



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 02:38 PM GMT

PDB ID : 3MZ9  
Title : X-ray structure of NikA in complex with HBED  
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Deposited on : 2010-05-12  
Resolution : 1.80 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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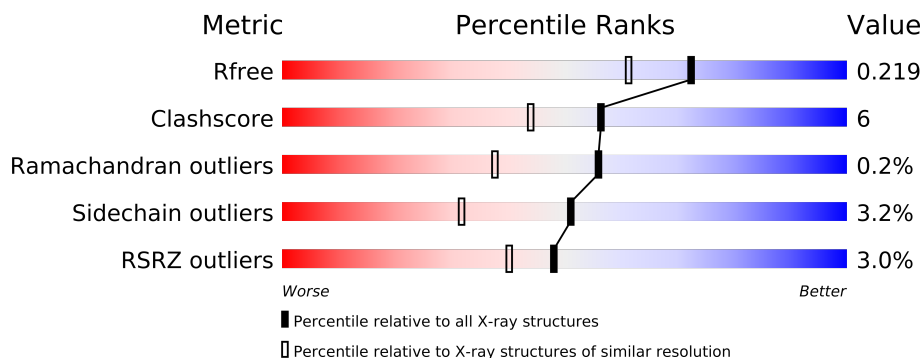
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.80 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	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (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 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	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	DTD	A	505	-	X
5	CL	A	525	-	X
5	CL	A	526	-	X
6	GOL	A	507	-	X
6	GOL	A	508	-	X
6	GOL	A	509	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	GOL	A	510	-	X
6	GOL	A	518	-	X
6	GOL	A	519	-	X
6	GOL	A	520	-	X
6	GOL	A	521	-	X
6	GOL	A	522	-	X
6	GOL	A	523	-	X
6	GOL	A	524	-	X
6	GOL	B	506	-	X
6	GOL	B	509	-	X
7	ACT	A	511	-	X
7	ACT	A	513	-	X
7	ACT	A	514	-	X
7	ACT	A	515	-	X
7	ACT	A	516	-	X
7	ACT	B	508	-	X

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 8867 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.

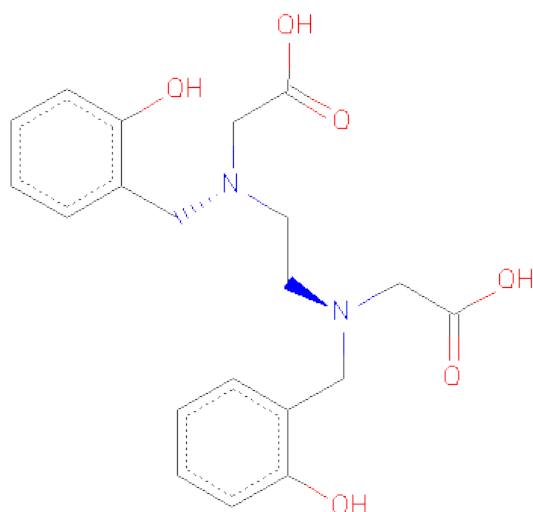
- Molecule 1 is a protein called Nickel-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	1	0
			3961	2539	668	744	10			
1	B	498	Total	C	N	O	S	7	0	0
			3951	2532	667	742	10			

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

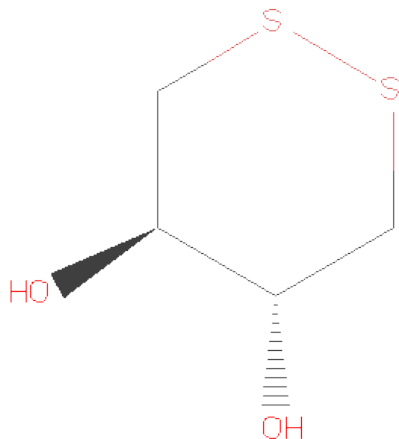
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		

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



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

- Molecule 4 is DITHIANE DIOL (three-letter code: DTD) (formula:  $C_4H_8O_2S_2$ ).



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

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

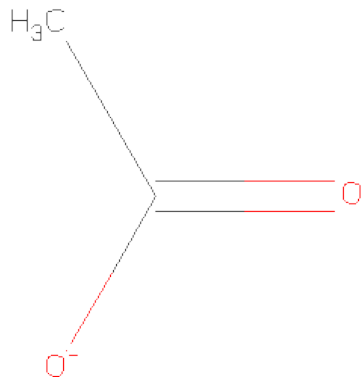
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	3	Total	Cl	0	0
			3	3		

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



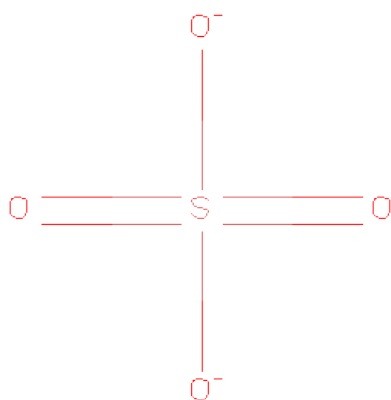
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total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

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 9 is water.

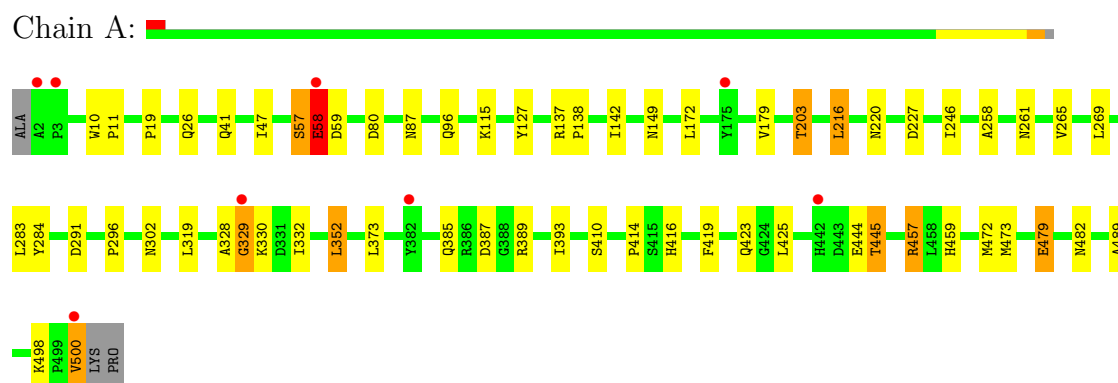
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	419	Total	O	0	0
			419	419		
9	B	343	Total	O	0	0
			343	343		



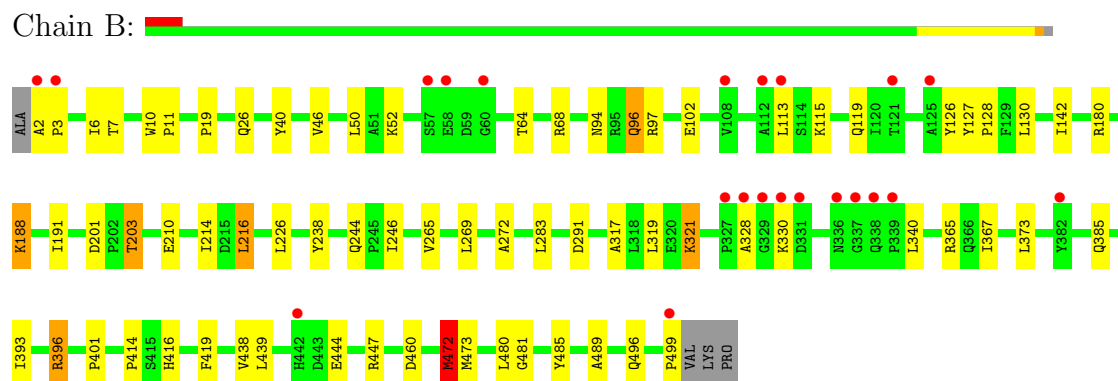
### 3 Residue-property plots

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



- 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, $\alpha$ , $\beta$ , $\gamma$	87.08Å 93.85Å 124.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.93 – 1.80 46.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.93-1.80) 99.9 (46.92-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.182 , 0.219 0.182 , 0.219	Depositor DCC
$R_{free}$ test set	4753 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 42.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 95053 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8867	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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, BHN, CL, DTD, FE, ACT, 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	0.57	0/4068	0.68	5/5543 (0.1%)
1	B	0.54	0/4055	0.66	4/5525 (0.1%)
All	All	0.56	0/8123	0.67	9/11068 (0.1%)

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	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	396	ARG	NE-CZ-NH1	-11.38	114.61	120.30
1	B	396	ARG	NE-CZ-NH2	11.33	125.96	120.30
1	A	457	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	216	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	457	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	472	MET	CG-SD-CE	5.28	108.64	100.20
1	A	216	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	329	GLY	N-CA-C	-5.25	99.98	113.10
1	A	291	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	GLU	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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3961	0	3912	55	1
1	B	3951	0	3898	46	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	20	0	0
3	B	28	0	20	0	0
4	A	8	0	8	1	0
4	B	8	0	8	1	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
6	A	66	0	88	17	0
6	B	12	0	16	1	0
7	A	24	0	18	1	0
7	B	8	0	6	0	0
8	A	5	0	0	0	0
9	A	419	0	0	17	2
9	B	343	0	0	11	0
All	All	8867	0	7994	104	3

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 6.

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:416:HIS:HD2	9:A:695:HOH:O	1.30	1.14
1:A:149:ASN:H	6:A:519:GOL:H11	1.13	1.06
1:A:387:ASP:HB3	6:A:507:GOL:O2	1.64	0.97
1:B:244:GLN:HG3	9:B:712:HOH:O	1.68	0.94
1:A:425:LEU:HA	6:A:524:GOL:H31	1.49	0.90
1:B:416:HIS:HD2	9:B:659:HOH:O	1.52	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:94:ASN:HD21	1:B:97:ARG:HE	1.26	0.82
1:A:203:THR:HG23	9:A:698:HOH:O	1.80	0.81
1:A:459:HIS:CE1	7:A:511:ACT:H3	2.17	0.79
6:A:510:GOL:H2	9:A:646:HOH:O	1.83	0.78
1:A:10:TRP:HE1	1:A:26:GLN:HE21	1.31	0.76
1:A:479:GLU:H	1:A:479:GLU:CD	1.90	0.75
1:A:58:GLU:HB2	1:A:59:ASP:HB3	1.68	0.74
1:B:10:TRP:HE1	1:B:26:GLN:HE21	1.34	0.74
1:A:149:ASN:N	6:A:519:GOL:H11	1.96	0.72
1:B:94:ASN:HD21	1:B:97:ARG:NE	1.88	0.72
6:A:521:GOL:H12	9:A:934:HOH:O	1.91	0.70
1:A:498:LYS:HG2	1:A:500:VAL:HG23	1.74	0.69
1:A:445:THR:HG23	9:A:920:HOH:O	1.91	0.69
6:A:507:GOL:C3	9:A:551:HOH:O	2.41	0.68
1:A:416:HIS:CD2	9:A:695:HOH:O	2.17	0.68
1:B:291:ASP:OD1	9:B:929:HOH:O	2.11	0.67
1:A:80:ASP:HB3	6:A:522:GOL:H32	1.75	0.67
1:B:485:TYR:HB3	6:B:509:GOL:H11	1.77	0.66
6:A:507:GOL:H31	9:A:551:HOH:O	1.96	0.65
1:A:227:ASP:HB3	1:A:284:TYR:CZ	2.31	0.65
1:A:58:GLU:HB2	1:A:59:ASP:CB	2.27	0.65
1:A:416:HIS:NE2	9:A:938:HOH:O	2.29	0.62
1:B:2:ALA:N	1:B:3:PRO:HD2	2.15	0.62
1:A:445:THR:HG21	9:B:744:HOH:O	1.99	0.61
1:B:210:GLU:OE2	9:B:932:HOH:O	2.16	0.61
1:A:87:ASN:HD21	1:A:142:ILE:H	1.48	0.60
1:B:321:LYS:HD3	9:B:803:HOH:O	2.01	0.60
1:A:482:ASN:HD21	6:A:510:GOL:C1	2.15	0.59
1:A:115:LYS:HD3	6:A:522:GOL:H31	1.85	0.59
1:A:10:TRP:HE1	1:A:26:GLN:NE2	2.02	0.56
1:B:180:ARG:HD2	1:B:188:LYS:HG3	1.87	0.56
1:B:113:LEU:HD11	1:B:119:GLN:HE21	1.71	0.56
1:A:11:PRO:HD3	4:A:505:DTD:S1	2.46	0.56
1:B:7:THR:HG22	1:B:214:ILE:HG22	1.88	0.56
1:B:265:VAL:O	1:B:269:LEU:HG	2.06	0.55
1:B:52:LYS:HG3	1:B:68:ARG:HG2	1.89	0.55
1:B:96:GLN:H	1:B:96:GLN:NE2	2.03	0.55
1:A:479:GLU:CD	1:A:479:GLU:N	2.60	0.55
1:B:416:HIS:CD2	9:B:659:HOH:O	2.39	0.55
1:B:444:GLU:HA	1:B:447:ARG:NH1	2.22	0.55
1:B:210:GLU:HG3	1:B:238:TYR:OH	2.06	0.54
1:A:296:PRO:HB3	1:A:302:ASN:HD22	1.72	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:317:ALA:O	1:B:321:LYS:HE2	2.08	0.54
1:B:480:LEU:HD23	1:B:499:PRO:HB3	1.90	0.53
1:B:246:ILE:HD13	1:B:472:MET:HE3	1.90	0.52
1:A:479:GLU:OE2	1:A:479:GLU:N	2.42	0.52
6:A:524:GOL:H32	9:A:677:HOH:O	2.10	0.51
1:B:226:LEU:HD12	1:B:283:LEU:HA	1.92	0.51
1:B:496:GLN:NE2	9:B:735:HOH:O	2.41	0.50
1:A:58:GLU:CB	1:A:59:ASP:HB3	2.39	0.50
1:B:102:GLU:HB3	1:B:126:TYR:OH	2.12	0.49
1:B:328:ALA:HA	1:B:330:LYS:H	1.77	0.49
1:B:19:PRO:HG3	1:B:142:ILE:HB	1.96	0.48
1:A:479:GLU:OE2	9:A:869:HOH:O	2.20	0.48
1:A:444:GLU:CG	1:B:481:GLY:HA2	2.45	0.47
1:B:191:ILE:HD11	1:B:499:PRO:HG3	1.95	0.47
1:A:489:ALA:HB3	9:A:765:HOH:O	2.14	0.47
1:A:444:GLU:HG2	1:B:481:GLY:HA2	1.96	0.47
1:A:389:ARG:HD3	9:A:709:HOH:O	2.15	0.46
1:A:58:GLU:CD	1:A:58:GLU:H	2.18	0.46
1:B:272:ALA:HB2	1:B:367:ILE:HD13	1.97	0.46
1:B:10:TRP:HE1	1:B:26:GLN:NE2	2.05	0.46
1:A:80:ASP:CB	6:A:522:GOL:H32	2.45	0.46
1:B:11:PRO:HD3	4:B:505:DTD:S4	2.54	0.46
1:A:414:PRO:HA	1:A:419:PHE:CG	2.51	0.46
1:A:385:GLN:HG2	1:A:393:ILE:HD13	1.98	0.46
1:B:385:GLN:HG2	1:B:393:ILE:HD13	1.98	0.45
6:A:507:GOL:H32	9:A:551:HOH:O	2.14	0.45
1:A:57:SER:OG	1:A:59:ASP:O	2.31	0.45
1:A:330:LYS:HG3	1:A:332:ILE:H	1.82	0.45
1:B:96:GLN:H	1:B:96:GLN:CD	2.20	0.45
1:A:283:LEU:HD23	1:A:352:LEU:HD21	1.99	0.45
1:A:482:ASN:HD21	6:A:510:GOL:H11	1.82	0.44
1:B:64:THR:HG22	1:B:119:GLN:HG3	1.99	0.44
1:B:40:TYR:CE1	1:B:401:PRO:HB3	2.53	0.44
1:B:489:ALA:HB3	9:B:777:HOH:O	2.17	0.44
1:B:6:ILE:HG23	1:B:191:ILE:HD12	2.00	0.43
1:B:94:ASN:ND2	1:B:97:ARG:HE	2.05	0.43
1:A:137:ARG:HB2	1:A:138:PRO:HA	2.00	0.43
1:A:328:ALA:HA	1:A:329:GLY:HA2	1.87	0.43
1:A:457:ARG:HH22	6:A:509:GOL:H2	1.83	0.43
1:B:396:ARG:CD	9:B:600:HOH:O	2.67	0.43
1:B:46:VAL:HG21	1:B:130:LEU:HB3	2.01	0.42
1:B:201:ASP:OD1	1:B:203:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:220:ASN:O	1:A:473:MET:HE2	2.18	0.42
1:A:410[A]:SER:OG	9:A:716:HOH:O	2.22	0.42
1:A:246:ILE:HG22	6:A:520:GOL:H2	2.00	0.42
1:B:414:PRO:HA	1:B:419:PHE:CD1	2.54	0.42
1:A:19:PRO:HG3	1:A:142:ILE:HB	2.02	0.42
1:B:128:PRO:HB3	9:B:820:HOH:O	2.20	0.42
1:A:472:MET:HE2	9:A:702:HOH:O	2.19	0.41
1:A:41:GLN:HG3	1:A:47:ILE:HG23	2.02	0.41
1:A:444:GLU:HG2	1:B:481:GLY:CA	2.51	0.41
1:A:96:GLN:HA	1:A:96:GLN:NE2	2.35	0.41
1:A:59:ASP:OD2	1:A:59:ASP:O	2.39	0.41
1:A:265:VAL:O	1:A:269:LEU:HG	2.21	0.41
1:A:416:HIS:HB3	9:A:580:HOH:O	2.21	0.41
1:A:258:ALA:HA	1:A:261:ASN:OD1	2.21	0.40

All (3) 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)
1:A:387:ASP:OD2	1:B:460:ASP:OD2[3_545]	2.07	0.13
1:B:365:ARG:NH2	9:A:696:HOH:O[4_555]	2.18	0.02
9:A:683:HOH:O	9:A:917:HOH:O[3_555]	2.18	0.02

## 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	498/502 (99%)	482 (97%)	14 (3%)	2 (0%)	43	25
1	B	496/502 (99%)	482 (97%)	14 (3%)	0	100	100
All	All	994/1004 (99%)	964 (97%)	28 (3%)	2 (0%)	56	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	57	SER

### 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	424/425 (100%)	412 (97%)	12 (3%)	56	38
1	B	422/425 (99%)	407 (96%)	15 (4%)	47	27
All	All	846/850 (100%)	819 (97%)	27 (3%)	51	32

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	TYR
1	A	172	LEU
1	A	179	VAL
1	A	203	THR
1	A	216	LEU
1	A	319	LEU
1	A	352	LEU
1	A	373	LEU
1	A	423	GLN
1	A	445	THR
1	A	479	GLU
1	A	500	VAL
1	B	50	LEU
1	B	96	GLN
1	B	115	LYS
1	B	127	TYR
1	B	188	LYS
1	B	203	THR
1	B	216	LEU
1	B	319	LEU
1	B	321	LYS
1	B	340	LEU
1	B	373	LEU
1	B	438	VAL

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Mol	Chain	Res	Type
1	B	439	LEU
1	B	472	MET
1	B	473	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	87	ASN
1	A	96	GLN
1	A	197	ASN
1	A	288	GLN
1	A	302	ASN
1	A	416	HIS
1	A	423	GLN
1	A	446	GLN
1	A	482	ASN
1	B	25	ASN
1	B	26	GLN
1	B	56	HIS
1	B	94	ASN
1	B	96	GLN
1	B	119	GLN
1	B	234	GLN
1	B	288	GLN
1	B	302	ASN
1	B	336	ASN
1	B	416	HIS

### 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 32 ligands modelled in this entry, 6 are monoatomic - leaving 26 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	BHN	A	504	2	29,29,29	0.61	0	38,38,38	1.70	8 (21%)
4	DTD	A	505	-	8,8,8	0.94	1 (12%)	10,10,10	1.78	3 (30%)
6	GOL	A	507	-	5,5,5	0.46	0	5,5,5	0.39	0
6	GOL	A	508	-	5,5,5	0.31	0	5,5,5	0.88	0
6	GOL	A	509	-	5,5,5	0.32	0	5,5,5	0.24	0
6	GOL	A	510	-	5,5,5	0.36	0	5,5,5	0.56	0
7	ACT	A	511	-	1,3,3	1.00	0	0,3,3	0.00	-
7	ACT	A	512	-	1,3,3	1.21	0	0,3,3	0.00	-
7	ACT	A	513	-	1,3,3	1.69	0	0,3,3	0.00	-
7	ACT	A	514	-	1,3,3	1.23	0	0,3,3	0.00	-
7	ACT	A	515	-	1,3,3	1.19	0	0,3,3	0.00	-
7	ACT	A	516	-	1,3,3	0.77	0	0,3,3	0.00	-
8	SO4	A	517	-	4,4,4	0.24	0	6,6,6	0.19	0
6	GOL	A	518	-	5,5,5	0.27	0	5,5,5	0.50	0
6	GOL	A	519	-	5,5,5	0.51	0	5,5,5	0.48	0
6	GOL	A	520	-	5,5,5	0.26	0	5,5,5	0.54	0
6	GOL	A	521	-	5,5,5	0.53	0	5,5,5	0.60	0
6	GOL	A	522	-	5,5,5	0.32	0	5,5,5	0.42	0
6	GOL	A	523	-	5,5,5	0.24	0	5,5,5	0.37	0
6	GOL	A	524	-	5,5,5	0.35	0	5,5,5	0.57	0
3	BHN	B	504	2	29,29,29	0.73	0	38,38,38	1.60	8 (21%)
4	DTD	B	505	-	8,8,8	1.26	1 (12%)	10,10,10	1.72	3 (30%)
6	GOL	B	506	-	5,5,5	0.32	0	5,5,5	0.31	0
7	ACT	B	507	-	1,3,3	0.76	0	0,3,3	0.00	-
7	ACT	B	508	-	1,3,3	1.46	0	0,3,3	0.00	-
6	GOL	B	509	-	5,5,5	0.31	0	5,5,5	0.54	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	BHN	A	504	2	-	0/21/21/21	0/2/2/2
4	DTD	A	505	-	-	0/0/11/11	0/1/1/1
6	GOL	A	507	-	-	0/4/4/4	0/0/0/0
6	GOL	A	508	-	-	0/4/4/4	0/0/0/0
6	GOL	A	509	-	-	0/4/4/4	0/0/0/0
6	GOL	A	510	-	-	0/4/4/4	0/0/0/0
7	ACT	A	511	-	-	0/0/0/0	0/0/0/0
7	ACT	A	512	-	-	0/0/0/0	0/0/0/0
7	ACT	A	513	-	-	0/0/0/0	0/0/0/0
7	ACT	A	514	-	-	0/0/0/0	0/0/0/0
7	ACT	A	515	-	-	0/0/0/0	0/0/0/0
7	ACT	A	516	-	-	0/0/0/0	0/0/0/0
8	SO4	A	517	-	-	0/0/0/0	0/0/0/0
6	GOL	A	518	-	-	0/4/4/4	0/0/0/0
6	GOL	A	519	-	-	0/4/4/4	0/0/0/0
6	GOL	A	520	-	-	0/4/4/4	0/0/0/0
6	GOL	A	521	-	-	0/4/4/4	0/0/0/0
6	GOL	A	522	-	-	0/4/4/4	0/0/0/0
6	GOL	A	523	-	-	0/4/4/4	0/0/0/0
6	GOL	A	524	-	-	0/4/4/4	0/0/0/0
3	BHN	B	504	2	-	0/21/21/21	0/2/2/2
4	DTD	B	505	-	-	0/0/11/11	0/1/1/1
6	GOL	B	506	-	-	0/4/4/4	0/0/0/0
7	ACT	B	507	-	-	0/0/0/0	0/0/0/0
7	ACT	B	508	-	-	0/0/0/0	0/0/0/0
6	GOL	B	509	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	505	DTD	C3-C2	3.09	1.56	1.52
4	A	505	DTD	C3-C2	2.26	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	504	BHN	C12-C13-C18	5.17	125.78	120.47
3	B	504	BHN	C7-C1-C6	4.61	125.21	120.47
3	A	504	BHN	C7-N8-C9	-3.85	102.93	111.20
3	A	504	BHN	C7-C1-C6	3.83	124.40	120.47
4	A	505	DTD	C4-S4-S1	3.75	102.54	98.70
3	A	504	BHN	C12-N11-C10	-3.39	103.91	111.20
3	A	504	BHN	C7-N8-C19	-3.27	105.79	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	504	BHN	C12-N11-C21	-3.12	106.09	112.58
3	A	504	BHN	C12-C13-C18	3.12	123.67	120.47
4	B	505	DTD	O3-C3-C4	-2.97	104.52	109.86
4	B	505	DTD	C1-S1-S4	2.97	101.73	98.70
4	A	505	DTD	C1-S1-S4	-2.94	95.68	98.70
3	B	504	BHN	C12-N11-C10	-2.84	105.10	111.20
3	A	504	BHN	C21-N11-C10	-2.75	105.45	112.34
4	B	505	DTD	C2-C1-S1	-2.34	109.34	112.61
3	B	504	BHN	C21-N11-C10	-2.28	106.62	112.34
3	B	504	BHN	C7-C1-C2	-2.28	115.60	120.19
3	B	504	BHN	C12-N11-C21	-2.28	107.83	112.58
3	A	504	BHN	C7-C1-C2	-2.27	115.61	120.19
3	B	504	BHN	C12-C13-C14	-2.26	115.65	120.19
4	A	505	DTD	O3-C3-C4	-2.03	106.21	109.86
3	B	504	BHN	C7-N8-C19	-2.02	108.38	112.58

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	499/502 (99%)	-0.09	8 (1%) 68 64	13, 21, 37, 50	0
1	B	498/502 (99%)	-0.02	22 (4%) 33 26	13, 25, 45, 55	3 (0%)
All	All	997/1004 (99%)	-0.05	30 (3%) 48 40	13, 23, 42, 55	3 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	6.3
1	B	3	PRO	5.1
1	A	3	PRO	4.7
1	B	329	GLY	4.3
1	B	58	GLU	4.1
1	A	500	VAL	3.9
1	A	442	HIS	3.9
1	B	125	ALA	3.8
1	B	337	GLY	3.8
1	B	328	ALA	3.7
1	A	58	GLU	3.7
1	B	327	PRO	3.6
1	B	60	GLY	3.5
1	B	113	LEU	3.4
1	B	338	GLN	3.4
1	A	382	TYR	3.3
1	B	336	ASN	3.1
1	B	108	VAL	3.1
1	A	175	TYR	3.0
1	B	57	SER	2.9
1	B	2	ALA	2.9
1	B	121	THR	2.7
1	B	442	HIS	2.6
1	B	112	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	330	LYS	2.4
1	A	329	GLY	2.3
1	B	331	ASP	2.3
1	B	382	TYR	2.1
1	B	499	PRO	2.0
1	B	339	PRO	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
6	GOL	A	509	6/6	0.22	32.00	55,55,55,56	0
6	GOL	A	524	6/6	0.33	15.79	29,34,35,36	0
7	ACT	A	516	4/4	0.29	14.70	44,44,44,45	0
6	GOL	B	509	6/6	0.30	11.80	47,48,49,50	0
6	GOL	A	522	6/6	0.42	10.64	44,46,47,50	0
7	ACT	A	511	4/4	0.21	8.91	34,36,36,36	0
6	GOL	B	506	6/6	0.23	7.78	59,60,61,62	0
6	GOL	A	510	6/6	0.22	7.21	45,48,49,50	0
7	ACT	A	514	4/4	0.19	6.95	44,45,45,45	0
7	ACT	A	513	4/4	0.15	6.66	40,40,40,40	0
6	GOL	A	507	6/6	0.29	6.64	47,51,51,52	0
5	CL	A	525	1/1	0.16	4.89	59,59,59,59	0
7	ACT	B	508	4/4	0.15	4.36	45,45,45,45	0
6	GOL	A	521	6/6	0.18	4.29	38,40,40,41	0
6	GOL	A	520	6/6	0.22	4.17	42,43,44,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	A	518	6/6	0.14	3.95	38,40,41,43	0
6	GOL	A	508	6/6	0.21	3.75	33,39,42,44	0
6	GOL	A	519	6/6	0.15	3.57	40,41,43,43	0
7	ACT	A	515	4/4	0.20	3.47	58,58,59,59	0
5	CL	A	526	1/1	0.18	2.86	58,58,58,58	0
4	DTD	A	505	8/8	0.14	2.28	22,25,25,30	0
6	GOL	A	523	6/6	0.17	2.26	35,37,40,43	0
3	BHN	A	504	28/28	0.15	1.44	22,31,35,36	0
7	ACT	B	507	4/4	0.12	1.28	43,43,43,44	0
7	ACT	A	512	4/4	0.18	1.25	61,61,61,61	0
5	CL	B	510	1/1	0.09	1.17	41,41,41,41	0
4	DTD	B	505	8/8	0.08	0.38	21,22,24,26	0
8	SO4	A	517	5/5	0.12	0.23	46,46,47,48	0
3	BHN	B	504	28/28	0.09	-0.47	19,26,32,32	0
5	CL	A	506	1/1	0.07	-1.28	68,68,68,68	0
2	FE	B	503	1/1	0.04	-	21,21,21,21	0
2	FE	A	503	1/1	0.08	-	27,27,27,27	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.