Full wwPDB X-ray Structure Validation Report (i)

Jan 30, 2024 – 09:17 PM EST

PDB ID	:	1K2S
Title	:	Structure of rat brain nNOS heme domain complexed with NG-allyl-L-arginine
Authors	:	Li, H.; Martasek, P.; Masters, B.S.S.; Poulos, T.L.; Raman, C.S.
Deposited on	:	2001-09-28
Resolution	:	2.55 Å(reported)

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

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

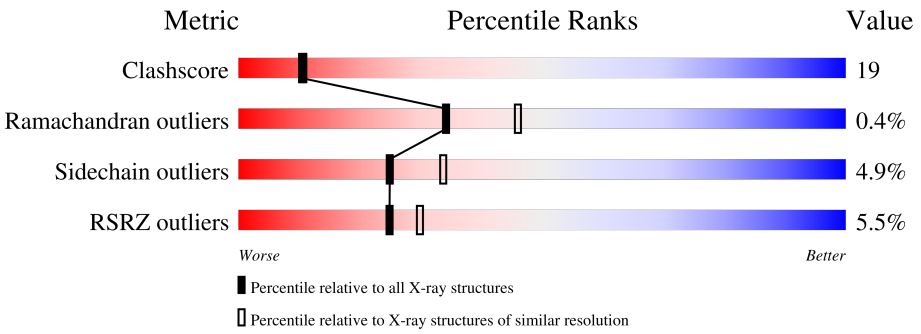
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.55 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	419	6% 59% 35%
1	B	419	5% 62% 34%

2 Entry composition (i)

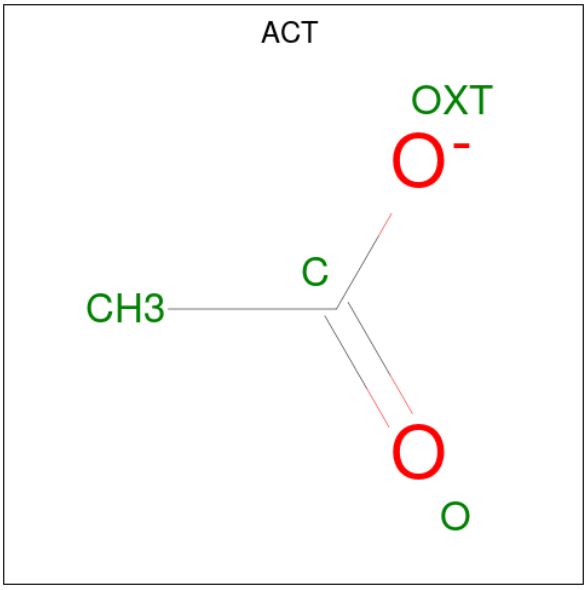
There are 7 unique types of molecules in this entry. The entry contains 7008 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	407	3313	2121	566	605	21	0	0	0
1	B	410	3341	2138	573	609	21	0	0	0

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

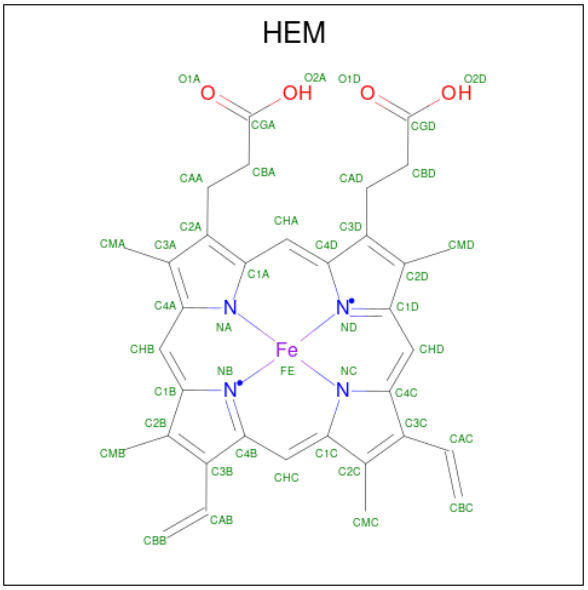


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0
2	B	1	4	2	2	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

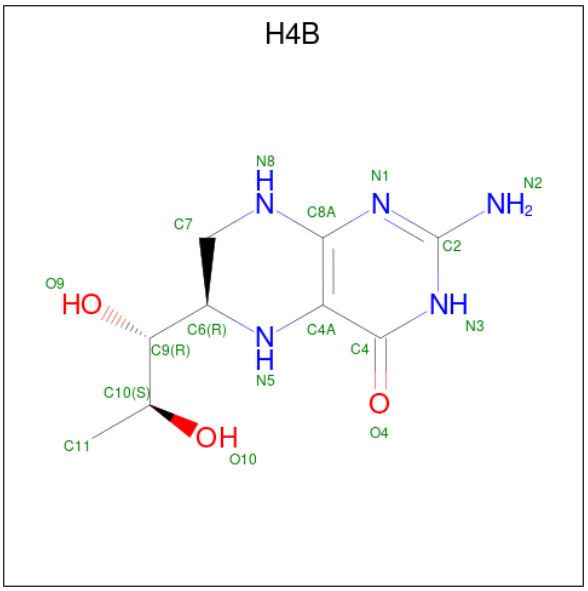
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



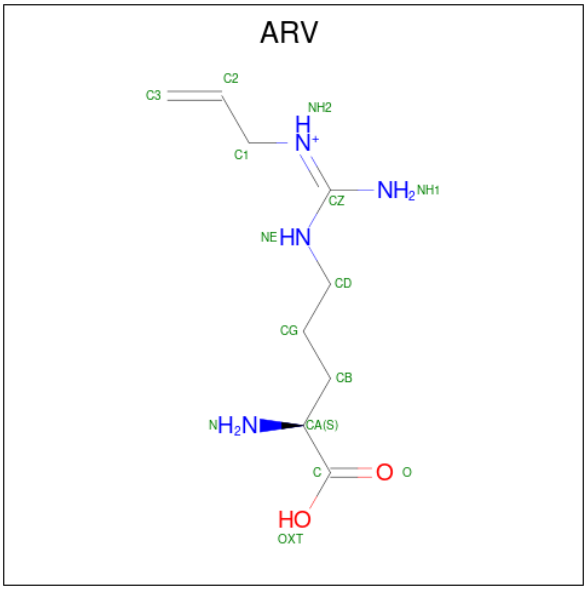
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
4	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	B	1	43	34	1	4	4	0	0

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



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

- Molecule 6 is 5-N-ALLYL-ARGININE (three-letter code: ARV) (formula: $C_9H_{19}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	15	9	4	2	0	0
6	B	1	15	9	4	2	0	0

- Molecule 7 is water.

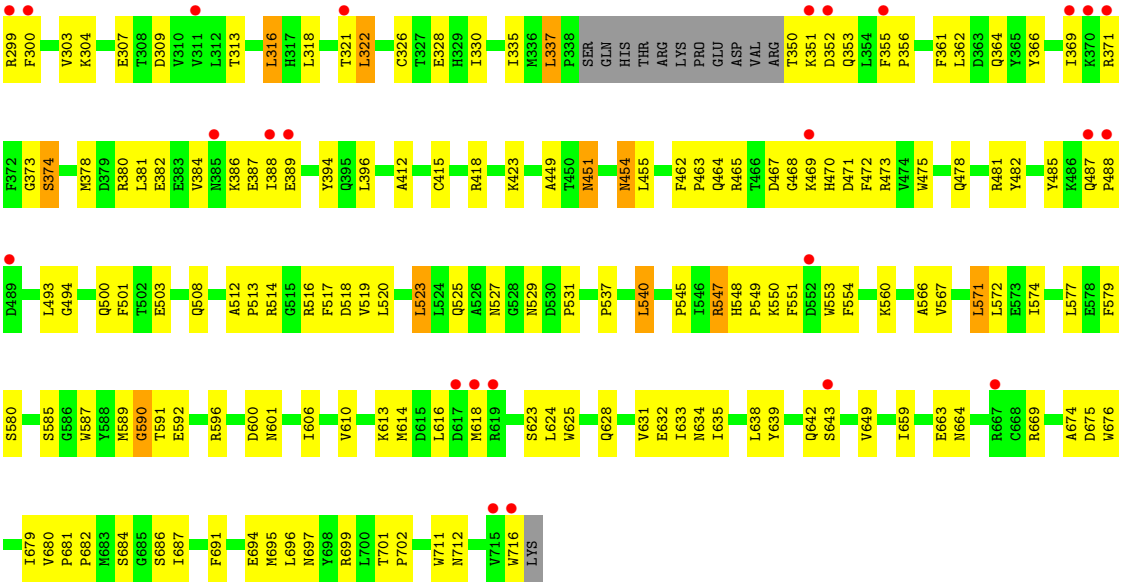
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	92	92	92	0	0
			Total	O		
7	B	103	103	103	0	0

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.

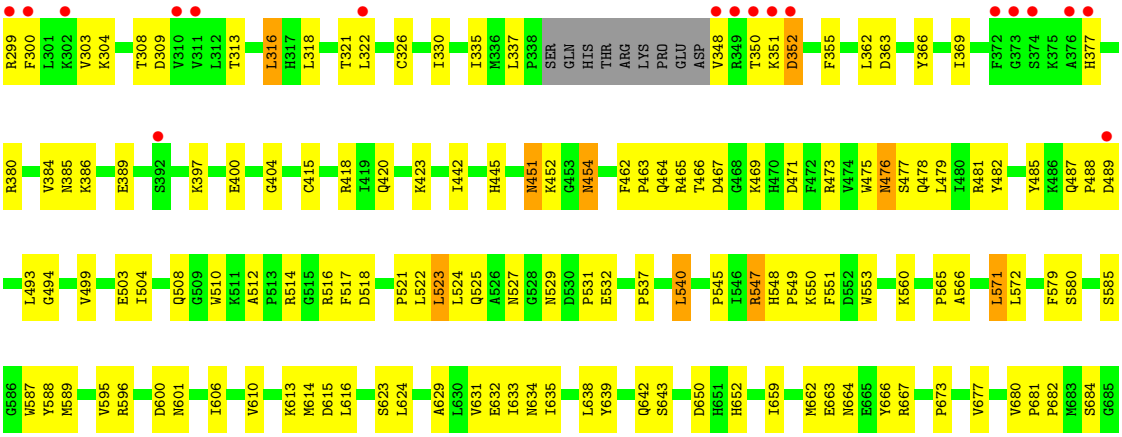
- Molecule 1: nitric-oxide synthase

Chain A:



- Molecule 1: nitric-oxide synthase

Chain B:



S686
I687
T688
P689
E694
M695
L696
N697
Y698
R699
L700
T701
P702
P710
W711
N712
V715
W716
K717

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.73Å 111.03Å 165.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.61 – 2.55 29.61 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.61-2.55) 88.4 (29.61-2.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.286 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	1.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7008	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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: ZN, ARV, ACT, H4B, 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	0.37	0/3406	0.65	1/4621 (0.0%)
1	B	0.39	0/3434	0.64	2/4656 (0.0%)
All	All	0.38	0/6840	0.64	3/9277 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	326	CYS	CA-CB-SG	7.00	126.60	114.00
1	B	326	CYS	CA-CB-SG	6.85	126.33	114.00
1	B	589	MET	N-CA-C	-5.20	96.97	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3313	0	3221	136	0
1	B	3341	0	3256	121	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
4	A	43	0	30	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	43	0	30	3	0
5	A	17	0	15	1	0
5	B	17	0	15	0	0
6	A	15	0	18	6	0
6	B	15	0	18	3	0
7	A	92	0	0	7	0
7	B	103	0	0	6	0
All	All	7008	0	6609	249	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 19.

All (249) 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:523:LEU:HD22	1:B:531:PRO:HB2	1.30	1.11
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.41	1.00
1:B:299:ARG:HB3	1:B:318:LEU:HD21	1.51	0.92
1:A:299:ARG:HB3	1:A:318:LEU:HD21	1.53	0.91
1:B:465:ARG:HG3	1:B:471:ASP:OD1	1.74	0.88
1:B:571:LEU:HD12	1:B:572:LEU:N	1.94	0.80
4:B:750:HEM:HMC2	4:B:750:HEM:HBC2	1.65	0.78
1:A:396:LEU:HD13	1:A:577:LEU:HD12	1.67	0.75
4:A:750:HEM:HBC2	4:A:750:HEM:HMC2	1.67	0.75
1:B:587:TRP:H	4:B:750:HEM:HAB	1.53	0.73
1:A:549:PRO:HG3	1:A:639:TYR:CG	2.23	0.73
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.04	0.73
1:A:635:ILE:HD11	1:B:624:LEU:HB2	1.71	0.73
1:A:624:LEU:HB2	1:B:635:ILE:HD11	1.71	0.73
1:B:348:VAL:O	1:B:348:VAL:CG1	2.36	0.73
1:B:549:PRO:HG3	1:B:639:TYR:CG	2.23	0.73
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.05	0.71
1:B:523:LEU:CD2	1:B:531:PRO:HB2	2.17	0.68
1:A:585:SER:HA	6:A:1780:ARV:HC32	1.76	0.68
1:B:585:SER:HA	6:B:2780:ARV:HC32	1.76	0.67
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.77	0.67
1:A:374:SER:HB2	7:A:130:HOH:O	1.96	0.66
1:A:624:LEU:HB2	1:B:635:ILE:CD1	2.26	0.66
6:B:2780:ARV:CD	6:B:2780:ARV:HC12	2.26	0.66
1:A:635:ILE:CD1	1:B:624:LEU:HB2	2.26	0.66
1:B:489:ASP:HB2	7:B:18:HOH:O	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1780:ARV:CD	6:A:1780:ARV:HC12	2.26	0.65
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.31	0.65
1:A:299:ARG:CB	1:A:318:LEU:HD21	2.25	0.63
1:B:596:ARG:O	1:B:600:ASP:HB2	1.98	0.63
1:A:362:LEU:HD11	1:A:384:VAL:HG21	1.81	0.62
1:B:348:VAL:O	1:B:348:VAL:HG12	1.99	0.62
1:B:452:LYS:HB2	7:B:78:HOH:O	2.00	0.62
1:A:487:GLN:HB3	1:A:488:PRO:HD2	1.82	0.61
1:A:711:TRP:CD1	1:A:712:ASN:ND2	2.69	0.60
1:B:595:VAL:HG23	1:B:634:ASN:HD21	1.66	0.60
1:A:493:LEU:HD12	1:A:494:GLY:H	1.66	0.60
1:A:493:LEU:HD12	1:A:494:GLY:N	2.16	0.60
1:A:396:LEU:HD21	1:A:574:ILE:HG21	1.82	0.60
1:B:299:ARG:CB	1:B:318:LEU:HD21	2.30	0.59
1:A:304:LYS:O	1:A:694:GLU:HG3	2.01	0.59
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.16	0.59
1:B:610:VAL:O	1:B:614:MET:HG3	2.02	0.59
1:B:664:ASN:O	1:B:667:ARG:HG2	2.03	0.59
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.84	0.59
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.85	0.59
1:A:465:ARG:HG3	1:A:471:ASP:OD1	2.02	0.59
1:B:571:LEU:HD12	1:B:571:LEU:C	2.23	0.59
1:B:350:THR:HG22	1:B:351:LYS:N	2.19	0.58
1:B:303:VAL:HG13	1:B:694:GLU:HB2	1.85	0.58
1:A:396:LEU:HD21	1:A:574:ILE:CG2	2.34	0.58
1:A:684:SER:O	1:A:687:ILE:HG12	2.03	0.58
1:B:631:VAL:O	1:B:635:ILE:HG12	2.04	0.58
1:A:537:PRO:HB2	1:A:540:LEU:HD22	1.84	0.58
1:A:396:LEU:HD13	1:A:577:LEU:CD1	2.34	0.57
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.87	0.57
1:B:467:ASP:OD2	1:B:469:LYS:HB2	2.05	0.57
1:A:571:LEU:HD12	1:A:572:LEU:N	2.20	0.56
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.35	0.56
1:A:596:ARG:O	1:A:600:ASP:HB2	2.05	0.56
1:A:701:THR:HA	1:A:702:PRO:C	2.26	0.56
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.69	0.56
1:A:463:PRO:HB2	1:A:472:PHE:CE1	2.41	0.55
1:A:451:ASN:HB3	1:A:454:ASN:O	2.06	0.55
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.88	0.55
1:A:355:PHE:N	1:A:356:PRO:HD2	2.21	0.55
1:A:386:LYS:O	1:A:389:GLU:HB3	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:ILE:HD11	1:A:633:ILE:HD13	1.87	0.55
1:B:363:ASP:HA	1:B:377:HIS:HE1	1.71	0.54
1:A:589:MET:HA	1:A:649:VAL:O	2.07	0.54
1:A:500:GLN:OE1	1:A:711:TRP:NE1	2.41	0.54
1:A:335:ILE:HD13	1:B:694:GLU:HB3	1.88	0.54
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.90	0.54
1:A:548:HIS:HD2	1:A:550:LYS:H	1.56	0.54
1:A:631:VAL:O	1:A:635:ILE:HG12	2.08	0.54
1:A:501:PHE:CD2	1:A:520:LEU:HD13	2.43	0.54
1:B:525:GLN:HG3	1:B:529:ASN:O	2.08	0.53
1:A:516:ARG:HD3	1:A:517:PHE:CE1	2.43	0.53
1:A:381:LEU:HG	7:A:149:HOH:O	2.08	0.53
1:A:686:SER:OG	1:B:682:PRO:HB2	2.09	0.53
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.43	0.53
1:A:485:TYR:HB3	1:A:514:ARG:NH1	2.24	0.53
1:A:638:LEU:O	1:A:642:GLN:HG3	2.08	0.53
1:B:476:ASN:HB3	7:B:71:HOH:O	2.08	0.53
1:A:380:ARG:O	1:A:384:VAL:HG23	2.09	0.53
1:A:350:THR:HB	1:A:353:GLN:HG3	1.91	0.52
1:A:659:ILE:O	1:A:663:GLU:HG3	2.10	0.52
1:B:701:THR:HA	1:B:702:PRO:C	2.28	0.52
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.91	0.52
1:A:675:ASP:O	1:A:679:ILE:HG12	2.10	0.52
1:A:682:PRO:HB2	1:B:686:SER:OG	2.10	0.52
1:B:684:SER:HB3	1:B:687:ILE:HG12	1.91	0.52
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.39	0.52
1:A:374:SER:O	1:A:378:MET:HG2	2.09	0.52
1:A:711:TRP:HD1	1:A:712:ASN:ND2	2.08	0.52
1:B:473:ARG:NH2	1:B:710:PRO:HD3	2.25	0.52
1:A:478:GLN:HA	1:A:566:ALA:O	2.09	0.51
1:A:567:VAL:HG23	6:A:1780:ARV:HC31	1.91	0.51
1:B:300:PHE:HD2	1:B:313:THR:HG21	1.75	0.51
1:B:451:ASN:HB3	1:B:454:ASN:O	2.10	0.51
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.75	0.51
1:B:464:GLN:HB3	1:B:579:PHE:CE2	2.45	0.51
1:A:686:SER:HA	1:A:691:PHE:CG	2.45	0.51
1:B:537:PRO:HB2	1:B:540:LEU:HD22	1.92	0.51
1:A:517:PHE:HB2	1:A:560:LYS:HE2	1.92	0.51
1:B:638:LEU:O	1:B:642:GLN:HG3	2.11	0.51
1:A:467:ASP:OD2	1:A:469:LYS:HB2	2.10	0.51
1:B:462:PHE:HB3	1:B:463:PRO:HD2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:GLU:HG3	7:A:146:HOH:O	2.10	0.50
1:A:614:MET:CE	1:A:632:GLU:HG3	2.42	0.50
1:A:523:LEU:HD22	1:A:531:PRO:CB	2.28	0.50
1:B:493:LEU:HD12	1:B:494:GLY:N	2.27	0.50
1:A:300:PHE:HD2	1:A:313:THR:HG21	1.77	0.50
1:A:571:LEU:HD12	1:A:571:LEU:C	2.33	0.50
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.41	0.50
1:A:614:MET:HE3	1:A:632:GLU:HG3	1.94	0.49
1:A:303:VAL:HG13	1:A:694:GLU:HB2	1.93	0.49
6:B:2780:ARV:HC12	6:B:2780:ARV:HD2	1.93	0.49
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.95	0.49
1:A:525:GLN:HG3	1:A:529:ASN:O	2.12	0.49
1:B:485:TYR:CE2	1:B:512:ALA:HB1	2.47	0.49
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.47	0.49
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.95	0.49
1:B:473:ARG:HD3	1:B:580:SER:HB2	1.95	0.49
1:B:420:GLN:HB3	7:B:69:HOH:O	2.13	0.49
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.95	0.49
1:A:316:LEU:HD11	1:A:669:ARG:HD3	1.95	0.48
1:A:467:ASP:OD1	1:A:470:HIS:ND1	2.45	0.48
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.47	0.48
1:B:442:ILE:HG23	1:B:479:LEU:HD13	1.95	0.48
1:B:445:HIS:HE1	1:B:585:SER:OG	1.96	0.48
1:A:353:GLN:O	1:A:356:PRO:HG2	2.13	0.48
1:A:366:TYR:HA	1:A:369:ILE:HG12	1.95	0.48
1:A:373:GLY:O	1:A:374:SER:O	2.31	0.48
1:A:482:TYR:HA	1:A:518:ASP:O	2.13	0.48
1:B:629:ALA:O	1:B:633:ILE:HG13	2.14	0.48
1:A:468:GLY:HA2	1:A:471:ASP:OD1	2.14	0.48
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.95	0.48
1:B:366:TYR:CD2	1:B:369:ILE:HD11	2.48	0.48
1:B:478:GLN:HB2	1:B:481:ARG:CG	2.44	0.47
1:B:659:ILE:HG13	1:B:689:PRO:HB2	1.95	0.47
1:A:361:PHE:O	1:A:364:GLN:HB2	2.13	0.47
1:A:606:ILE:O	1:A:610:VAL:HG23	2.15	0.47
1:B:415:CYS:HB3	1:B:418:ARG:HG3	1.95	0.47
1:A:371:ARG:HH11	1:A:371:ARG:HG2	1.78	0.47
1:A:545:PRO:HG2	1:A:547:ARG:HH11	1.79	0.47
1:B:606:ILE:HD11	1:B:633:ILE:HD13	1.97	0.47
1:B:615:ASP:HA	7:B:131:HOH:O	2.14	0.47
1:B:547:ARG:NH2	1:B:643:SER:HB2	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:GLU:HG3	7:A:135:HOH:O	2.15	0.47
1:A:635:ILE:HD12	1:B:623:SER:O	2.14	0.47
1:B:553:TRP:CE3	1:B:613:LYS:HD3	2.49	0.47
1:A:547:ARG:NH2	1:A:643:SER:HB2	2.30	0.47
1:B:523:LEU:HA	1:B:532:GLU:O	2.15	0.47
1:A:519:VAL:HG23	7:A:8:HOH:O	2.14	0.46
1:B:380:ARG:O	1:B:384:VAL:HG23	2.14	0.46
1:B:493:LEU:HD12	1:B:494:GLY:H	1.80	0.46
1:A:415:CYS:HB3	1:A:418:ARG:HG3	1.97	0.46
1:B:350:THR:HG22	1:B:351:LYS:H	1.79	0.46
1:B:632:GLU:O	1:B:635:ILE:HB	2.15	0.46
1:A:553:TRP:CE3	1:A:613:LYS:HD3	2.50	0.46
1:A:350:THR:HG22	1:A:351:LYS:N	2.30	0.46
1:A:548:HIS:CD2	1:A:550:LYS:H	2.33	0.45
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.97	0.45
1:B:350:THR:CG2	1:B:352:ASP:OD1	2.65	0.45
1:B:524:LEU:O	1:B:531:PRO:HA	2.16	0.45
1:B:565:PRO:HB3	1:B:588:TYR:CZ	2.52	0.45
1:B:350:THR:HG21	1:B:352:ASP:OD1	2.16	0.45
1:B:516:ARG:HD3	1:B:517:PHE:CE1	2.51	0.45
1:A:384:VAL:O	1:A:388:ILE:HG13	2.16	0.45
1:A:500:GLN:O	1:A:503:GLU:HB2	2.17	0.45
1:B:537:PRO:O	1:B:540:LEU:HB2	2.17	0.45
1:A:366:TYR:CD2	1:A:369:ILE:HD11	2.52	0.44
1:A:501:PHE:HD2	1:A:520:LEU:HD13	1.81	0.44
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.31	0.44
1:A:591:THR:HA	1:A:634:ASN:HD21	1.82	0.44
1:A:610:VAL:HG21	1:A:633:ILE:HD11	1.99	0.44
1:A:623:SER:O	1:B:635:ILE:CD1	2.64	0.44
1:B:466:THR:OG1	1:B:467:ASP:N	2.49	0.44
1:A:396:LEU:CD1	1:A:577:LEU:HD12	2.44	0.44
1:B:684:SER:O	1:B:687:ILE:HG12	2.17	0.44
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.48	0.44
1:B:548:HIS:CD2	1:B:550:LYS:H	2.35	0.44
1:A:462:PHE:HB3	1:A:463:PRO:HD2	1.98	0.44
1:B:610:VAL:HG21	1:B:633:ILE:CD1	2.48	0.44
1:A:610:VAL:O	1:A:614:MET:HG3	2.17	0.44
1:B:478:GLN:HA	1:B:566:ALA:O	2.18	0.44
1:A:454:ASN:C	1:A:454:ASN:HD22	2.21	0.44
1:A:508:GLN:HE22	1:A:716:TRP:HZ3	1.64	0.44
1:A:596:ARG:HH12	5:A:1760:H4B:C4	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:VAL:O	1:B:503:GLU:HG3	2.18	0.44
1:B:711:TRP:CD1	1:B:712:ASN:ND2	2.86	0.44
1:A:473:ARG:HD3	1:A:580:SER:HB2	2.00	0.43
1:A:606:ILE:CD1	1:A:633:ILE:HD13	2.48	0.43
1:B:545:PRO:HG2	1:B:547:ARG:HH11	1.83	0.43
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.89	0.43
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.53	0.43
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.54	0.43
1:B:684:SER:HB3	1:B:687:ILE:CD1	2.48	0.43
1:B:504:ILE:O	1:B:508:GLN:HB2	2.17	0.43
1:B:587:TRP:N	4:B:750:HEM:HAB	2.27	0.43
1:B:473:ARG:CD	1:B:580:SER:HB2	2.49	0.43
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.82	0.43
1:B:548:HIS:HB3	1:B:551:PHE:HB2	2.01	0.43
1:A:465:ARG:CZ	7:A:11:HOH:O	2.66	0.42
1:B:304:LYS:O	1:B:694:GLU:HG3	2.19	0.42
1:B:523:LEU:HD23	1:B:532:GLU:O	2.19	0.42
1:A:485:TYR:CE1	1:A:514:ARG:HA	2.54	0.42
1:B:348:VAL:O	1:B:348:VAL:HG13	2.15	0.42
1:A:548:HIS:HB2	1:A:554:PHE:CG	2.55	0.42
1:B:517:PHE:HB2	1:B:560:LYS:HE2	2.01	0.42
1:B:650:ASP:OD2	1:B:652:HIS:HB2	2.18	0.42
1:A:449:ALA:O	1:A:455:LEU:HA	2.20	0.42
6:A:1780:ARV:HC12	6:A:1780:ARV:HD3	2.02	0.42
1:B:614:MET:HE3	1:B:632:GLU:HG3	2.00	0.42
1:A:592:GLU:OE2	6:A:1780:ARV:NH1	2.52	0.42
1:B:303:VAL:CG1	1:B:694:GLU:O	2.68	0.42
1:B:673:PRO:HA	1:B:696:LEU:O	2.20	0.42
1:A:590:GLY:HA3	7:A:16:HOH:O	2.18	0.42
1:A:337:LEU:HD12	1:A:337:LEU:O	2.21	0.41
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.01	0.41
1:A:485:TYR:HB3	1:A:514:ARG:HH12	1.84	0.41
4:A:750:HEM:HBC2	4:A:750:HEM:CMC	2.45	0.41
6:A:1780:ARV:HC12	6:A:1780:ARV:HD2	2.00	0.41
1:B:482:TYR:HA	1:B:518:ASP:O	2.20	0.41
1:A:387:GLU:OE2	1:A:394:TYR:HA	2.20	0.41
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.51	0.41
1:A:494:GLY:HA2	1:A:516:ARG:O	2.21	0.41
1:A:676:TRP:CE3	1:B:677:VAL:HG22	2.55	0.41
1:B:404:GLY:HA2	1:B:702:PRO:HG2	2.03	0.41
1:B:508:GLN:HG3	7:B:22:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:ILE:O	1:B:663:GLU:HG3	2.21	0.41
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.54	0.41
1:B:701:THR:HA	1:B:702:PRO:O	2.21	0.41
1:A:330:ILE:CD1	1:B:696:LEU:HD22	2.50	0.41
1:A:299:ARG:C	1:A:300:PHE:CD1	2.94	0.41
1:B:397:LYS:HB2	1:B:400:GLU:HG3	2.03	0.41
1:A:618:MET:HG2	1:A:625:TRP:CD2	2.56	0.40
1:B:308:THR:O	1:B:309:ASP:HB2	2.21	0.40
1:A:537:PRO:O	1:A:540:LEU:HB2	2.22	0.40
1:B:662:MET:O	1:B:666:TYR:HD1	2.05	0.40
1:A:674:ALA:HB3	1:A:695:MET:HB3	2.02	0.40
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.88	0.40
1:B:386:LYS:O	1:B:389:GLU:HB3	2.22	0.40
1:A:635:ILE:HD13	1:B:624:LEU:HG	2.02	0.40
1:B:442:ILE:HG21	1:B:522:LEU:HD11	2.03	0.40
1:A:454:ASN:C	1:A:454:ASN:ND2	2.75	0.40
1:B:316:LEU:HD22	1:B:700:LEU:HD11	2.04	0.40
1:B:487:GLN:HB3	1:B:488:PRO:HD2	2.03	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	403/419 (96%)	358 (89%)	42 (10%)	3 (1%)	22 30
1	B	406/419 (97%)	372 (92%)	34 (8%)	0	100 100
All	All	809/838 (96%)	730 (90%)	76 (9%)	3 (0%)	34 46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	SER
1	A	412	ALA
1	A	590	GLY

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	363/375 (97%)	344 (95%)	19 (5%)	23	30
1	B	366/375 (98%)	349 (95%)	17 (5%)	27	36
All	All	729/750 (97%)	693 (95%)	36 (5%)	25	34

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	ASP
1	A	316	LEU
1	A	321	THR
1	A	322	LEU
1	A	328	GLU
1	A	337	LEU
1	A	352	ASP
1	A	423	LYS
1	A	451	ASN
1	A	454	ASN
1	A	523	LEU
1	A	527	ASN
1	A	540	LEU
1	A	547	ARG
1	A	571	LEU
1	A	601	ASN
1	A	616	LEU
1	A	664	ASN
1	A	697	ASN
1	B	316	LEU
1	B	321	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	337	LEU
1	B	352	ASP
1	B	423	LYS
1	B	451	ASN
1	B	454	ASN
1	B	476	ASN
1	B	477	SER
1	B	523	LEU
1	B	527	ASN
1	B	540	LEU
1	B	547	ARG
1	B	571	LEU
1	B	601	ASN
1	B	616	LEU
1	B	697	ASN

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	425	GLN
1	A	451	ASN
1	A	454	ASN
1	A	487	GLN
1	A	548	HIS
1	A	634	ASN
1	A	697	ASN
1	A	712	ASN
1	A	714	HIS
1	B	445	HIS
1	B	451	ASN
1	B	454	ASN
1	B	487	GLN
1	B	548	HIS
1	B	634	ASN
1	B	697	ASN
1	B	712	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\#\|Z\| > 2$
2	ACT	B	2860	-	3,3,3	0.86	0	3,3,3	0.71	0
5	H4B	A	1760	-	16,18,18	2.31	4 (25%)	11,26,26	4.04	7 (63%)
4	HEM	A	750	1	41,50,50	1.30	4 (9%)	45,82,82	1.44	9 (20%)
2	ACT	A	1860	-	3,3,3	0.96	0	3,3,3	0.76	0
6	ARV	B	2780	-	11,14,14	1.75	3 (27%)	10,16,16	1.50	3 (30%)
4	HEM	B	750	1	41,50,50	1.30	4 (9%)	45,82,82	1.50	8 (17%)
5	H4B	B	2760	-	16,18,18	2.13	4 (25%)	11,26,26	4.26	9 (81%)
6	ARV	A	1780	-	11,14,14	1.88	4 (36%)	10,16,16	1.54	3 (30%)

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	H4B	A	1760	-	-	0/8/17/17	0/2/2/2
4	HEM	A	750	1	-	2/12/54/54	-
6	ARV	B	2780	-	-	1/13/15/15	-
4	HEM	B	750	1	-	4/12/54/54	-
5	H4B	B	2760	-	-	0/8/17/17	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ARV	A	1780	-	-	1/13/15/15	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1760	H4B	C4-N3	5.63	1.42	1.33
5	B	2760	H4B	C4-N3	5.62	1.42	1.33
5	A	1760	H4B	C4A-N5	4.67	1.47	1.38
5	A	1760	H4B	C6-N5	4.44	1.54	1.45
4	A	750	HEM	C3C-CAC	-4.04	1.39	1.47
5	B	2760	H4B	C6-N5	4.03	1.53	1.45
6	A	1780	ARV	OXT-C	-3.76	1.18	1.30
6	B	2780	ARV	OXT-C	-3.74	1.18	1.30
5	B	2760	H4B	C4A-N5	3.70	1.45	1.38
4	B	750	HEM	C3C-CAC	-3.28	1.41	1.47
6	A	1780	ARV	O-C	3.01	1.31	1.22
4	B	750	HEM	C3C-C2C	-2.95	1.36	1.40
4	B	750	HEM	CAB-C3B	-2.86	1.39	1.47
4	A	750	HEM	C3C-C2C	-2.83	1.36	1.40
6	B	2780	ARV	O-C	2.70	1.30	1.22
4	A	750	HEM	C4D-ND	-2.67	1.35	1.40
6	A	1780	ARV	CZ-NH1	-2.65	1.28	1.34
5	A	1760	H4B	C8A-N1	2.44	1.39	1.34
4	B	750	HEM	CHB-C1B	2.29	1.40	1.35
4	A	750	HEM	CAB-C3B	-2.28	1.41	1.47
6	B	2780	ARV	CZ-NH1	-2.15	1.29	1.34
5	B	2760	H4B	C8A-N1	2.15	1.38	1.34
6	A	1780	ARV	CD-NE	2.02	1.50	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	2760	H4B	C8A-C4A-C4	9.51	123.02	114.57
5	A	1760	H4B	C8A-C4A-C4	8.54	122.16	114.57
5	A	1760	H4B	C2-N3-C4	5.77	125.09	115.93
5	B	2760	H4B	C2-N3-C4	5.62	124.87	115.93
5	A	1760	H4B	N1-C2-N3	-4.69	118.06	125.42
5	B	2760	H4B	N1-C2-N3	-4.47	118.41	125.42
4	B	750	HEM	CBA-CAA-C2A	-4.07	105.68	112.62
5	B	2760	H4B	C4A-C4-N3	-3.77	113.31	124.01
5	A	1760	H4B	C4A-C4-N3	-3.71	113.47	124.01
5	A	1760	H4B	C2-N1-C8A	3.59	122.58	114.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	2760	H4B	C2-N1-C8A	3.36	122.06	114.54
5	A	1760	H4B	N2-C2-N1	3.19	122.21	117.25
5	B	2760	H4B	N2-C2-N1	3.14	122.13	117.25
5	B	2760	H4B	C4-C4A-N5	-2.87	116.71	119.12
6	A	1780	ARV	OXT-C-CA	2.78	122.86	113.38
4	A	750	HEM	C2C-C3C-C4C	-2.73	104.99	106.90
6	B	2780	ARV	OXT-C-CA	2.73	122.69	113.38
4	A	750	HEM	CMD-C2D-C1D	2.73	129.19	125.04
4	A	750	HEM	C1D-C2D-C3D	-2.72	104.09	106.96
5	A	1760	H4B	C4A-N5-C6	-2.72	113.75	121.16
4	A	750	HEM	CBA-CAA-C2A	-2.68	108.06	112.62
5	B	2760	H4B	C4A-N5-C6	-2.64	113.97	121.16
4	B	750	HEM	C1B-NB-C4B	-2.44	102.55	105.07
4	B	750	HEM	C2C-C3C-C4C	-2.36	105.25	106.90
4	A	750	HEM	C4B-C3B-C2B	-2.31	105.28	107.11
6	A	1780	ARV	OXT-C-O	-2.26	118.96	124.09
4	B	750	HEM	CMA-C3A-C4A	-2.25	125.00	128.46
4	A	750	HEM	C4B-CHC-C1C	2.23	125.50	122.56
4	B	750	HEM	C2B-C1B-NB	2.22	112.47	109.84
4	A	750	HEM	C3B-C2B-C1B	2.19	108.11	106.49
4	B	750	HEM	C1D-C2D-C3D	-2.18	104.67	106.96
4	B	750	HEM	CMC-C2C-C3C	2.17	128.75	124.68
5	B	2760	H4B	O9-C9-C6	2.17	114.18	108.98
4	B	750	HEM	C4B-CHC-C1C	2.15	125.40	122.56
6	B	2780	ARV	NH1-CZ-NH2	-2.14	114.73	122.79
4	A	750	HEM	C4A-C3A-C2A	2.13	108.48	107.00
6	A	1780	ARV	NH1-CZ-NH2	-2.09	114.95	122.79
4	A	750	HEM	C2D-C1D-ND	2.08	112.38	109.88
6	B	2780	ARV	OXT-C-O	-2.07	119.39	124.09

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	750	HEM	C4B-C3B-CAB-CBB
4	A	750	HEM	C2B-C3B-CAB-CBB
4	B	750	HEM	C2B-C3B-CAB-CBB
4	A	750	HEM	C4B-C3B-CAB-CBB
6	A	1780	ARV	O-C-CA-N
6	B	2780	ARV	O-C-CA-N
4	B	750	HEM	CAA-CBA-CGA-O2A
4	B	750	HEM	CAA-CBA-CGA-O1A

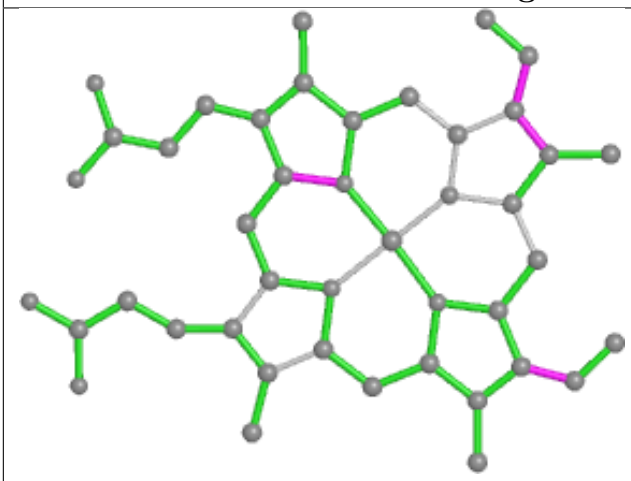
There are no ring outliers.

5 monomers are involved in 15 short contacts:

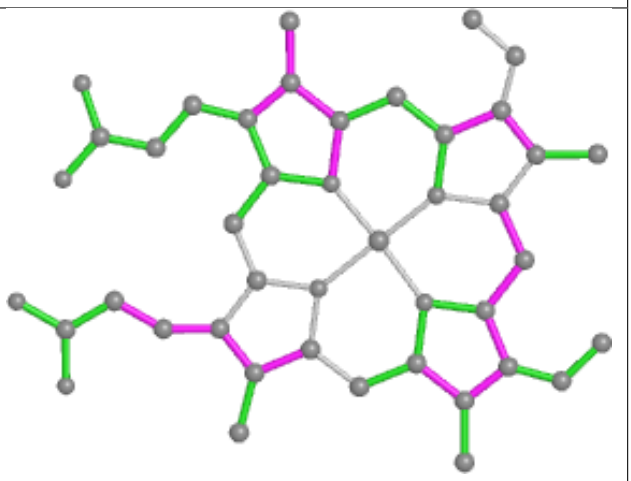
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1760	H4B	1	0
4	A	750	HEM	2	0
6	B	2780	ARV	3	0
4	B	750	HEM	3	0
6	A	1780	ARV	6	0

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 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.

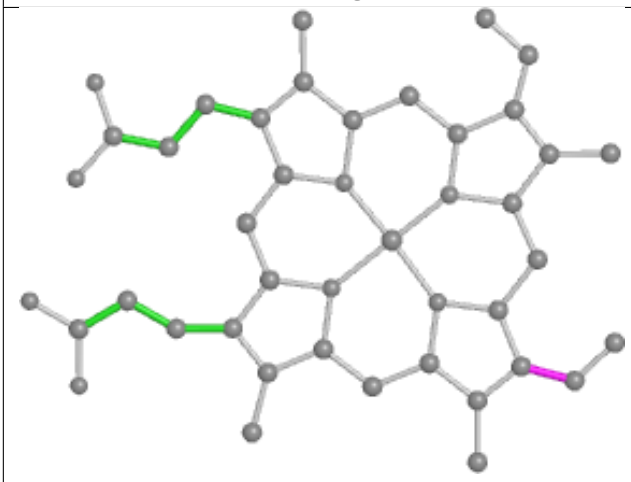
Ligand HEM A 750



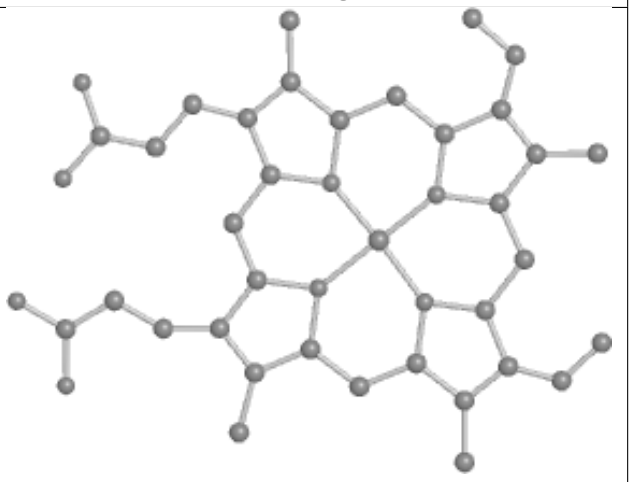
Bond lengths



Bond angles

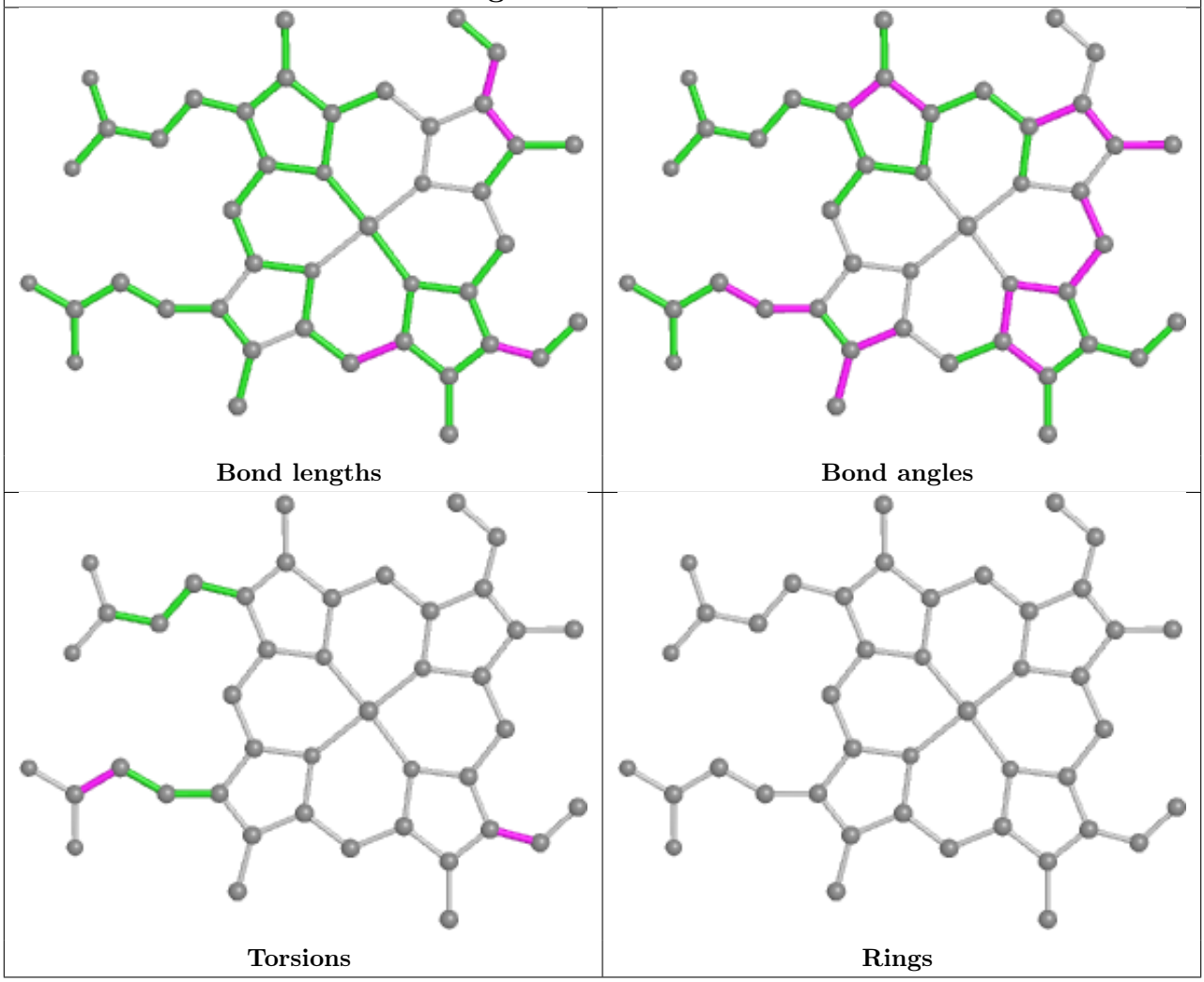


Torsions



Rings

Ligand HEM B 750



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 (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	407/419 (97%)	0.48	25 (6%)	21	25	24, 51, 85, 102	0
1	B	410/419 (97%)	0.30	20 (4%)	29	35	21, 48, 78, 101	0
All	All	817/838 (97%)	0.39	45 (5%)	25	30	21, 49, 82, 102	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	488	PRO	6.2
1	A	715	VAL	5.7
1	A	619	ARG	4.2
1	B	392	SER	4.1
1	A	299	ARG	3.7
1	A	351	LYS	3.6
1	B	348	VAL	3.6
1	A	321	THR	3.4
1	B	352	ASP	3.3
1	B	350	THR	3.3
1	A	370	LYS	3.2
1	A	311	VAL	3.2
1	A	352	ASP	3.2
1	B	351	LYS	3.1
1	B	715	VAL	3.0
1	A	371	ARG	3.0
1	A	487	GLN	2.9
1	B	300	PHE	2.9
1	A	716	TRP	2.9
1	A	469	LYS	2.8
1	A	355	PHE	2.8
1	B	299	ARG	2.8
1	A	667	ARG	2.8
1	B	322	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	374	SER	2.8
1	B	373	GLY	2.7
1	A	389	GLU	2.7
1	B	717	LYS	2.6
1	A	385	ASN	2.6
1	A	618	MET	2.5
1	B	372	PHE	2.5
1	B	349	ARG	2.5
1	B	311	VAL	2.4
1	A	388	ILE	2.4
1	A	369	ILE	2.3
1	B	310	VAL	2.3
1	A	617	ASP	2.2
1	A	643	SER	2.2
1	B	302	LYS	2.2
1	A	489	ASP	2.1
1	A	552	ASP	2.1
1	B	377	HIS	2.1
1	A	300	PHE	2.1
1	B	489	ASP	2.1
1	B	376	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	H4B	A	1760	17/17	0.95	0.18	24,34,41,41	0
5	H4B	B	2760	17/17	0.95	0.18	29,35,43,45	0

Continued on next page...

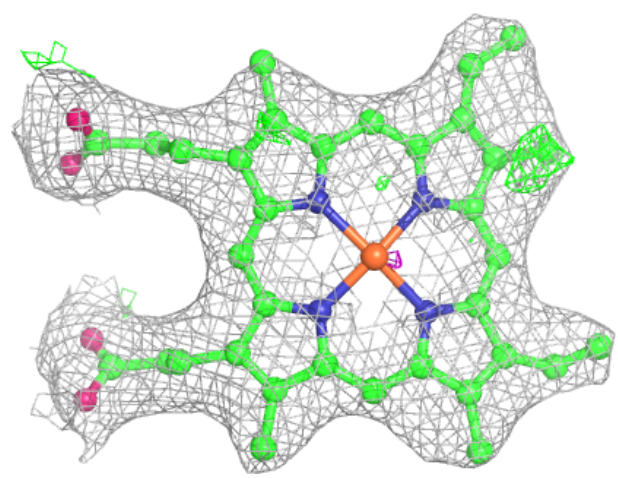
Continued from previous page...

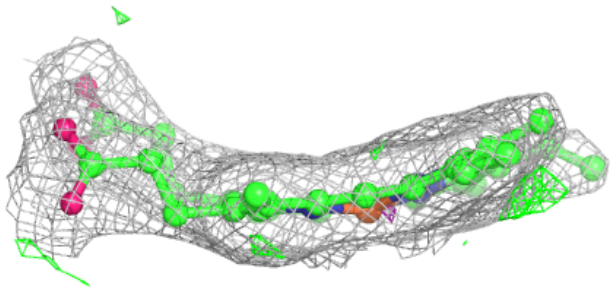
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ARV	A	1780	15/15	0.95	0.24	26,35,41,42	0
6	ARV	B	2780	15/15	0.95	0.25	34,41,54,55	0
2	ACT	A	1860	4/4	0.96	0.16	48,54,55,58	0
4	HEM	A	750	43/43	0.96	0.22	20,34,43,45	0
4	HEM	B	750	43/43	0.97	0.19	10,29,39,41	0
2	ACT	B	2860	4/4	0.98	0.11	35,39,40,44	0
3	ZN	A	900	1/1	0.99	0.07	44,44,44,44	0

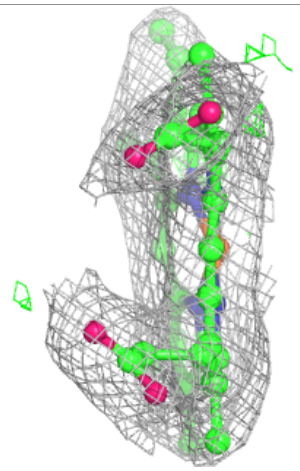
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM A 750:

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

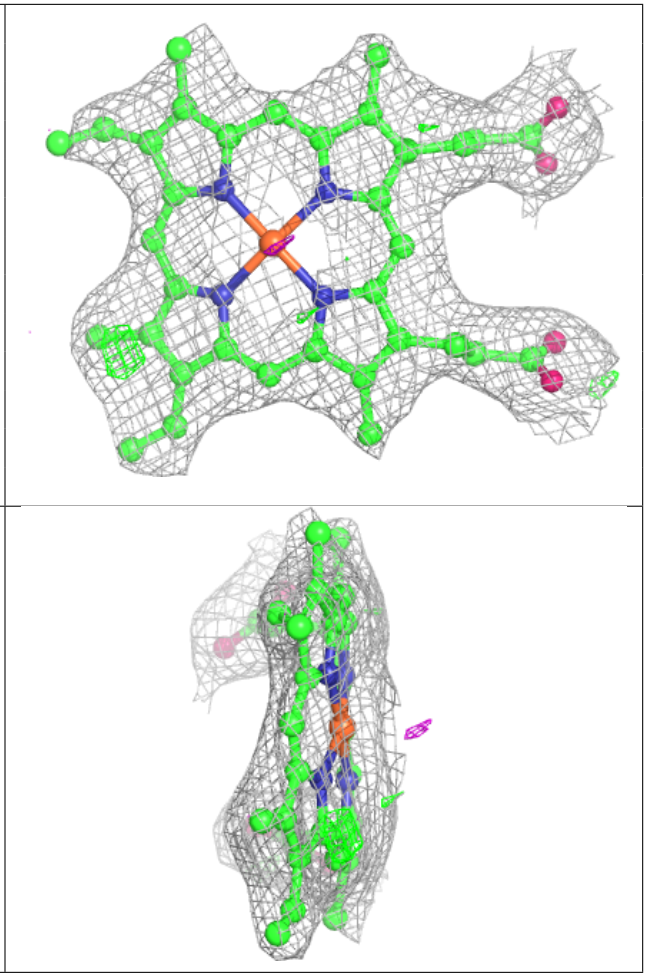






Electron density around HEM B 750:

$2mF_o$-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.