



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:00 pm BST

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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

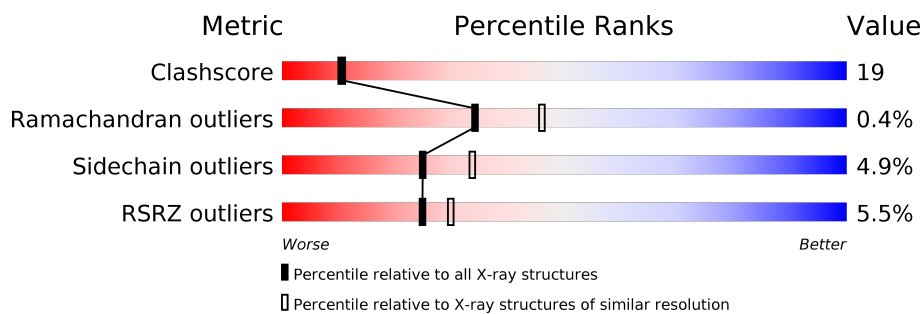
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	419	
1	B	419	

## 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
1	A	407	Total	C	N	O	S	0	0	0
			3313	2121	566	605	21			
1	B	410	Total	C	N	O	S	0	0	0
			3341	2138	573	609	21			

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



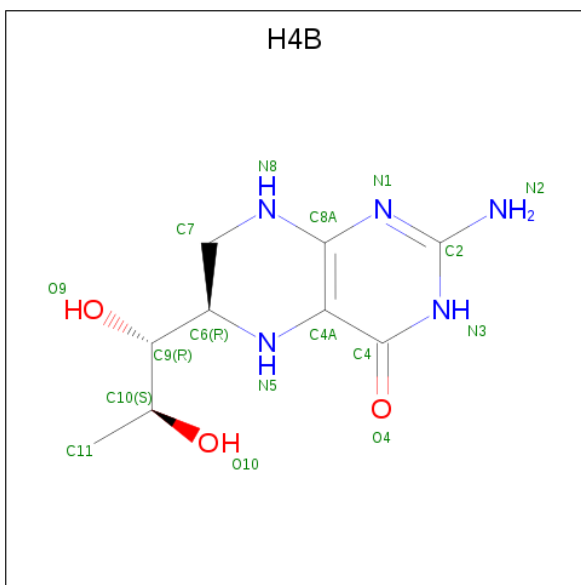
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

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

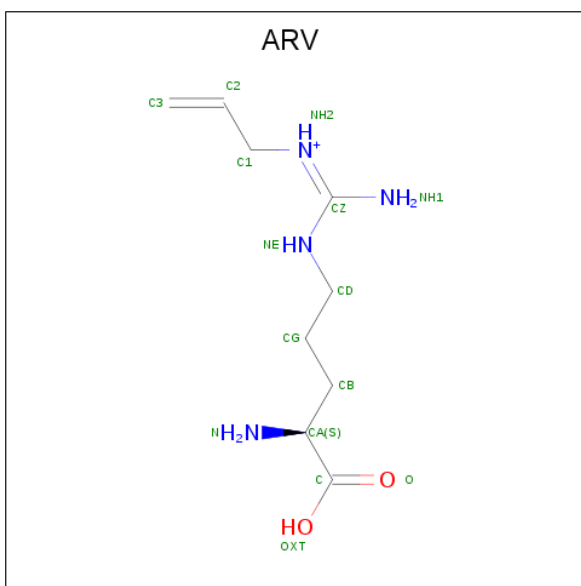
- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





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

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



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

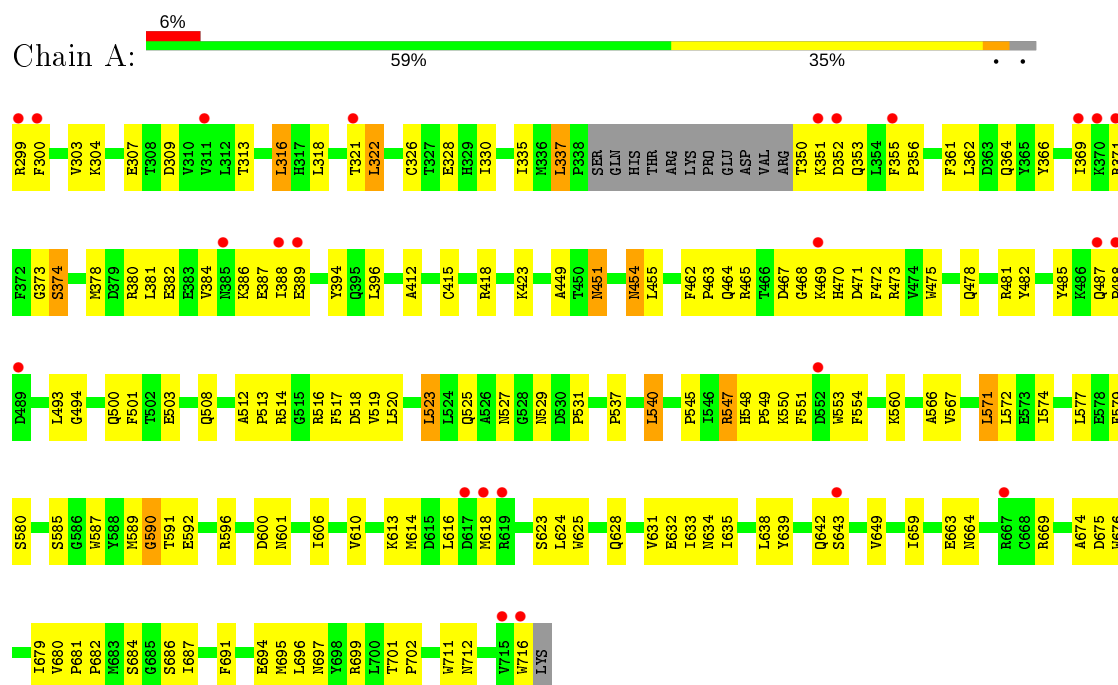
- Molecule 7 is water.

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

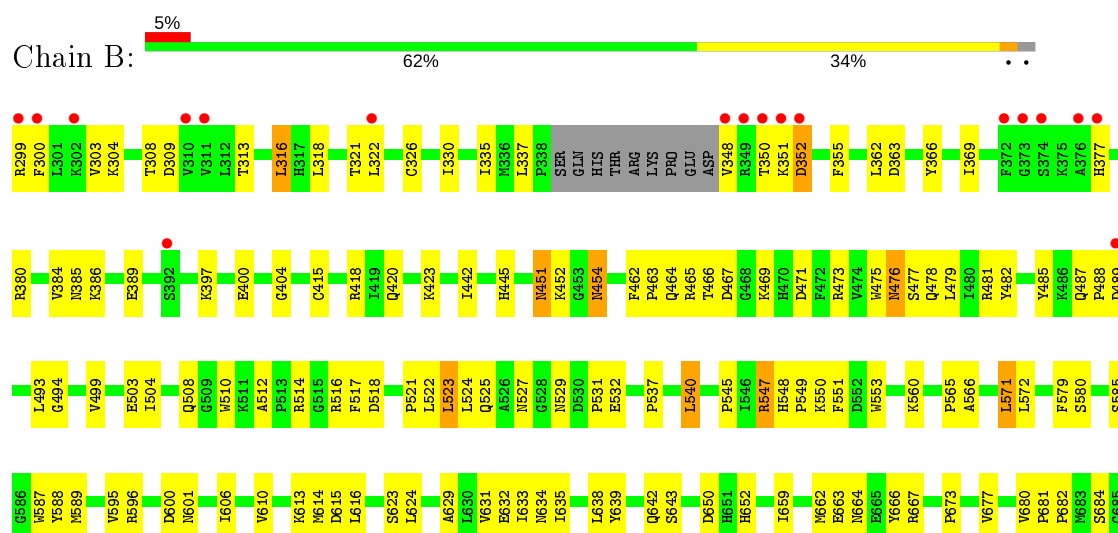
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



#### • Molecule 1: nitric-oxide synthase



S686	I687	T688	P689	E694	Y695	L696	N697	Y698	R699	L700	T701	P702	P710	W711	N712	Y715	W716	K717



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	34.3	Xtriage
Anisotropy	1.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7008	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZN, H4B, ARV, ACT

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(°)	Ideal(°)
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

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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:HMC2	4:A:750:HEM:HBC2	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:HC12	6:B:2780:ARV:CD	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

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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

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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:567:VAL:HG23	6:A:1780:ARV:HC31	1.91	0.51
1:A:478:GLN:HA	1:A:566:ALA:O	2.09	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

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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:HD2	6:B:2780:ARV:HC12	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:467:ASP:OD1	1:A:470:HIS:ND1	2.45	0.48
1:A:316:LEU:HD11	1:A:669:ARG:HD3	1.95	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:HG2	1:A:371:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:TRP:CE3	1:B:613:LYS:HD3	2.49	0.47
1:A:635:ILE:HD12	1:B:623:SER:O	2.14	0.47
1:A:382:GLU:HG3	7:A:135:HOH:O	2.15	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:B:466:THR:OG1	1:B:467:ASP:N	2.49	0.44
1:A:623:SER:O	1:B:635:ILE:CD1	2.64	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:596:ARG:HH12	5:A:1760:H4B:C4	2.31	0.44
1:A:454:ASN:HD22	1:A:454:ASN:C	2.21	0.44
1:A:508:GLN:HE22	1:A:716:TRP:HZ3	1.64	0.44

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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
6:A:1780:ARV:HD3	6:A:1780:ARV:HC12	2.02	0.42
1:A:449:ALA:O	1:A:455:LEU:HA	2.20	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:485:TYR:HB3	1:A:514:ARG:HH12	1.84	0.41
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.01	0.41
4:A:750:HEM:CMC	4:A:750:HEM:HBC2	2.45	0.41
6:A:1780:ARV:HD2	6:A:1780:ARV:HC12	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:B:508:GLN:HG3	7:B:22:HOH:O	2.20	0.41
1:B:659:ILE:O	1:B:663:GLU:HG3	2.21	0.41
1:A:676:TRP:CE3	1:B:677:VAL:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:GLY:HA2	1:B:702:PRO:HG2	2.03	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:680:VAL:HA	1:A:681:PRO:HD3	1.88	0.40
1:A:674:ALA:HB3	1:A:695:MET:HB3	2.02	0.40
1:B:386:LYS:O	1:B:389:GLU:HB3	2.22	0.40
1:B:442:ILE:HG21	1:B:522:LEU:HD11	2.03	0.40
1:A:635:ILE:HD13	1:B:624:LEU:HG	2.02	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 ⓘ

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

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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

Some 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 ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	-	1,3,3	2.40	1 (100%)	0,3,3	0.00	-
5	H4B	B	2760	-	16,18,18	2.13	4 (25%)	11,26,26	4.26	9 (81%)
6	ARV	A	1780	-	8,14,14	1.40	2 (25%)	5,16,16	1.35	1 (20%)
6	ARV	B	2780	-	8,14,14	1.22	1 (12%)	5,16,16	1.34	1 (20%)
4	HEM	A	750	1	27,50,50	1.62	6 (22%)	17,82,82	1.60	4 (23%)
5	H4B	A	1760	-	16,18,18	2.31	4 (25%)	11,26,26	4.04	7 (63%)
4	HEM	B	750	1	27,50,50	1.66	5 (18%)	17,82,82	1.88	5 (29%)
2	ACT	A	1860	-	1,3,3	3.49	1 (100%)	0,3,3	0.00	-

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	B	2760	-	-	0/8/17/17	0/2/2/2
6	ARV	A	1780	-	-	0/9/15/15	-
6	ARV	B	2780	-	-	0/9/15/15	-
4	HEM	A	750	1	-	0/6/54/54	-
5	H4B	A	1760	-	-	0/8/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	B	750	1	-	0/6/54/54	-

All (24) 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	B	750	HEM	C3B-C2B	-4.11	1.34	1.40
4	B	750	HEM	C3B-CAB	-4.07	1.39	1.47
4	A	750	HEM	C3C-CAC	-4.04	1.39	1.47
5	B	2760	H4B	C6-N5	4.03	1.53	1.45
5	B	2760	H4B	C4A-N5	3.70	1.45	1.38
2	A	1860	ACT	CH3-C	3.49	1.53	1.48
4	A	750	HEM	C3B-CAB	-3.30	1.41	1.47
4	B	750	HEM	C3C-CAC	-3.28	1.41	1.47
4	B	750	HEM	C3C-C2C	-2.95	1.36	1.40
4	A	750	HEM	C3C-C2C	-2.83	1.36	1.40
4	A	750	HEM	C3B-C2B	-2.79	1.36	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
2	B	2860	ACT	CH3-C	2.40	1.51	1.48
4	A	750	HEM	C1D-ND	2.39	1.41	1.36
4	A	750	HEM	C4B-NB	2.26	1.40	1.36
6	B	2780	ARV	CZ-NH1	-2.15	1.29	1.34
5	B	2760	H4B	C8A-N1	2.15	1.38	1.34
4	B	750	HEM	C1D-ND	2.07	1.40	1.36
6	A	1780	ARV	CD-NE	2.02	1.50	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2760	H4B	C4-C4A-C8A	9.51	123.02	114.57
5	A	1760	H4B	C4-C4A-C8A	8.54	122.16	114.57
5	A	1760	H4B	C4-N3-C2	5.77	125.09	115.93
5	B	2760	H4B	C4-N3-C2	5.62	124.87	115.93
5	A	1760	H4B	N3-C2-N1	-4.69	118.06	125.42
5	B	2760	H4B	N3-C2-N1	-4.47	118.41	125.42
4	A	750	HEM	C1D-C2D-C3D	-4.17	104.09	107.00
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	750	HEM	CBA-CAA-C2A	-3.69	105.68	112.49
5	A	1760	H4B	C2-N1-C8A	3.59	122.58	114.54
5	B	2760	H4B	C2-N1-C8A	3.36	122.06	114.54
4	B	750	HEM	C1D-C2D-C3D	-3.34	104.67	107.00
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
4	A	750	HEM	C4C-C3C-C2C	-2.73	104.99	106.90
5	A	1760	H4B	C4A-N5-C6	-2.72	113.75	121.16
5	B	2760	H4B	C4A-N5-C6	-2.64	113.97	121.16
4	A	750	HEM	CBA-CAA-C2A	-2.40	108.06	112.49
4	B	750	HEM	C4C-C3C-C2C	-2.36	105.25	106.90
4	B	750	HEM	CMA-C3A-C4A	-2.25	125.00	128.46
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
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

There are no chirality outliers.

There are no torsion outliers.

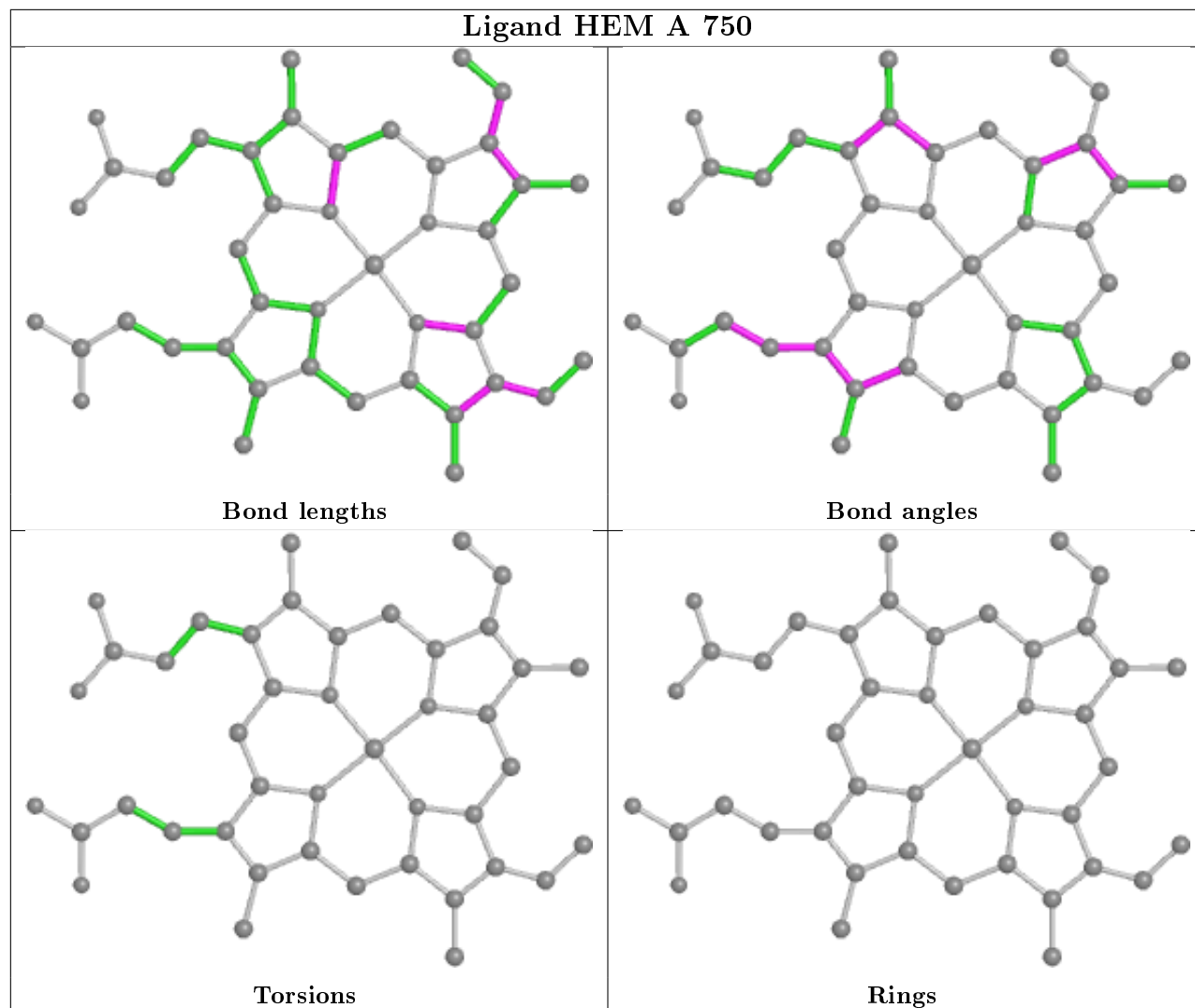
There are no ring outliers.

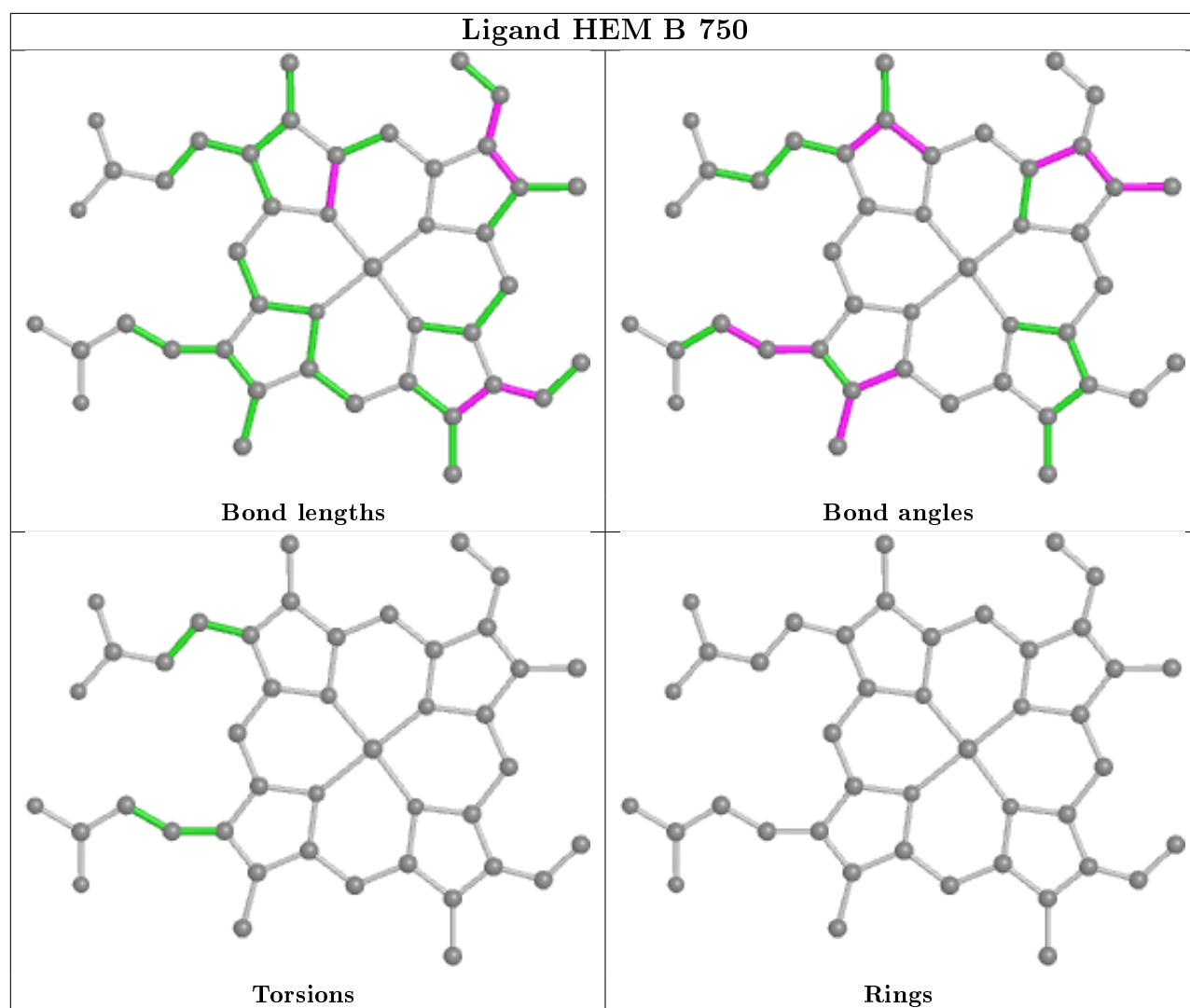
5 monomers are involved in 15 short contacts:

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





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	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

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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 ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	H4B	B	2760	17/17	0.95	0.18	29,35,43,45	0
6	ARV	A	1780	15/15	0.95	0.24	26,35,41,42	0

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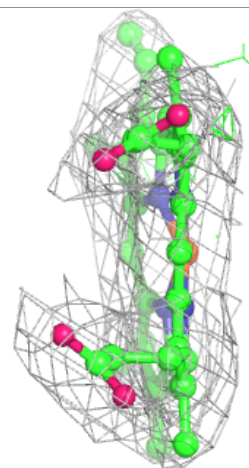
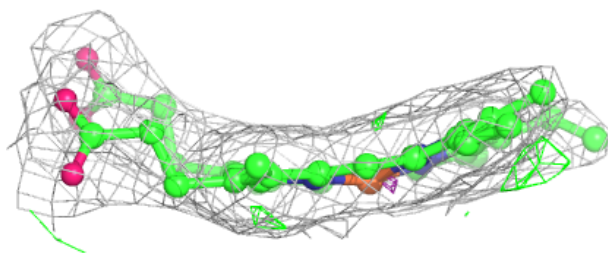
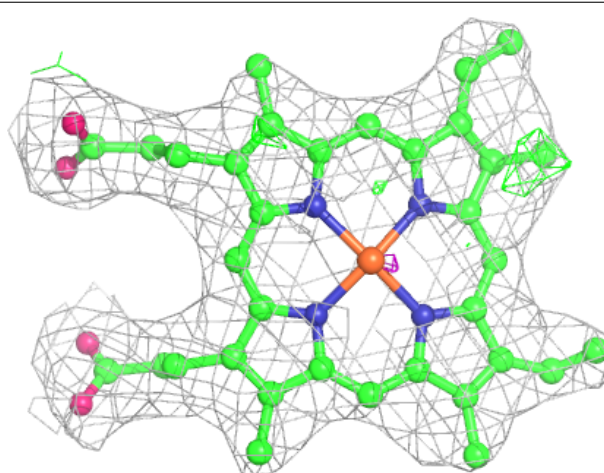
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	ARV	B	2780	15/15	0.95	0.25	34,41,54,55	0
5	H4B	A	1760	17/17	0.95	0.18	24,34,41,41	0
4	HEM	A	750	43/43	0.96	0.22	20,34,43,45	0
2	ACT	A	1860	4/4	0.96	0.16	48,54,55,58	0
4	HEM	B	750	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.

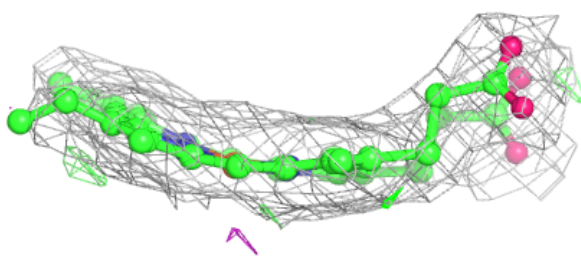
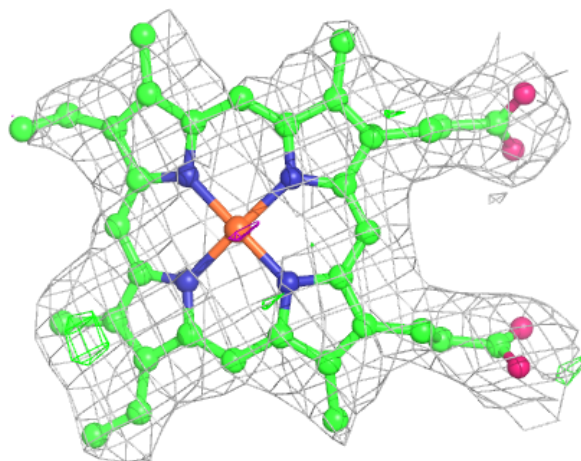
**Electron density around HEM A 750:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (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.