



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:25 PM UTC

PDB ID : 3MVW / pdb_00003mvw
Title : X-ray structure of a "NikA+Iron complex" hybrid, NikA/1
Authors : Cavazza, C.; Bochot, C.; Rousselot-Pailley, P.; Carpentier, P.; Cherrier, M.V.;
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Deposited on : 2010-05-05
Resolution : 1.79 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

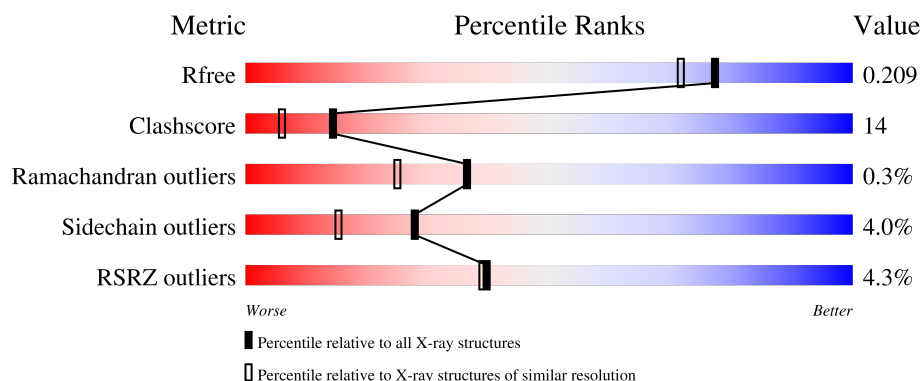
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	3% 75% 22% ..
1	B	502	5% 76% 19% ..

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
4	ACT	B	505	-	-	X	-
6	GOL	A	509	-	-	X	-
6	GOL	A	512	-	-	X	-
7	CL	A	516	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9006 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.

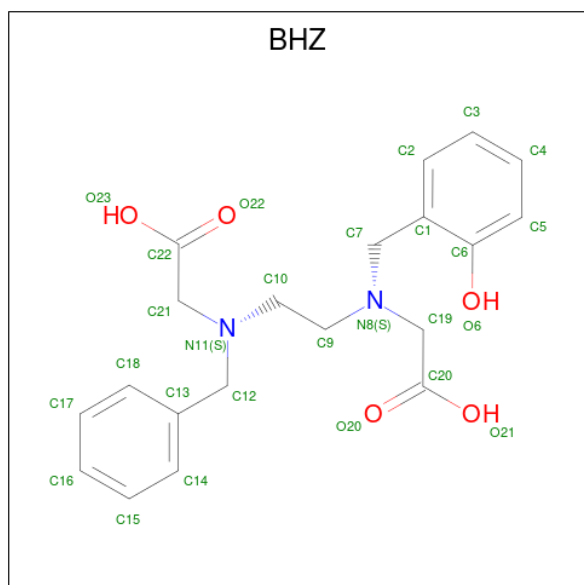
- Molecule 1 is a protein called Nickel-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	4	10	0
			3998	2563	672	753	10			
1	B	498	Total	C	N	O	S	0	5	0
			3970	2546	668	745	11			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

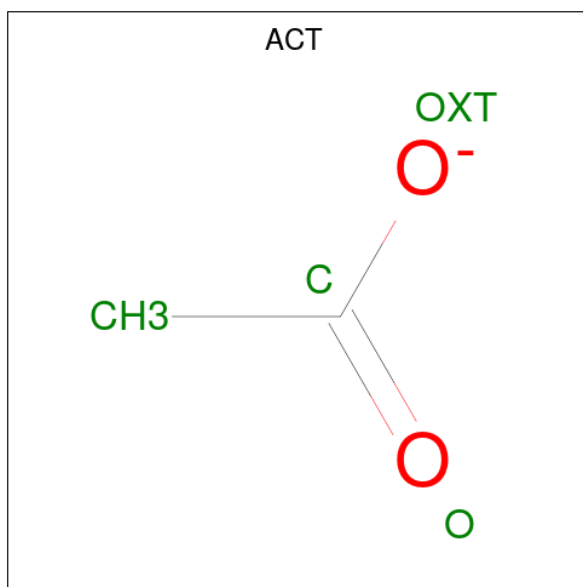
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 2-[2-[carboxymethyl(phenylmethyl)amino]ethyl-[(2-hydroxyphenyl)methyl]amino]ethanoic acid (CCD ID: BHZ) (formula: C₂₀H₂₄N₂O₅).



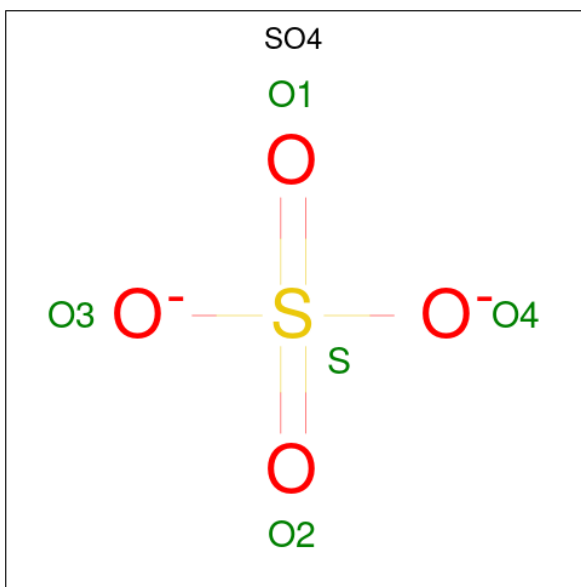
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	20	2	5		
3	B	1	Total	C	N	O	0	0
			27	20	2	5		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



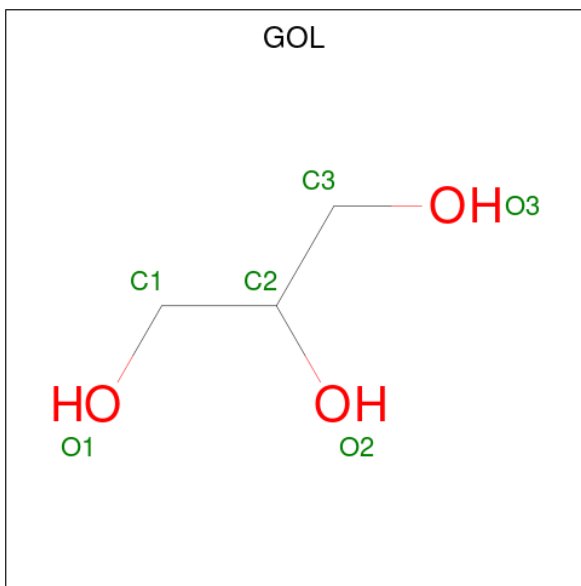
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

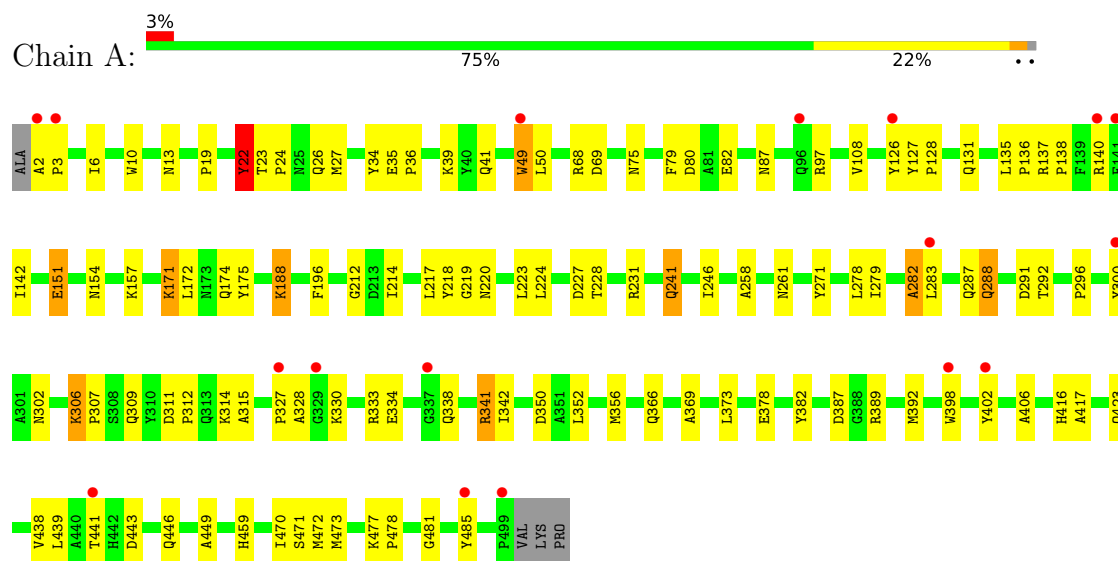
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	483	Total	O	0	0
			483	483		
8	B	416	Total	O	0	0
			416	416		

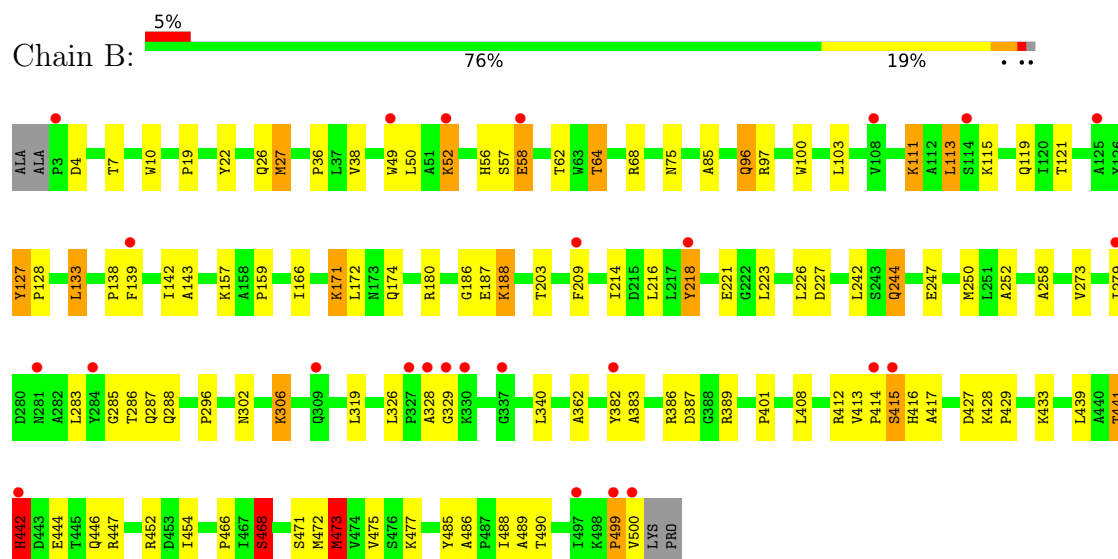
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 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	86.97Å 94.58Å 124.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.29 – 1.79 47.29 – 1.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.29-1.79) 99.6 (47.29-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.47 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.159 , 0.204 0.174 , 0.209	Depositor DCC
R_{free} test set	4853 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9006	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.44	17/4123 (0.4%)	1.19	11/5620 (0.2%)
1	B	1.44	13/4086 (0.3%)	1.23	23/5565 (0.4%)
All	All	1.44	30/8209 (0.4%)	1.21	34/11185 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
All	All	0	6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	LEU	C-O	-8.57	1.13	1.23
1	B	258	ALA	CA-CB	7.13	1.63	1.53
1	B	38	VAL	C-O	-6.90	1.16	1.23
1	B	22	TYR	C-O	-6.66	1.15	1.24
1	A	108	VAL	CA-CB	6.60	1.64	1.54
1	A	417	ALA	CA-CB	6.32	1.63	1.53
1	B	252	ALA	N-CA	6.03	1.53	1.46
1	B	273	VAL	CA-CB	6.03	1.61	1.54
1	A	13	ASN	N-CA	5.99	1.54	1.45
1	B	166	ILE	CA-CB	5.89	1.62	1.54
1	A	311	ASP	C-O	-5.83	1.17	1.24
1	A	449	ALA	CA-CB	5.82	1.62	1.53
1	B	75	ASN	N-CA	5.71	1.54	1.46
1	A	224	LEU	N-CA	5.57	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	GLY	N-CA	5.56	1.52	1.45
1	A	50	LEU	C-O	5.45	1.30	1.24
1	A	369	ALA	CA-CB	5.43	1.61	1.53
1	B	247	GLU	N-CA	5.37	1.52	1.46
1	B	85	ALA	CA-CB	5.34	1.62	1.53
1	A	241	GLN	N-CA	5.33	1.52	1.45
1	A	75	ASN	N-CA	5.32	1.53	1.46
1	A	315	ALA	N-CA	5.31	1.52	1.46
1	A	312	PRO	C-O	-5.27	1.17	1.24
1	A	6	ILE	CA-CB	-5.27	1.46	1.54
1	B	383	ALA	CA-CB	5.23	1.61	1.53
1	B	417	ALA	CA-CB	5.21	1.61	1.53
1	B	159	PRO	CA-C	5.18	1.57	1.52
1	A	157	LYS	C-O	-5.17	1.17	1.24
1	A	279	ILE	CA-CB	-5.09	1.47	1.54
1	A	406	ALA	CA-C	-5.03	1.46	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151[A]	GLU	CA-C-O	-8.08	112.21	121.58
1	A	151[B]	GLU	CA-C-O	-8.08	112.21	121.58
1	B	244[A]	GLN	CA-C-O	-7.01	113.06	120.70
1	B	244[B]	GLN	CA-C-O	-7.01	113.06	120.70
1	B	285	GLY	N-CA-C	6.98	125.02	114.61
1	B	486	ALA	CA-C-N	6.68	126.93	119.32
1	B	486	ALA	C-N-CA	6.68	126.93	119.32
1	B	441	THR	CA-C-N	6.51	130.21	120.31
1	B	441	THR	C-N-CA	6.51	130.21	120.31
1	A	282	ALA	CA-C-N	-6.42	112.05	122.26
1	A	282	ALA	C-N-CA	-6.42	112.05	122.26
1	B	446	GLN	N-CA-C	-6.31	104.48	111.36
1	B	143	ALA	CA-C-N	-6.10	113.34	119.56
1	B	143	ALA	C-N-CA	-6.10	113.34	119.56
1	A	288[A]	GLN	CA-C-O	-5.82	114.58	121.16
1	A	288[B]	GLN	CA-C-O	-5.82	114.58	121.16
1	B	362	ALA	N-CA-C	-5.78	105.06	111.36
1	B	466	PRO	CA-C-N	-5.74	117.35	122.97
1	B	466	PRO	C-N-CA	-5.74	117.35	122.97
1	B	113	LEU	N-CA-C	-5.58	106.31	113.23
1	A	22	TYR	O-C-N	-5.50	115.27	122.59
1	A	35	GLU	CA-C-N	5.46	126.67	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	GLU	C-N-CA	5.46	126.67	119.84
1	B	286	THR	N-CA-C	5.41	119.88	113.28
1	A	333	ARG	N-CA-C	5.32	117.39	110.43
1	B	442	HIS	N-CA-CB	-5.32	102.04	110.28
1	B	468[A]	SER	CA-C-O	-5.22	115.86	121.45
1	B	468[B]	SER	CA-C-O	-5.22	115.86	121.45
1	B	203	THR	N-CA-C	-5.08	105.82	111.36
1	B	326	LEU	CA-C-N	-5.08	114.55	119.78
1	B	326	LEU	C-N-CA	-5.08	114.55	119.78
1	A	443	ASP	N-CA-C	-5.07	101.85	109.15
1	B	468[A]	SER	N-CA-C	5.04	116.85	109.24
1	B	468[B]	SER	N-CA-C	5.04	116.85	109.24

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	TYR	Mainchain
1	A	288[A]	GLN	Mainchain
1	B	244[A]	GLN	Mainchain
1	B	468[A]	SER	Mainchain
1	B	473[A]	MET	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	3998	0	3947	116	0
1	B	3970	0	3923	107	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	21	6	0
3	B	27	0	21	1	0
4	A	12	0	9	0	0
4	B	8	0	6	4	1
5	A	5	0	0	0	0
6	A	36	0	48	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	18	0	23	2	0
7	A	2	0	0	3	0
7	B	2	0	0	0	0
8	A	483	0	0	25	1
8	B	416	0	0	21	0
All	All	9006	0	7998	227	1

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 14.

All (227) 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:209:PHE:CZ	1:B:475:VAL:HG12	1.62	1.34
1:B:306:LYS:N	1:B:306:LYS:HD3	1.55	1.16
1:B:306:LYS:H	1:B:306:LYS:CD	1.53	1.14
1:A:477:LYS:HE2	6:A:509:GOL:C3	1.80	1.11
1:A:387[B]:ASP:OD2	1:A:389:ARG:HG3	1.51	1.10
1:A:341:ARG:HH11	1:A:341:ARG:HG3	0.97	1.10
1:B:209:PHE:CZ	1:B:475:VAL:CG1	2.37	1.07
1:A:69:ASP:HA	6:A:512:GOL:H12	1.34	1.05
1:B:209:PHE:CE2	1:B:475:VAL:CG1	2.40	1.04
1:A:477:LYS:HE2	6:A:509:GOL:H31	1.04	1.03
1:B:287:GLN:HE22	1:B:473[B]:MET:HE1	1.20	1.02
1:B:442:HIS:H	1:B:442:HIS:CD2	1.76	1.02
1:A:27:MET:HG3	8:A:600:HOH:O	1.61	1.00
1:B:414:PRO:O	8:B:943:HOH:O	1.79	1.00
1:B:287:GLN:NE2	1:B:473[B]:MET:HE1	1.75	1.00
6:A:509:GOL:H12	8:A:536:HOH:O	1.62	0.99
1:B:64:THR:HG23	8:B:1063:HOH:O	1.62	0.98
1:A:341:ARG:HG3	1:A:341:ARG:NH1	1.68	0.97
1:B:306:LYS:HD3	1:B:306:LYS:H	0.84	0.97
1:A:477:LYS:CE	6:A:509:GOL:H31	1.96	0.95
1:A:188:LYS:HD2	1:A:188:LYS:H	1.32	0.94
1:B:287:GLN:HE22	1:B:473[B]:MET:CE	1.79	0.94
1:A:135:LEU:HD22	1:A:402:TYR:CZ	2.03	0.93
6:A:509:GOL:C1	8:A:536:HOH:O	2.15	0.92
1:B:414:PRO:O	1:B:415:SER:HB2	1.67	0.91
1:A:341:ARG:HH11	1:A:341:ARG:CG	1.84	0.91
1:B:209:PHE:CE1	1:B:475:VAL:HG12	2.07	0.88
1:B:485:TYR:HB3	6:B:506:GOL:H11	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:510:GOL:H12	8:A:860:HOH:O	1.72	0.87
1:B:427:ASP:HB3	8:B:675:HOH:O	1.73	0.87
1:B:477:LYS:HE3	8:B:1050:HOH:O	1.76	0.86
1:B:180:ARG:HD2	1:B:188:LYS:HG2	1.59	0.83
1:A:172:LEU:HD11	8:A:878:HOH:O	1.78	0.83
1:B:209:PHE:CE2	1:B:475:VAL:HG11	2.14	0.83
1:B:287:GLN:HG3	8:B:795:HOH:O	1.77	0.82
1:B:64:THR:CG2	8:B:1063:HOH:O	2.20	0.81
1:A:387[B]:ASP:CG	1:A:389:ARG:HG3	2.05	0.80
1:A:23[A]:THR:HG22	7:A:516:CL:CL	2.21	0.78
1:A:151[B]:GLU:OE2	1:A:154:ASN:ND2	2.17	0.78
6:A:510:GOL:C1	8:A:860:HOH:O	2.27	0.78
1:B:414:PRO:O	1:B:415:SER:CB	2.32	0.78
1:B:171:LYS:HG2	1:B:174:GLN:HG3	1.66	0.77
1:A:23[A]:THR:HG23	8:A:1037:HOH:O	1.86	0.76
1:A:171:LYS:HG3	1:A:175:TYR:CZ	2.20	0.75
1:B:58:GLU:H	1:B:58:GLU:CD	1.94	0.75
1:A:23[A]:THR:CG2	7:A:516:CL:CL	2.72	0.75
1:B:287:GLN:CD	1:B:473[B]:MET:HE1	2.13	0.74
1:A:10:TRP:HE1	1:A:26:GLN:HE21	1.36	0.74
1:B:386:ARG:HA	1:B:415:SER:O	1.89	0.73
1:B:52:LYS:HG3	1:B:68:ARG:HG2	1.69	0.72
1:B:242:LEU:CD1	1:B:473[B]:MET:SD	2.78	0.72
1:B:27:MET:HG3	8:B:602:HOH:O	1.88	0.72
1:A:23[B]:THR:CG2	1:A:24:PRO:HA	2.20	0.71
1:A:23[B]:THR:HG23	1:A:24:PRO:HA	1.71	0.70
1:A:87:ASN:HD21	1:A:142:ILE:H	1.38	0.70
1:A:97:ARG:HH11	3:A:504:BHZ:C16	2.04	0.70
1:B:10:TRP:HE1	1:B:26:GLN:HE21	1.40	0.70
6:A:512:GOL:H31	8:A:794:HOH:O	1.89	0.70
1:A:416:HIS:HB2	8:A:1023:HOH:O	1.91	0.69
1:A:378:GLU:HG2	1:A:382:TYR:CE2	2.28	0.69
1:A:126:TYR:CE1	1:A:439:LEU:HB3	2.29	0.68
1:A:39:LYS:HE2	8:A:904:HOH:O	1.94	0.67
1:A:36:PRO:HD2	1:A:49:TRP:CD1	2.30	0.67
1:A:287:GLN:HE22	1:A:471:SER:H	1.43	0.67
1:B:64:THR:HG21	8:B:598:HOH:O	1.94	0.67
1:A:97:ARG:CZ	8:A:552:HOH:O	2.42	0.66
1:A:231[B]:ARG:HH21	6:A:515:GOL:HO3	1.44	0.66
1:A:126:TYR:CE2	1:A:128:PRO:HD2	2.31	0.66
1:B:36:PRO:HD2	1:B:49:TRP:CD1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:VAL:O	1:A:441:THR:HG22	1.98	0.64
1:A:223:LEU:HB3	1:A:473:MET:HE3	1.79	0.64
1:A:79:PHE:O	6:A:512:GOL:H11	1.97	0.64
1:B:218:TYR:CZ	1:B:472:MET:HG2	2.33	0.64
1:B:287:GLN:NE2	1:B:473[B]:MET:CE	2.49	0.63
1:A:126:TYR:CD2	1:A:128:PRO:HD2	2.34	0.63
1:B:221:GLU:HA	1:B:473[B]:MET:HE3	1.78	0.63
1:B:416:HIS:HB2	8:B:812:HOH:O	1.98	0.63
1:A:416:HIS:HE1	8:A:882:HOH:O	1.81	0.63
1:B:58:GLU:CD	1:B:58:GLU:N	2.55	0.63
1:A:140:ARG:HG3	8:A:659:HOH:O	1.99	0.62
1:A:135:LEU:HD22	1:A:402:TYR:CE2	2.35	0.62
1:B:4:ASP:N	1:B:4:ASP:OD1	2.29	0.61
1:A:212:GLY:HA2	6:A:509:GOL:O3	1.99	0.61
4:B:511:ACT:H1	8:B:688:HOH:O	2.01	0.60
6:A:512:GOL:C3	8:A:794:HOH:O	2.48	0.60
1:B:442:HIS:CD2	1:B:442:HIS:N	2.60	0.60
1:A:34:TYR:HB3	1:A:140:ARG:HB3	1.84	0.59
1:A:136:PRO:HD2	1:A:402:TYR:OH	2.03	0.59
1:B:218:TYR:C	1:B:218:TYR:CD2	2.81	0.59
1:B:490:THR:HG22	6:B:508:GOL:O2	2.04	0.58
1:B:96:GLN:HG2	8:B:629:HOH:O	2.03	0.57
1:B:287:GLN:OE1	1:B:473[B]:MET:HE1	2.04	0.57
1:B:96:GLN:NE2	1:B:96:GLN:H	2.03	0.57
1:B:444[A]:GLU:HA	1:B:447:ARG:NH1	2.20	0.57
1:A:481:GLY:HA2	1:B:444[B]:GLU:HG2	1.86	0.57
1:A:287:GLN:HE21	1:A:470:ILE:HA	1.69	0.57
1:B:121:THR:HG23	8:B:612:HOH:O	2.05	0.56
1:A:97:ARG:NH1	3:A:504:BHZ:C16	2.69	0.56
1:B:227:ASP:OD2	4:B:505:ACT:H2	2.05	0.56
1:B:62:THR:HG23	1:B:121:THR:HG22	1.88	0.56
1:B:444[A]:GLU:HA	1:B:447:ARG:HH11	1.71	0.56
1:A:446:GLN:HE21	1:A:446:GLN:HA	1.71	0.55
1:B:209:PHE:CE2	1:B:475:VAL:HG12	2.10	0.55
1:B:10:TRP:HE1	1:B:26:GLN:NE2	2.03	0.55
1:B:283:LEU:HD13	8:B:795:HOH:O	2.06	0.55
1:B:444[B]:GLU:HA	1:B:447:ARG:HH11	1.72	0.55
6:A:509:GOL:H11	8:A:536:HOH:O	1.91	0.55
1:A:23[A]:THR:HG21	7:A:516:CL:CL	2.44	0.55
1:A:220:ASN:O	1:A:473:MET:HE2	2.06	0.55
1:B:444[B]:GLU:HA	1:B:447:ARG:NH1	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:HIS:CE1	8:A:882:HOH:O	2.59	0.54
1:A:97:ARG:HH11	3:A:504:BHZ:C15	2.19	0.54
1:A:271:TYR:CZ	1:A:314:LYS:HD3	2.43	0.54
1:B:242:LEU:HD12	1:B:473[B]:MET:SD	2.47	0.54
1:B:499:PRO:O	1:B:500:VAL:CB	2.55	0.54
1:A:278:LEU:HD21	1:A:356:MET:HE3	1.88	0.53
1:B:382:TYR:CZ	1:B:386:ARG:HD2	2.42	0.53
1:A:49:TRP:HA	1:A:49:TRP:CE3	2.42	0.53
1:A:172:LEU:CD1	8:A:878:HOH:O	2.45	0.53
1:A:300:TYR:OH	8:A:775:HOH:O	2.13	0.53
1:B:296:PRO:HB3	1:B:302:ASN:HD22	1.73	0.53
1:A:241:GLN:HB3	1:A:485:TYR:OH	2.08	0.52
1:B:227:ASP:CG	4:B:505:ACT:H2	2.34	0.52
1:A:231[B]:ARG:NH2	6:A:515:GOL:O3	2.35	0.52
1:B:100:TRP:HA	1:B:413:VAL:HG21	1.92	0.52
1:B:242:LEU:HD11	1:B:473[B]:MET:SD	2.49	0.52
1:A:287:GLN:NE2	1:A:471:SER:H	2.08	0.52
1:A:296:PRO:HB3	1:A:302:ASN:HD22	1.75	0.52
1:B:416:HIS:CB	8:B:812:HOH:O	2.57	0.51
1:B:288:GLN:O	1:B:468[B]:SER:HB2	2.10	0.51
1:A:10:TRP:HE1	1:A:26:GLN:NE2	2.07	0.51
1:A:292:THR:HG22	1:A:459:HIS:CE1	2.45	0.51
1:A:387[B]:ASP:OD2	1:A:389:ARG:CG	2.42	0.51
1:B:171:LYS:CG	1:B:174:GLN:HG3	2.40	0.50
1:A:41:GLN:NE2	8:A:917:HOH:O	2.44	0.50
1:A:68:ARG:O	6:A:512:GOL:H12	2.11	0.50
1:B:127:TYR:N	1:B:128:PRO:HD3	2.27	0.50
1:B:387:ASP:OD2	1:B:389:ARG:NH1	2.41	0.50
1:B:226:LEU:HD12	1:B:283:LEU:HA	1.92	0.50
1:B:103:LEU:HD21	1:B:133:LEU:HD13	1.93	0.50
1:A:241:GLN:CB	1:A:485:TYR:OH	2.60	0.50
1:A:416:HIS:HD2	8:A:827:HOH:O	1.94	0.50
1:B:49:TRP:HA	1:B:49:TRP:CE3	2.46	0.49
1:A:126:TYR:HE1	1:A:439:LEU:HB3	1.76	0.49
1:B:7:THR:HG22	1:B:214:ILE:HG22	1.95	0.49
1:B:52:LYS:HE3	1:B:68:ARG:HG2	1.93	0.49
1:B:412:ARG:O	1:B:414:PRO:HD3	2.12	0.49
1:B:452:ARG:HD2	8:B:735:HOH:O	2.12	0.49
1:B:227:ASP:OD1	4:B:505:ACT:H2	2.12	0.49
1:B:471:SER:O	1:B:473[B]:MET:HE2	2.11	0.49
1:A:366:GLN:NE2	8:A:809:HOH:O	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:MET:HG2	8:A:578:HOH:O	2.14	0.47
1:B:127:TYR:N	1:B:128:PRO:CD	2.77	0.47
1:A:477:LYS:HE2	6:A:509:GOL:O3	2.14	0.47
1:A:398:TRP:HB3	3:A:504:BHZ:C2	2.45	0.47
1:A:477:LYS:CE	6:A:509:GOL:C3	2.72	0.47
1:A:80:ASP:HB3	6:A:512:GOL:H2	1.97	0.47
1:A:175:TYR:C	1:A:175:TYR:CD2	2.92	0.47
1:A:241:GLN:NE2	1:A:485:TYR:OH	2.32	0.47
1:A:423:GLN:NE2	8:A:943:HOH:O	2.48	0.47
1:B:19:PRO:HG3	1:B:142:ILE:HB	1.97	0.47
1:A:477:LYS:CG	6:A:509:GOL:H31	2.45	0.47
1:A:481:GLY:HA2	1:B:444[B]:GLU:CG	2.44	0.47
1:B:209:PHE:CD2	1:B:475:VAL:HG11	2.48	0.47
1:A:223:LEU:HB3	1:A:473:MET:CE	2.46	0.46
1:A:416:HIS:CB	8:A:1023:HOH:O	2.56	0.46
1:B:433:LYS:HE3	8:B:600:HOH:O	2.16	0.46
1:A:171:LYS:HG3	1:A:175:TYR:CE2	2.51	0.45
1:A:227:ASP:OD1	1:A:228:THR:N	2.48	0.45
1:A:22:TYR:O	1:A:23[A]:THR:C	2.58	0.45
1:A:137:ARG:HB2	1:A:138:PRO:HA	1.98	0.45
1:A:39:LYS:HD2	1:A:49:TRP:CZ2	2.52	0.45
1:B:96:GLN:H	1:B:96:GLN:CD	2.25	0.45
1:A:278:LEU:HD23	1:A:278:LEU:C	2.42	0.45
1:A:477:LYS:HG2	6:A:509:GOL:H31	1.99	0.45
1:B:306:LYS:N	1:B:306:LYS:CD	2.33	0.44
1:A:97:ARG:O	3:A:504:BHZ:H15	2.16	0.44
1:B:226:LEU:CD1	1:B:283:LEU:HA	2.47	0.44
1:A:342:ILE:HG21	1:A:392:MET:HG3	1.99	0.44
1:A:438:VAL:HA	1:A:441:THR:HG22	2.00	0.44
1:B:386:ARG:HD3	8:B:527:HOH:O	2.16	0.44
1:A:171:LYS:HB2	1:A:174:GLN:HB2	1.99	0.44
1:B:499:PRO:HG2	1:B:500:VAL:H	1.83	0.44
1:A:22:TYR:O	1:A:23[B]:THR:C	2.60	0.43
1:A:282:ALA:C	1:A:283[A]:LEU:HD22	2.43	0.43
1:A:327:PRO:HG2	1:A:330:LYS:HB2	2.00	0.43
1:A:327:PRO:O	1:A:328:ALA:C	2.60	0.43
1:B:401:PRO:HD3	1:B:488:ILE:HG12	2.00	0.43
1:A:82:GLU:HB2	8:A:717:HOH:O	2.18	0.43
1:A:218:TYR:CE2	1:A:472:MET:HE2	2.53	0.43
1:A:350:ASP:C	1:A:350:ASP:OD1	2.62	0.43
1:B:328:ALA:HA	1:B:329:GLY:HA2	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ALA:HA	1:A:261:ASN:OD1	2.17	0.43
1:A:423:GLN:HE21	1:A:423:GLN:HB3	1.73	0.43
1:B:103:LEU:HD23	1:B:139:PHE:CE2	2.54	0.43
1:A:19:PRO:HG3	1:A:142:ILE:HB	2.01	0.43
1:A:291:ASP:HB3	1:A:307:PRO:HB3	2.00	0.43
1:B:389:ARG:NH2	8:B:628:HOH:O	2.51	0.42
1:A:481:GLY:CA	1:B:444[B]:GLU:HG2	2.48	0.42
1:B:56:HIS:HD2	1:B:57:SER:O	2.02	0.42
1:B:218:TYR:C	1:B:218:TYR:HD2	2.25	0.42
1:B:119:GLN:NE2	8:B:598:HOH:O	2.23	0.42
1:B:4:ASP:HA	1:B:499:PRO:HB3	2.02	0.42
1:A:342:ILE:CG2	1:A:392:MET:HG3	2.49	0.42
1:A:334:GLU:HA	1:A:338:GLN:O	2.20	0.42
1:A:188:LYS:H	1:A:188:LYS:CD	2.13	0.42
1:A:246:ILE:HD13	1:A:472:MET:HG2	2.00	0.42
1:A:481:GLY:HA2	1:B:444[B]:GLU:CD	2.44	0.42
1:A:214:ILE:CD1	1:A:217:LEU:HD21	2.50	0.41
1:B:111:LYS:HD2	1:B:113:LEU:HD23	2.02	0.41
1:B:223:LEU:HD23	1:B:473[A]:MET:HG3	2.02	0.41
1:A:175:TYR:HA	1:A:196:PHE:O	2.20	0.41
1:A:306:LYS:HE3	1:A:306:LYS:HB2	1.49	0.41
1:B:186:GLY:HA3	8:B:847:HOH:O	2.21	0.41
1:A:23[B]:THR:HG22	1:A:24:PRO:HA	2.02	0.41
1:A:398:TRP:HB3	3:A:504:BHZ:H2	2.02	0.41
1:B:389:ARG:NE	8:B:840:HOH:O	2.47	0.41
1:B:441:THR:O	1:B:447:ARG:NH2	2.53	0.41
1:B:408:LEU:HD13	1:B:454:ILE:HG21	2.03	0.41
1:B:472:MET:HE1	1:B:489:ALA:O	2.21	0.41
1:B:442:HIS:H	1:B:442:HIS:HD2	1.51	0.41
1:B:428:LYS:N	1:B:429:PRO:CD	2.85	0.40
1:B:97:ARG:O	3:B:504:BHZ:H15	2.21	0.40
1:A:2:ALA:N	1:A:3:PRO:HD3	2.36	0.40
1:A:126:TYR:CZ	1:A:128:PRO:HD2	2.56	0.40
1:B:279:ILE:HA	1:B:283:LEU:HD12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:505:ACT:CH3	8:A:592:HOH:O[2_554]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone

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	506/502 (101%)	488 (96%)	18 (4%)	0	100	100
1	B	500/502 (100%)	486 (97%)	11 (2%)	3 (1%)	21	11
All	All	1006/1004 (100%)	974 (97%)	29 (3%)	3 (0%)	36	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	499	PRO
1	B	415	SER
1	B	157	LYS

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	429/425 (101%)	418 (97%)	11 (3%)	40	28
1	B	426/425 (100%)	402 (94%)	24 (6%)	19	8
All	All	855/850 (101%)	820 (96%)	35 (4%)	28	15

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	TRP
1	A	127	TYR
1	A	131	GLN

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Mol	Chain	Res	Type
1	A	171	LYS
1	A	188	LYS
1	A	306	LYS
1	A	309	GLN
1	A	341	ARG
1	A	352	LEU
1	A	373	LEU
1	A	478	PRO
1	B	27	MET
1	B	50	LEU
1	B	52	LYS
1	B	58	GLU
1	B	64	THR
1	B	96	GLN
1	B	111	LYS
1	B	115	LYS
1	B	127	TYR
1	B	133	LEU
1	B	138	PRO
1	B	171	LYS
1	B	172	LEU
1	B	187	GLU
1	B	188	LYS
1	B	218	TYR
1	B	250	MET
1	B	306	LYS
1	B	319	LEU
1	B	340	LEU
1	B	439	LEU
1	B	442	HIS
1	B	473[A]	MET
1	B	473[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	41	GLN
1	A	87	ASN
1	A	131	GLN
1	A	154	ASN
1	A	197	ASN

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Mol	Chain	Res	Type
1	A	234	GLN
1	A	287	GLN
1	A	302	ASN
1	A	385	GLN
1	A	416	HIS
1	A	423	GLN
1	A	446	GLN
1	A	482	ASN
1	A	496	GLN
1	B	25	ASN
1	B	26	GLN
1	B	41	GLN
1	B	56	HIS
1	B	96	GLN
1	B	168	GLN
1	B	234	GLN
1	B	288	GLN
1	B	302	ASN
1	B	336	ASN
1	B	385	GLN
1	B	442	HIS
1	B	496	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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
4	ACT	A	506	-	3,3,3	1.05	0	3,3,3	2.39	2 (66%)
3	BHZ	A	504	2	28,28,28	1.73	5 (17%)	36,36,36	1.80	8 (22%)
6	GOL	A	512	-	5,5,5	0.56	0	5,5,5	1.17	0
3	BHZ	B	504	2	28,28,28	1.90	6 (21%)	36,36,36	1.24	4 (11%)
6	GOL	A	513	-	5,5,5	0.74	0	5,5,5	0.58	0
4	ACT	B	511	-	3,3,3	0.79	0	3,3,3	1.80	2 (66%)
6	GOL	B	508	-	5,5,5	0.38	0	5,5,5	0.31	0
4	ACT	A	507	-	3,3,3	0.49	0	3,3,3	0.92	0
4	ACT	A	505	-	3,3,3	0.96	0	3,3,3	1.92	1 (33%)
6	GOL	B	507	-	5,5,5	0.37	0	5,5,5	0.31	0
6	GOL	A	515	-	5,5,5	0.44	0	5,5,5	0.88	0
6	GOL	A	509	-	5,5,5	0.38	0	5,5,5	0.31	0
6	GOL	B	506	-	5,5,5	1.10	0	5,5,5	0.87	0
5	SO4	A	508	-	4,4,4	0.25	0	6,6,6	0.23	0
4	ACT	B	505	-	3,3,3	0.79	0	3,3,3	0.97	0
6	GOL	A	510	-	5,5,5	0.38	0	5,5,5	0.32	0
6	GOL	A	514	-	5,5,5	0.38	0	5,5,5	1.39	1 (20%)

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
3	BHZ	A	504	2	-	0/21/21/21	0/2/2/2
6	GOL	A	512	-	-	2/4/4/4	-
3	BHZ	B	504	2	-	1/21/21/21	0/2/2/2
6	GOL	B	508	-	-	0/4/4/4	-
6	GOL	B	507	-	-	4/4/4/4	-
6	GOL	A	515	-	-	0/4/4/4	-
6	GOL	A	509	-	-	0/4/4/4	-
6	GOL	B	506	-	-	0/4/4/4	-
6	GOL	A	513	-	-	0/4/4/4	-
6	GOL	A	510	-	-	2/4/4/4	-
6	GOL	A	514	-	-	2/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	504	BHZ	C12-C13	4.45	1.59	1.51
3	B	504	BHZ	C12-N11	4.00	1.55	1.47
3	B	504	BHZ	C21-C22	4.00	1.59	1.51
3	B	504	BHZ	C12-C13	3.83	1.58	1.51
3	A	504	BHZ	C21-N11	3.36	1.54	1.47
3	B	504	BHZ	C19-C20	3.20	1.57	1.51
3	A	504	BHZ	C19-C20	3.02	1.57	1.51
3	B	504	BHZ	C15-C14	2.56	1.43	1.38
3	A	504	BHZ	C7-C1	2.40	1.55	1.51
3	B	504	BHZ	C17-C18	2.29	1.42	1.38
3	A	504	BHZ	C3-C2	2.25	1.42	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	504	BHZ	C12-N11-C10	4.40	120.45	111.28
3	A	504	BHZ	C7-N8-C19	-3.93	103.86	111.77
3	A	504	BHZ	C21-N11-C10	-3.48	103.52	111.91
4	A	506	ACT	OXT-C-O	-3.32	109.71	122.03
3	B	504	BHZ	C7-C1-C6	3.28	123.69	120.45
3	A	504	BHZ	C7-C1-C6	3.19	123.60	120.45
3	A	504	BHZ	C16-C15-C14	-2.82	116.76	120.24
3	B	504	BHZ	C7-N8-C19	-2.76	106.22	111.77
3	A	504	BHZ	C7-N8-C9	-2.70	105.64	111.28
6	A	514	GOL	O3-C3-C2	-2.65	98.44	110.38
4	A	505	ACT	OXT-C-CH3	2.65	126.15	115.05
3	B	504	BHZ	C13-C12-N11	-2.62	107.79	113.15
3	A	504	BHZ	C17-C16-C15	2.41	123.17	119.87
4	A	506	ACT	OXT-C-CH3	2.38	125.05	115.05
3	A	504	BHZ	C4-C5-C6	2.23	122.80	120.05
4	B	511	ACT	OXT-C-O	-2.20	113.86	122.03
4	B	511	ACT	OXT-C-CH3	2.20	124.28	115.05
3	B	504	BHZ	C12-N11-C10	2.00	115.45	111.28

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	510	GOL	O1-C1-C2-C3
6	A	512	GOL	C1-C2-C3-O3
6	A	514	GOL	C1-C2-C3-O3

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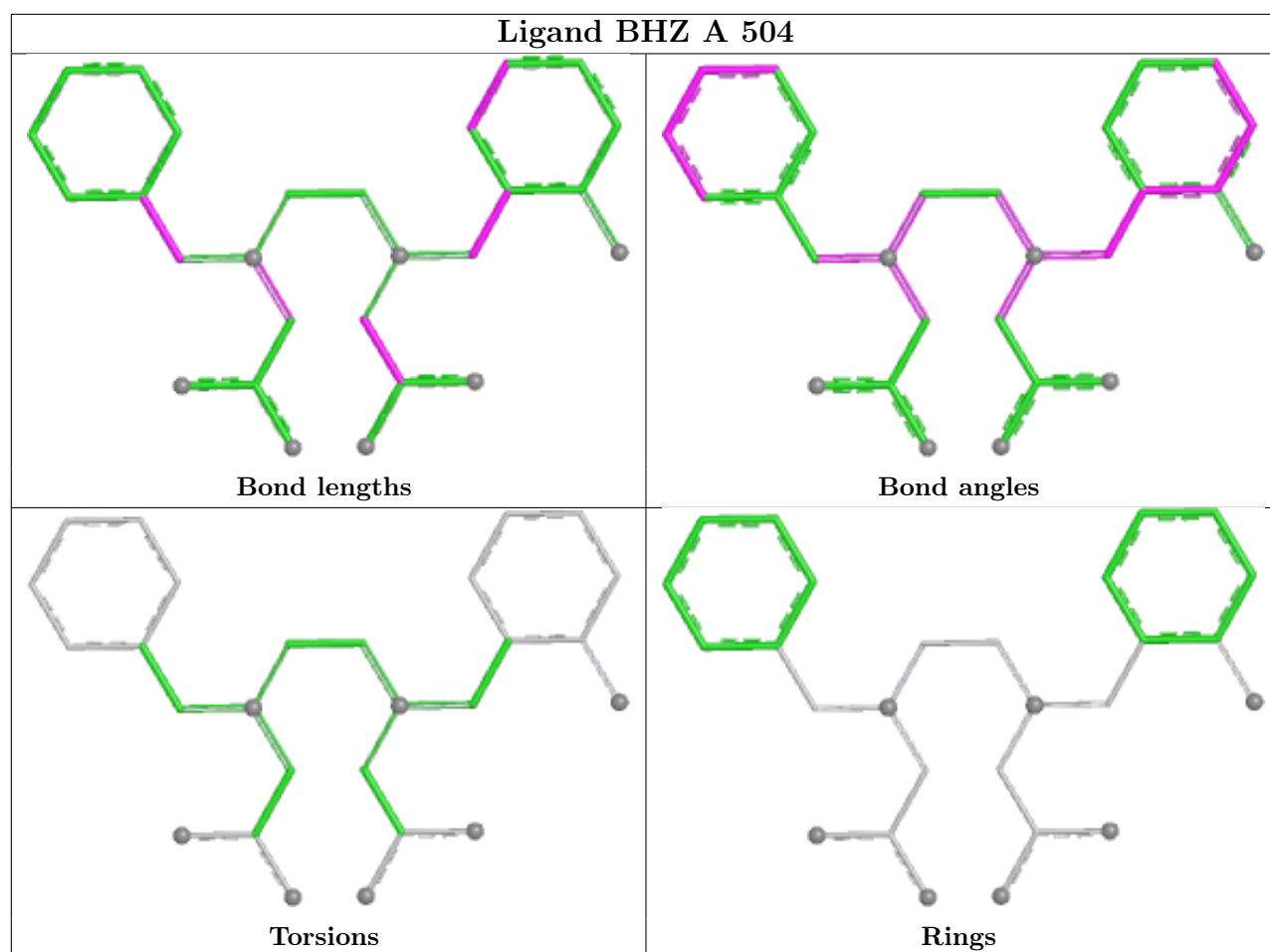
Mol	Chain	Res	Type	Atoms
6	B	507	GOL	C1-C2-C3-O3
6	A	510	GOL	O1-C1-C2-O2
6	A	514	GOL	O2-C2-C3-O3
6	B	507	GOL	O2-C2-C3-O3
6	B	507	GOL	O1-C1-C2-O2
3	B	504	BHZ	C22-C21-N11-C12
6	B	507	GOL	O1-C1-C2-C3
6	A	512	GOL	O2-C2-C3-O3

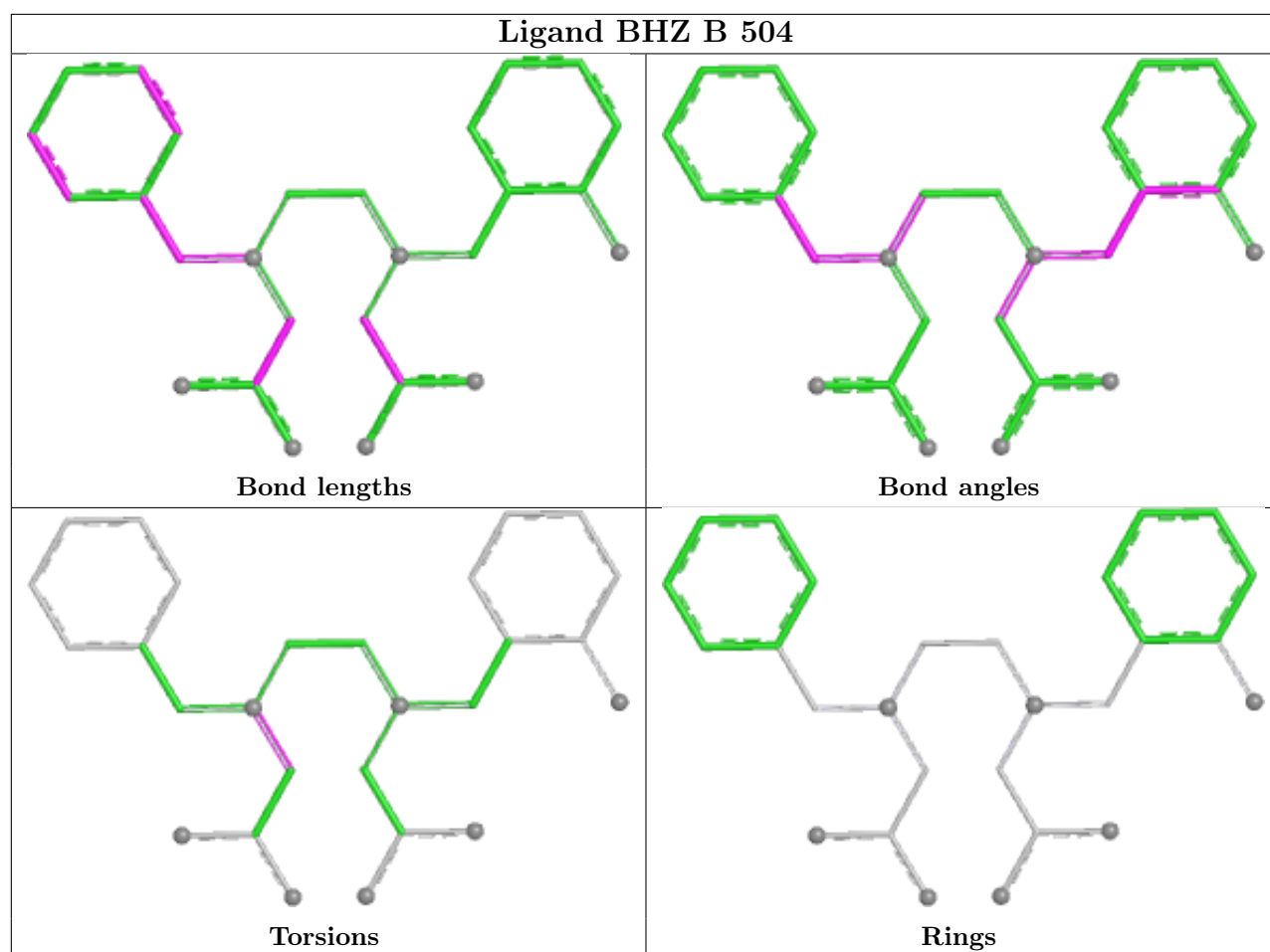
There are no ring outliers.

10 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	BHZ	6	0
6	A	512	GOL	6	0
3	B	504	BHZ	1	0
4	B	511	ACT	1	0
6	B	508	GOL	1	0
6	A	515	GOL	2	0
6	A	509	GOL	11	0
6	B	506	GOL	1	0
4	B	505	ACT	3	1
6	A	510	GOL	2	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%)	-0.30	17 (3%)	48	48	5, 13, 26, 45	11 (2%)
1	B	498/502 (99%)	0.07	26 (5%)	33	31	6, 17, 39, 51	4 (0%)
All	All	996/1004 (99%)	-0.12	43 (4%)	40	39	5, 15, 35, 51	15 (1%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	500	VAL	6.5
1	B	209	PHE	6.3
1	A	49	TRP	5.8
1	B	49	TRP	5.7
1	B	499	PRO	5.7
1	A	485	TYR	5.4
1	B	218	TYR	5.2
1	A	2	ALA	4.8
1	A	141	PHE	4.6
1	A	300	TYR	4.5
1	B	328	ALA	4.5
1	B	3	PRO	4.2
1	B	125	ALA	4.0
1	B	415	SER	3.9
1	B	414	PRO	3.8
1	B	329	GLY	3.7
1	A	140	ARG	3.5
1	B	139	PHE	3.5
1	A	126	TYR	3.4
1	A	402	TYR	3.3
1	B	337	GLY	3.1
1	B	382	TYR	3.0
1	A	283[A]	LEU	3.0
1	A	441	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	327	PRO	2.7
1	B	284	TYR	2.6
1	A	329	GLY	2.5
1	B	58	GLU	2.5
1	A	3	PRO	2.5
1	A	499	PRO	2.5
1	B	281	ASN	2.4
1	B	52	LYS	2.4
1	B	330	LYS	2.2
1	B	279	ILE	2.2
1	B	442	HIS	2.2
1	A	337	GLY	2.1
1	A	96	GLN	2.1
1	B	497	ILE	2.1
1	B	327	PRO	2.0
1	A	398	TRP	2.0
1	B	309	GLN	2.0
1	B	114	SER	2.0
1	B	108	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	A	509	6/6	0.60	0.28	20,20,20,20	0
4	ACT	B	511	4/4	0.65	0.29	20,20,20,20	0
6	GOL	B	506	6/6	0.66	0.26	55,56,56,61	0
6	GOL	A	510	6/6	0.67	0.22	40,49,51,51	0

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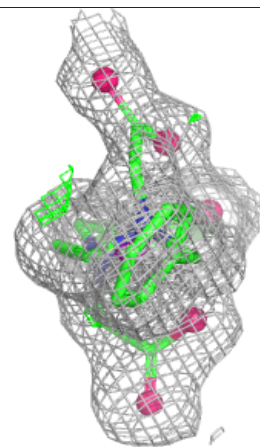
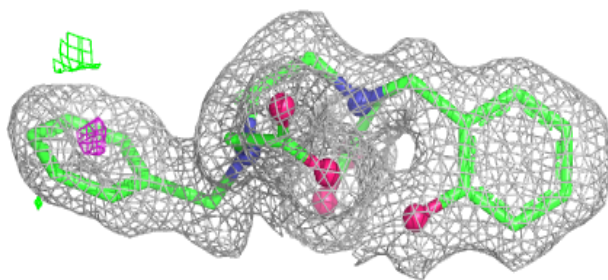
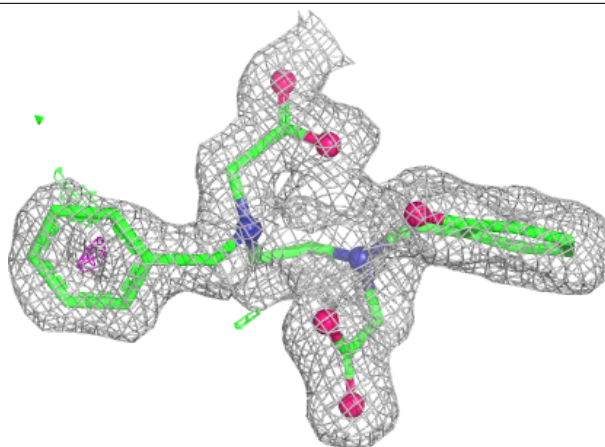
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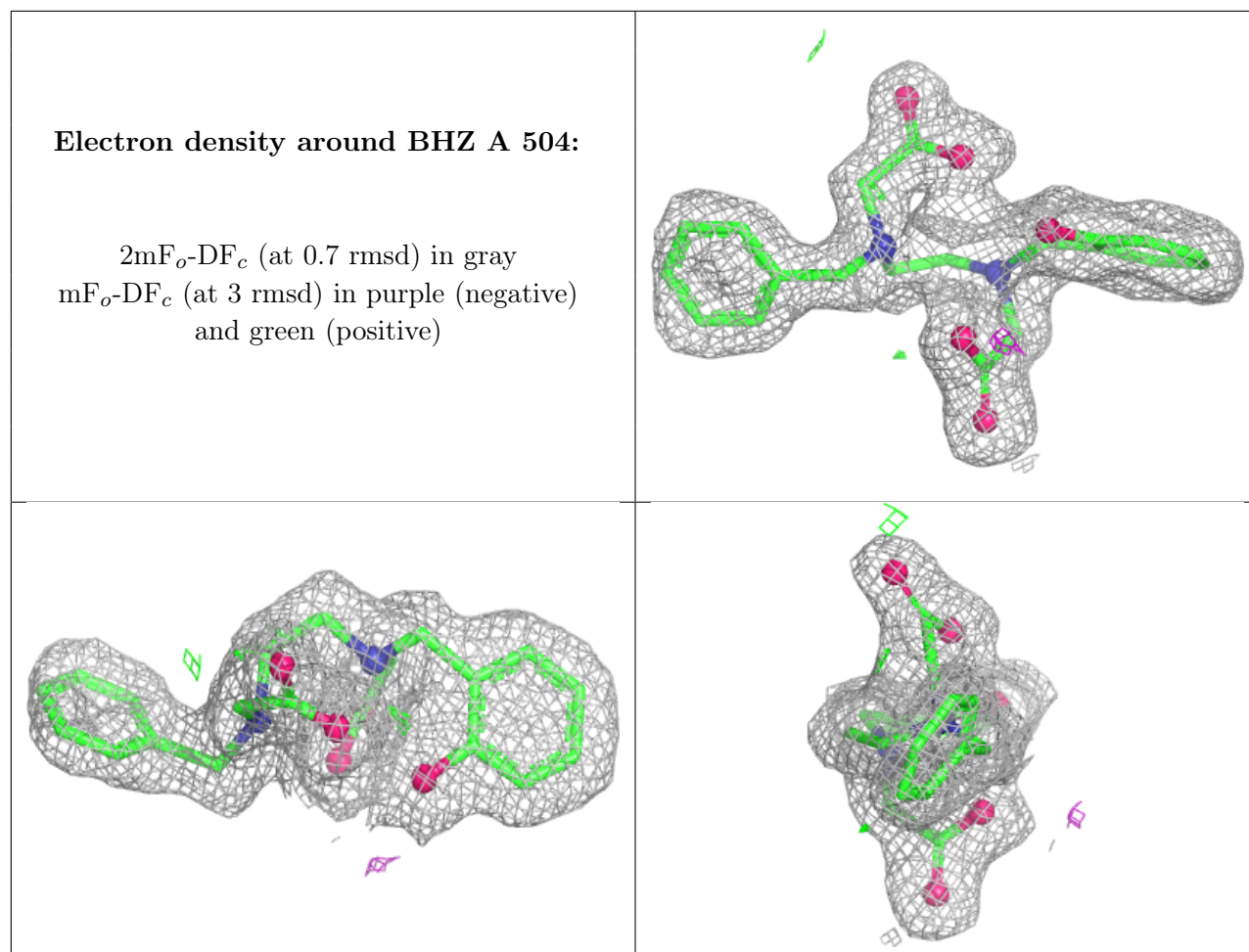
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	A	505	4/4	0.69	0.20	37,39,40,40	0
4	ACT	A	507	4/4	0.72	0.20	31,35,36,36	0
5	SO4	A	508	5/5	0.77	0.17	92,93,94,95	0
4	ACT	A	506	4/4	0.79	0.15	37,38,38,40	0
6	GOL	B	507	6/6	0.80	0.14	18,22,28,34	0
6	GOL	A	515	6/6	0.81	0.12	27,29,34,37	0
4	ACT	B	505	4/4	0.84	0.15	55,55,56,56	0
6	GOL	A	514	6/6	0.90	0.09	19,28,32,36	0
7	CL	A	517	1/1	0.90	0.11	46,46,46,46	0
6	GOL	A	512	6/6	0.91	0.11	21,37,39,45	0
7	CL	A	516	1/1	0.92	0.12	51,51,51,51	0
7	CL	B	509	1/1	0.93	0.16	40,40,40,40	0
6	GOL	B	508	6/6	0.94	0.09	14,17,20,23	0
6	GOL	A	513	6/6	0.95	0.08	12,20,22,24	0
3	BHZ	B	504	27/27	0.95	0.07	12,17,25,29	0
7	CL	B	510	1/1	0.95	0.10	41,41,41,41	0
3	BHZ	A	504	27/27	0.96	0.07	11,16,26,28	0
2	FE	B	503	1/1	0.99	0.02	15,15,15,15	0
2	FE	A	503	1/1	1.00	0.02	14,14,14,14	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 BHZ B 504:

$2mF_o-DF_c$ (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.