



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:30 PM GMT

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.;
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Deposited on : 2010-05-05
Resolution : 1.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

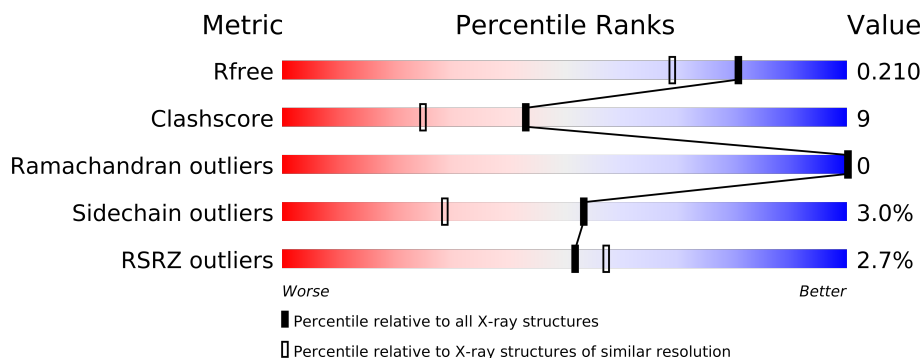
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	502	
1	B	502	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	ACT	A	505	-	X
4	ACT	A	506	-	X
4	ACT	A	507	-	X
4	ACT	A	517	-	X
6	GOL	A	510	-	X
6	GOL	A	515	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	GOL	B	508	-	X
6	GOL	B	509	-	X
7	CL	B	506	-	X
8	DTU	A	513	-	X
9	DTV	B	507	-	X

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 8831 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

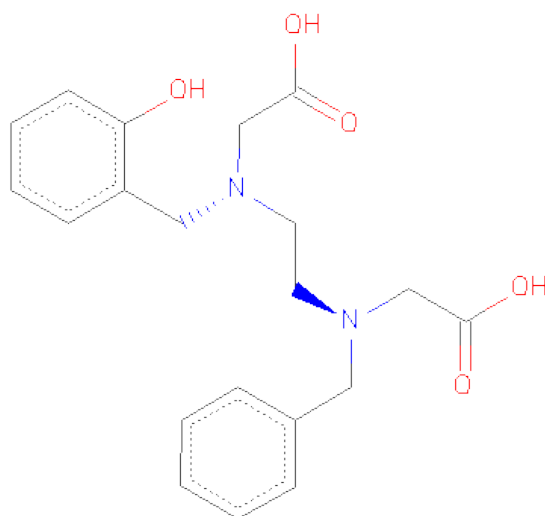
- Molecule 1 is a protein called Nickel-binding periplasmic protein.

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

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

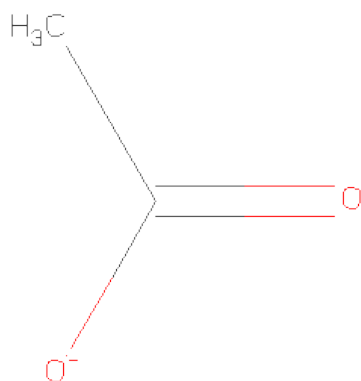
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 2-[2-[CARBOXYMETHYL(PHENYLMETHYL)AMINO]ETHYL-[(2-HYDROXYPHENYL)METHYL]AMINO]ETHANOICACID (three-letter code: 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 (three-letter code: ACT) (formula: $C_2H_3O_2$).



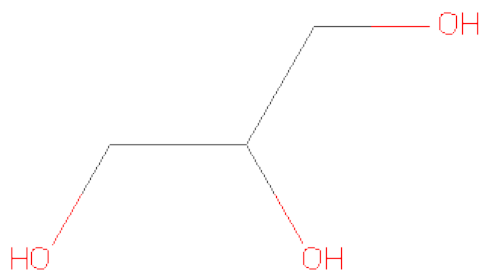
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SULFATE ION (three-letter code: 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 (three-letter code: 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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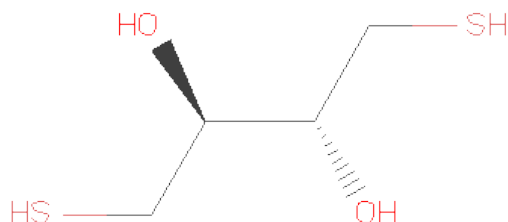
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

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

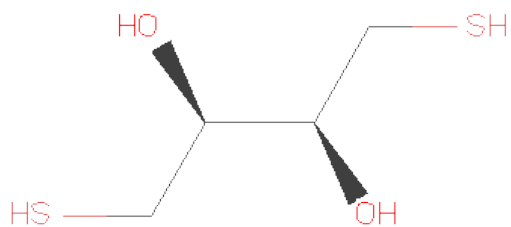
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is (2R,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTU) (formula: C₄H₁₀O₂S₂).



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

- Molecule 9 is (2S,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTV) (formula: C₄H₁₀O₂S₂).



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

- Molecule 10 is water.

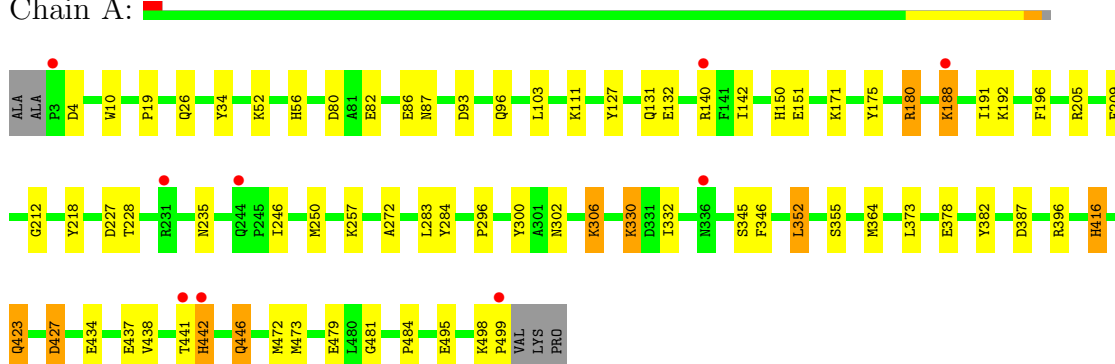
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	404	Total	O	0	0
			404	404		
10	B	331	Total	O	0	0
			331	331		

3 Residue-property plots i

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

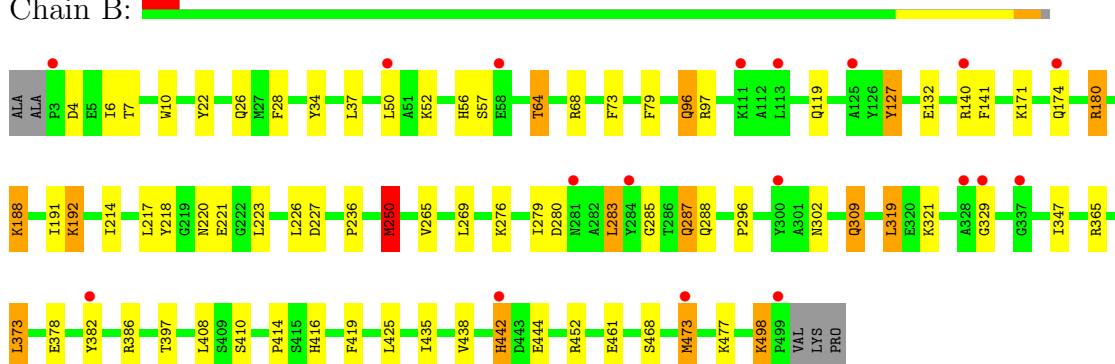
- Molecule 1: Nickel-binding periplasmic protein

Chain A:



- Molecule 1: Nickel-binding periplasmic protein

Chain B:



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	4.39 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.164 , 0.204 0.175 , 0.210	Depositor DCC
R_{free} test set	5682 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 31.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 113637 reflections	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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(°)	Ideal(°)
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 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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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
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (142) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:CD2	1:B:442:HIS:H	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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:H	1:B:309:GLN:HE21	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:N	1:A:442:HIS:ND1	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:309:GLN:H	1:B:309:GLN:NE2	1.93	0.67
1:B:180:ARG:HD2	1:B:188:LYS:HG3	1.77	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:HD2	1:B:442:HIS:N	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:272:ALA:HB3	1:A:364[B]:MET:CE	2.33	0.58
1:A:479:GLU:H	1:A:479:GLU:CD	2.06	0.58
1:B:365:ARG:HH11	1:B:365:ARG:HG3	1.68	0.58
6:B:509:GOL:H32	10:B:570:HOH:O	2.03	0.57
1:B:10:TRP:HE1	1:B:26:GLN:NE2	2.01	0.57
1:A:498:LYS:O	1:A:499:PRO:O	2.22	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:HA	1:A:446:GLN:HE21	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:B:221:GLU:HA	1:B:473:MET:SD	2.46	0.55
1:A:330:LYS:HD3	1:A:332:ILE:H	1.71	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:287:GLN:HG3	10:B:554:HOH:O	2.06	0.55
1:B:140:ARG:O	1:B:141:PHE:CD2	2.59	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:423:GLN:NE2	10:A:885:HOH:O	2.45	0.49
1:A:180:ARG:NH2	1:A:188:LYS:NZ	2.59	0.49
1:A:150:HIS:C	1:A:151:GLU:HG2	2.33	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:B:220:ASN:O	1:B:473:MET:SD	2.71	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:481:GLY:HA2	1:B:444:GLU:HG2	1.95	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:347:ILE:CD1	1:B:378:GLU:HG3	2.45	0.47
1:B:288:GLN:O	1:B:468[B]:SER:HB2	2.14	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:HB3	1:B:52:LYS:HE3	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:B:4:ASP:OD2	1:B:192:LYS:CD	2.56	0.41
1:A:481:GLY:CA	1:B:444:GLU:HG2	2.51	0.41
1:A:175:TYR:HA	1:A:196:PHE:O	2.20	0.41
1:B:217:LEU:HB3	1:B:223:LEU:HD11	2.02	0.41
1:A:495[B]:GLU:H	1:A:495[B]:GLU:CD	2.23	0.41
1:A:330:LYS:HE3	1:A:332:ILE:HG12	2.03	0.40
1:B:435:ILE:O	1:B:438:VAL:HG12	2.22	0.40
1:B:28:PHE:C	1:B:28:PHE:CD2	2.95	0.40

There are no symmetry-related clashes.

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	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 ⓘ

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%)	63	41
1	B	426/425 (100%)	410 (96%)	16 (4%)	44	19
All	All	857/850 (101%)	831 (97%)	26 (3%)	53	29

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
1	A	423	GLN
1	A	446	GLN
1	B	64	THR

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Mol	Chain	Res	Type
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

Some 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 ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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$
3	BHZ	A	504	2	28,28,28	1.42	4 (14%)	36,36,36	1.71	9 (25%)
4	ACT	A	505	-	1,3,3	1.75	0	0,3,3	0.00	-
4	ACT	A	506	-	1,3,3	2.61	1 (100%)	0,3,3	0.00	-
4	ACT	A	507	-	1,3,3	3.20	1 (100%)	0,3,3	0.00	-
4	ACT	A	508	-	1,3,3	1.11	0	0,3,3	0.00	-
5	SO4	A	509	-	4,4,4	0.21	0	6,6,6	0.07	0
6	GOL	A	510	-	5,5,5	0.33	0	5,5,5	0.25	0
8	DTU	A	513	-	7,7,7	1.28	1 (14%)	8,8,8	2.48	3 (37%)
8	DTU	A	514	-	7,7,7	5.47	2 (28%)	8,8,8	4.46	4 (50%)
6	GOL	A	515	-	5,5,5	0.96	0	5,5,5	1.11	0
6	GOL	A	516	-	5,5,5	0.78	0	5,5,5	0.86	0
4	ACT	A	517	-	1,3,3	1.14	0	0,3,3	0.00	-
3	BHZ	B	504	2	28,28,28	1.37	3 (10%)	36,36,36	1.40	4 (11%)
9	DTV	B	507	-	7,7,7	1.44	2 (28%)	8,8,8	1.62	1 (12%)
6	GOL	B	508	-	5,5,5	0.33	0	5,5,5	0.25	0
6	GOL	B	509	-	5,5,5	0.66	0	5,5,5	0.75	0

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
4	ACT	A	505	-	-	0/0/0/0	0/0/0/0
4	ACT	A	506	-	-	0/0/0/0	0/0/0/0
4	ACT	A	507	-	-	0/0/0/0	0/0/0/0
4	ACT	A	508	-	-	0/0/0/0	0/0/0/0
5	SO4	A	509	-	-	0/0/0/0	0/0/0/0
6	GOL	A	510	-	-	0/4/4/4	0/0/0/0
8	DTU	A	513	-	2/2/2/2	0/8/8/8	0/0/0/0
8	DTU	A	514	-	2/2/2/2	0/8/8/8	0/0/0/0
6	GOL	A	515	-	-	0/4/4/4	0/0/0/0
6	GOL	A	516	-	-	0/4/4/4	0/0/0/0
4	ACT	A	517	-	-	0/0/0/0	0/0/0/0
3	BHZ	B	504	2	-	0/21/21/21	0/2/2/2
9	DTV	B	507	-	-	0/8/8/8	0/0/0/0
6	GOL	B	508	-	-	0/4/4/4	0/0/0/0
6	GOL	B	509	-	-	0/4/4/4	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	514	DTU	O2-C2	-14.01	1.11	1.43
3	B	504	BHZ	C12-N11	3.75	1.54	1.47
8	A	514	DTU	C1-C2	3.24	1.58	1.50
4	A	507	ACT	CH3-C	3.20	1.53	1.48
3	A	504	BHZ	C19-N8	3.07	1.53	1.46
3	B	504	BHZ	C21-C22	3.04	1.58	1.51
8	A	513	DTU	C1-C2	2.80	1.57	1.50
4	A	506	ACT	CH3-C	2.61	1.52	1.48
3	A	504	BHZ	C5-C6	2.40	1.44	1.39
3	B	504	BHZ	C4-C5	2.38	1.44	1.39
9	B	507	DTV	C4-S4	2.33	1.86	1.81
3	A	504	BHZ	C2-C1	2.28	1.43	1.39
3	A	504	BHZ	C10-N11	2.27	1.52	1.47
9	B	507	DTV	O3-C3	2.16	1.48	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	514	DTU	C3-C4-S4	-9.04	100.42	114.66
8	A	514	DTU	C2-C1-S1	-6.56	104.32	114.66
3	B	504	BHZ	C21-N11-C10	-4.62	100.76	112.34
8	A	513	DTU	C3-C4-S4	-4.56	107.47	114.66
8	A	514	DTU	O2-C2-C3	-4.26	101.52	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	513	DTU	O2-C2-C3	-4.21	101.61	109.83
3	A	504	BHZ	C12-N11-C10	-3.86	102.91	111.20
3	A	504	BHZ	C20-C19-N8	-3.28	101.58	113.73
3	A	504	BHZ	C21-N11-C10	-3.06	104.67	112.34
3	B	504	BHZ	C7-N8-C19	-3.03	106.27	112.58
8	A	514	DTU	C1-C2-C3	2.88	119.66	113.07
9	B	507	DTV	O2-C2-C1	-2.75	104.69	109.87
3	A	504	BHZ	O6-C6-C1	2.62	125.08	118.78
3	A	504	BHZ	C2-C1-C6	2.55	121.23	118.16
8	A	513	DTU	O3-C3-C2	2.43	114.58	109.83
3	A	504	BHZ	C19-N8-C9	-2.42	106.27	112.34
3	B	504	BHZ	C22-C21-N11	-2.42	104.78	113.73
3	B	504	BHZ	O23-C22-O22	2.30	129.14	123.30
3	A	504	BHZ	C3-C2-C1	-2.15	117.50	120.90
3	A	504	BHZ	C18-C13-C14	2.06	121.64	118.16
3	A	504	BHZ	C15-C14-C13	-2.01	117.27	120.64

All (4) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	497/502 (99%)	-0.27	9 (1%) 65 71	8, 13, 26, 44	0
1	B	497/502 (99%)	-0.13	18 (3%) 41 46	8, 17, 35, 50	1 (0%)
All	All	994/1004 (99%)	-0.20	27 (2%) 52 57	8, 15, 32, 50	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	PRO	6.5
1	B	328	ALA	5.3
1	B	442	HIS	4.9
1	B	58	GLU	4.3
1	B	473	MET	4.0
1	A	442	HIS	4.0
1	B	284	TYR	3.9
1	A	3	PRO	3.6
1	A	499	PRO	3.3
1	B	499	PRO	3.2
1	B	140	ARG	3.2
1	B	125	ALA	3.1
1	B	382	TYR	3.1
1	A	336	ASN	2.8
1	B	329	GLY	2.7
1	B	337	GLY	2.6
1	B	281	ASN	2.6
1	A	140	ARG	2.5
1	A	188	LYS	2.5
1	A	231	ARG	2.4
1	B	113	LEU	2.3
1	B	111	LYS	2.2
1	A	244	GLN	2.2
1	A	441	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	300	TYR	2.1
1	B	50	LEU	2.0
1	B	174	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	GOL	A	510	6/6	0.19	7.77	26,38,42,44	0
6	GOL	A	515	6/6	0.15	7.00	20,20,20,20	0
6	GOL	B	508	6/6	0.13	4.91	20,20,20,20	0
8	DTU	A	513	8/8	0.14	4.40	18,33,44,44	0
4	ACT	A	505	4/4	0.18	4.08	30,35,35,36	0
4	ACT	A	506	4/4	0.12	3.88	39,40,41,42	0
4	ACT	A	507	4/4	0.17	3.61	37,40,41,42	0
6	GOL	B	509	6/6	0.16	3.27	28,33,35,36	0
9	DTV	B	507	8/8	0.09	2.89	16,26,30,35	0
7	CL	B	506	1/1	0.10	2.46	39,39,39,39	0
4	ACT	A	517	4/4	0.16	2.40	22,24,26,29	0
5	SO4	A	509	5/5	0.15	1.93	60,62,64,65	0
4	ACT	A	508	4/4	0.21	1.55	54,55,55,55	0
8	DTU	A	514	8/8	0.19	0.64	9,33,47,49	0
7	CL	A	512	1/1	0.10	0.49	53,53,53,53	0
3	BHZ	B	504	27/27	0.07	0.23	9,12,17,18	0
6	GOL	A	516	6/6	0.09	-0.19	16,22,22,24	0
3	BHZ	A	504	27/27	0.09	-0.46	8,11,15,16	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FE2	A	503	1/1	0.07	-2.43	11,11,11,11	0
2	FE2	B	503	1/1	0.04	-19.00	12,12,12,12	0

6.5 Other polymers ⓘ

There are no such residues in this entry.