Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 11:47 PM EDT

PDB ID	:	3MVX
Title	:	X-ray structure of the reduced NikA/1 hybrid, NikA/1-Red
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

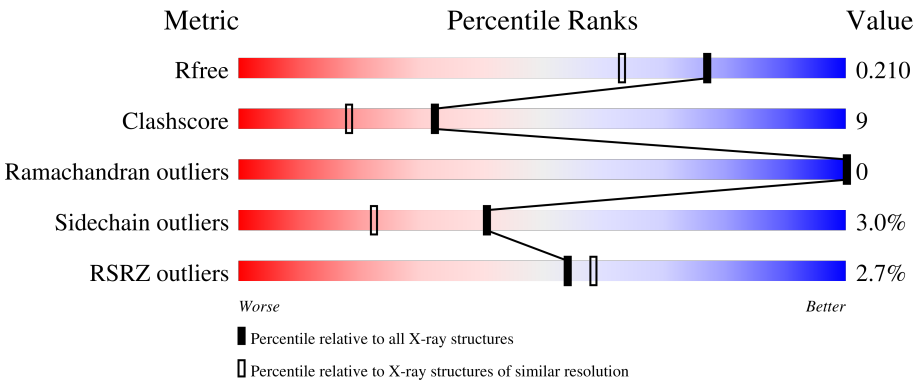
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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 <=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% 84% 13% • •
1	B	502	4% 83% 13% • •

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	A	505	-	-	X	-
4	ACT	A	517	-	-	X	-
6	GOL	B	509	-	-	X	-
8	DTU	A	513	X	-	-	-
8	DTU	A	514	X	-	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 8831 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.

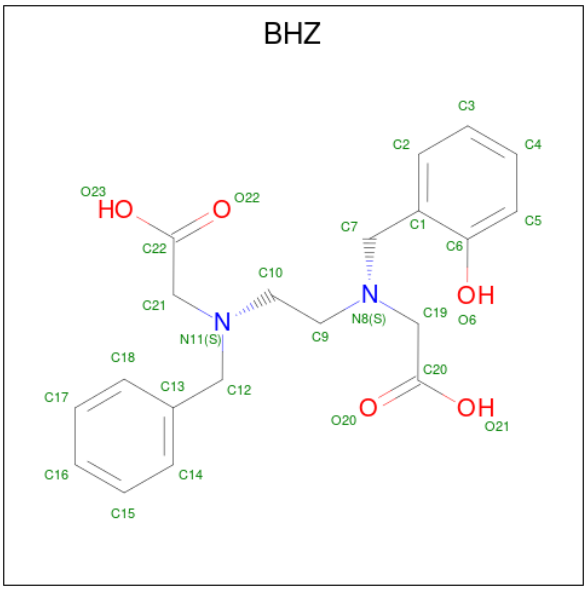
- Molecule 1 is a protein called Nickel-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	497	3993	2559	669	754	11	0	10	0
1	B	497	3966	2543	667	745	11	0	4	0

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

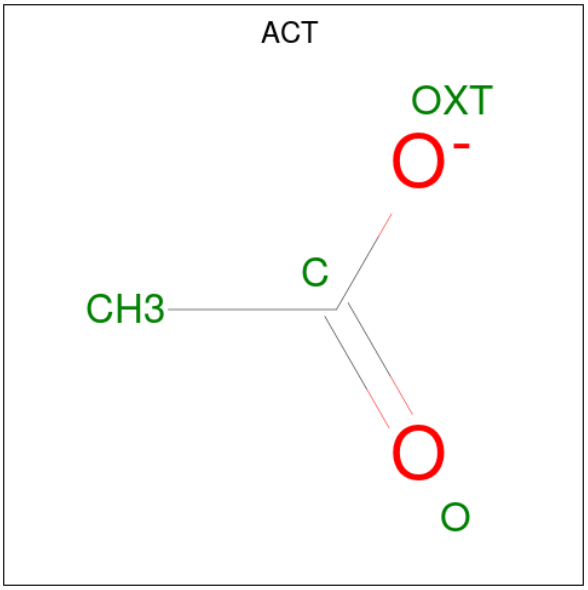
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is 2-[2-[carboxymethyl(phenylmethyl)amino]ethyl-[(2-hydroxyphenyl)methyl]amino]ethanoic acid (three-letter code: BHZ) (formula: $C_{20}H_{24}N_2O_5$).



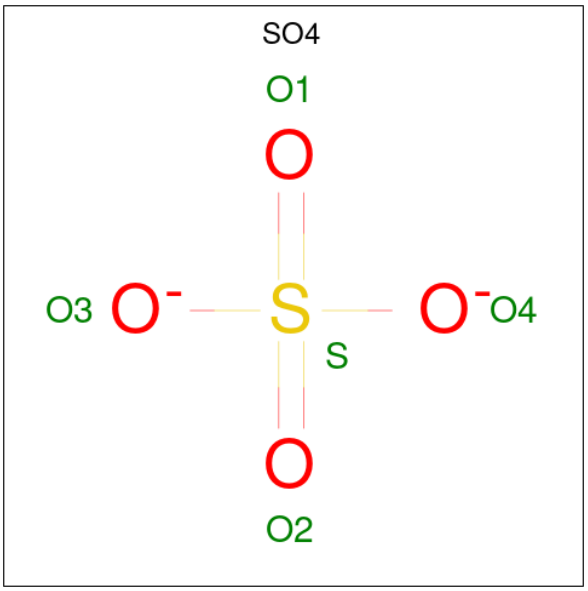
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	27	20	2	5	0	0
			Total	C	N	O		
3	B	1	27	20	2	5	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



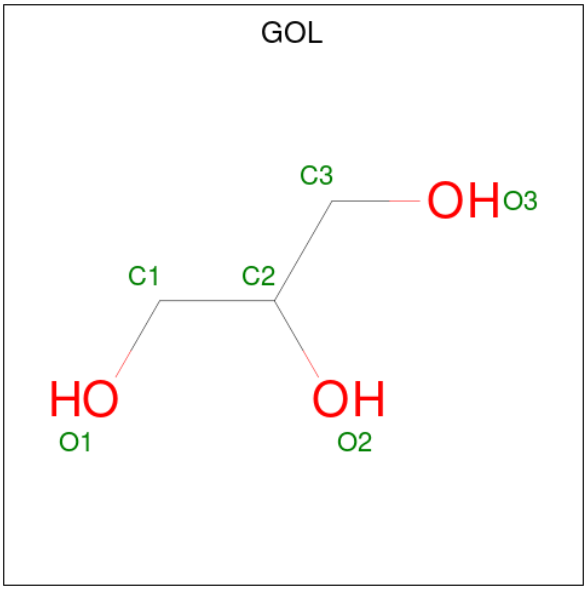
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	A	1	4	2	2		0	0
			Total	C	O			
4	A	1	4	2	2		0	0
			Total	C	O			
4	A	1	4	2	2		0	0
			Total	C	O			
4	A	1	4	2	2		0	0
			Total	C	O			
4	A	1	4	2	2		0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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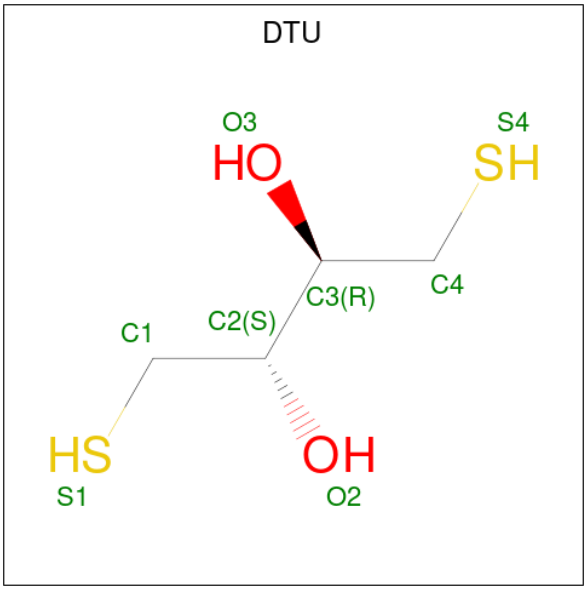
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

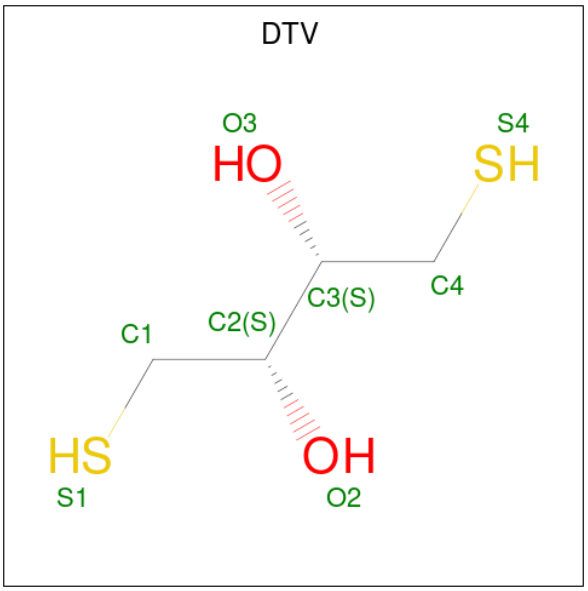
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0
7	B	1	Total Cl 1 1	0	0

- Molecule 8 is (2R,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTU) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O S 8 4 2 2	0	0
8	A	1	Total C O S 8 4 2 2	0	0

- Molecule 9 is (2S,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTV) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
9	B	1	8	4	2	2	0	0

- Molecule 10 is water.

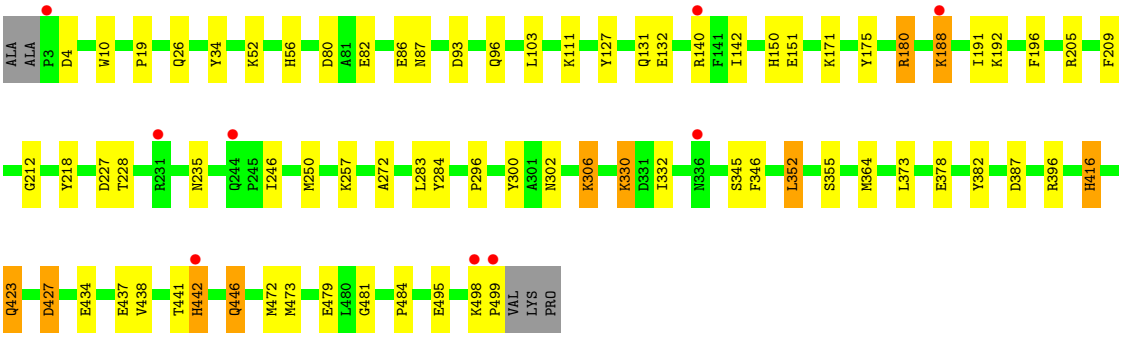
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	404	404	404	0	0
			Total	O		
10	B	331	331	331	0	0

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.

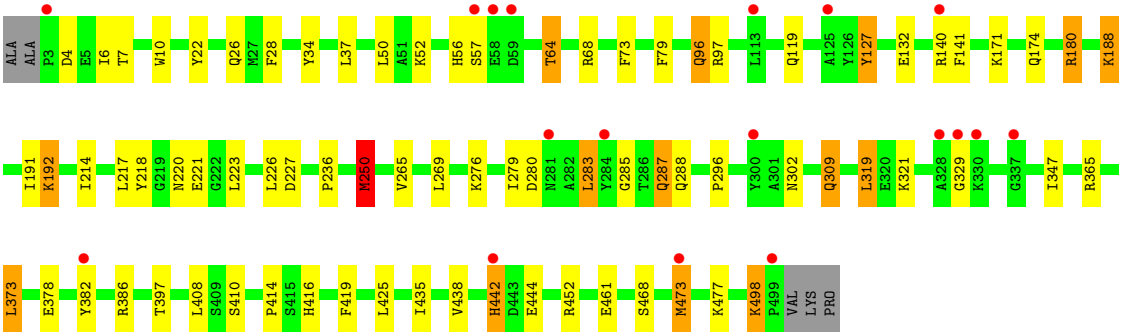
• Molecule 1: Nickel-binding periplasmic protein

Chain A:



• Molecule 1: Nickel-binding periplasmic protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.97Å 94.62Å 125.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.30 – 1.70 47.31 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.30-1.70) 99.8 (47.31-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.39 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.164 , 0.204 0.174 , 0.210	Depositor DCC
R_{free} test set	5682 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	15.9	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8831	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FE2, ACT, CL, BHZ, DTU, SO4, DTV

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	1.30	10/4121 (0.2%)	1.10	10/5612 (0.2%)
1	B	1.25	6/4082 (0.1%)	1.06	12/5560 (0.2%)
All	All	1.28	16/8203 (0.2%)	1.08	22/11172 (0.2%)

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	4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	LYS	CE-NZ	-5.86	1.34	1.49
1	B	132	GLU	CD-OE2	-5.69	1.19	1.25
1	A	218	TYR	CE1-CZ	-5.67	1.31	1.38
1	B	127	TYR	CB-CG	5.55	1.59	1.51
1	A	209	PHE	CE1-CZ	5.54	1.47	1.37
1	B	218	TYR	CE1-CZ	-5.54	1.31	1.38
1	A	434	GLU	CD-OE2	5.51	1.31	1.25
1	A	111	LYS	CB-CG	-5.41	1.38	1.52
1	B	73	PHE	CE1-CZ	5.35	1.47	1.37
1	A	345	SER	CB-OG	-5.34	1.35	1.42
1	A	355[A]	SER	CA-C	-5.27	1.39	1.52
1	A	355[B]	SER	CA-C	-5.27	1.39	1.52
1	B	22	TYR	CD2-CE2	-5.12	1.31	1.39
1	A	205	ARG	CZ-NH1	5.11	1.39	1.33
1	A	438	VAL	CB-CG2	5.03	1.63	1.52
1	B	287	GLN	CB-CG	5.01	1.66	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	250[A]	MET	CB-CA-C	6.66	123.72	110.40
1	B	250[B]	MET	CB-CA-C	6.66	123.72	110.40
1	B	329	GLY	N-CA-C	-5.81	98.57	113.10
1	B	283	LEU	CA-CB-CG	-5.70	102.19	115.30
1	B	285	GLY	N-CA-C	5.68	127.31	113.10
1	B	68	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	300	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	A	188	LYS	CD-CE-NZ	-5.53	98.98	111.70
1	A	427[A]	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	427[B]	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	B	227	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	373	LEU	CB-CG-CD2	5.47	120.31	111.00
1	B	319	LEU	CB-CG-CD1	5.45	120.26	111.00
1	A	131[A]	GLN	CA-C-O	-5.44	108.67	120.10
1	A	131[B]	GLN	CA-C-O	-5.44	108.67	120.10
1	B	408	LEU	CB-CG-CD2	5.44	120.24	111.00
1	A	396	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	442	HIS	N-CA-CB	-5.21	101.22	110.60
1	A	180	ARG	CG-CD-NE	-5.20	100.88	111.80
1	B	452	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	A	80	ASP	CB-CG-OD1	5.05	122.84	118.30
1	B	97	ARG	NE-CZ-NH1	-5.04	117.78	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	250[A]	MET	Mainchain,Peptide
1	B	250[B]	MET	Mainchain,Peptide

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	3993	0	3946	72	0
1	B	3966	0	3922	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	21	0	0
3	B	27	0	21	0	0
4	A	20	0	15	6	0
5	A	5	0	0	0	0
6	A	18	0	23	0	0
6	B	12	0	16	5	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	16	0	19	4	0
9	B	8	0	10	0	0
10	A	404	0	0	19	0
10	B	331	0	0	16	0
All	All	8831	0	7993	142	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 9.

All (142) 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:56:HIS:NE2	8:A:514:DTU:H2	1.39	1.34
6:B:509:GOL:H12	10:B:879:HOH:O	1.51	1.09
1:A:82:GLU:HG3	10:A:865:HOH:O	1.52	1.07
1:B:287:GLN:HG3	10:B:658:HOH:O	1.52	1.06
4:A:517:ACT:H3	10:A:708:HOH:O	1.58	1.04
1:A:423:GLN:HG2	10:A:626:HOH:O	1.59	1.03
1:B:279:ILE:HA	1:B:283:LEU:HD12	1.38	1.03
1:A:56:HIS:NE2	8:A:514:DTU:C2	2.22	1.02
1:B:442:HIS:H	1:B:442:HIS:CD2	1.61	1.02
1:B:425:LEU:HD22	1:B:461[B]:GLU:OE1	1.67	0.94
1:B:477:LYS:HE3	10:B:827:HOH:O	1.64	0.94
1:A:180:ARG:HH22	1:A:192:LYS:HE3	1.33	0.93
1:A:56:HIS:CE1	8:A:514:DTU:H2	2.05	0.91
1:B:4:ASP:OD2	1:B:192:LYS:HD3	1.72	0.89
1:B:442:HIS:CD2	1:B:442:HIS:N	2.42	0.87
4:A:517:ACT:CH3	10:A:708:HOH:O	2.18	0.87
1:B:442:HIS:H	1:B:442:HIS:HD2	1.15	0.87
1:B:425:LEU:HD13	1:B:461[B]:GLU:OE1	1.76	0.84
1:A:180:ARG:NH2	1:A:192:LYS:HE3	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LEU:HD12	1:B:283:LEU:HA	1.61	0.80
1:A:4:ASP:OD2	1:A:192:LYS:HD2	1.80	0.79
1:A:180:ARG:CZ	1:A:188:LYS:NZ	2.46	0.78
1:B:498:LYS:HG2	10:B:813:HOH:O	1.84	0.77
1:A:82:GLU:CG	10:A:865:HOH:O	2.22	0.76
1:A:10:TRP:HE1	1:A:26:GLN:HE21	1.34	0.75
1:B:309:GLN:HE21	1:B:309:GLN:H	1.35	0.75
1:B:10:TRP:HE1	1:B:26:GLN:HE21	1.33	0.75
1:A:423:GLN:HA	10:A:626:HOH:O	1.87	0.74
1:B:64:THR:HG21	10:B:560:HOH:O	1.87	0.74
1:A:87:ASN:HD21	1:A:142:ILE:H	1.38	0.72
1:B:425:LEU:CD2	1:B:461[B]:GLU:OE1	2.39	0.71
1:A:442:HIS:ND1	1:A:442:HIS:N	2.29	0.71
1:B:50:LEU:HD13	1:B:79:PHE:CZ	2.27	0.70
1:B:283:LEU:HD22	10:B:658:HOH:O	1.91	0.70
1:B:226:LEU:CD1	1:B:283:LEU:HA	2.23	0.68
1:B:416:HIS:HE1	10:B:763:HOH:O	1.76	0.68
6:B:509:GOL:C1	10:B:879:HOH:O	2.21	0.68
1:A:416:HIS:HD2	10:A:853:HOH:O	1.78	0.67
1:B:180:ARG:HD2	1:B:188:LYS:HG3	1.77	0.67
1:B:309:GLN:H	1:B:309:GLN:NE2	1.93	0.67
1:B:96:GLN:H	1:B:96:GLN:CD	1.99	0.66
1:A:272:ALA:CB	1:A:364[B]:MET:HE3	2.25	0.66
1:B:34:TYR:HB3	1:B:140:ARG:HB3	1.77	0.66
1:A:378:GLU:HG2	1:A:382:TYR:CE2	2.31	0.65
10:A:749:HOH:O	1:B:236:PRO:HB3	1.95	0.65
8:A:513:DTU:H4C2	10:A:826:HOH:O	1.95	0.64
1:A:416:HIS:HE1	10:A:846:HOH:O	1.79	0.64
1:B:498:LYS:CG	10:B:813:HOH:O	2.43	0.64
1:B:425:LEU:CD1	1:B:461[B]:GLU:OE1	2.44	0.64
1:A:423:GLN:CG	10:A:626:HOH:O	2.32	0.64
1:B:171:LYS:HB3	1:B:174:GLN:HB2	1.80	0.63
1:A:34:TYR:HB3	1:A:140:ARG:HB3	1.82	0.62
1:A:235:ASN:OD1	4:A:507:ACT:H3	2.01	0.61
1:B:442:HIS:N	1:B:442:HIS:HD2	1.90	0.61
1:A:103:LEU:HD22	1:A:132:GLU:HB2	1.83	0.60
1:B:250[B]:MET:HE2	1:B:397:THR:HG23	1.84	0.60
1:B:37:LEU:HA	1:B:50:LEU:HB2	1.84	0.59
1:A:272:ALA:CB	1:A:364[B]:MET:CE	2.81	0.59
1:B:296:PRO:HB3	1:B:302:ASN:HD22	1.68	0.58
1:A:272:ALA:HB3	1:A:364[B]:MET:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:GLU:H	1:A:479:GLU:CD	2.06	0.58
1:B:365:ARG:HG3	1:B:365:ARG:HH11	1.68	0.58
6:B:509:GOL:H32	10:B:570:HOH:O	2.03	0.57
1:A:498:LYS:O	1:A:499:PRO:O	2.22	0.57
1:B:10:TRP:HE1	1:B:26:GLN:NE2	2.01	0.57
1:A:484:PRO:HG3	4:A:508:ACT:H3	1.85	0.57
1:B:220:ASN:HB3	6:B:508:GOL:H11	1.85	0.57
1:A:283:LEU:HD23	1:A:352:LEU:HD21	1.85	0.57
1:A:180:ARG:CZ	1:A:192:LYS:HG2	2.34	0.57
1:A:446:GLN:HE21	1:A:446:GLN:HA	1.68	0.57
1:B:56:HIS:HD2	1:B:57:SER:O	1.88	0.56
1:B:382:TYR:CE2	1:B:386:ARG:HD2	2.40	0.56
1:A:330:LYS:HD3	1:A:332:ILE:H	1.71	0.55
1:B:221:GLU:HA	1:B:473:MET:SD	2.46	0.55
1:A:180:ARG:NE	1:A:188:LYS:HZ2	2.04	0.55
1:B:280:ASP:HB3	10:B:588:HOH:O	2.05	0.55
1:B:140:ARG:O	1:B:141:PHE:CD2	2.59	0.55
1:B:287:GLN:HG3	10:B:554:HOH:O	2.06	0.55
1:B:414:PRO:HA	1:B:419:PHE:CD1	2.42	0.55
1:B:347:ILE:HD13	1:B:378:GLU:HG3	1.88	0.55
1:B:171:LYS:HD2	1:B:174:GLN:CD	2.28	0.54
1:B:140:ARG:HG3	10:B:655:HOH:O	2.09	0.53
6:B:509:GOL:C3	10:B:570:HOH:O	2.56	0.53
1:A:180:ARG:NH2	1:A:188:LYS:HZ3	2.07	0.53
1:B:64:THR:HG23	10:B:585:HOH:O	2.09	0.53
1:A:52:LYS:NZ	4:A:505:ACT:H1	2.25	0.52
1:B:4:ASP:N	1:B:4:ASP:OD1	2.30	0.52
1:A:103:LEU:HB2	1:A:132:GLU:OE2	2.10	0.52
1:B:382:TYR:CZ	1:B:386:ARG:HD2	2.45	0.52
1:B:140:ARG:O	1:B:141:PHE:CG	2.63	0.51
1:A:171:LYS:HG3	1:A:175:TYR:CZ	2.47	0.50
1:A:246:ILE:HD13	1:A:472:MET:HG2	1.92	0.50
1:A:140:ARG:HG3	10:A:640:HOH:O	2.12	0.49
1:A:473:MET:CE	10:A:809:HOH:O	2.60	0.49
1:B:119:GLN:NE2	10:B:560:HOH:O	2.30	0.49
1:A:150:HIS:C	1:A:151:GLU:HG2	2.33	0.49
1:A:180:ARG:NH2	1:A:188:LYS:NZ	2.59	0.49
1:A:423:GLN:NE2	10:A:885:HOH:O	2.45	0.49
1:A:346:PHE:HA	10:A:811:HOH:O	2.12	0.49
1:A:481:GLY:HA2	1:B:444:GLU:CG	2.42	0.49
1:A:481:GLY:HA2	1:B:444:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ASN:O	1:B:473:MET:SD	2.71	0.48
1:B:410:SER:OG	1:B:416:HIS:CD2	2.65	0.48
1:A:180:ARG:CZ	1:A:188:LYS:HZ1	2.24	0.48
1:B:7:THR:HG22	1:B:214:ILE:HG22	1.95	0.48
1:A:180:ARG:NE	1:A:188:LYS:NZ	2.61	0.47
1:B:410:SER:OG	1:B:416:HIS:HD2	1.96	0.47
1:B:265:VAL:O	1:B:269:LEU:HG	2.14	0.47
1:A:481:GLY:HA2	1:B:444:GLU:CD	2.35	0.47
1:A:4:ASP:OD2	1:A:192:LYS:CD	2.57	0.47
1:B:288:GLN:O	1:B:468[B]:SER:HB2	2.14	0.47
1:B:347:ILE:CD1	1:B:378:GLU:HG3	2.45	0.47
1:A:103:LEU:CB	1:A:132:GLU:OE2	2.63	0.47
1:A:498:LYS:HB3	1:A:498:LYS:HE2	1.62	0.46
1:A:19:PRO:HG3	1:A:142:ILE:HB	1.97	0.46
1:A:257:LYS:HB2	1:A:257:LYS:HE2	1.76	0.46
1:A:272:ALA:HB3	1:A:364[B]:MET:HE1	1.97	0.45
1:B:192:LYS:HB3	1:B:192:LYS:NZ	2.31	0.45
1:A:180:ARG:HH12	1:A:192:LYS:HZ2	1.65	0.45
1:A:212:GLY:HA2	10:A:829:HOH:O	2.17	0.45
1:A:227:ASP:OD1	1:A:228:THR:N	2.49	0.44
1:A:52:LYS:HZ3	4:A:505:ACT:H1	1.81	0.44
1:A:96:GLN:NE2	10:A:750:HOH:O	2.43	0.44
1:A:296:PRO:HB3	1:A:302:ASN:HD22	1.82	0.43
1:A:191:ILE:HD13	1:A:191:ILE:HG21	1.82	0.43
1:A:473:MET:HE3	10:A:809:HOH:O	2.16	0.43
1:A:82:GLU:O	1:A:86:GLU:HG2	2.18	0.42
1:B:6:ILE:HG23	1:B:191:ILE:HD12	2.02	0.42
1:A:93:ASP:OD2	1:A:151:GLU:OE1	2.37	0.42
1:B:52:LYS:HE3	1:B:52:LYS:HB3	1.85	0.42
1:A:306:LYS:HD3	10:A:609:HOH:O	2.19	0.42
1:A:437:GLU:O	1:A:441:THR:HG23	2.20	0.41
1:A:481:GLY:CA	1:B:444:GLU:HG2	2.51	0.41
1:B:4:ASP:OD2	1:B:192:LYS:CD	2.56	0.41
1:A:175:TYR:HA	1:A:196:PHE:O	2.20	0.41
1:A:495[B]:GLU:CD	1:A:495[B]:GLU:H	2.23	0.41
1:B:217:LEU:HB3	1:B:223:LEU:HD11	2.02	0.41
1:A:330:LYS:HE3	1:A:332:ILE:HG12	2.03	0.40
1:B:28:PHE:CD2	1:B:28:PHE:C	2.95	0.40
1:B:435:ILE:O	1:B:438:VAL:HG12	2.22	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	504/502 (100%)	492 (98%)	12 (2%)	0	100	100
1	B	499/502 (99%)	486 (97%)	13 (3%)	0	100	100
All	All	1003/1004 (100%)	978 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	431/425 (101%)	421 (98%)	10 (2%)	50	33
1	B	426/425 (100%)	410 (96%)	16 (4%)	33	14
All	All	857/850 (101%)	831 (97%)	26 (3%)	41	22

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	TYR
1	A	250	MET
1	A	284	TYR
1	A	306	LYS
1	A	330	LYS
1	A	352	LEU
1	A	373	LEU
1	A	416	HIS

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Mol	Chain	Res	Type
1	A	423	GLN
1	A	446	GLN
1	B	64	THR
1	B	96	GLN
1	B	127	TYR
1	B	180	ARG
1	B	188	LYS
1	B	192	LYS
1	B	250[A]	MET
1	B	250[B]	MET
1	B	276	LYS
1	B	309	GLN
1	B	319	LEU
1	B	321	LYS
1	B	373	LEU
1	B	442	HIS
1	B	473	MET
1	B	498	LYS

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	87	ASN
1	A	302	ASN
1	A	385	GLN
1	A	416	HIS
1	A	423	GLN
1	A	446	GLN
1	B	25	ASN
1	B	26	GLN
1	B	56	HIS
1	B	234	GLN
1	B	288	GLN
1	B	302	ASN
1	B	309	GLN
1	B	336	ASN
1	B	416	HIS
1	B	442	HIS
1	B	482	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
8	DTU	A	513	-	7,7,7	1.08	1 (14%)	4,8,8	2.60	3 (75%)
8	DTU	A	514	-	7,7,7	5.85	2 (28%)	4,8,8	3.66	3 (75%)
6	GOL	B	508	-	5,5,5	0.36	0	5,5,5	0.28	0
4	ACT	A	505	-	3,3,3	0.65	0	3,3,3	1.83	1 (33%)
4	ACT	A	508	-	3,3,3	0.73	0	3,3,3	1.40	0
3	BHZ	B	504	2	28,28,28	1.47	4 (14%)	36,36,36	1.40	4 (11%)
6	GOL	A	516	-	5,5,5	0.85	0	5,5,5	0.89	0
5	SO4	A	509	-	4,4,4	0.14	0	6,6,6	0.05	0
6	GOL	A	510	-	5,5,5	0.36	0	5,5,5	0.28	0
4	ACT	A	517	-	3,3,3	0.77	0	3,3,3	1.34	0
9	DTV	B	507	-	7,7,7	1.47	2 (28%)	4,8,8	1.25	0
4	ACT	A	507	-	3,3,3	1.53	1 (33%)	3,3,3	1.39	0
6	GOL	B	509	-	5,5,5	0.69	0	5,5,5	0.76	0
6	GOL	A	515	-	5,5,5	0.98	0	5,5,5	1.21	0
3	BHZ	A	504	2	28,28,28	1.48	4 (14%)	36,36,36	1.77	10 (27%)
4	ACT	A	506	-	3,3,3	1.11	0	3,3,3	2.37	2 (66%)

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
8	DTU	A	514	-	2/2/2/2	3/8/8/8	-
6	GOL	B	508	-	-	0/4/4/4	-
6	GOL	A	516	-	-	0/4/4/4	-
3	BHZ	B	504	2	-	2/21/21/21	0/2/2/2
6	GOL	A	515	-	-	3/4/4/4	-
9	DTV	B	507	-	-	0/8/8/8	-
6	GOL	A	510	-	-	0/4/4/4	-
6	GOL	B	509	-	-	2/4/4/4	-
8	DTU	A	513	-	2/2/2/2	5/8/8/8	-
3	BHZ	A	504	2	-	2/21/21/21	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	514	DTU	O2-C2	-15.18	1.11	1.43
3	B	504	BHZ	C12-N11	3.60	1.54	1.47
3	B	504	BHZ	C21-C22	3.56	1.58	1.51
3	A	504	BHZ	C19-N8	2.83	1.53	1.47
3	B	504	BHZ	C4-C5	2.65	1.44	1.38
3	A	504	BHZ	C5-C6	2.56	1.44	1.39
8	A	514	DTU	C1-C2	2.53	1.58	1.51
9	B	507	DTV	C4-S4	2.49	1.86	1.81
4	A	507	ACT	OXT-C	-2.45	1.19	1.30
3	A	504	BHZ	C2-C1	2.43	1.43	1.39
9	B	507	DTV	O3-C3	2.37	1.48	1.43
3	A	504	BHZ	C10-N11	2.33	1.52	1.47
3	B	504	BHZ	C17-C18	2.23	1.43	1.38
8	A	513	DTU	C1-C2	2.16	1.57	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	514	DTU	C3-C4-S4	-4.83	100.42	114.47
3	B	504	BHZ	C21-N11-C10	-4.60	100.76	111.94
8	A	514	DTU	O2-C2-C3	-3.99	101.52	109.72
3	A	504	BHZ	C12-N11-C10	-3.97	102.91	111.29
8	A	513	DTU	O2-C2-C3	-3.95	101.61	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	504	BHZ	C20-C19-N8	-3.69	101.58	113.63
8	A	514	DTU	C2-C1-S1	-3.49	104.32	114.47
4	A	506	ACT	OXT-C-O	-3.36	109.65	122.05
3	A	504	BHZ	C21-N11-C10	-2.99	104.67	111.94
3	A	504	BHZ	C2-C1-C6	2.88	121.23	118.16
3	B	504	BHZ	C22-C21-N11	-2.71	104.78	113.63
3	B	504	BHZ	C7-N8-C19	-2.69	106.27	112.02
4	A	505	ACT	OXT-C-CH3	2.52	125.58	115.18
3	A	504	BHZ	O6-C6-C1	2.41	125.08	118.89
8	A	513	DTU	C3-C4-S4	-2.41	107.47	114.47
8	A	513	DTU	O3-C3-C2	2.36	114.58	109.72
3	B	504	BHZ	O23-C22-O22	2.35	129.14	123.30
3	A	504	BHZ	C19-N8-C9	-2.34	106.27	111.94
3	A	504	BHZ	C3-C2-C1	-2.27	117.50	120.89
3	A	504	BHZ	C18-C13-C14	2.21	121.64	118.17
3	A	504	BHZ	C15-C14-C13	-2.19	117.27	120.63
4	A	506	ACT	OXT-C-CH3	2.13	123.97	115.18
3	A	504	BHZ	C22-C21-N11	-2.03	106.99	113.63

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	513	DTU	C3
8	A	513	DTU	C2
8	A	514	DTU	C3
8	A	514	DTU	C2

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	515	GOL	C1-C2-C3-O3
6	B	509	GOL	C1-C2-C3-O3
8	A	513	DTU	S1-C1-C2-O2
8	A	513	DTU	S1-C1-C2-C3
8	A	513	DTU	C1-C2-C3-C4
8	A	513	DTU	C2-C3-C4-S4
8	A	513	DTU	O3-C3-C4-S4
8	A	514	DTU	S1-C1-C2-O2
8	A	514	DTU	S1-C1-C2-C3
8	A	514	DTU	O3-C3-C4-S4
6	B	509	GOL	O2-C2-C3-O3
6	A	515	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	515	GOL	O2-C2-C3-O3
3	A	504	BHZ	N8-C19-C20-O20
3	A	504	BHZ	N8-C19-C20-O21
3	B	504	BHZ	N8-C19-C20-O21
3	B	504	BHZ	N8-C19-C20-O20

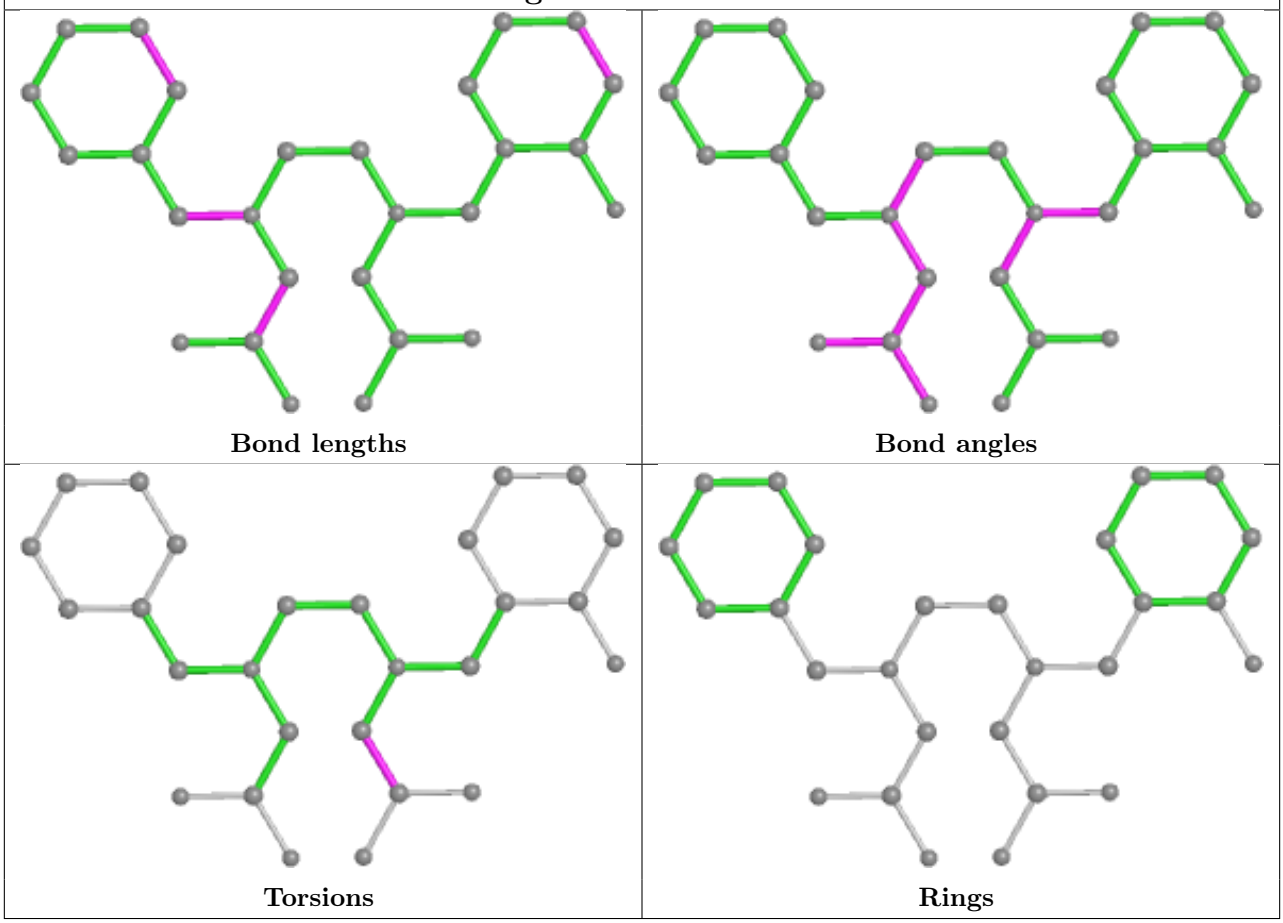
There are no ring outliers.

8 monomers are involved in 15 short contacts:

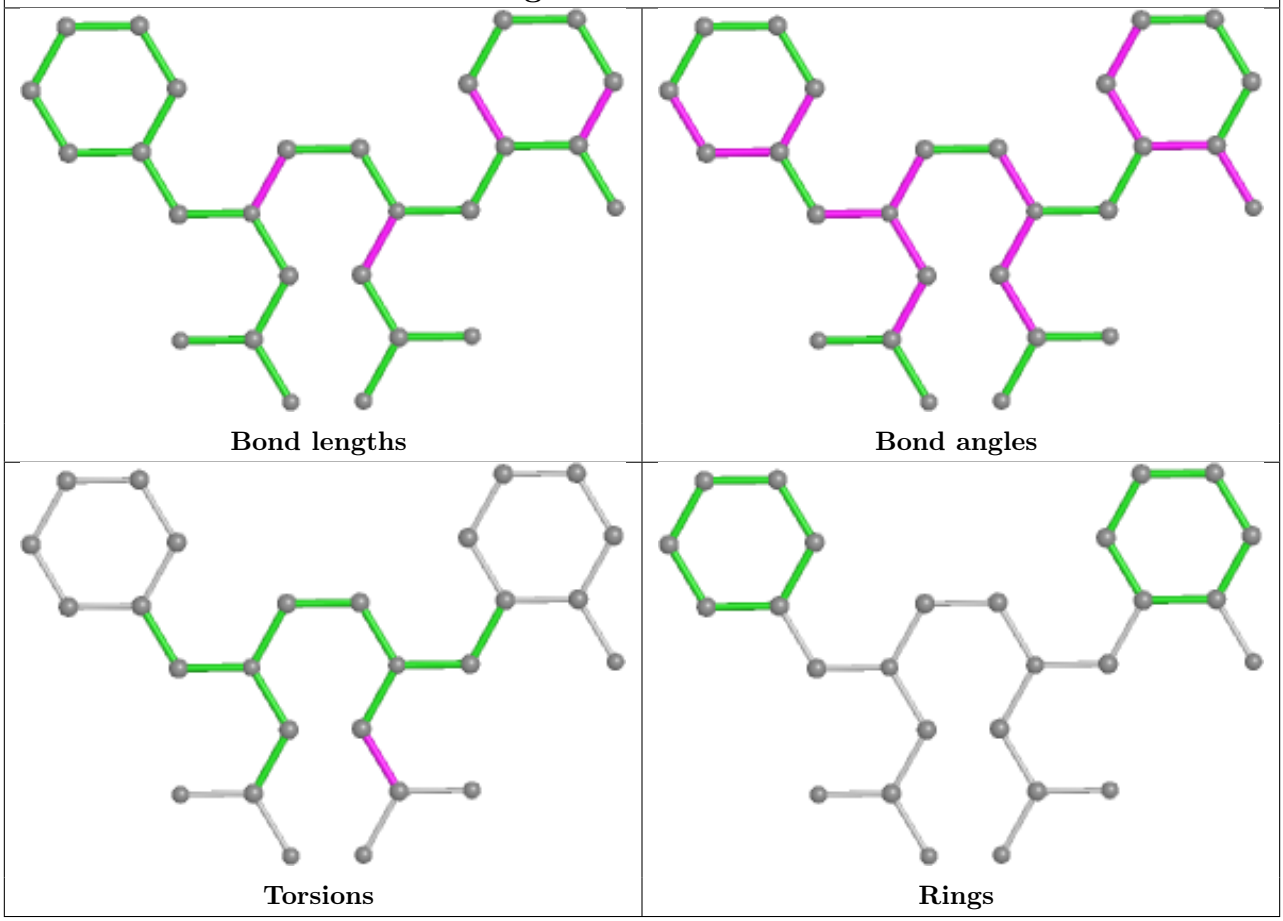
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	513	DTU	1	0
8	A	514	DTU	3	0
6	B	508	GOL	1	0
4	A	505	ACT	2	0
4	A	508	ACT	1	0
4	A	517	ACT	2	0
4	A	507	ACT	1	0
6	B	509	GOL	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand BHZ B 504



Ligand BHZ A 504



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	497/502 (99%)	-0.20	9 (1%)	68	72	8, 13, 26, 44	0
1	B	497/502 (99%)	-0.01	18 (3%)	42	47	8, 17, 35, 50	1 (0%)
All	All	994/1004 (99%)	-0.10	27 (2%)	54	58	8, 15, 32, 50	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	PRO	7.3
1	B	328	ALA	5.5
1	B	442	HIS	4.8
1	A	442	HIS	4.3
1	B	473	MET	4.3
1	B	58	GLU	4.2
1	B	337	GLY	4.1
1	B	499	PRO	4.0
1	A	499	PRO	3.8
1	B	329	GLY	3.6
1	B	284	TYR	3.6
1	B	140	ARG	3.3
1	B	125	ALA	3.2
1	A	3	PRO	3.1
1	A	188	LYS	3.0
1	B	113	LEU	3.0
1	B	382	TYR	2.7
1	A	231	ARG	2.7
1	B	330	LYS	2.7
1	A	140	ARG	2.6
1	A	336	ASN	2.5
1	A	498	LYS	2.5
1	B	300	TYR	2.4
1	B	59	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	281	ASN	2.4
1	B	57	SER	2.1
1	A	244	GLN	2.1

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)

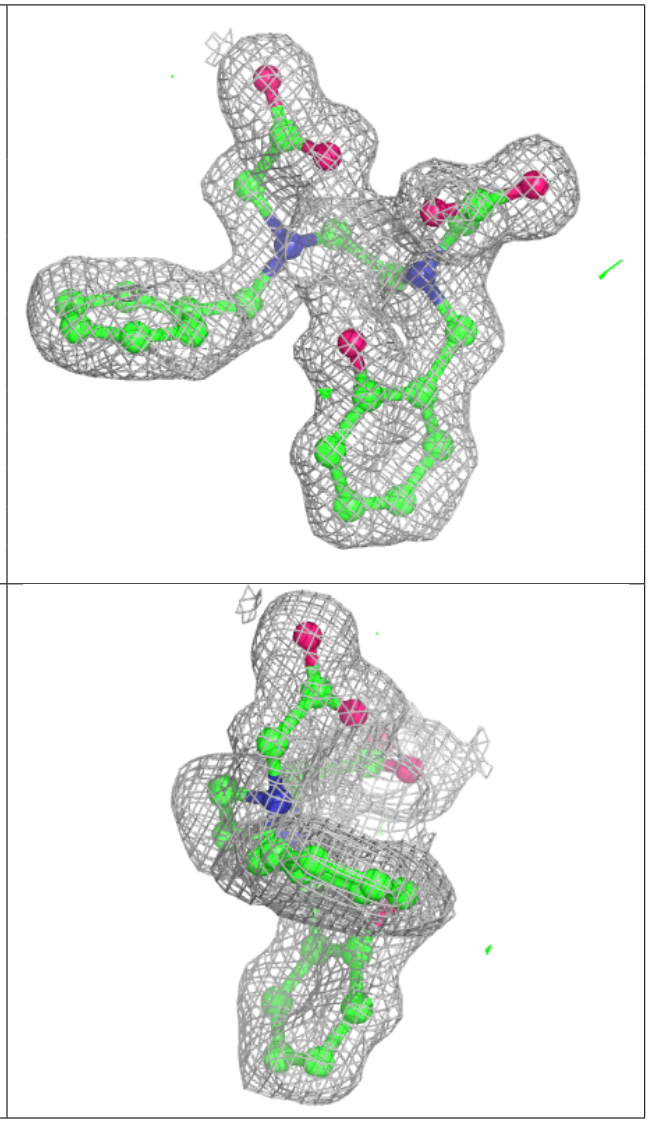
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	A	510	6/6	0.66	0.20	26,38,42,44	0
4	ACT	A	507	4/4	0.68	0.18	37,40,41,42	0
4	ACT	A	508	4/4	0.73	0.21	54,55,55,55	0
4	ACT	A	505	4/4	0.73	0.20	30,35,35,36	0
6	GOL	B	509	6/6	0.83	0.15	28,33,35,36	0
8	DTU	A	514	8/8	0.84	0.19	9,33,47,49	0
4	ACT	A	506	4/4	0.85	0.13	39,40,41,42	0
6	GOL	B	508	6/6	0.86	0.14	20,20,20,20	0
5	SO4	A	509	5/5	0.86	0.19	60,62,64,65	0
6	GOL	A	515	6/6	0.88	0.14	20,20,20,20	0
4	ACT	A	517	4/4	0.91	0.16	22,24,26,29	0
8	DTU	A	513	8/8	0.92	0.14	18,33,44,44	0
6	GOL	A	516	6/6	0.93	0.12	16,22,22,24	0
7	CL	B	506	1/1	0.93	0.09	39,39,39,39	0
9	DTV	B	507	8/8	0.93	0.09	16,26,30,35	0
7	CL	A	512	1/1	0.94	0.08	53,53,53,53	0
3	BHZ	B	504	27/27	0.96	0.08	9,12,17,18	0
3	BHZ	A	504	27/27	0.97	0.09	8,11,15,16	0
2	FE2	A	503	1/1	1.00	0.07	11,11,11,11	0
2	FE2	B	503	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.

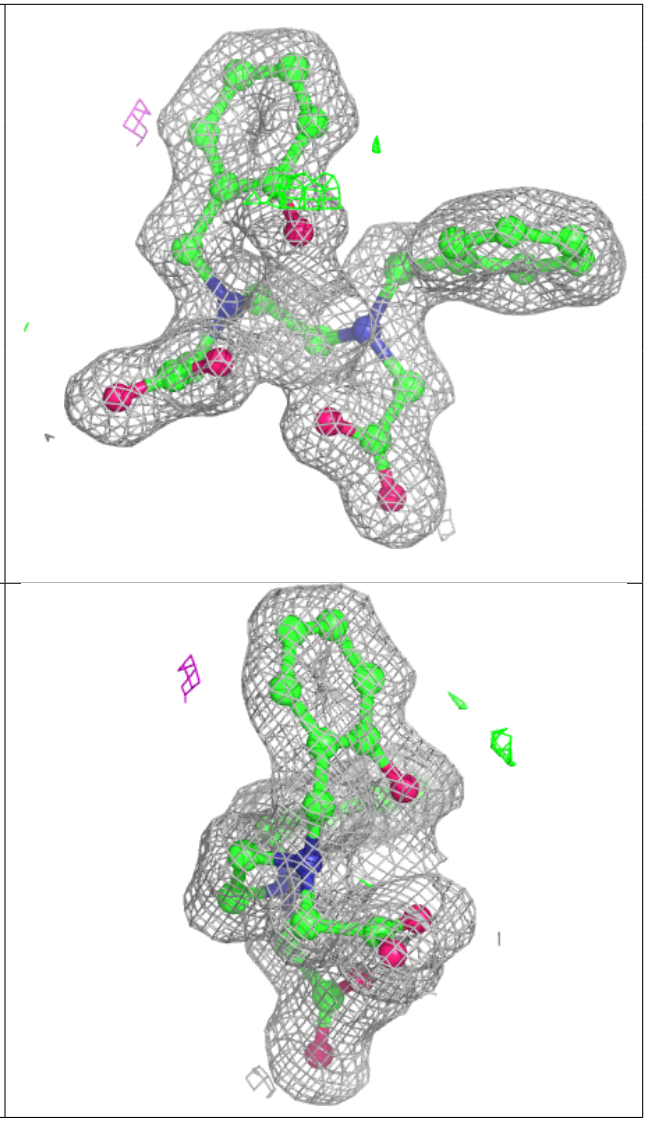
Electron density around BHZ B 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BHZ A 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.