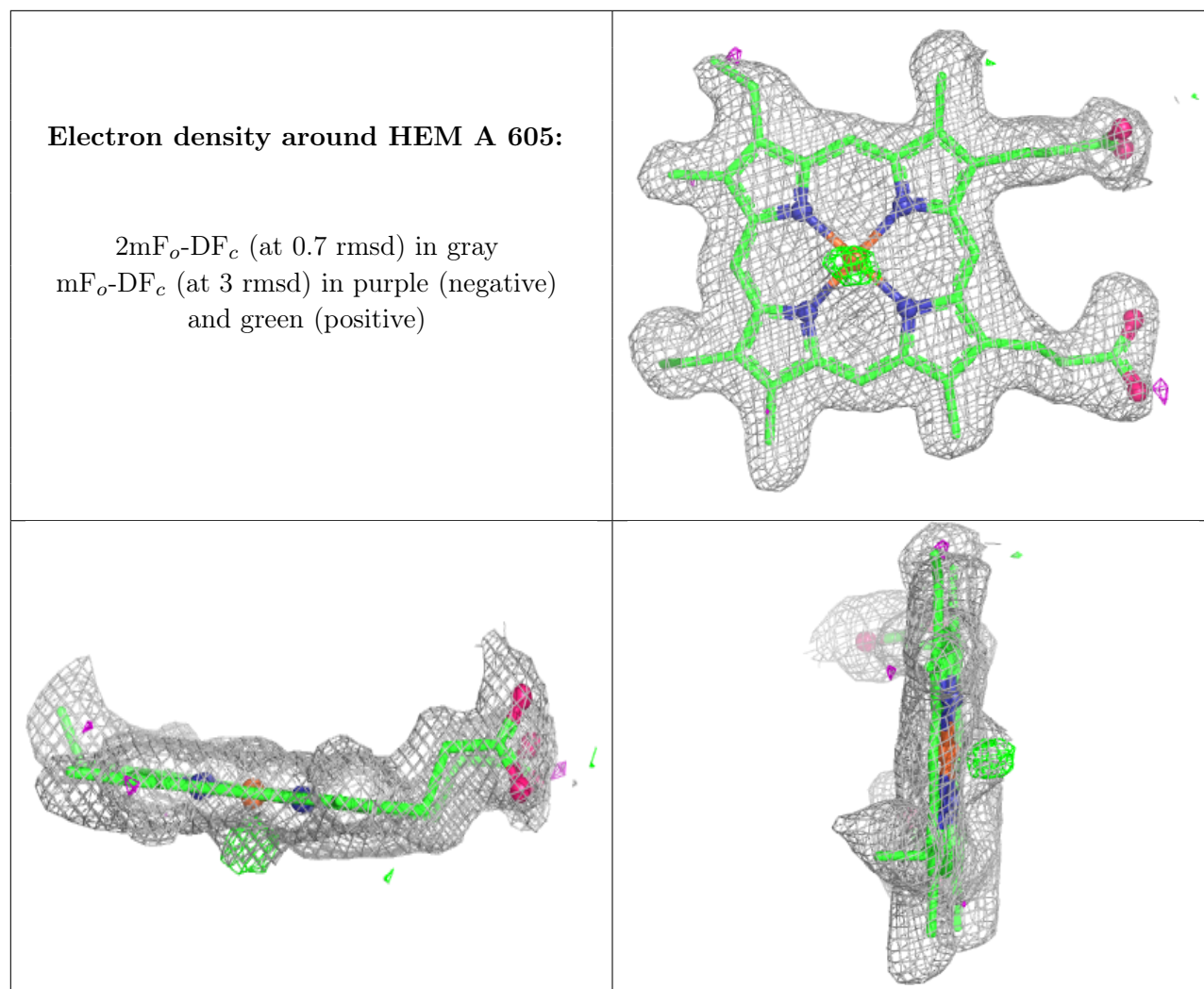
There are no oligosaccharides in this entry.

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
2	MYR	A	1004	16/16	0.77	0.29	63,64,70,70	0
2	MYR	A	1005	16/16	0.83	0.16	37,41,45,46	0
2	MYR	A	1006	16/16	0.84	0.16	47,48,52,52	0
2	MYR	A	1002	16/16	0.86	0.13	24,31,45,47	0
2	MYR	A	1003	16/16	0.90	0.12	21,29,42,42	0
3	HEM	A	605	43/43	0.94	0.11	23,26,36,38	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.