



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 02:39 PM GMT

PDB ID : 3MZB  
Title : X-ray structure of NikA in complex with the doubly hydroxylated iron complex, 1-O2  
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 : 2010-05-12  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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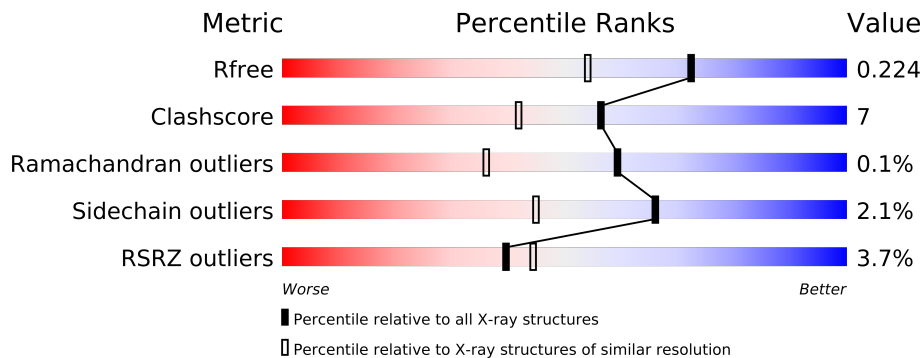
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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  $\geq 3$ , 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	501	
1	B	501	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	ACT	A	502	-	X
2	ACT	A	503	-	X
2	ACT	A	504	-	X
2	ACT	A	505	-	X
2	ACT	A	506	-	X
2	ACT	A	508	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	ACT	B	502	-	X
2	ACT	B	503	-	X
2	ACT	B	512	-	X
4	GOL	A	511	-	X
4	GOL	A	512	-	X
4	GOL	A	513	-	X
4	GOL	A	514	-	X
4	GOL	A	515	-	X
4	GOL	A	516	-	X
4	GOL	A	525	-	X
4	GOL	A	526	-	X
4	GOL	A	527	-	X
4	GOL	B	504	-	X
4	GOL	B	509	-	X
4	GOL	B	510	-	X
5	CL	A	517	-	X
5	CL	A	518	-	X
5	CL	A	519	-	X
8	DTD	A	522	-	X

## 2 Entry composition i

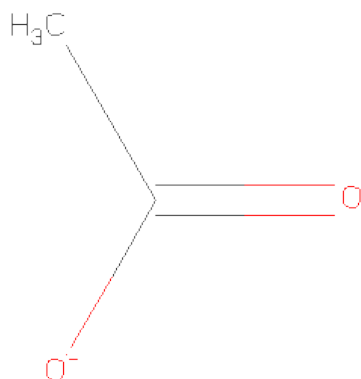
There are 9 unique types of molecules in this entry. The entry contains 8820 atoms, of which 0 are hydrogen and 0 are deuterium.

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	498	Total	C	N	O	S	20	0	0
			3951	2532	667	742	10			
1	B	496	Total	C	N	O	S	21	1	0
			3939	2524	665	740	10			

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



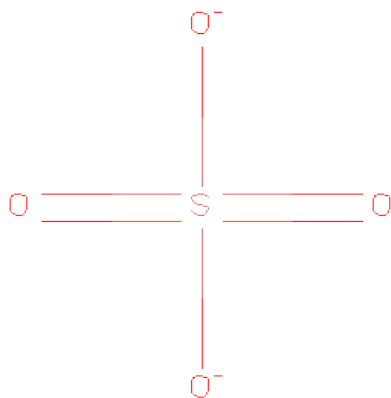
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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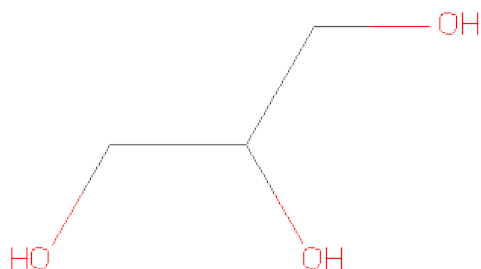
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

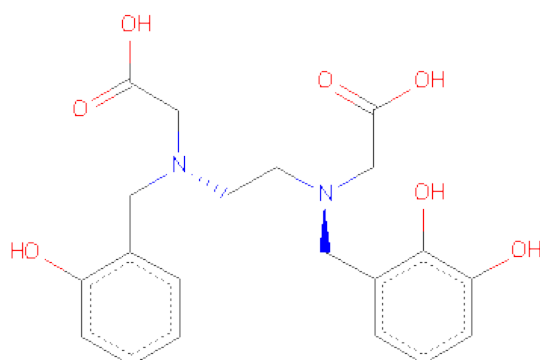


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0
5	A	4	Total Cl 4 4	0	0

- Molecule 6 is 2-[2-[CARBOXYMETHYL-[(2-HYDROXYPHENYL)METHYL]AMINO]ETHYL-[(2,3-DIHYDROXYPHENYL)METHYL]AMINO]ETHANOICACID (three-letter code: BHR) (formula: C<sub>20</sub>H<sub>24</sub>N<sub>2</sub>O<sub>7</sub>).

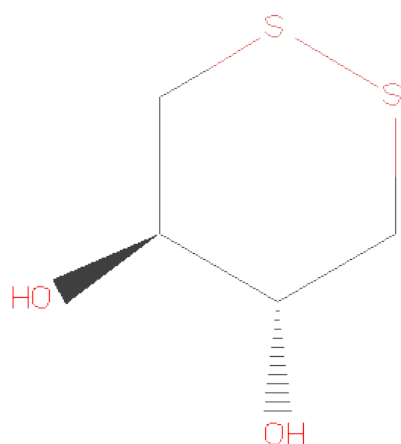


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 29 20 2 7	0	0
6	B	1	Total C N O 29 20 2 7	0	0

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 8 is DITHIANE DIOL (three-letter code: DTD) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>S<sub>2</sub>).



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

- Molecule 9 is water.

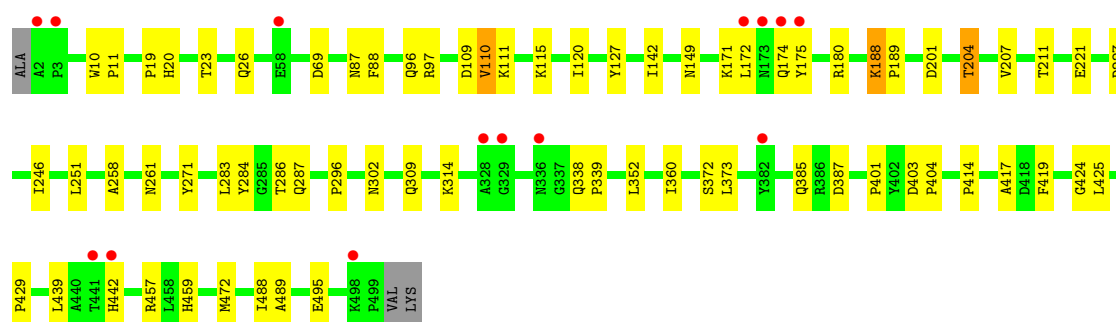
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	408	Total	O	0	0
			408	408		
9	B	314	Total	O	0	0
			314	314		

### 3 Residue-property plots

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

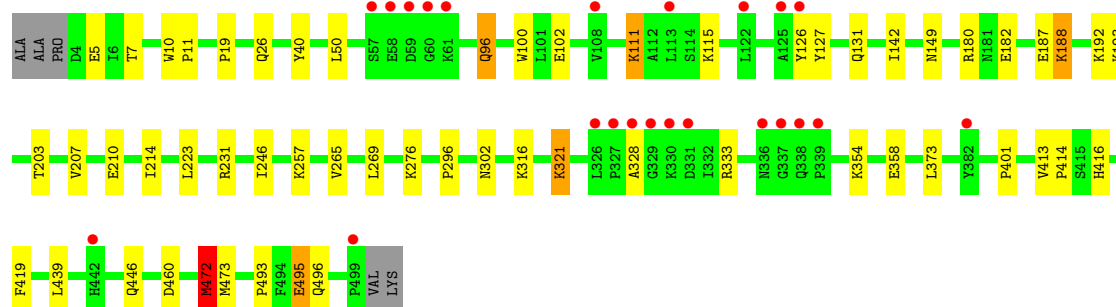
- Molecule 1: Nickel-binding periplasmic protein

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, $\alpha$ , $\beta$ , $\gamma$	87.04Å 93.87Å 124.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.93 – 1.70 46.94 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.93-1.70) 98.7 (46.94-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.22 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.187 , 0.223 0.187 , 0.224	Depositor DCC
$R_{free}$ test set	5562 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.8	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 40.9	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	1 of 111236 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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, DTD, FE, ACT, BHR, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.56	3/4055 (0.1%)	0.66	0/5525
1	B	0.60	5/4042 (0.1%)	0.68	3/5506 (0.1%)
All	All	0.58	8/8097 (0.1%)	0.67	3/11031 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	LYS	CG-CD	-13.90	1.05	1.52
1	A	188	LYS	CE-NZ	10.93	1.76	1.49
1	B	115	LYS	CB-CG	10.48	1.80	1.52
1	B	321	LYS	CE-NZ	-9.40	1.25	1.49
1	B	187	GLU	CB-CG	-9.06	1.34	1.52
1	B	276	LYS	CB-CG	-7.06	1.33	1.52
1	A	115	LYS	CG-CD	-5.43	1.33	1.52
1	A	96	GLN	CB-CG	5.14	1.66	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	LYS	CB-CG-CD	19.86	163.25	111.60
1	B	276	LYS	CA-CB-CG	6.42	127.51	113.40
1	B	472	MET	CG-SD-CE	5.40	108.83	100.20

There are no chirality outliers.

There are no planarity outliers.

## 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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3951	0	3897	59	1
1	B	3939	0	3879	36	1
2	A	28	0	21	3	0
2	B	16	0	12	1	0
3	A	5	0	0	0	0
4	A	60	0	80	14	0
4	B	18	0	24	3	0
5	A	4	0	0	0	0
5	B	1	0	0	0	0
6	A	29	0	20	13	0
6	B	29	0	20	1	0
7	A	1	0	0	2	0
7	B	1	0	0	1	0
8	A	8	0	8	1	0
8	B	8	0	8	1	0
9	A	408	0	0	10	1
9	B	314	0	0	8	1
All	All	8820	0	7969	104	2

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 7.

All (104) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:287:GLN:NE2	9:A:868:HOH:O	1.87	1.06
1:A:69:ASP:HA	4:A:514:GOL:H12	1.39	1.03
1:A:149:ASN:H	4:A:511:GOL:H11	1.20	1.03
1:A:97:ARG:HH22	6:A:520:BHR:C14	1.77	0.97
1:A:201:ASP:HB3	1:A:204:THR:HG23	1.46	0.95
1:A:97:ARG:HH22	6:A:520:BHR:H14	1.32	0.91
6:A:520:BHR:O6	7:A:521:FE:FE	1.22	0.90
6:A:520:BHR:H17	9:A:582:HOH:O	1.77	0.83
6:A:520:BHR:O18	7:A:521:FE:FE	1.29	0.83
1:A:97:ARG:HH22	6:A:520:BHR:C15	1.93	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:231:ARG:NH2	9:B:861:HOH:O	2.15	0.79
4:A:511:GOL:H31	9:A:932:HOH:O	1.84	0.78
6:A:520:BHR:O6	6:A:520:BHR:O18	2.02	0.78
1:A:459:HIS:CE1	2:A:502:ACT:H3	2.20	0.77
1:A:283:LEU:HD23	1:A:352:LEU:HD11	1.67	0.76
1:A:97:ARG:NH2	6:A:520:BHR:H15	2.01	0.76
1:A:10:TRP:HE1	1:A:26:GLN:HE21	1.35	0.74
1:B:149:ASN:OD1	9:B:848:HOH:O	2.06	0.73
1:A:109:ASP:OD1	1:A:111:LYS:HE3	1.89	0.72
1:A:110:VAL:HG12	1:A:120:ILE:HG12	1.72	0.72
1:B:10:TRP:HE1	1:B:26:GLN:HE21	1.36	0.71
1:A:495:GLU:OE2	9:A:865:HOH:O	2.08	0.71
1:B:180:ARG:NH1	1:B:182:GLU:OE1	2.23	0.70
1:B:416:HIS:HD2	9:B:798:HOH:O	1.76	0.69
1:B:180:ARG:HH21	1:B:192:LYS:HG2	1.58	0.68
1:A:221:GLU:HB2	9:A:868:HOH:O	1.93	0.68
1:B:131:GLN:OE1	9:B:854:HOH:O	2.13	0.67
1:A:149:ASN:N	4:A:511:GOL:H11	2.03	0.66
1:A:283:LEU:CD2	1:A:352:LEU:HD11	2.26	0.65
1:A:87:ASN:HD21	1:A:142:ILE:H	1.45	0.63
1:B:180:ARG:HD2	1:B:188:LYS:HG3	1.78	0.63
1:A:171:LYS:HB2	1:A:174:GLN:HB2	1.81	0.63
1:B:246:ILE:HD13	1:B:472:MET:HE3	1.81	0.61
1:A:97:ARG:NH2	6:A:520:BHR:C15	2.57	0.60
1:A:227:ASP:HB3	1:A:284:TYR:CZ	2.36	0.60
4:A:516:GOL:H32	9:A:660:HOH:O	2.02	0.60
1:B:495:GLU:CD	1:B:495:GLU:H	2.05	0.59
1:B:203:THR:HG22	2:B:503:ACT:H2	1.85	0.59
1:A:425:LEU:HD23	4:A:516:GOL:H31	1.85	0.59
1:A:172:LEU:O	1:A:174:GLN:OE1	2.21	0.59
1:A:296:PRO:HB3	1:A:302:ASN:HD22	1.68	0.58
6:B:506:BHR:O18	7:B:507:FE:FE	1.52	0.58
1:A:97:ARG:NH2	6:A:520:BHR:H14	2.12	0.58
1:B:10:TRP:HE1	1:B:26:GLN:NE2	2.03	0.57
1:B:354:LYS:HE3	1:B:358:GLU:OE1	2.04	0.56
1:A:171:LYS:HG3	1:A:175:TYR:CE1	2.41	0.56
1:A:425:LEU:HA	4:A:516:GOL:H31	1.86	0.55
1:A:211:THR:CG2	4:A:525:GOL:H32	2.36	0.55
6:A:520:BHR:O6	6:A:520:BHR:N8	2.40	0.54
1:A:429:PRO:HB2	9:A:571:HOH:O	2.08	0.53
1:B:19:PRO:HG3	1:B:142:ILE:HB	1.91	0.53
1:A:11:PRO:HD3	8:A:522:DTD:S1	2.50	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:211:THR:HG22	4:A:525:GOL:H32	1.90	0.52
1:A:10:TRP:HE1	1:A:26:GLN:NE2	2.06	0.52
1:A:286:THR:HG22	4:A:527:GOL:H11	1.92	0.52
1:B:446:GLN:HG2	9:B:612:HOH:O	2.10	0.51
1:A:23:THR:HG22	6:A:520:BHR:H16	1.91	0.51
6:A:520:BHR:N11	6:A:520:BHR:O18	2.45	0.50
1:B:257:LYS:HE2	9:B:705:HOH:O	2.11	0.49
1:A:424:GLY:O	4:A:516:GOL:H11	2.13	0.49
1:A:302:ASN:HD21	2:A:504:ACT:CH3	2.27	0.48
1:B:223:LEU:HB3	1:B:473:MET:HE2	1.96	0.48
1:B:414:PRO:HA	1:B:419:PHE:CD1	2.48	0.48
1:B:102:GLU:HB3	1:B:126:TYR:OH	2.13	0.48
1:B:223:LEU:HB3	1:B:473:MET:CE	2.43	0.47
1:A:414:PRO:HA	1:A:419:PHE:CG	2.50	0.47
1:A:88:PHE:HB3	1:A:110:VAL:HG21	1.97	0.46
1:A:211:THR:HG22	4:A:525:GOL:C3	2.45	0.46
1:A:258:ALA:HA	1:A:261:ASN:OD1	2.15	0.46
1:A:457:ARG:HG2	4:A:526:GOL:H2	1.98	0.46
1:A:385:GLN:HB3	1:A:417:ALA:HB2	1.98	0.45
1:B:11:PRO:HD3	8:B:508:DTD:S4	2.56	0.45
1:B:493:PRO:HA	4:B:509:GOL:H12	1.99	0.44
1:A:302:ASN:HD21	2:A:504:ACT:H3	1.82	0.44
1:A:110:VAL:HG23	9:A:793:HOH:O	2.17	0.44
1:A:207:VAL:O	1:A:211:THR:HG23	2.17	0.44
1:B:296:PRO:HB3	1:B:302:ASN:HD22	1.82	0.44
1:B:5:GLU:HG2	1:B:193:LYS:HB3	1.99	0.44
1:B:246:ILE:HD13	1:B:472:MET:CE	2.47	0.44
1:A:19:PRO:HG3	1:A:142:ILE:HB	1.99	0.43
1:A:338:GLN:HA	1:A:339:PRO:HD3	1.84	0.43
1:B:207:VAL:HA	1:B:210:GLU:HG2	2.00	0.43
1:B:265:VAL:O	1:B:269:LEU:HG	2.18	0.43
1:B:321:LYS:NZ	9:B:766:HOH:O	2.51	0.43
1:A:251:LEU:HD11	1:A:360:ILE:HD13	2.01	0.43
1:A:489:ALA:HB3	9:A:783:HOH:O	2.17	0.43
1:B:7:THR:HG22	1:B:214:ILE:HG22	2.01	0.43
1:A:211:THR:HG22	4:A:525:GOL:C2	2.49	0.42
1:B:246:ILE:CG2	4:B:504:GOL:H12	2.49	0.42
1:A:271:TYR:CZ	1:A:314:LYS:HD3	2.55	0.42
1:B:246:ILE:HG21	4:B:504:GOL:H12	2.01	0.42
1:B:496:GLN:NE2	9:B:742:HOH:O	2.44	0.42
1:A:387:ASP:HB3	9:A:809:HOH:O	2.20	0.41
1:A:414:PRO:HA	1:A:419:PHE:CD1	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:180:ARG:HG3	1:A:189:PRO:HD2	2.02	0.41
1:A:401:PRO:HD3	1:A:488:ILE:HG12	2.03	0.41
1:B:40:TYR:CE1	1:B:401:PRO:HB3	2.56	0.41
1:B:100:TRP:HA	1:B:413:VAL:HG21	2.02	0.41
1:A:246:ILE:HD13	1:A:472:MET:HG2	2.03	0.41
1:A:201:ASP:HB3	1:A:204:THR:CG2	2.32	0.40
1:B:316:LYS:HG2	1:B:333:ARG:HH11	1.86	0.40
1:A:403:ASP:HA	1:A:404:PRO:HA	1.93	0.40
1:A:20:HIS:CE1	1:A:87:ASN:HD22	2.40	0.40

All (2) 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	Distance(Å)	Clash(Å)
9:A:880:HOH:O	9:B:770:HOH:O[4_455]	1.80	0.40
1:A:387:ASP:OD2	1:B:460:ASP:OD2[3_545]	1.93	0.27

## 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	496/501 (99%)	483 (97%)	13 (3%)	0	100	100
1	B	494/501 (99%)	482 (98%)	11 (2%)	1 (0%)	56	33
All	All	990/1002 (99%)	965 (98%)	24 (2%)	1 (0%)	59	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	328	ALA

### 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	422/424 (100%)	413 (98%)	9 (2%)	66	45
1	B	421/424 (99%)	412 (98%)	9 (2%)	66	45
All	All	843/848 (99%)	825 (98%)	18 (2%)	66	45

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	VAL
1	A	127	TYR
1	A	188	LYS
1	A	204	THR
1	A	309	GLN
1	A	372	SER
1	A	373	LEU
1	A	439	LEU
1	A	442	HIS
1	B	50	LEU
1	B	96[A]	GLN
1	B	111	LYS
1	B	127	TYR
1	B	188	LYS
1	B	373	LEU
1	B	439	LEU
1	B	472	MET
1	B	495	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	87	ASN
1	A	131	GLN
1	A	197	ASN
1	A	302	ASN
1	A	446	GLN
1	B	25	ASN
1	B	26	GLN
1	B	174	GLN

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Mol	Chain	Res	Type
1	B	234	GLN
1	B	302	ASN
1	B	336	ASN
1	B	416	HIS
1	B	442	HIS
1	B	496	GLN

### 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 36 ligands modelled in this entry, 7 are monoatomic - leaving 29 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ACT	A	502	-	1,3,3	0.83	0	0,3,3	0.00	-
2	ACT	A	503	-	1,3,3	1.25	0	0,3,3	0.00	-
2	ACT	A	504	-	1,3,3	1.13	0	0,3,3	0.00	-
2	ACT	A	505	-	1,3,3	0.83	0	0,3,3	0.00	-
2	ACT	A	506	-	1,3,3	1.55	0	0,3,3	0.00	-
2	ACT	A	507	-	1,3,3	1.18	0	0,3,3	0.00	-
2	ACT	A	508	-	1,3,3	0.49	0	0,3,3	0.00	-
3	SO4	A	509	-	4,4,4	0.28	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	A	510	-	5,5,5	0.29	0	5,5,5	0.49	0
4	GOL	A	511	-	5,5,5	0.42	0	5,5,5	0.54	0
4	GOL	A	512	-	5,5,5	0.32	0	5,5,5	0.53	0
4	GOL	A	513	-	5,5,5	0.44	0	5,5,5	0.56	0
4	GOL	A	514	-	5,5,5	0.41	0	5,5,5	0.57	0
4	GOL	A	515	-	5,5,5	0.30	0	5,5,5	0.57	0
4	GOL	A	516	-	5,5,5	0.29	0	5,5,5	0.47	0
6	BHR	A	520	7	30,30,30	1.02	1 (3%)	40,40,40	1.49	6 (15%)
8	DTD	A	522	-	8,8,8	0.65	0	10,10,10	1.68	1 (10%)
4	GOL	A	525	-	5,5,5	0.39	0	5,5,5	0.84	0
4	GOL	A	526	-	5,5,5	0.28	0	5,5,5	0.49	0
4	GOL	A	527	-	5,5,5	0.45	0	5,5,5	0.53	0
2	ACT	B	502	-	1,3,3	1.05	0	0,3,3	0.00	-
2	ACT	B	503	-	1,3,3	0.67	0	0,3,3	0.00	-
4	GOL	B	504	-	5,5,5	0.29	0	5,5,5	0.54	0
6	BHR	B	506	7	30,30,30	0.63	0	40,40,40	1.54	7 (17%)
8	DTD	B	508	-	8,8,8	1.00	1 (12%)	10,10,10	1.40	2 (20%)
4	GOL	B	509	-	5,5,5	0.28	0	5,5,5	0.54	0
4	GOL	B	510	-	5,5,5	0.34	0	5,5,5	0.36	0
2	ACT	B	511	-	1,3,3	1.29	0	0,3,3	0.00	-
2	ACT	B	512	-	1,3,3	0.28	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACT	A	502	-	-	0/0/0/0	0/0/0/0
2	ACT	A	503	-	-	0/0/0/0	0/0/0/0
2	ACT	A	504	-	-	0/0/0/0	0/0/0/0
2	ACT	A	505	-	-	0/0/0/0	0/0/0/0
2	ACT	A	506	-	-	0/0/0/0	0/0/0/0
2	ACT	A	507	-	-	0/0/0/0	0/0/0/0
2	ACT	A	508	-	-	0/0/0/0	0/0/0/0
3	SO4	A	509	-	-	0/0/0/0	0/0/0/0
4	GOL	A	510	-	-	0/4/4/4	0/0/0/0
4	GOL	A	511	-	-	0/4/4/4	0/0/0/0
4	GOL	A	512	-	-	0/4/4/4	0/0/0/0
4	GOL	A	513	-	-	0/4/4/4	0/0/0/0
4	GOL	A	514	-	-	0/4/4/4	0/0/0/0
4	GOL	A	515	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	516	-	-	0/4/4/4	0/0/0/0
6	BHR	A	520	7	-	0/21/21/21	0/2/2/2
8	DTD	A	522	-	-	0/0/11/11	0/1/1/1
4	GOL	A	525	-	-	0/4/4/4	0/0/0/0
4	GOL	A	526	-	-	0/4/4/4	0/0/0/0
4	GOL	A	527	-	-	0/4/4/4	0/0/0/0
2	ACT	B	502	-	-	0/0/0/0	0/0/0/0
2	ACT	B	503	-	-	0/0/0/0	0/0/0/0
4	GOL	B	504	-	-	0/4/4/4	0/0/0/0
6	BHR	B	506	7	-	0/21/21/21	0/2/2/2
8	DTD	B	508	-	-	0/0/11/11	0/1/1/1
4	GOL	B	509	-	-	0/4/4/4	0/0/0/0
4	GOL	B	510	-	-	0/4/4/4	0/0/0/0
2	ACT	B	511	-	-	0/0/0/0	0/0/0/0
2	ACT	B	512	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	508	DTD	C3-C2	2.60	1.55	1.52
6	A	520	BHR	C7-C1	2.41	1.55	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	520	BHR	C5-C6-C1	5.19	123.59	120.45
8	A	522	DTD	C4-S4-S1	4.51	103.32	98.70
6	B	506	BHR	C12-C13-C18	4.21	124.80	120.47
6	B	506	BHR	C7-C1-C6	4.18	126.33	120.31
6	B	506	BHR	C7-N8-C9	-3.12	104.50	111.20
6	A	520	BHR	C7-N8-C19	-3.04	106.26	112.58
6	A	520	BHR	C17-C18-C13	2.93	123.25	120.45
6	A	520	BHR	C19-N8-C9	-2.77	105.41	112.34
6	B	506	BHR	C7-C1-C2	-2.71	114.74	120.19
6	B	506	BHR	C7-N8-C19	-2.54	107.29	112.58
6	B	506	BHR	C12-N11-C10	-2.32	106.22	111.20
6	A	520	BHR	C12-C13-C18	2.31	122.85	120.47
8	B	508	DTD	O3-C3-C4	-2.19	105.92	109.86
6	B	506	BHR	C19-N8-C9	-2.10	107.08	112.34
6	A	520	BHR	O20-C20-C19	-2.08	114.13	122.10
8	B	508	DTD	C1-S1-S4	2.07	100.82	98.70

There are no chirality outliers.

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	498/501 (99%)	-0.02	14 (2%)	50	56	11, 19, 31, 40	7 (1%)
1	B	496/501 (99%)	0.16	23 (4%)	31	35	11, 23, 43, 54	6 (1%)
All	All	994/1002 (99%)	0.07	37 (3%)	39	44	11, 21, 38, 54	13 (1%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	326	LEU	6.6
1	B	329	GLY	6.2
1	B	125	ALA	5.8
1	B	337	GLY	5.4
1	A	3	PRO	5.4
1	B	328	ALA	5.2
1	A	2	ALA	5.0
1	B	338	GLN	4.9
1	B	327	PRO	4.8
1	A	442	HIS	4.6
1	A	175	TYR	4.2
1	B	382	TYR	4.1
1	B	57	SER	4.1
1	B	113	LEU	4.0
1	B	58	GLU	3.9
1	B	108	VAL	3.9
1	A	172	LEU	3.8
1	B	331	ASP	3.6
1	B	330	LYS	3.5
1	A	329	GLY	3.4
1	B	60	GLY	3.3
1	A	382	TYR	3.3
1	B	336	ASN	3.2
1	A	174	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	58	GLU	2.7
1	A	336	ASN	2.5
1	B	339	PRO	2.5
1	A	498	LYS	2.5
1	B	442	HIS	2.4
1	B	61	LYS	2.3
1	B	59	ASP	2.3
1	A	173	ASN	2.2
1	A	328	ALA	2.2
1	B	499	PRO	2.2
1	A	441	THR	2.1
1	B	122	LEU	2.0
1	B	126	TYR	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ACT	A	502	4/4	0.25	17.08	28,30,31,31	0
4	GOL	A	511	6/6	0.19	14.50	38,39,41,42	0
4	GOL	A	526	6/6	0.25	14.36	39,41,41,43	0
4	GOL	A	514	6/6	0.27	13.81	30,37,39,41	0
2	ACT	B	503	4/4	0.15	12.08	43,44,44,44	0
4	GOL	A	516	6/6	0.26	10.84	27,33,34,35	0
4	GOL	A	525	6/6	0.34	10.02	80,81,82,82	0
2	ACT	A	508	4/4	0.19	6.33	40,40,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	527	6/6	0.25	5.89	35,36,38,40	0
2	ACT	A	506	4/4	0.18	4.92	35,35,36,36	0
4	GOL	B	509	6/6	0.21	4.81	35,39,41,42	0
4	GOL	B	510	6/6	0.20	4.53	40,41,41,43	0
2	ACT	B	512	4/4	0.17	4.37	38,38,39,39	0
5	CL	A	519	1/1	0.23	4.36	86,86,86,86	0
2	ACT	A	505	4/4	0.17	4.30	35,36,36,36	0
2	ACT	A	503	4/4	0.22	3.80	59,59,59,59	0
4	GOL	A	515	6/6	0.20	3.29	35,39,40,43	0
5	CL	A	518	1/1	0.19	3.05	48,48,48,48	0
4	GOL	A	512	6/6	0.15	3.03	37,39,40,42	0
4	GOL	A	513	6/6	0.19	3.01	33,35,35,35	0
2	ACT	A	504	4/4	0.12	2.95	38,39,39,39	0
2	ACT	B	502	4/4	0.14	2.71	38,38,38,38	0
5	CL	A	517	1/1	0.12	2.56	64,64,64,64	0
4	GOL	B	504	6/6	0.15	2.54	32,37,39,39	0
8	DTD	A	522	8/8	0.11	2.38	23,25,26,28	0
4	GOL	A	510	6/6	0.12	1.84	37,37,38,39	0
6	BHR	B	506	29/29	0.12	1.25	15,29,32,32	0
5	CL	B	505	1/1	0.09	1.11	47,47,47,47	0
2	ACT	A	507	4/4	0.20	1.05	62,62,62,62	0
6	BHR	A	520	29/29	0.14	0.64	18,31,34,37	0
2	ACT	B	511	4/4	0.15	0.44	39,40,40,40	0
3	SO4	A	509	5/5	0.10	0.37	36,37,38,38	0
8	DTD	B	508	8/8	0.08	0.28	21,25,26,29	0
5	CL	A	523	1/1	0.08	-0.47	51,51,51,51	0
7	FE	A	521	1/1	0.05	-3.69	19,19,19,19	1
7	FE	B	507	1/1	0.06	-	19,19,19,19	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.