



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 02:11 PM EDT

PDB ID : 3MVZ
Title : X-ray structure of the (hydro)peroxo intermediate NikA/1-Int", after mono-hydroxylation of the iron complex
Authors : Cavazza, C.; Bochot, C.; Rousselot-Pailley, P.; Carpentier, P.; Cherrier, M.V.; Martin, L.; Marchi-Delapierre, C.; Fontecilla-Camps, J.C.; Menage, S.
Deposited on : 2010-05-05
Resolution : 1.70 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 : 4.02b-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

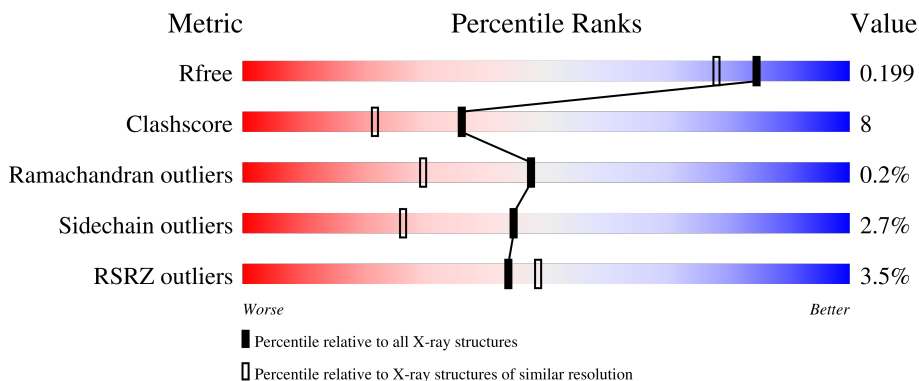
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


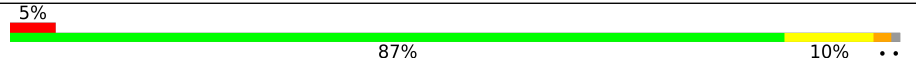
The reported resolution of this entry is 1.70 Å.

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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	502	 2% 86% 13% .
1	B	502	 5% 87% 10% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	523	-	-	X	-
4	GOL	A	517	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9282 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 Nickel-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	498	Total 4026	C 2584	N 673	O 757	S 12	3	15	0
1	B	497	Total 3974	C 2548	N 671	O 742	S 13	4	6	0

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



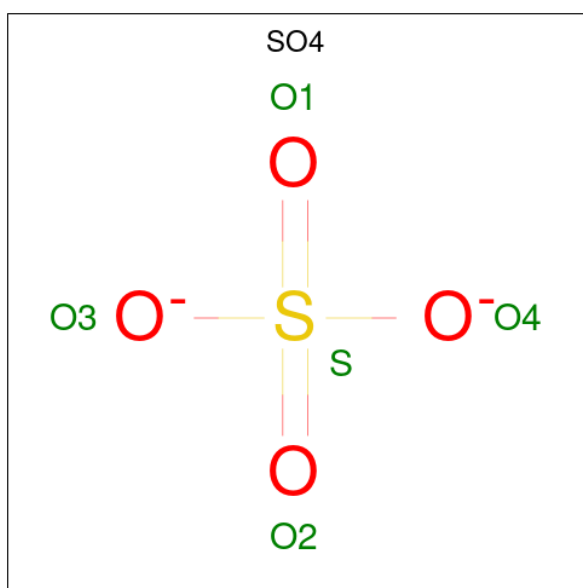
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

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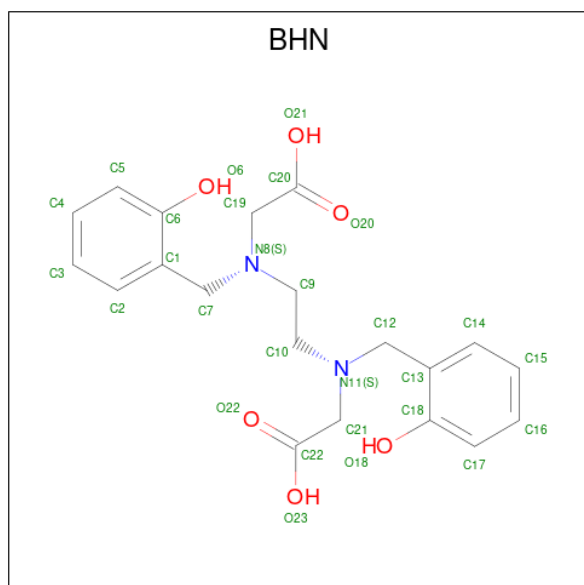
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

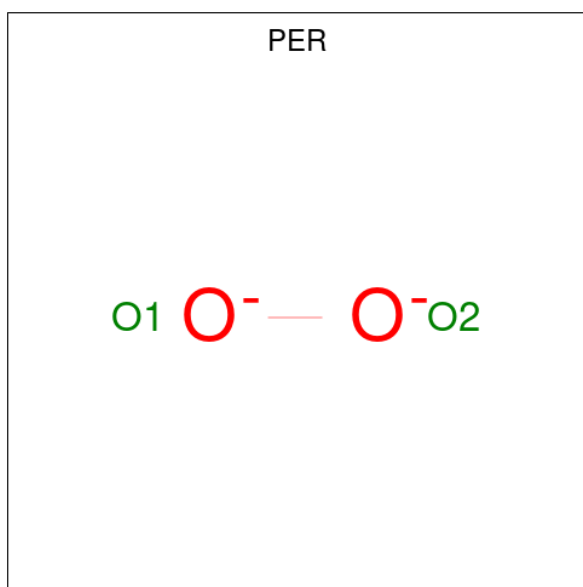
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe		0	0
			1	1			
5	B	1	Total	Fe		0	0
			1	1			

- Molecule 6 is 2-[2-[carboxymethyl-[(2-hydroxyphenyl)methyl]amino]ethyl-[(2-hydroxyphenyl)methyl]amino]ethanoic acid (three-letter code: BHN) (formula: C₂₀H₂₄N₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			28	20	2	6		
6	B	1	Total	C	N	O	0	0
			28	20	2	6		

- Molecule 7 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



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

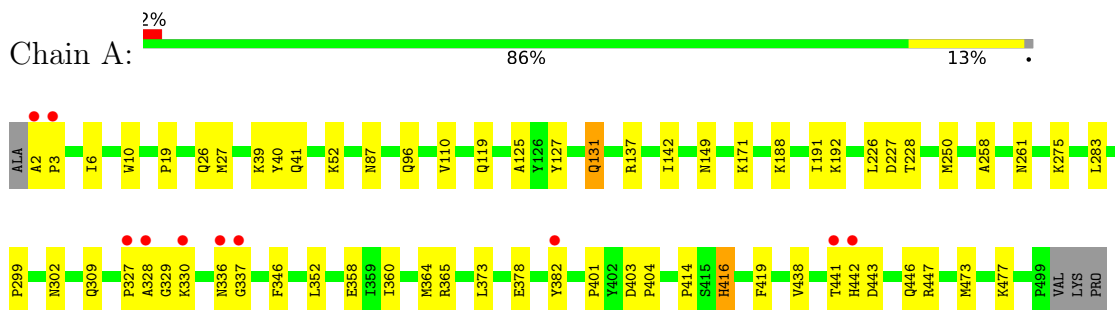
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	595	Total O 595 595	0	0
8	B	494	Total O 494 494	0	0

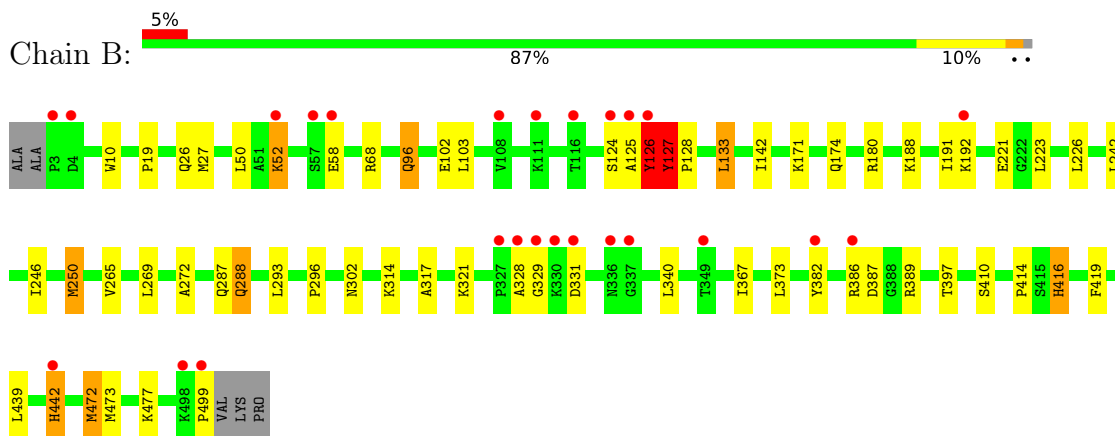
3 Residue-property plots [i](#)

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: Nickel-binding periplasmic protein



- Molecule 1: Nickel-binding periplasmic protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.73Å 94.30Å 124.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.15 – 1.70 47.15 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.15-1.70) 99.0 (47.15-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.164 , 0.200 0.167 , 0.199	Depositor DCC
R_{free} test set	5576 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtrriage
Anisotropy	0.331	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9282	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACT, FE, PER, BHN, SO4

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	0.62	1/4166 (0.0%)	0.66	0/5674
1	B	0.59	1/4090 (0.0%)	0.66	1/5570 (0.0%)
All	All	0.60	2/8256 (0.0%)	0.66	1/11244 (0.0%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	127	TYR	N-CA	-5.55	1.35	1.46
1	A	171	LYS	CD-CE	5.14	1.64	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	472	MET	CG-SD-CE	5.54	109.07	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	288[A]	GLN	Mainchain
1	B	288[B]	GLN	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4026	0	3997	67	0
1	B	3974	0	3922	59	0
2	A	28	0	21	8	0
2	B	8	0	6	0	0
3	A	5	0	0	0	0
4	A	60	0	80	11	0
4	B	30	0	40	5	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	28	0	20	1	0
6	B	28	0	20	1	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	A	595	0	0	12	0
8	B	494	0	0	13	0
All	All	9282	0	8106	130	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 8.

All (130) 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:149:ASN:H	4:A:509:GOL:H11	1.18	1.02
1:B:242:LEU:CD1	1:B:473[B]:MET:SD	2.50	1.00
1:A:188:LYS:HD3	8:A:942:HOH:O	1.61	0.98
1:B:242:LEU:HD12	1:B:473[B]:MET:SD	2.05	0.95
1:A:27[A]:MET:HG3	8:A:780:HOH:O	1.70	0.92
1:A:26:GLN:OE1	2:A:520:ACT:H3	1.71	0.91
1:B:477:LYS:HE3	8:B:1214:HOH:O	1.75	0.86
1:B:250[B]:MET:CE	1:B:293:LEU:HD12	2.11	0.80
4:B:511:GOL:H32	8:B:526:HOH:O	1.81	0.80
1:A:125:ALA:O	1:A:442:HIS:HE1	1.64	0.80
1:A:110:VAL:N	4:A:515:GOL:H32	1.97	0.79
1:B:250[B]:MET:HE1	1:B:293:LEU:HD12	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LEU:HD11	1:B:473[B]:MET:SD	2.24	0.77
1:A:10:TRP:HE1	1:A:26:GLN:HE21	1.33	0.75
1:A:110:VAL:H	4:A:515:GOL:H32	1.49	0.75
1:B:389[A]:ARG:NH1	8:B:791:HOH:O	2.21	0.74
1:A:416:HIS:HB2	8:A:806:HOH:O	1.87	0.73
1:B:27[A]:MET:HG3	8:B:570:HOH:O	1.88	0.72
1:B:387:ASP:OD2	1:B:389[A]:ARG:NH2	2.23	0.71
6:A:512:BHN:O18	6:A:512:BHN:O6	2.08	0.70
1:A:438:VAL:O	1:A:441:THR:HG22	1.92	0.70
1:A:299:PRO:HG3	4:B:511:GOL:H11	1.74	0.69
1:B:102:GLU:HB3	1:B:126:TYR:OH	1.93	0.68
1:B:125:ALA:O	1:B:126:TYR:O	2.14	0.66
1:A:87:ASN:HD21	1:A:142:ILE:H	1.44	0.66
1:A:2:ALA:N	1:A:3:PRO:HD2	2.10	0.65
1:A:358:GLU:HG3	8:A:825:HOH:O	1.97	0.64
1:B:10:TRP:HE1	1:B:26:GLN:HE21	1.45	0.64
1:A:360:ILE:O	1:A:364[B]:MET:HG2	1.99	0.63
1:A:110:VAL:H	4:A:515:GOL:C3	2.12	0.62
1:A:327:PRO:HG2	1:A:330:LYS:HB2	1.81	0.62
1:B:382:TYR:CE2	1:B:386:ARG:HD2	2.35	0.61
1:B:288[B]:GLN:NE2	8:B:1058:HOH:O	2.34	0.60
1:B:221:GLU:OE2	4:B:512:GOL:H31	2.02	0.60
1:A:416:HIS:HE1	8:A:610:HOH:O	1.83	0.59
1:A:446:GLN:HE21	1:A:446:GLN:HA	1.66	0.59
1:B:321:LYS:HD3	8:B:1022:HOH:O	2.01	0.59
1:B:52:LYS:HG3	1:B:68:ARG:HG2	1.84	0.59
1:A:275:LYS:H	4:A:517:GOL:C3	2.15	0.59
1:B:221:GLU:HA	1:B:473[B]:MET:CE	2.32	0.59
1:B:246:ILE:HD13	1:B:472:MET:CE	2.33	0.59
4:B:510:GOL:H32	8:B:657:HOH:O	2.01	0.59
1:B:382:TYR:CZ	1:B:386:ARG:HD2	2.38	0.58
1:B:246:ILE:HD13	1:B:472:MET:HE2	1.85	0.58
1:A:441:THR:HG21	1:A:447:ARG:HG3	1.85	0.58
6:B:507:BHN:O18	6:B:507:BHN:O6	2.21	0.58
1:A:443:ASP:CB	2:A:523:ACT:H2	2.34	0.58
1:A:275:LYS:H	4:A:517:GOL:H31	1.68	0.57
1:B:246:ILE:CD1	1:B:472:MET:CE	2.83	0.57
1:A:275:LYS:N	4:A:517:GOL:H31	2.20	0.57
1:B:250[B]:MET:CE	1:B:293:LEU:CD1	2.82	0.57
1:B:103:LEU:HD21	1:B:133:LEU:HD13	1.87	0.57
1:B:416:HIS:HB2	8:B:1071:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:HIS:CB	8:B:1071:HOH:O	2.54	0.56
1:B:191:ILE:HD11	1:B:499:PRO:HG3	1.88	0.56
1:A:125:ALA:O	1:A:442:HIS:CE1	2.54	0.55
1:B:410:SER:OG	1:B:416:HIS:HD2	1.91	0.53
1:A:442:HIS:H	2:A:523:ACT:H3	1.73	0.53
1:B:221:GLU:HA	1:B:473[B]:MET:HE2	1.90	0.53
1:A:10:TRP:HE1	1:A:26:GLN:NE2	2.06	0.53
1:A:149:ASN:N	4:A:509:GOL:H11	2.03	0.52
1:A:283[B]:LEU:HD23	1:A:352:LEU:HD11	1.91	0.52
1:B:414:PRO:HA	1:B:419:PHE:CD1	2.43	0.52
1:A:441:THR:O	1:A:441:THR:HG23	2.09	0.52
1:A:275:LYS:HB2	4:A:517:GOL:H32	1.91	0.51
1:A:2:ALA:N	1:A:3:PRO:CD	2.73	0.51
1:B:265:VAL:O	1:B:269:LEU:HG	2.11	0.51
1:A:443:ASP:HB3	2:A:523:ACT:H2	1.93	0.50
1:B:127:TYR:N	1:B:128:PRO:CD	2.75	0.49
1:B:19:PRO:HG3	1:B:142:ILE:HB	1.95	0.49
1:A:378:GLU:HG2	1:A:382:TYR:CE2	2.47	0.49
1:A:131[A]:GLN:NE2	1:A:131[A]:GLN:H	2.10	0.48
1:A:414:PRO:HA	1:A:419:PHE:CG	2.48	0.48
1:A:41:GLN:NE2	8:A:1031:HOH:O	2.46	0.48
1:B:296:PRO:HB3	1:B:302:ASN:HD22	1.79	0.48
1:B:328:ALA:HA	1:B:329:GLY:HA2	1.66	0.47
1:A:119:GLN:OE1	8:A:1131:HOH:O	2.20	0.47
1:B:410:SER:OG	1:B:416:HIS:CD2	2.68	0.47
1:A:227:ASP:OD1	1:A:228:THR:N	2.47	0.47
1:A:441:THR:O	1:A:441:THR:CG2	2.63	0.46
1:B:442:HIS:HD2	8:B:1224:HOH:O	1.98	0.46
1:A:52:LYS:HD2	2:A:503:ACT:H1	1.97	0.46
1:B:96:GLN:O	1:B:96:GLN:NE2	2.48	0.46
1:B:226:LEU:HD21	1:B:473[A]:MET:HE1	1.96	0.46
1:B:287:GLN:HE22	1:B:473[B]:MET:CE	2.29	0.46
1:B:10:TRP:HE1	1:B:26:GLN:NE2	2.12	0.46
1:B:442:HIS:N	1:B:442:HIS:CD2	2.84	0.45
1:B:191:ILE:HD11	1:B:499:PRO:CG	2.47	0.45
1:A:258:ALA:HA	1:A:261:ASN:OD1	2.16	0.45
1:A:441:THR:HG23	1:A:447:ARG:HE	1.81	0.44
1:B:416:HIS:HE1	8:B:789:HOH:O	2.01	0.44
1:B:442:HIS:CD2	8:B:1224:HOH:O	2.71	0.44
1:A:346:PHE:HA	8:A:898:HOH:O	2.17	0.44
1:B:52:LYS:HE2	8:B:886:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250[B]:MET:HE3	1:B:397:THR:HG23	1.99	0.44
1:A:19:PRO:HG3	1:A:142:ILE:HB	1.99	0.44
1:B:317:ALA:O	1:B:321:LYS:HG2	2.17	0.43
1:B:127:TYR:N	1:B:128:PRO:HD3	2.33	0.43
1:B:246:ILE:CD1	1:B:472:MET:HE3	2.48	0.43
1:A:360:ILE:O	1:A:364[A]:MET:HG3	2.18	0.43
1:A:365:ARG:HH21	2:A:522:ACT:H3	1.84	0.43
1:A:477:LYS:HE2	8:A:901:HOH:O	2.17	0.43
1:A:414:PRO:HA	1:A:419:PHE:CD1	2.53	0.43
1:A:125:ALA:HB1	1:A:442:HIS:CE1	2.54	0.43
1:B:246:ILE:HD11	1:B:472:MET:CE	2.49	0.42
1:A:27[B]:MET:HB2	1:A:27[B]:MET:HE2	1.82	0.42
1:A:39:LYS:HE3	8:A:840:HOH:O	2.19	0.42
1:B:314:LYS:NZ	4:B:510:GOL:H32	2.35	0.42
1:B:272:ALA:HB2	1:B:367:ILE:HD13	2.01	0.42
1:B:246:ILE:CD1	1:B:472:MET:HE2	2.48	0.42
1:A:443:ASP:HB2	2:A:523:ACT:H2	2.00	0.41
1:A:27[A]:MET:HG2	1:A:137:ARG:CZ	2.50	0.41
1:A:226:LEU:CD2	1:A:473:MET:HE1	2.51	0.41
1:A:302:ASN:CG	4:A:519:GOL:H31	2.41	0.41
1:B:171:LYS:HB3	1:B:174:GLN:HB2	2.02	0.41
1:A:302:ASN:OD1	4:A:519:GOL:H31	2.20	0.41
1:B:223:LEU:HD23	1:B:473[A]:MET:HG3	2.02	0.41
1:A:446:GLN:HA	1:A:446:GLN:NE2	2.33	0.41
1:B:250[B]:MET:SD	1:B:293:LEU:CD1	3.08	0.41
1:A:96[B]:GLN:CG	8:A:915:HOH:O	2.69	0.41
1:B:180:ARG:CZ	1:B:192:LYS:HG2	2.50	0.41
1:A:403:ASP:HA	1:A:404:PRO:HA	1.91	0.41
1:B:127:TYR:H	1:B:128:PRO:HD3	1.86	0.40
1:A:416:HIS:CB	8:A:806:HOH:O	2.58	0.40
1:A:441:THR:CG2	1:A:447:ARG:HG3	2.51	0.40
1:A:441:THR:HA	2:A:523:ACT:H3	2.03	0.40
1:A:40:TYR:CE1	1:A:401:PRO:HB3	2.56	0.40
1:A:6:ILE:HD13	1:A:191[A]:ILE:HD13	2.04	0.40
1:A:328:ALA:HA	1:A:329:GLY:HA2	1.78	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	510/502 (102%)	491 (96%)	18 (4%)	1 (0%)	47	30
1	B	501/502 (100%)	485 (97%)	15 (3%)	1 (0%)	47	30
All	All	1011/1004 (101%)	976 (96%)	33 (3%)	2 (0%)	47	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	126	TYR
1	A	337	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	436/425 (103%)	428 (98%)	8 (2%)	59	43
1	B	424/425 (100%)	407 (96%)	17 (4%)	31	13
All	All	860/850 (101%)	835 (97%)	25 (3%)	44	23

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	TYR
1	A	131[A]	GLN
1	A	131[B]	GLN
1	A	192	LYS

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Mol	Chain	Res	Type
1	A	250	MET
1	A	309	GLN
1	A	373	LEU
1	A	416	HIS
1	B	50	LEU
1	B	52	LYS
1	B	58	GLU
1	B	96	GLN
1	B	124	SER
1	B	126	TYR
1	B	127	TYR
1	B	133	LEU
1	B	188	LYS
1	B	250[A]	MET
1	B	250[B]	MET
1	B	331	ASP
1	B	340	LEU
1	B	373	LEU
1	B	416	HIS
1	B	439	LEU
1	B	442	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	41	GLN
1	A	87	ASN
1	A	119	GLN
1	A	416	HIS
1	A	442	HIS
1	A	446	GLN
1	B	25	ASN
1	B	26	GLN
1	B	56	HIS
1	B	96	GLN
1	B	234	GLN
1	B	244	GLN
1	B	302	ASN
1	B	336	ASN
1	B	385	GLN
1	B	416	HIS

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Mol	Chain	Res	Type
1	B	442	HIS

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 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 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	A	522	-	3,3,3	0.72	0	3,3,3	1.43	0
4	GOL	A	508	-	5,5,5	1.12	1 (20%)	5,5,5	1.34	1 (20%)
6	BHN	A	512	5	29,29,29	0.69	1 (3%)	38,38,38	1.47	4 (10%)
2	ACT	A	505	-	3,3,3	0.77	0	3,3,3	1.10	0
3	SO4	A	507	-	4,4,4	0.11	0	6,6,6	0.09	0
4	GOL	A	510	-	5,5,5	0.36	0	5,5,5	0.27	0
4	GOL	A	517	-	5,5,5	0.41	0	5,5,5	0.70	0
2	ACT	A	523	-	3,3,3	0.75	0	3,3,3	1.20	0
2	ACT	A	504	-	3,3,3	0.82	0	3,3,3	1.50	0
2	ACT	A	503	-	3,3,3	0.67	0	3,3,3	1.39	0
7	PER	A	513	5	0,1,1	-	-	-	-	-
4	GOL	A	521	-	5,5,5	0.36	0	5,5,5	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	515	-	5,5,5	0.50	0	5,5,5	0.66	0
4	GOL	B	505	-	5,5,5	0.32	0	5,5,5	0.75	0
4	GOL	B	510	-	5,5,5	0.36	0	5,5,5	0.28	0
2	ACT	A	506	-	3,3,3	0.79	0	3,3,3	1.29	0
4	GOL	A	519	-	5,5,5	0.39	0	5,5,5	0.95	0
4	GOL	A	509	-	5,5,5	0.37	0	5,5,5	0.50	0
4	GOL	A	518	-	5,5,5	0.34	0	5,5,5	0.72	0
2	ACT	A	520	-	3,3,3	0.77	0	3,3,3	1.35	0
4	GOL	B	509	-	5,5,5	0.39	0	5,5,5	0.40	0
4	GOL	A	516	-	5,5,5	0.26	0	5,5,5	0.79	0
6	BHN	B	507	5	29,29,29	0.79	0	38,38,38	1.20	4 (10%)
2	ACT	B	504	-	3,3,3	0.80	0	3,3,3	1.18	0
4	GOL	A	514	-	5,5,5	0.37	0	5,5,5	0.28	0
4	GOL	B	511	-	5,5,5	0.40	0	5,5,5	0.60	0
2	ACT	B	503	-	3,3,3	0.76	0	3,3,3	1.39	0
4	GOL	B	512	-	5,5,5	0.28	0	5,5,5	0.28	0
7	PER	B	508	5	0,1,1	-	-	-	-	-

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
6	BHN	A	512	5	-	2/21/21/21	0/2/2/2
4	GOL	A	508	-	-	1/4/4/4	-
4	GOL	B	509	-	-	0/4/4/4	-
4	GOL	A	516	-	-	4/4/4/4	-
6	BHN	B	507	5	-	3/21/21/21	0/2/2/2
4	GOL	A	521	-	-	1/4/4/4	-
4	GOL	A	519	-	-	1/4/4/4	-
4	GOL	A	515	-	-	4/4/4/4	-
4	GOL	B	505	-	-	1/4/4/4	-
4	GOL	B	510	-	-	2/4/4/4	-
4	GOL	A	514	-	-	0/4/4/4	-
4	GOL	A	509	-	-	2/4/4/4	-
4	GOL	B	511	-	-	2/4/4/4	-
4	GOL	A	518	-	-	4/4/4/4	-
4	GOL	B	512	-	-	4/4/4/4	-
4	GOL	A	510	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	517	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	508	GOL	O2-C2	-2.13	1.37	1.43
6	A	512	BHN	O23-C22	-2.02	1.23	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	512	BHN	C12-N11-C10	-4.72	101.32	111.29
6	A	512	BHN	C21-N11-C10	-4.01	102.20	111.94
6	A	512	BHN	C7-C1-C6	3.13	123.58	120.45
6	B	507	BHN	C7-C1-C6	3.00	123.45	120.45
6	B	507	BHN	C21-N11-C10	-2.28	106.40	111.94
6	B	507	BHN	C1-C7-N8	-2.28	108.77	112.75
4	A	508	GOL	C3-C2-C1	2.25	120.47	111.70
6	A	512	BHN	C22-C21-N11	-2.06	106.90	113.63
6	B	507	BHN	C20-C19-N8	-2.05	106.93	113.63

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	509	GOL	C1-C2-C3-O3
4	A	510	GOL	O1-C1-C2-C3
4	A	510	GOL	C1-C2-C3-O3
4	A	515	GOL	O1-C1-C2-C3
4	A	515	GOL	C1-C2-C3-O3
4	A	516	GOL	O1-C1-C2-C3
4	B	510	GOL	O1-C1-C2-C3
4	B	511	GOL	O1-C1-C2-C3
4	A	515	GOL	O1-C1-C2-O2
4	A	516	GOL	O1-C1-C2-O2
4	A	518	GOL	O2-C2-C3-O3
6	B	507	BHN	N8-C19-C20-O21
4	A	516	GOL	C1-C2-C3-O3
4	A	517	GOL	O1-C1-C2-C3
4	A	517	GOL	C1-C2-C3-O3
4	A	518	GOL	O1-C1-C2-C3

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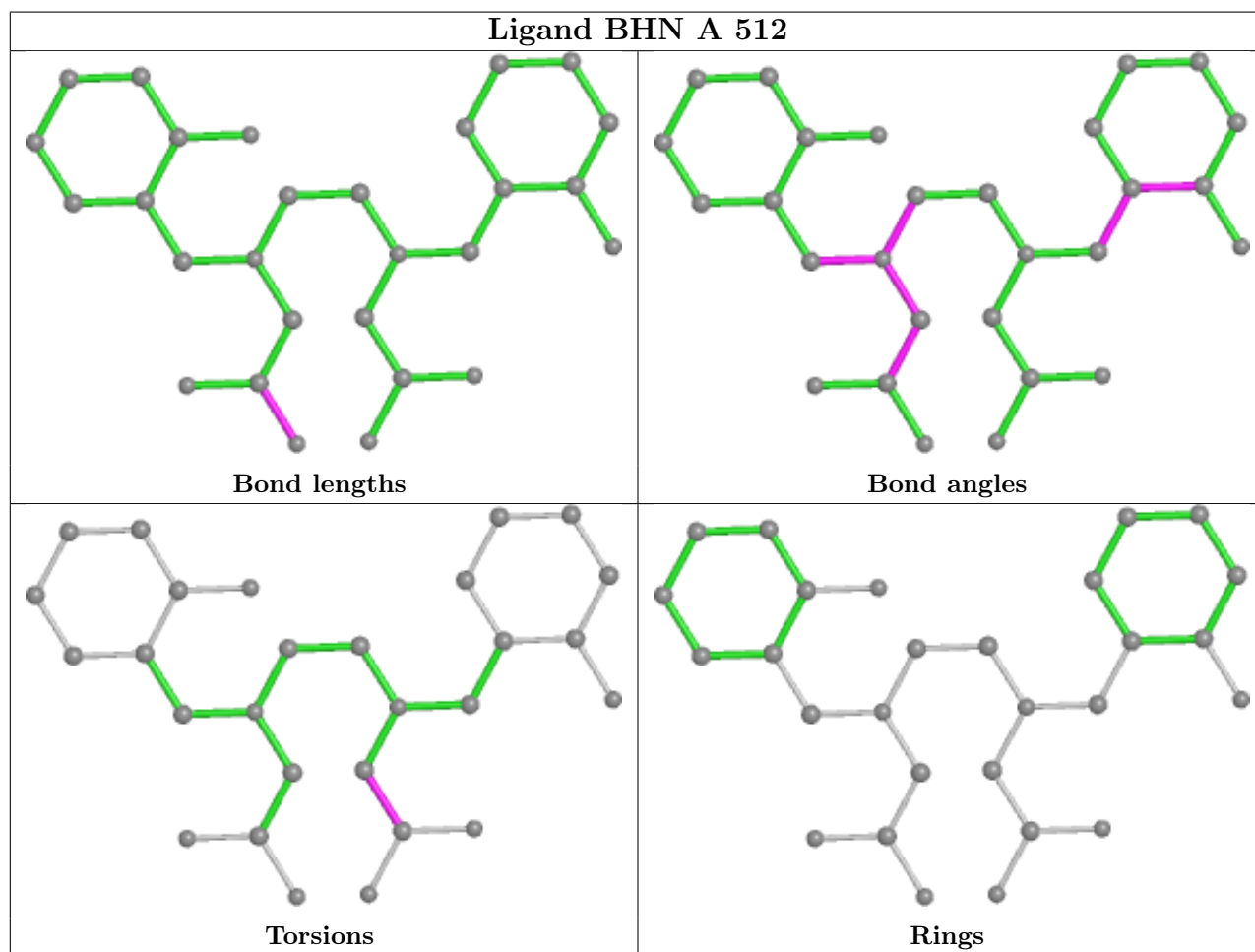
Mol	Chain	Res	Type	Atoms
4	A	518	GOL	C1-C2-C3-O3
4	A	519	GOL	O1-C1-C2-C3
4	B	512	GOL	O1-C1-C2-C3
4	B	512	GOL	C1-C2-C3-O3
6	A	512	BHN	N8-C19-C20-O21
4	A	509	GOL	O2-C2-C3-O3
4	A	510	GOL	O1-C1-C2-O2
4	A	510	GOL	O2-C2-C3-O3
4	A	515	GOL	O2-C2-C3-O3
4	B	510	GOL	O1-C1-C2-O2
4	B	511	GOL	O1-C1-C2-O2
6	B	507	BHN	N8-C19-C20-O20
4	A	508	GOL	O1-C1-C2-O2
4	A	517	GOL	O1-C1-C2-O2
4	B	512	GOL	O2-C2-C3-O3
6	A	512	BHN	N8-C19-C20-O20
4	A	518	GOL	O1-C1-C2-O2
4	B	505	GOL	C1-C2-C3-O3
4	B	512	GOL	O1-C1-C2-O2
4	A	521	GOL	O1-C1-C2-C3
6	B	507	BHN	C13-C12-N11-C21
4	A	516	GOL	O2-C2-C3-O3
4	A	517	GOL	O2-C2-C3-O3

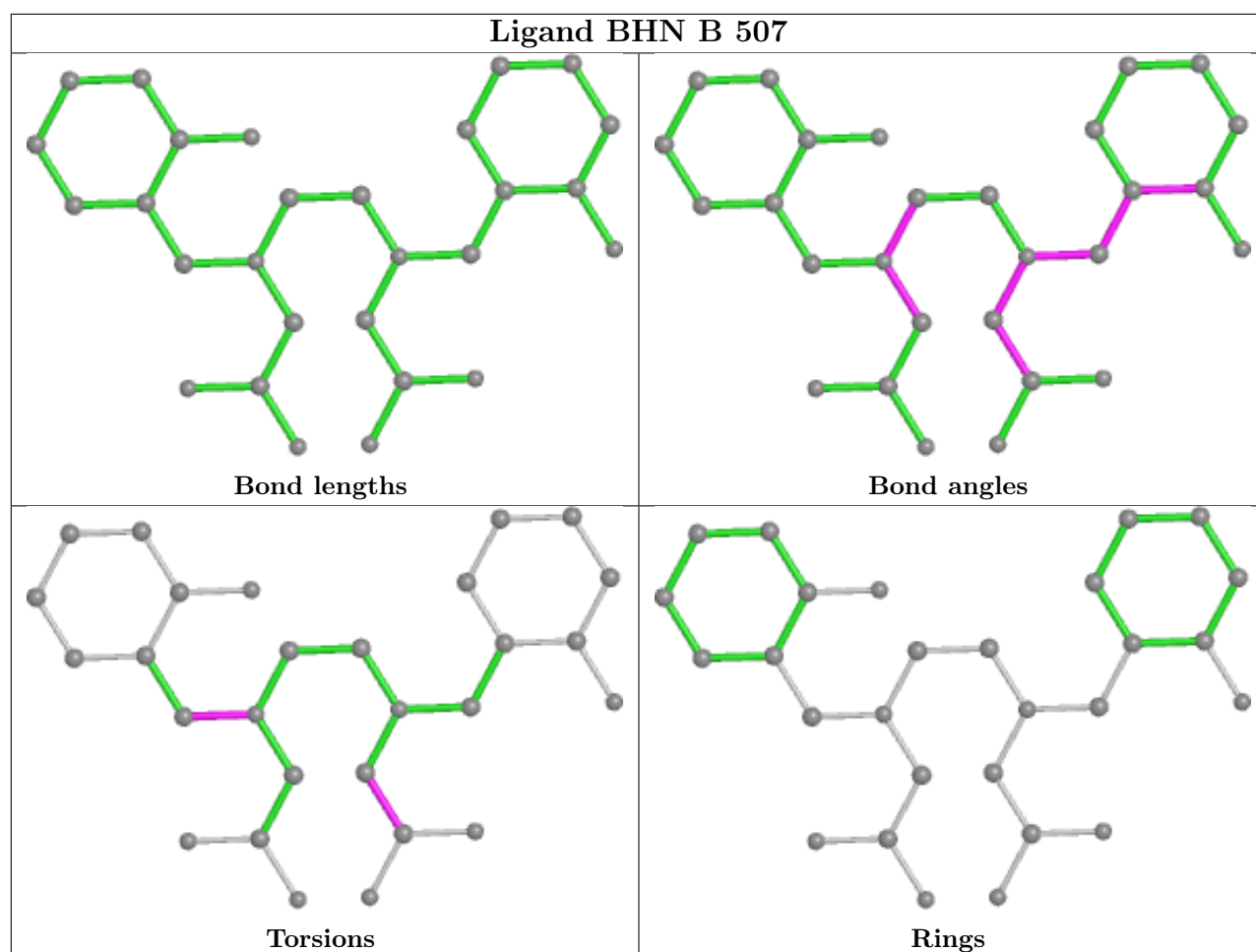
There are no ring outliers.

13 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	522	ACT	1	0
6	A	512	BHN	1	0
4	A	517	GOL	4	0
2	A	523	ACT	5	0
2	A	503	ACT	1	0
4	A	515	GOL	3	0
4	B	510	GOL	2	0
4	A	519	GOL	2	0
4	A	509	GOL	2	0
2	A	520	ACT	1	0
6	B	507	BHN	1	0
4	B	511	GOL	2	0
4	B	512	GOL	1	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	498/502 (99%)	-0.21	10 (2%) 65 69	7, 12, 23, 35	2 (0%)
1	B	497/502 (99%)	-0.01	25 (5%) 28 32	7, 16, 31, 43	1 (0%)
All	All	995/1004 (99%)	-0.11	35 (3%) 44 49	7, 14, 29, 43	3 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	125	ALA	6.8
1	B	328	ALA	5.1
1	A	2	ALA	5.0
1	A	3	PRO	4.9
1	B	442	HIS	4.8
1	B	58	GLU	4.7
1	A	328	ALA	4.6
1	B	499	PRO	4.2
1	B	3	PRO	4.1
1	B	329	GLY	4.1
1	B	126	TYR	3.8
1	B	382	TYR	3.6
1	B	327	PRO	3.4
1	B	498	LYS	3.3
1	B	337	GLY	3.1
1	A	336[A]	ASN	2.9
1	A	442	HIS	2.9
1	B	330	LYS	2.9
1	B	331	ASP	2.9
1	B	52	LYS	2.7
1	A	382	TYR	2.7
1	A	330	LYS	2.6
1	B	336	ASN	2.5
1	B	349	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	327	PRO	2.5
1	B	4	ASP	2.4
1	A	337	GLY	2.4
1	A	441	THR	2.4
1	B	124	SER	2.2
1	B	192	LYS	2.2
1	B	111	LYS	2.2
1	B	116	THR	2.2
1	B	386	ARG	2.1
1	B	108	VAL	2.0
1	B	57	SER	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
4	GOL	A	510	6/6	0.36	0.26	35,40,41,42	0
2	ACT	A	506	4/4	0.52	0.23	55,55,55,55	0
4	GOL	B	510	6/6	0.63	0.35	48,50,51,52	0
2	ACT	A	505	4/4	0.64	0.17	29,29,29,30	0
2	ACT	B	504	4/4	0.65	0.22	33,33,34,34	0
4	GOL	A	509	6/6	0.72	0.21	32,34,36,36	0
4	GOL	A	516	6/6	0.76	0.15	25,27,30,33	0
2	ACT	A	523	4/4	0.77	0.19	34,34,34,35	0
4	GOL	A	519	6/6	0.79	0.18	25,29,30,31	0
2	ACT	A	503	4/4	0.79	0.18	34,36,36,36	0
4	GOL	A	515	6/6	0.80	0.22	24,28,28,29	0
4	GOL	A	508	6/6	0.82	0.17	25,32,34,34	0

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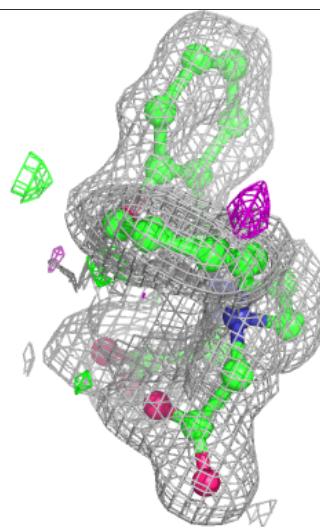
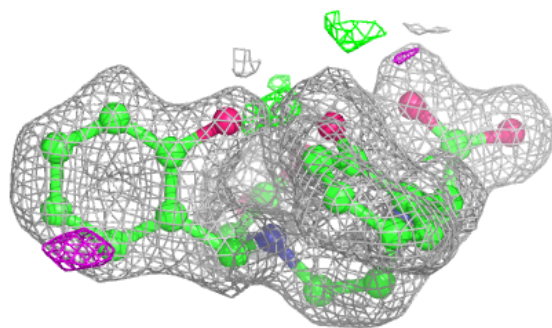
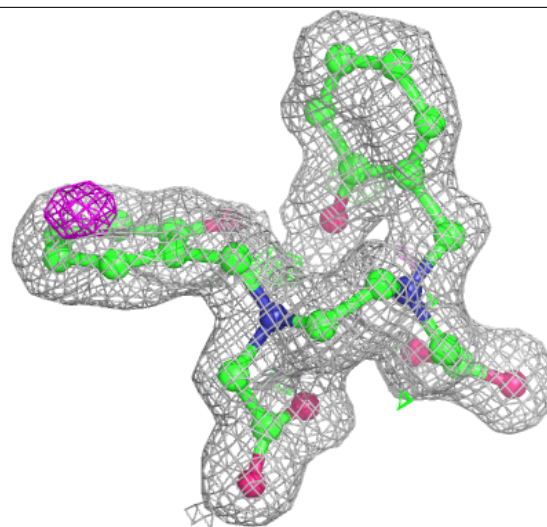
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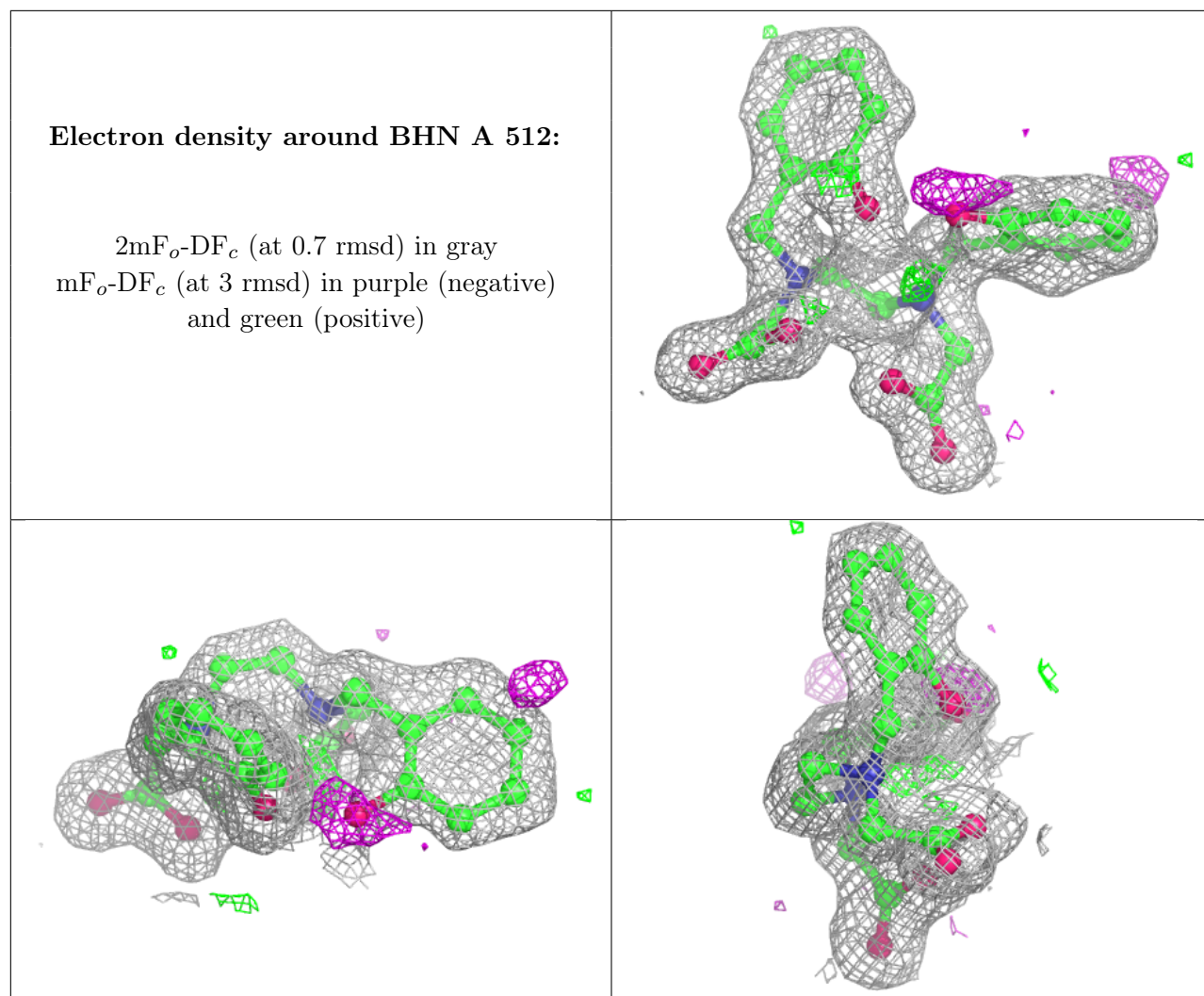
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ACT	A	522	4/4	0.83	0.14	38,38,38,38	0
4	GOL	B	512	6/6	0.84	0.12	40,42,42,44	0
4	GOL	A	518	6/6	0.87	0.15	23,28,30,31	0
4	GOL	B	505	6/6	0.87	0.13	19,22,26,27	0
2	ACT	B	503	4/4	0.88	0.12	44,44,44,44	0
4	GOL	B	511	6/6	0.88	0.17	21,29,30,30	0
2	ACT	A	520	4/4	0.88	0.25	37,37,38,38	0
4	GOL	A	514	6/6	0.90	0.13	13,19,20,21	0
4	GOL	A	521	6/6	0.90	0.10	16,22,23,24	0
2	ACT	A	504	4/4	0.91	0.13	32,32,32,33	0
4	GOL	A	517	6/6	0.92	0.18	19,26,28,31	0
7	PER	A	513	2/2	0.92	0.15	26,26,26,29	0
4	GOL	B	509	6/6	0.93	0.10	15,17,18,19	0
7	PER	B	508	2/2	0.93	0.12	21,21,21,21	2
6	BHN	B	507	28/28	0.95	0.09	11,15,19,19	1
3	SO4	A	507	5/5	0.95	0.13	41,41,41,42	0
6	BHN	A	512	28/28	0.95	0.10	10,15,19,20	1
5	FE	A	511	1/1	0.99	0.07	12,12,12,12	0
5	FE	B	506	1/1	1.00	0.04	12,12,12,12	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 BHN B 507:

$2mF_o-DF_c$ (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.