



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:20 pm GMT

PDB ID : 3MZ9  
Title : X-ray structure of NikA in complex with HBED  
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 : 1.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

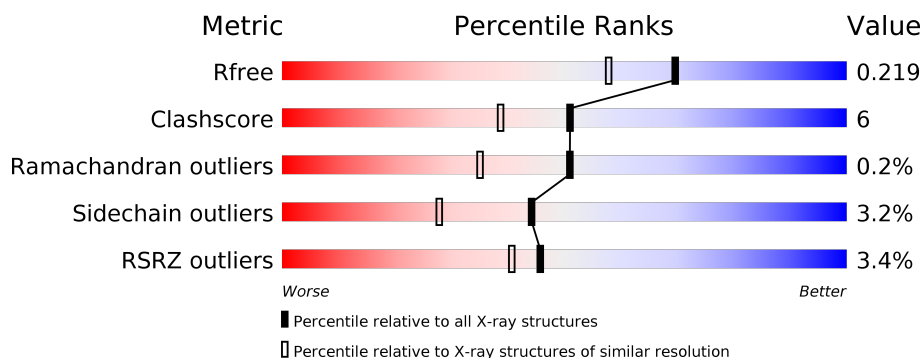
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	502	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	502	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>..</div> </div> </div>

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	DTD	A	505	-	-	-	X
5	CL	A	526	-	-	-	X
6	GOL	A	507	-	-	X	X
6	GOL	A	508	-	-	-	X
6	GOL	A	510	-	-	-	X
6	GOL	A	518	-	-	-	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	514	-	-	-	X
7	ACT	A	515	-	-	-	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 hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

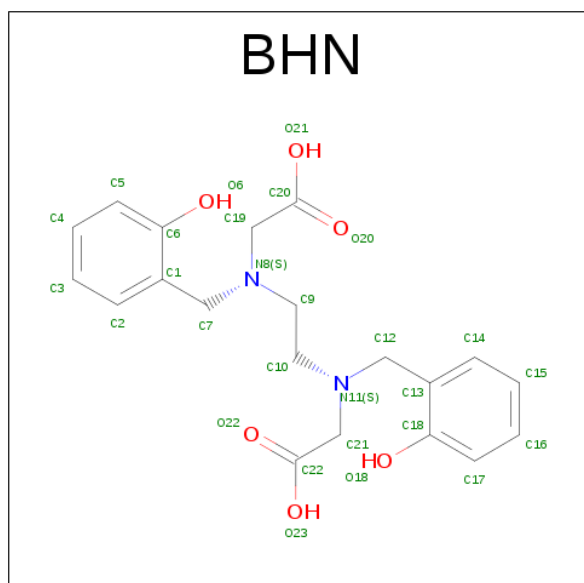
- Molecule 1 is a protein called Nickel-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	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).

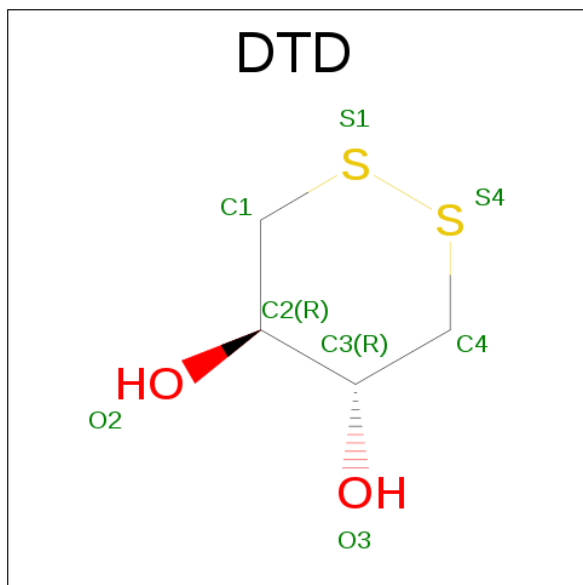
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 2-[2-[CARBOXYMETHYL-[(2-HYDROXYPHENYL)METHYL]AMINO]ETHYL-[(2-HYDROXYPHENYL)METHYL]AMINO]ETHANOIC ACID (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:  $C_3H_8O_3$ ).



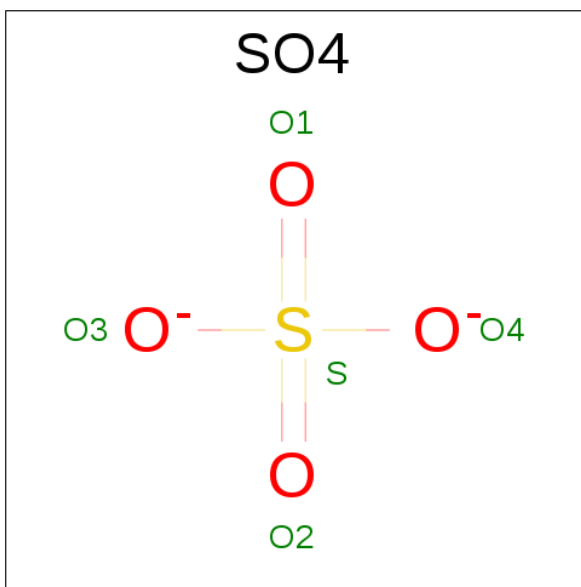
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total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

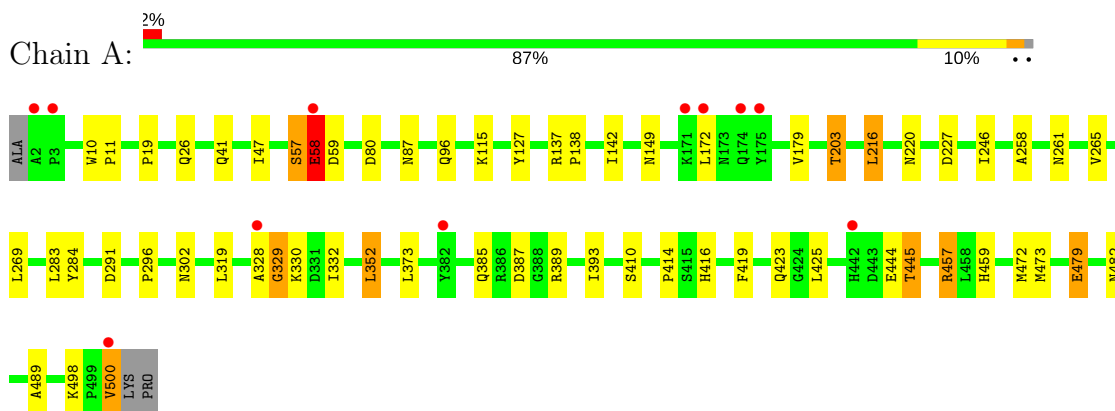
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	419	Total	O	0	0
			419	419		
9	B	343	Total	O	0	0
			343	343		



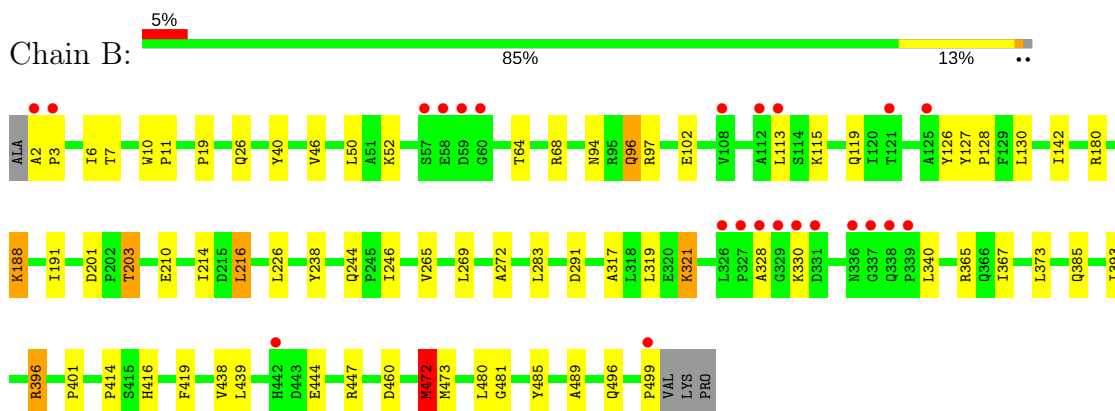
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: Nickel-binding periplasmic protein



#### • Molecule 1: Nickel-binding periplasmic protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(°)	Ideal(°)
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 Too-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 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	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

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 6.

All (104) 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: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	Interatomic distance (Å)	Clash overlap (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:115:LYS:HD3	6:A:522:GOL:H31	1.85	0.59
1:A:482:ASN:HD21	6:A:510:GOL:C1	2.15	0.59
1:B:180:ARG:HD2	1:B:188:LYS:HG3	1.87	0.56
1:A:10:TRP:HE1	1:A:26:GLN:NE2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:PRO:HB3	1:A:302:ASN:HD22	1.72	0.54
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:385:GLN:HG2	1:A:393:ILE:HD13	1.98	0.46
1:A:414:PRO:HA	1:A:419:PHE:CG	2.51	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:330:LYS:HG3	1:A:332:ILE:H	1.82	0.45
1:A:57:SER:OG	1:A:59:ASP:O	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	Interatomic distance (Å)	Clash overlap (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 [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	498/502 (99%)	482 (97%)	14 (3%)	2 (0%)	38	23
1	B	496/502 (99%)	482 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	994/1004 (99%)	964 (97%)	28 (3%)	2 (0%)	51 35

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%)	49 34
1	B	422/425 (99%)	407 (96%)	15 (4%)	40 23
All	All	846/850 (100%)	819 (97%)	27 (3%)	44 28

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

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Mol	Chain	Res	Type
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
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 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	23,29,29	0.45	0	32,38,38	1.76	8 (25%)
4	DTD	A	505	-	6,8,8	1.08	1 (16%)	6,10,10	1.14	1 (16%)
6	GOL	A	507	-	5,5,5	0.48	0	5,5,5	0.40	0
6	GOL	A	508	-	5,5,5	0.32	0	5,5,5	0.80	0
6	GOL	A	509	-	5,5,5	0.32	0	5,5,5	0.20	0
6	GOL	A	510	-	5,5,5	0.38	0	5,5,5	0.47	0
7	ACT	A	511	-	1,3,3	1.17	0	0,3,3	0.00	-
7	ACT	A	512	-	1,3,3	1.40	0	0,3,3	0.00	-
7	ACT	A	513	-	1,3,3	1.93	0	0,3,3	0.00	-
7	ACT	A	514	-	1,3,3	1.42	0	0,3,3	0.00	-
7	ACT	A	515	-	1,3,3	1.39	0	0,3,3	0.00	-
7	ACT	A	516	-	1,3,3	0.92	0	0,3,3	0.00	-
8	SO4	A	517	-	4,4,4	0.08	0	6,6,6	0.19	0
6	GOL	A	518	-	5,5,5	0.29	0	5,5,5	0.40	0
6	GOL	A	519	-	5,5,5	0.53	0	5,5,5	0.48	0
6	GOL	A	520	-	5,5,5	0.26	0	5,5,5	0.50	0
6	GOL	A	521	-	5,5,5	0.56	0	5,5,5	0.59	0
6	GOL	A	522	-	5,5,5	0.35	0	5,5,5	0.33	0
6	GOL	A	523	-	5,5,5	0.26	0	5,5,5	0.33	0
6	GOL	A	524	-	5,5,5	0.38	0	5,5,5	0.58	0
3	BHN	B	504	2	23,29,29	0.59	0	32,38,38	1.79	8 (25%)
4	DTD	B	505	-	6,8,8	1.40	1 (16%)	6,10,10	1.51	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	B	506	-	5,5,5	0.34	0	5,5,5	0.23	0
7	ACT	B	507	-	1,3,3	0.91	0	0,3,3	0.00	-
7	ACT	B	508	-	1,3,3	1.68	0	0,3,3	0.00	-
6	GOL	B	509	-	5,5,5	0.33	0	5,5,5	0.48	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	-	0/17/21/21	0/2/2/2
4	DTD	A	505	-	-	0/0/11/11	0/0/1/1
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	-	0/17/21/21	0/2/2/2
4	DTD	B	505	-	-	0/0/11/11	0/0/1/1
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	A	505	DTD	C3-C2	2.32	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	505	DTD	C3-C2	3.17	1.56	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	504	BHN	C7-N8-C9	-3.92	102.93	111.29
3	B	504	BHN	C20-C19-N8	-3.54	108.44	113.48
3	A	504	BHN	C12-N11-C10	-3.46	103.91	111.29
4	B	505	DTD	O3-C3-C4	-3.07	104.52	109.91
3	B	504	BHN	C12-N11-C10	-2.90	105.10	111.29
3	A	504	BHN	C19-N8-C7	-2.88	105.79	110.73
3	A	504	BHN	C21-N11-C10	-2.74	105.45	111.29
3	A	504	BHN	C21-N11-C12	-2.70	106.09	110.73
3	B	504	BHN	C7-C1-C2	-2.28	115.60	120.14
3	A	504	BHN	C7-C1-C2	-2.27	115.61	120.14
3	B	504	BHN	C12-C13-C14	-2.25	115.65	120.14
3	B	504	BHN	C21-N11-C10	-2.19	106.62	111.29
4	A	505	DTD	O3-C3-C4	-2.11	106.21	109.91
3	B	504	BHN	C22-C21-N11	-2.08	110.52	113.48
3	A	504	BHN	C12-C13-C18	3.26	123.67	120.45
3	A	504	BHN	C7-C1-C6	4.00	124.40	120.45
3	B	504	BHN	C7-C1-C6	4.82	125.21	120.45
3	B	504	BHN	C12-C13-C18	5.39	125.78	120.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	505	DTD	1	0
6	A	507	GOL	4	0
6	A	509	GOL	1	0
6	A	510	GOL	3	0
7	A	511	ACT	1	0
6	A	519	GOL	2	0
6	A	520	GOL	1	0
6	A	521	GOL	1	0
6	A	522	GOL	3	0
6	A	524	GOL	2	0
4	B	505	DTD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	509	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.08	11 (2%) 62 58	13, 21, 37, 50	0
1	B	498/502 (99%)	0.04	23 (4%) 33 28	13, 25, 45, 55	3 (0%)
All	All	997/1004 (99%)	-0.02	34 (3%) 46 41	13, 23, 42, 55	3 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	6.7
1	B	3	PRO	5.8
1	A	3	PRO	5.2
1	B	329	GLY	4.9
1	B	328	ALA	4.8
1	B	327	PRO	4.7
1	A	442	HIS	4.5
1	B	113	LEU	4.5
1	B	338	GLN	4.4
1	B	337	GLY	4.4
1	B	58	GLU	4.3
1	A	500	VAL	4.2
1	B	336	ASN	4.0
1	B	60	GLY	4.0
1	B	125	ALA	4.0
1	A	58	GLU	3.9
1	A	175	TYR	3.7
1	A	382	TYR	3.7
1	B	2	ALA	3.3
1	B	108	VAL	3.3
1	B	330	LYS	3.1
1	A	172	LEU	2.9
1	B	57	SER	2.9
1	B	442	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	326	LEU	2.7
1	B	499	PRO	2.7
1	B	331	ASP	2.6
1	B	112	ALA	2.5
1	B	339	PRO	2.4
1	B	121	THR	2.4
1	A	174	GLN	2.3
1	A	328	ALA	2.3
1	A	171	LYS	2.3
1	B	59	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	A	524	6/6	0.81	0.31	15.60	29,34,35,36	0
6	GOL	B	509	6/6	0.49	0.29	12.59	47,48,49,50	0
6	GOL	A	522	6/6	0.61	0.45	10.83	44,46,47,50	0
7	ACT	A	514	4/4	0.73	0.22	10.53	44,45,45,45	0
6	GOL	A	507	6/6	0.83	0.32	9.59	47,51,51,52	0
7	ACT	A	511	4/4	0.71	0.20	9.23	34,36,36,36	0
6	GOL	B	506	6/6	0.78	0.23	8.53	59,60,61,62	0
6	GOL	A	510	6/6	0.69	0.24	6.04	45,48,49,50	0
6	GOL	A	521	6/6	0.80	0.21	5.76	38,40,40,41	0
6	GOL	A	520	6/6	0.81	0.22	4.89	42,43,44,45	0
5	CL	A	526	1/1	0.93	0.21	4.70	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	ACT	A	515	4/4	0.69	0.23	4.55	58,58,59,59	0
6	GOL	A	508	6/6	0.80	0.21	3.72	33,39,42,44	0
7	ACT	B	508	4/4	0.84	0.14	3.60	45,45,45,45	0
6	GOL	A	518	6/6	0.80	0.15	3.35	38,40,41,43	0
6	GOL	A	523	6/6	0.81	0.19	2.90	35,37,40,43	0
4	DTD	A	505	8/8	0.90	0.15	2.13	22,25,25,30	0
4	DTD	B	505	8/8	0.97	0.09	1.29	21,22,24,26	0
8	SO4	A	517	5/5	0.95	0.14	1.07	46,46,47,48	0
7	ACT	B	507	4/4	0.90	0.12	1.03	43,43,43,44	0
3	BHN	A	504	28/28	0.93	0.14	0.85	22,31,35,36	0
3	BHN	B	504	28/28	0.96	0.09	-0.40	19,26,32,32	0
7	ACT	A	512	4/4	0.82	0.21	-	61,61,61,61	0
5	CL	A	525	1/1	0.94	0.16	-	59,59,59,59	0
6	GOL	A	519	6/6	0.88	0.15	-	40,41,43,43	0
5	CL	B	510	1/1	0.96	0.08	-	41,41,41,41	0
2	FE	A	503	1/1	0.98	0.08	-	27,27,27,27	0
6	GOL	A	509	6/6	0.79	0.23	-	55,55,55,56	0
7	ACT	A	513	4/4	0.91	0.15	-	40,40,40,40	0
5	CL	A	506	1/1	0.84	0.07	-	68,68,68,68	0
2	FE	B	503	1/1	0.99	0.05	-	21,21,21,21	0
7	ACT	A	516	4/4	0.84	0.26	-	44,44,44,45	0

## 6.5 Other polymers

There are no such residues in this entry.