



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:31 AM EST

PDB ID : 5MWU  
Title : Crystal structure of the periplasmic nickel-binding protein NikA from Escherichia coli in complex with Ru(bpza)(CO)<sub>2</sub>Cl  
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Deposited on : 2017-01-20  
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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	rb-20028442

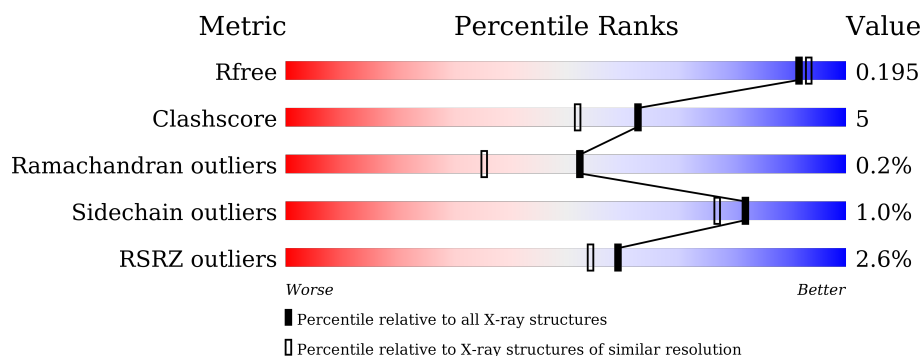
## 1 Overall quality at a glance

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 <sub>free</sub>	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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>89% 9% ..</div>
1	B	502	 <div>5% 92% 7% .</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
2	ACT	A	603	-	-	-	X
2	ACT	B	601	-	-	-	X
2	ACT	B	613	-	-	X	X
4	GOL	A	605	-	-	-	X
4	GOL	A	607	-	-	-	X
4	GOL	A	613	-	-	-	X
4	GOL	A	616	-	-	-	X
4	GOL	B	602	-	-	-	X
4	GOL	B	603	-	-	-	X
4	GOL	B	611	-	-	-	X
4	GOL	B	614	-	-	X	X

## 2 Entry composition [i](#)

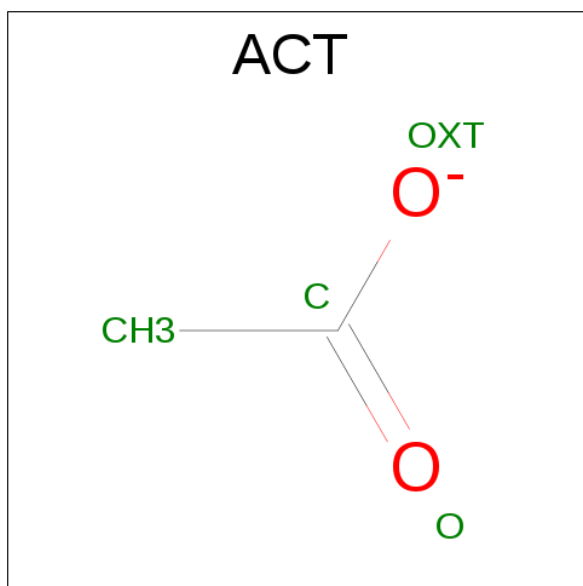
There are 11 unique types of molecules in this entry. The entry contains 8823 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	498	Total	C	N	O	S	0	18	0
			4031	2590	673	754	14			
1	B	498	Total	C	N	O	S	0	13	0
			3967	2554	660	741	12			

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



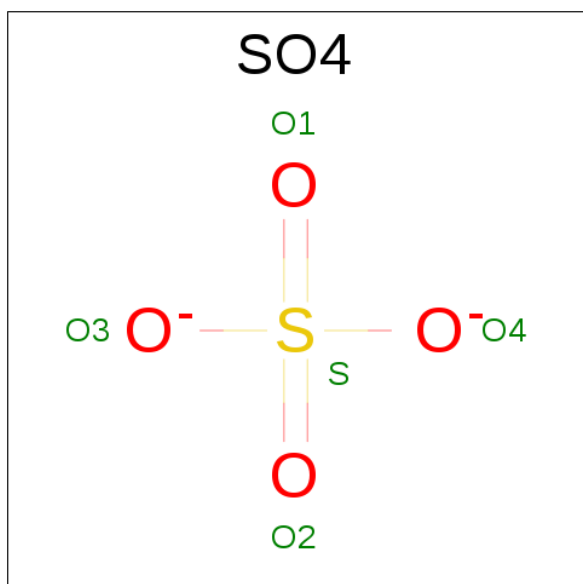
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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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>).

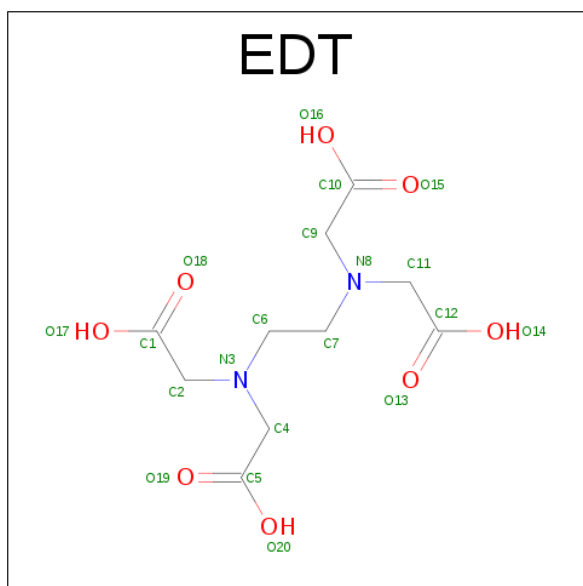


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total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

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe		0	0
			1	1			

- Molecule 6 is {[-(BIS-CARBOXYMETHYL-AMINO)-ETHYL]-CARBOXYMETHYL-AMINO}-ACETIC ACID (three-letter code: EDT) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			20	10	2	8		

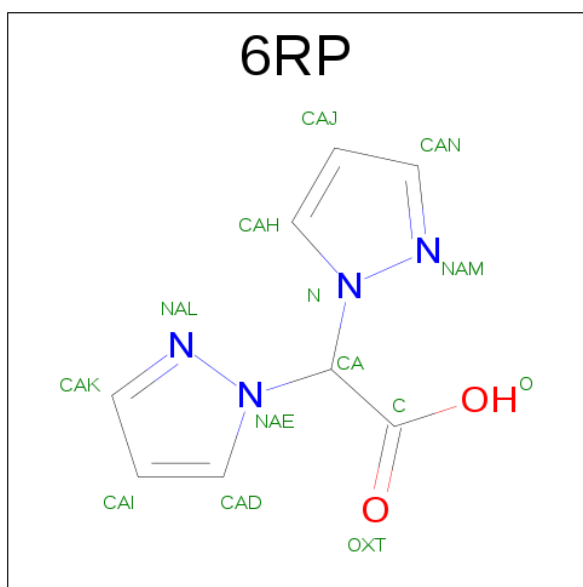
- Molecule 7 is RUTHENIUM ION (three-letter code: RU) (formula: Ru).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ru	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

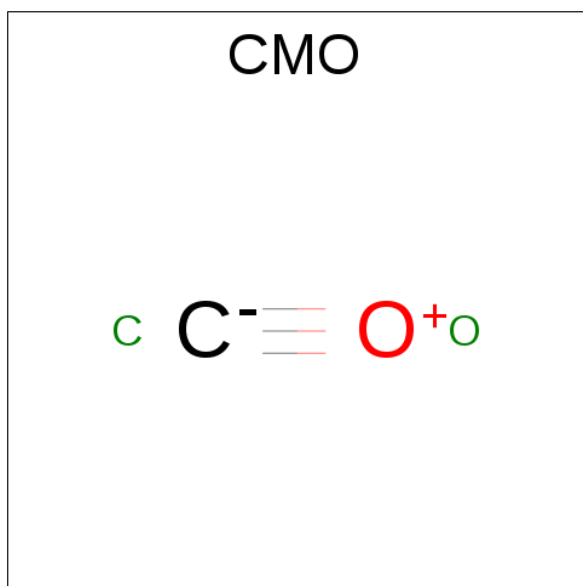
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Cl	0	0
			2	2		

- Molecule 9 is bis(pyrzol-1-yl)acetate scorpionate (three-letter code: 6RP) (formula: C<sub>8</sub>H<sub>8</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			14	8	4	2		

- Molecule 10 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



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

- Molecule 11 is water.

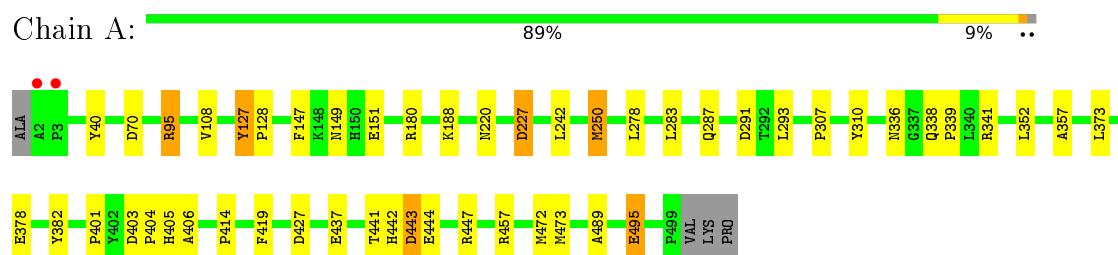


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	365	Total 365	O 365	0	0
11	B	301	Total 301	O 301	0	0

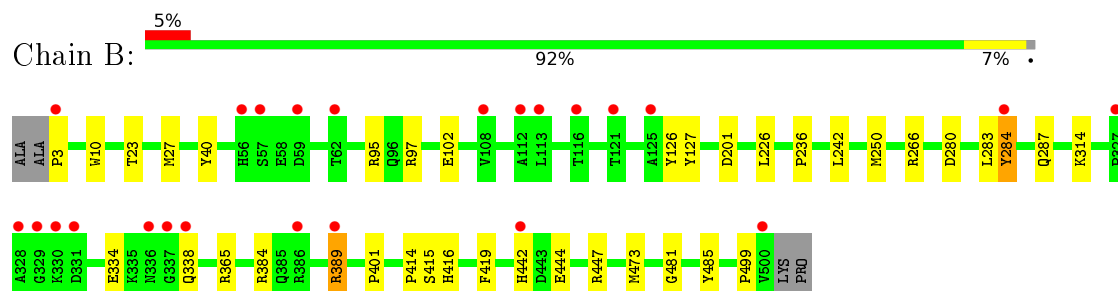
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	86.30Å 93.61Å 124.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.80 – 1.80 46.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.80-1.80) 98.8 (46.80-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	5.70	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.168 , 0.208 0.179 , 0.195	Depositor DCC
$R_{free}$ test set	4628 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CMO, GOL, 6RP, RU, CL, FE, EDT, 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	1.01	2/4187 (0.0%)	0.96	9/5701 (0.2%)
1	B	0.99	2/4105 (0.0%)	0.92	6/5599 (0.1%)
All	All	1.00	4/8292 (0.0%)	0.94	15/11300 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	389[A]	ARG	C-O	10.38	1.43	1.23
1	B	389[B]	ARG	C-O	10.38	1.43	1.23
1	A	310	TYR	CD1-CE1	-5.57	1.31	1.39
1	A	495	GLU	CD-OE1	5.51	1.31	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	A	95	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	B	27	MET	CG-SD-CE	-7.45	88.29	100.20
1	B	201	ASP	CB-CG-OD1	5.88	123.60	118.30
1	B	97	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	95	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	227	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	151[A]	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	A	151[B]	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	A	70	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	443	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	266	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	447	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	147	PHE	CB-CG-CD1	5.09	124.36	120.80
1	B	365	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	4031	0	3999	45	0
1	B	3967	0	3892	38	0
2	A	28	0	21	1	0
2	B	12	0	9	2	0
3	A	5	0	0	0	0
4	A	42	0	56	3	0
4	B	30	0	40	12	0
5	A	1	0	0	0	0
6	A	20	0	12	0	0
7	B	1	0	0	0	0
8	B	2	0	0	0	0
9	B	14	0	0	0	0
10	B	4	0	0	0	0
11	A	365	0	0	9	0
11	B	301	0	0	9	0
All	All	8823	0	8029	86	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (86) 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)
4:B:604:GOL:H31	11:B:706:HOH:O	1.23	1.35
1:B:314:LYS:NZ	4:B:614:GOL:H2	1.93	0.82
1:B:242:LEU:HD12	1:B:473[B]:MET:SD	2.22	0.80
1:A:341:ARG:NH1	11:A:701:HOH:O	2.16	0.77
1:A:472[B]:MET:CE	11:A:1001:HOH:O	2.32	0.77
1:A:472[B]:MET:HE2	11:A:1001:HOH:O	1.84	0.77
1:B:314:LYS:HZ3	4:B:614:GOL:H2	1.51	0.75
1:B:23[B]:THR:HG23	11:B:920:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LEU:CD1	1:B:473[B]:MET:SD	2.76	0.73
1:A:442[B]:HIS:CD2	1:A:443:ASP:H	2.07	0.72
1:B:287:GLN:HE22	1:B:473[B]:MET:CE	2.04	0.71
1:A:287:GLN:HE22	1:A:473[B]:MET:CE	2.04	0.70
1:A:149:ASN:ND2	2:A:611:ACT:H3	2.08	0.69
1:A:442[B]:HIS:HD2	1:A:443:ASP:H	1.42	0.66
4:B:604:GOL:C3	11:B:706:HOH:O	2.04	0.65
1:A:242:LEU:CD1	1:A:473[B]:MET:SD	2.85	0.65
1:B:485:TYR:HB3	4:B:602:GOL:H11	1.78	0.64
1:B:23[B]:THR:HG22	2:B:613:ACT:OXT	1.98	0.62
1:B:314:LYS:HZ3	4:B:614:GOL:C2	2.12	0.62
1:A:336:ASN:N	11:A:705:HOH:O	2.31	0.62
1:A:287:GLN:HE22	1:A:473[B]:MET:HE3	1.65	0.61
1:B:287:GLN:HE22	1:B:473[B]:MET:HE3	1.64	0.61
1:A:95:ARG:HD3	11:A:876:HOH:O	2.01	0.59
1:A:242:LEU:HD12	1:A:473[B]:MET:SD	2.42	0.59
1:B:314:LYS:HZ3	4:B:614:GOL:H31	1.68	0.58
1:B:416:HIS:HB2	11:B:833:HOH:O	2.03	0.57
1:B:314:LYS:HZ1	4:B:614:GOL:H2	1.69	0.56
1:A:283[B]:LEU:HD12	1:A:352:LEU:HD11	1.87	0.56
1:B:280:ASP:O	1:B:284[B]:TYR:HA	2.06	0.55
1:B:414:PRO:O	1:B:415:SER:CB	2.53	0.54
1:B:314:LYS:HZ3	4:B:614:GOL:C3	2.21	0.53
1:A:414:PRO:HA	1:A:419:PHE:CG	2.43	0.53
1:B:287:GLN:NE2	1:B:473[B]:MET:HE3	2.23	0.53
1:A:220:ASN:HB3	4:A:605:GOL:H11	1.91	0.52
1:B:23[B]:THR:HG23	11:B:951:HOH:O	2.08	0.52
4:B:614:GOL:O3	11:B:701:HOH:O	1.97	0.52
1:A:378:GLU:HG2	1:A:382:TYR:CE2	2.45	0.51
1:B:416:HIS:CB	11:B:833:HOH:O	2.57	0.51
1:B:444:GLU:OE1	1:B:447:ARG:NH1	2.44	0.51
1:B:10:TRP:CZ3	4:B:603:GOL:H31	2.47	0.50
1:A:472[A]:MET:HG3	11:A:1001:HOH:O	2.10	0.50
1:B:414:PRO:HA	1:B:419:PHE:CD2	2.47	0.49
1:A:338:GLN:NE2	1:A:339:PRO:HD2	2.28	0.49
1:A:283[B]:LEU:CD1	1:A:352:LEU:HD11	2.42	0.49
1:A:40:TYR:CE1	1:A:401:PRO:HB3	2.47	0.49
2:B:613:ACT:H1	11:B:951:HOH:O	2.12	0.49
1:B:23[B]:THR:CG2	11:B:951:HOH:O	2.60	0.48
1:A:227:ASP:OD2	4:A:607:GOL:H12	2.14	0.47
1:A:278:LEU:C	1:A:278:LEU:HD23	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ASP:HB3	1:A:307:PRO:HB3	1.97	0.47
1:A:180:ARG:HD2	1:A:188:LYS:HG2	1.97	0.47
1:A:250[B]:MET:SD	1:A:293:LEU:CD1	3.03	0.47
1:A:287:GLN:NE2	1:A:473[B]:MET:HE3	2.31	0.45
1:B:40:TYR:CE1	1:B:401:PRO:HB3	2.51	0.45
1:A:437:GLU:OE1	11:A:702:HOH:O	2.20	0.45
1:B:287:GLN:NE2	1:B:473[B]:MET:CE	2.76	0.45
4:A:613:GOL:H32	11:A:759:HOH:O	2.16	0.44
1:A:427:ASP:OD2	1:A:457:ARG:NH1	2.51	0.44
1:A:442[B]:HIS:CD2	1:A:442[B]:HIS:H	2.32	0.44
1:B:102:GLU:HB3	1:B:126:TYR:OH	2.18	0.44
1:B:334:GLU:HA	1:B:338:GLN:O	2.17	0.44
1:B:384:ARG:NH1	1:B:389[B]:ARG:HD2	2.33	0.44
1:A:441:THR:OG1	1:A:442[B]:HIS:CD2	2.71	0.44
1:A:180:ARG:HD2	1:A:188:LYS:CG	2.49	0.43
1:A:489:ALA:HB3	11:A:901:HOH:O	2.19	0.43
1:A:414:PRO:HA	1:A:419:PHE:CD1	2.54	0.43
1:A:441:THR:OG1	1:A:442[B]:HIS:HD2	2.00	0.42
1:A:405:HIS:CG	1:A:406:ALA:N	2.87	0.42
1:A:287:GLN:HE22	1:A:473[B]:MET:HE1	1.84	0.42
1:A:378:GLU:CG	1:A:382:TYR:CE2	3.02	0.42
1:A:403:ASP:HA	1:A:404:PRO:HA	1.87	0.42
1:B:242:LEU:HD11	1:B:473[B]:MET:SD	2.59	0.42
1:A:357:ALA:HB1	1:A:373:LEU:HD22	2.02	0.42
1:A:444:GLU:HG2	1:B:481:GLY:HA2	2.01	0.42
1:A:495:GLU:CD	1:A:495:GLU:H	2.24	0.41
1:A:127:TYR:N	1:A:128:PRO:CD	2.84	0.41
1:B:314:LYS:NZ	4:B:614:GOL:C2	2.70	0.41
1:A:283[A]:LEU:HD13	1:A:352:LEU:HD11	2.03	0.41
1:B:226:LEU:HD12	1:B:283:LEU:HA	2.03	0.41
1:B:473[A]:MET:HB3	1:B:473[A]:MET:HE3	1.70	0.40
1:A:444:GLU:CG	1:B:481:GLY:HA2	2.52	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	514/502 (102%)	499 (97%)	15 (3%)	0	100	100
1	B	507/502 (101%)	492 (97%)	12 (2%)	3 (1%)	30	14
All	All	1021/1004 (102%)	991 (97%)	27 (3%)	3 (0%)	52	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	284[A]	TYR
1	B	284[B]	TYR
1	B	499	PRO

### 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	435/425 (102%)	431 (99%)	4 (1%)	84	80
1	B	419/425 (99%)	413 (99%)	6 (1%)	74	65
All	All	854/850 (100%)	844 (99%)	10 (1%)	82	71

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	VAL
1	A	127	TYR
1	A	250[A]	MET
1	A	250[B]	MET
1	B	3	PRO
1	B	127	TYR
1	B	236	PRO
1	B	250[A]	MET
1	B	250[B]	MET

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Mol	Chain	Res	Type
1	B	442	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	A	174	GLN
1	A	302	ASN
1	A	338	GLN
1	A	416	HIS
1	A	482	ASN
1	B	423	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 4 are monoatomic - leaving 27 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	601	-	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ACT	A	602	-	0,3,3	0.00	-	0,3,3	0.00	-
2	ACT	A	603	-	0,3,3	0.00	-	0,3,3	0.00	-
3	SO4	A	604	-	4,4,4	0.64	0	6,6,6	0.54	0
4	GOL	A	605	-	5,5,5	0.67	0	5,5,5	0.58	0
4	GOL	A	606	-	5,5,5	0.60	0	5,5,5	1.21	0
4	GOL	A	607	-	5,5,5	0.72	0	5,5,5	0.54	0
6	EDT	A	609	5	7,19,19	0.57	0	12,24,24	1.78	2 (16%)
2	ACT	A	610	-	0,3,3	0.00	-	0,3,3	0.00	-
2	ACT	A	611	-	0,3,3	0.00	-	0,3,3	0.00	-
2	ACT	A	612	-	0,3,3	0.00	-	0,3,3	0.00	-
4	GOL	A	613	-	5,5,5	0.91	0	5,5,5	1.30	1 (20%)
4	GOL	A	614	-	5,5,5	0.54	0	5,5,5	0.73	0
4	GOL	A	615	-	5,5,5	0.29	0	5,5,5	0.67	0
4	GOL	A	616	-	5,5,5	0.31	0	5,5,5	0.79	0
2	ACT	A	617	-	0,3,3	0.00	-	0,3,3	0.00	-
2	ACT	B	601	-	0,3,3	0.00	-	0,3,3	0.00	-
4	GOL	B	602	-	5,5,5	0.49	0	5,5,5	1.16	0
4	GOL	B	603	-	5,5,5	0.93	0	5,5,5	1.44	0
4	GOL	B	604	-	5,5,5	0.51	0	5,5,5	0.69	0
2	ACT	B	605	-	0,3,3	0.00	-	0,3,3	0.00	-
9	6RP	B	608	7	12,15,15	3.07	5 (41%)	7,20,20	3.01	5 (71%)
10	CMO	B	609	-	0,1,1	0.00	-	0,0,0	0.00	-
10	CMO	B	610	-	0,1,1	0.00	-	0,0,0	0.00	-
4	GOL	B	611	-	5,5,5	0.35	0	5,5,5	0.52	0
2	ACT	B	613	-	0,3,3	0.00	-	0,3,3	0.00	-
4	GOL	B	614	-	5,5,5	1.19	0	5,5,5	1.05	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
2	ACT	A	601	-	-	0/0/0/0	0/0/0/0
2	ACT	A	602	-	-	0/0/0/0	0/0/0/0
2	ACT	A	603	-	-	0/0/0/0	0/0/0/0
3	SO4	A	604	-	-	0/0/0/0	0/0/0/0
4	GOL	A	605	-	-	0/4/4/4	0/0/0/0
4	GOL	A	606	-	-	0/4/4/4	0/0/0/0
4	GOL	A	607	-	-	0/4/4/4	0/0/0/0
6	EDT	A	609	5	-	0/13/21/21	0/0/0/0
2	ACT	A	610	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACT	A	611	-	-	0/0/0/0	0/0/0/0
2	ACT	A	612	-	-	0/0/0/0	0/0/0/0
4	GOL	A	613	-	-	0/4/4/4	0/0/0/0
4	GOL	A	614	-	-	0/4/4/4	0/0/0/0
4	GOL	A	615	-	-	0/4/4/4	0/0/0/0
4	GOL	A	616	-	-	0/4/4/4	0/0/0/0
2	ACT	A	617	-	-	0/0/0/0	0/0/0/0
2	ACT	B	601	-	-	0/0/0/0	0/0/0/0
4	GOL	B	602	-	-	0/4/4/4	0/0/0/0
4	GOL	B	603	-	-	0/4/4/4	0/0/0/0
4	GOL	B	604	-	-	0/4/4/4	0/0/0/0
2	ACT	B	605	-	-	0/0/0/0	0/0/0/0
9	6RP	B	608	7	-	0/2/12/12	0/2/2/2
10	CMO	B	609	-	-	0/0/0/0	0/0/0/0
10	CMO	B	610	-	-	0/0/0/0	0/0/0/0
4	GOL	B	611	-	-	0/4/4/4	0/0/0/0
2	ACT	B	613	-	-	0/0/0/0	0/0/0/0
4	GOL	B	614	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	608	6RP	NAL-NAE	-8.88	1.24	1.35
9	B	608	6RP	CAD-NAE	-3.38	1.31	1.35
9	B	608	6RP	CAD-CAI	-2.28	1.32	1.38
9	B	608	6RP	CAN-NAM	-2.27	1.29	1.33
9	B	608	6RP	CAJ-CAN	-2.09	1.32	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	609	EDT	C6-C7-N8	-3.42	104.61	113.13
6	A	609	EDT	C5-C4-N3	-3.40	108.49	113.53
9	B	608	6RP	CAI-CAK-NAL	-3.06	104.43	111.47
9	B	608	6RP	CAJ-CAN-NAM	-2.76	105.10	111.47
9	B	608	6RP	CAH-CAJ-CAN	2.42	110.40	105.30
4	A	613	GOL	O2-C2-C3	2.48	120.35	108.47
9	B	608	6RP	CA-NAE-NAL	3.34	128.34	119.38
9	B	608	6RP	CA-N-NAM	5.31	133.64	119.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	GOL	1	0
4	A	607	GOL	1	0
2	A	611	ACT	1	0
4	A	613	GOL	1	0
4	B	602	GOL	1	0
4	B	603	GOL	1	0
4	B	604	GOL	2	0
2	B	613	ACT	2	0
4	B	614	GOL	8	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	498/502 (99%)	-0.28	2 (0%) 93 91	15, 23, 41, 62	0
1	B	498/502 (99%)	-0.14	24 (4%) 34 28	15, 26, 48, 77	0
All	All	996/1004 (99%)	-0.21	26 (2%) 59 54	15, 24, 44, 77	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	500	VAL	6.1
1	A	2	ALA	4.8
1	A	3	PRO	4.3
1	B	328	ALA	4.1
1	B	125	ALA	3.5
1	B	442	HIS	3.5
1	B	57	SER	3.5
1	B	59	ASP	3.0
1	B	284[A]	TYR	3.0
1	B	330	LYS	3.0
1	B	121	THR	2.7
1	B	3	PRO	2.7
1	B	337	GLY	2.7
1	B	329	GLY	2.6
1	B	331	ASP	2.6
1	B	327	PRO	2.5
1	B	116	THR	2.4
1	B	112	ALA	2.4
1	B	113	LEU	2.3
1	B	62	THR	2.3
1	B	336	ASN	2.3
1	B	389[A]	ARG	2.2
1	B	386	ARG	2.2
1	B	338	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	56	HIS	2.1
1	B	108	VAL	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no 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
2	ACT	B	601	4/4	0.40	0.27	35.06	43,59,59,61	0
2	ACT	B	613	4/4	0.93	0.14	14.91	45,46,50,56	0
4	GOL	B	602	6/6	0.80	0.21	5.84	37,50,54,64	0
4	GOL	B	611	6/6	0.64	0.34	5.74	53,60,63,65	0
4	GOL	A	616	6/6	0.85	0.18	5.68	46,53,55,60	0
4	GOL	A	613	6/6	0.86	0.16	5.19	35,46,46,58	0
4	GOL	B	603	6/6	0.89	0.14	4.61	31,42,45,53	0
4	GOL	B	614	6/6	0.76	0.26	3.46	28,32,34,34	0
2	ACT	A	603	4/4	0.86	0.12	2.75	31,35,41,43	0
4	GOL	A	607	6/6	0.73	0.19	2.52	47,52,54,55	0
4	GOL	A	605	6/6	0.88	0.19	2.11	25,41,47,52	0
2	ACT	A	610	4/4	0.92	0.12	1.63	36,43,44,48	0
4	GOL	A	606	6/6	0.89	0.15	1.36	27,38,42,43	0
3	SO4	A	604	5/5	0.96	0.15	1.15	53,56,58,59	0
4	GOL	B	604	6/6	0.96	0.10	0.83	22,31,32,36	0
9	6RP	B	608	14/14	0.97	0.08	-0.27	19,28,32,33	0
6	EDT	A	609	20/20	0.95	0.09	-0.59	21,27,31,33	0
7	RU	B	606	1/1	0.99	0.03	-	28,28,28,28	0
4	GOL	A	614	6/6	0.50	0.31	-	61,74,79,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
10	CMO	B	609	2/2	0.98	0.14	-	34,34,34,42	0
2	ACT	A	611	4/4	0.95	0.14	-	39,48,52,58	0
2	ACT	A	602	4/4	0.96	0.13	-	33,35,42,50	0
2	ACT	A	612	4/4	0.84	0.10	-	43,54,55,62	0
2	ACT	A	601	4/4	0.83	0.17	-	48,49,59,62	0
8	CL	B	612	1/1	0.95	0.11	-	46,46,46,46	0
5	FE	A	608	1/1	1.00	0.09	-	23,23,23,23	0
2	ACT	A	617	4/4	0.94	0.17	-	27,31,32,32	0
10	CMO	B	610	2/2	0.88	0.20	-	32,32,32,39	2
8	CL	B	607	1/1	0.93	0.09	-	42,42,42,42	0
2	ACT	B	605	4/4	0.88	0.18	-	54,65,68,79	0
4	GOL	A	615	6/6	0.53	0.32	-	57,65,71,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.