



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 04:55 PM BST

PDB ID : 4I8C  
Title : X-ray structure of NikA in complex with Ni-(L-His)<sub>2</sub>  
Authors : Lebrette, H.; Iannello, M.; Fontecilla-Camps, J.C.; Cavazza, C.  
Deposited on : 2012-12-03  
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

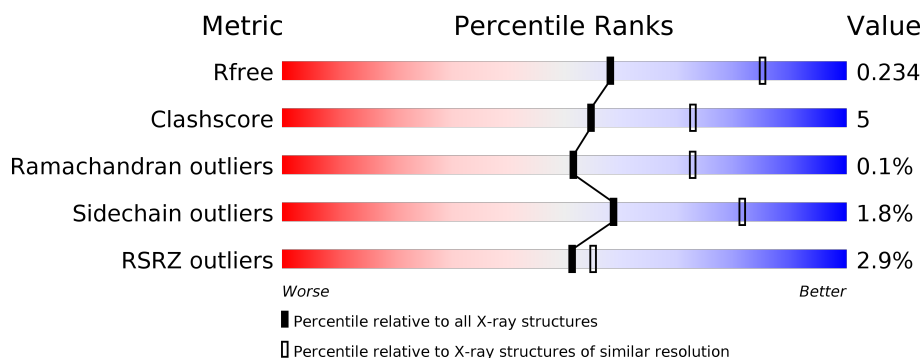
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 respectively. 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	
1	B	502	
1	C	502	

## 2 Entry composition [i](#)

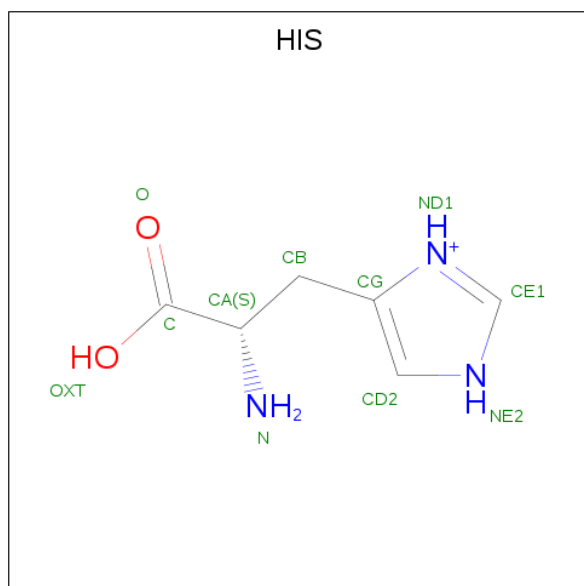
There are 8 unique types of molecules in this entry. The entry contains 12432 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	3	3	0
			3982	2552	672	748	10			
1	B	499	Total	C	N	O	S	3	2	0
			3982	2551	674	747	10			
1	C	496	Total	C	N	O	S	24	1	0
			3947	2528	667	742	10			

- Molecule 2 is HISTIDINE (three-letter code: HIS) (formula: C<sub>6</sub>H<sub>10</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	3	2		
2	A	1	Total	C	N	O	0	0
			11	6	3	2		
2	B	1	Total	C	N	O	0	0
			11	6	3	2		

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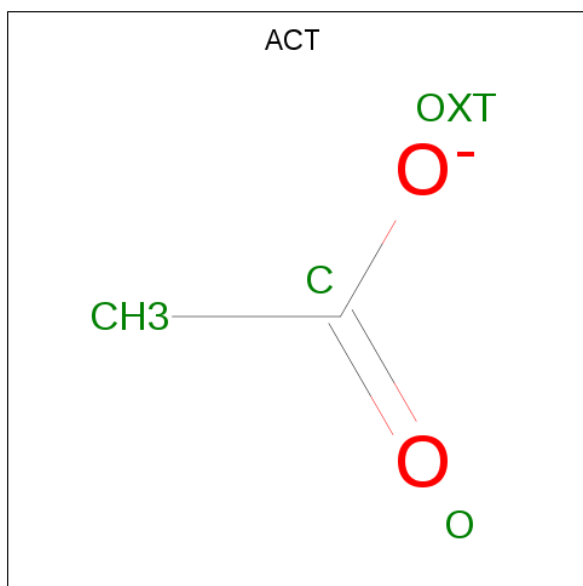
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			11	6	3	2		
2	C	1	Total	C	N	O	0	0
			11	6	3	2		
2	C	1	Total	C	N	O	0	0
			11	6	3	2		

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 4 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
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 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
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		

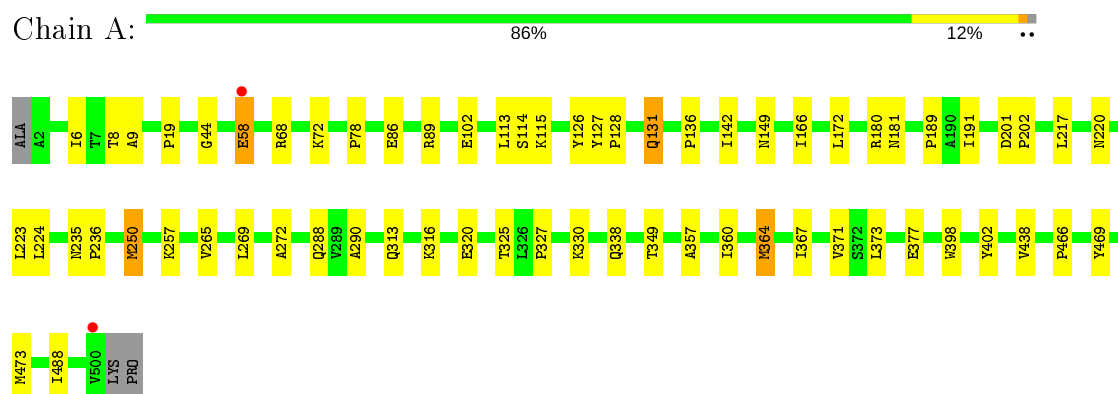
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	148	Total	O	0	0
			148	148		
8	B	125	Total	O	0	0
			125	125		
8	C	56	Total	O	0	0
			56	56		

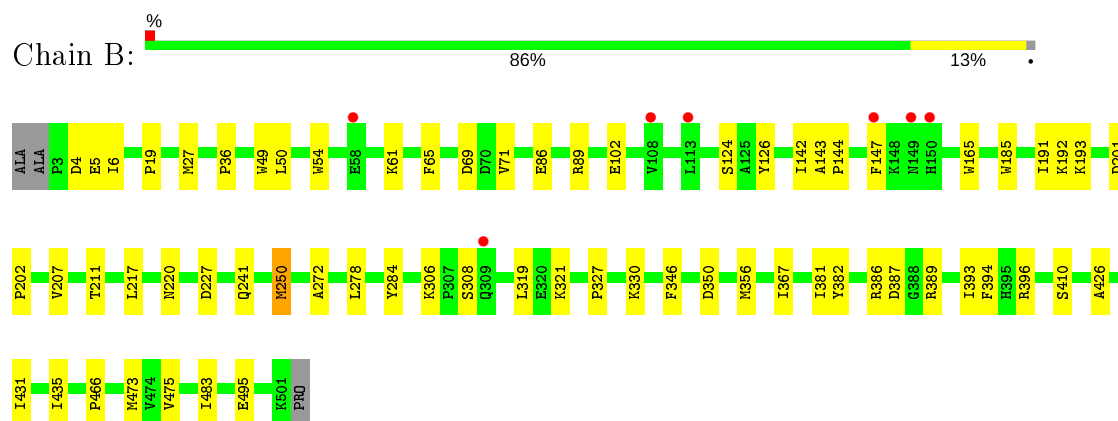
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

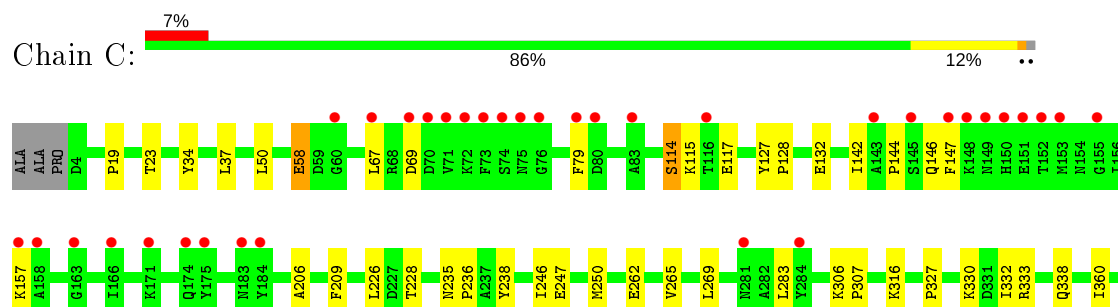
#### • Molecule 1: Nickel-binding periplasmic protein



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







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.63Å 158.63Å 135.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.50 – 2.50 48.50 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.50-2.50) 99.6 (48.50-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.41 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.189 , 0.234 0.189 , 0.234	Depositor DCC
$R_{free}$ test set	3327 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.8	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: ACT, GOL, CL, SO4, NI

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	0.45	0/4089	0.56	0/5570
1	B	0.45	0/4086	0.56	0/5564
1	C	0.38	0/4050	0.51	0/5517
All	All	0.43	0/12225	0.54	0/16651

There are no bond length outliers.

There are no bond angle outliers.

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	3982	0	3932	41	0
1	B	3982	0	3933	42	0
1	C	3947	0	3891	38	0
2	A	22	0	12	0	0
2	B	22	0	12	4	0
2	C	22	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	28	0	21	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	18	0	0
4	C	12	0	9	1	0
5	A	18	0	24	3	0
5	B	18	0	24	0	0
5	C	12	0	16	3	0
6	B	1	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
8	A	148	0	0	2	0
8	B	125	0	0	1	0
8	C	56	0	0	1	0
All	All	12432	0	11904	124	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 (124) 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:C:409:SER:HB2	1:C:439:LEU:HD11	1.67	0.76
1:A:250:MET:HB3	1:A:466:PRO:HA	1.66	0.76
1:A:220:ASN:H	5:A:611:GOL:H32	1.53	0.72
1:B:165:TRP:HE1	1:B:495[B]:GLU:HG3	1.59	0.67
1:B:327:PRO:HG2	1:B:330:LYS:HB2	1.77	0.66
1:C:438:VAL:HG12	1:C:447:ARG:HG3	1.77	0.65
1:C:114:SER:OG	1:C:115:LYS:N	2.30	0.64
1:C:373:LEU:H	5:C:607:GOL:H32	1.65	0.62
1:B:217:LEU:HB2	1:B:475:VAL:HG12	1.82	0.62
1:B:5:GLU:HG2	1:B:193:LYS:HB3	1.81	0.61
1:A:327:PRO:HG2	1:A:330:LYS:HB2	1.81	0.60
1:A:86:GLU:OE1	1:A:89:ARG:NH2	2.24	0.60
1:B:86:GLU:OE1	1:B:89:ARG:NH2	2.26	0.57
1:B:6:ILE:HD13	1:B:191:ILE:HD13	1.86	0.57
1:C:19:PRO:HG3	1:C:34:TYR:CZ	2.39	0.57
1:B:250:MET:HB2	1:B:466:PRO:HA	1.87	0.57
1:C:262:GLU:HG2	5:C:608:GOL:H11	1.88	0.56
1:B:220:ASN:HD22	1:B:396:ARG:NH1	2.02	0.56
1:C:246:ILE:HG13	1:C:247:GLU:HG2	1.89	0.55
1:C:364:MET:HG3	1:C:371:VAL:HG21	1.88	0.55
1:C:19:PRO:HG2	1:C:142:ILE:HB	1.88	0.54
1:A:360:ILE:O	1:A:364:MET:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLY:O	1:A:131:GLN:NE2	2.41	0.53
1:A:19:PRO:HG3	1:A:142:ILE:HB	1.89	0.53
1:A:136:PRO:HD3	1:A:488:ILE:HD13	1.89	0.53
1:C:360:ILE:O	1:C:364:MET:HG2	2.09	0.53
1:A:217:LEU:HB3	1:A:223:LEU:HD21	1.91	0.52
1:C:209:PHE:HE1	1:C:238:TYR:CD1	2.28	0.52
1:A:220:ASN:H	5:A:611:GOL:C3	2.23	0.51
1:B:144:PRO:HA	1:B:147:PHE:CE1	2.45	0.51
1:B:19:PRO:HG3	1:B:142:ILE:HB	1.91	0.51
1:B:386[A]:ARG:NH2	2:B:602:HIS:O	2.43	0.51
1:C:226:LEU:HD13	1:C:283:LEU:HD23	1.93	0.51
1:B:165:TRP:NE1	1:B:495[B]:GLU:HG3	2.27	0.50
1:A:102:GLU:HB3	1:A:126:TYR:OH	2.11	0.50
1:B:4:ASP:HB2	1:B:192:LYS:HG3	1.94	0.50
1:B:241:GLN:HE22	1:B:483:ILE:H	1.60	0.50
1:B:350:ASP:OD2	1:B:396:ARG:NH2	2.45	0.49
1:A:149:ASN:HA	4:A:610:ACT:H2	1.95	0.49
1:C:127:TYR:CG	1:C:128:PRO:HD3	2.48	0.49
1:A:68:ARG:NH2	4:A:609:ACT:O	2.36	0.49
1:A:72:LYS:HD3	1:A:78:PRO:HA	1.95	0.49
1:B:61:LYS:HD3	1:B:124:SER:HA	1.95	0.49
1:A:272:ALA:HB2	1:A:367:ILE:HD13	1.95	0.48
1:A:377[B]:GLU:CD	1:A:377[B]:GLU:H	2.17	0.48
1:A:349:THR:HG23	8:A:838:HOH:O	2.12	0.48
2:B:601:HIS:CE1	2:B:602:HIS:CE1	3.01	0.48
1:A:224:LEU:H	1:A:473:MET:HE3	1.78	0.47
1:A:320:GLU:OE1	1:A:325:THR:HG22	2.14	0.47
1:B:27:MET:HB3	1:B:27:MET:HE2	1.75	0.47
1:C:209:PHE:CZ	1:C:475:VAL:HG12	2.49	0.47
2:C:601:HIS:CE1	2:C:602:HIS:CE1	3.02	0.47
1:C:69:ASP:N	1:C:69:ASP:OD1	2.48	0.46
1:C:146:GLN:HA	1:C:157:LYS:HD2	1.96	0.46
1:A:364:MET:HG3	1:A:371:VAL:HG21	1.96	0.46
1:A:127:TYR:CD2	1:A:128:PRO:HD3	2.50	0.46
1:C:206:ALA:HB1	1:C:228:THR:HG21	1.98	0.46
1:B:387:ASP:OD1	1:B:389:ARG:HB2	2.16	0.46
1:C:405:HIS:CG	1:C:406:ALA:N	2.84	0.46
1:B:346:PHE:HB3	1:B:394:PHE:CD2	2.50	0.45
1:B:426:ALA:O	1:C:338:GLN:HG2	2.16	0.45
1:B:71:VAL:HG22	1:B:185:TRP:CG	2.51	0.45
5:C:608:GOL:H12	8:C:738:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:PRO:HG2	1:C:330:LYS:HB2	1.99	0.45
1:A:114:SER:OG	1:A:115:LYS:N	2.50	0.45
1:A:180:ARG:HG3	1:A:189:PRO:HG2	1.98	0.45
1:B:386[A]:ARG:HH21	2:B:602:HIS:C	2.20	0.45
1:C:438:VAL:HG13	1:C:450:LEU:HB2	1.97	0.45
1:C:483:ILE:HD12	1:C:497:ILE:HD12	1.99	0.45
1:B:381:ILE:HG23	1:B:393:ILE:HD11	1.98	0.44
1:B:250:MET:CB	1:B:466:PRO:HA	2.47	0.44
1:A:290:ALA:HA	1:A:469:TYR:CE2	2.52	0.44
1:A:373:LEU:H	5:A:612:GOL:H2	1.83	0.44
1:B:69:ASP:OD1	1:B:69:ASP:N	2.41	0.44
1:A:58:GLU:CD	1:A:58:GLU:H	2.20	0.44
1:C:58:GLU:H	1:C:58:GLU:CD	2.20	0.44
1:A:223:LEU:HB3	1:A:473:MET:HE3	1.99	0.44
1:A:72:LYS:NZ	1:A:78:PRO:HB3	2.32	0.44
1:B:207:VAL:O	1:B:211:THR:HG23	2.18	0.44
1:A:8:THR:OG1	1:A:9:ALA:N	2.50	0.43
1:B:54:TRP:HB3	1:B:65:PHE:CD2	2.54	0.43
1:B:382:TYR:CE2	2:B:602:HIS:HD2	2.36	0.43
1:C:316:LYS:HG2	1:C:333:ARG:HH11	1.83	0.43
1:B:27:MET:HG3	8:B:796:HOH:O	2.18	0.43
1:A:201:ASP:HA	1:A:202:PRO:HD3	1.90	0.43
1:C:332:ILE:HD12	1:C:370:ASP:HB2	2.01	0.43
1:B:102:GLU:HB3	1:B:126:TYR:OH	2.19	0.43
1:B:382:TYR:O	1:B:386[A]:ARG:HG3	2.19	0.43
1:B:272:ALA:HB2	1:B:367:ILE:HD13	2.01	0.42
1:A:6:ILE:HD13	1:A:191:ILE:HD13	2.01	0.42
1:B:278:LEU:HD21	1:B:356:MET:HG2	2.00	0.42
1:C:144:PRO:HA	1:C:147:PHE:CE1	2.54	0.42
1:A:131:GLN:HG2	8:A:786:HOH:O	2.19	0.42
1:B:321:LYS:HD3	1:B:321:LYS:HA	1.82	0.42
1:C:265:VAL:O	1:C:269:LEU:HG	2.20	0.42
1:C:403:ASP:HA	1:C:404:PRO:HA	1.82	0.42
1:A:265:VAL:O	1:A:269:LEU:HG	2.19	0.42
1:B:227:ASP:HB3	1:B:284:TYR:CZ	2.55	0.42
1:B:319:LEU:HA	1:B:319:LEU:HD23	1.87	0.41
1:C:373:LEU:O	1:C:374:ILE:HD13	2.19	0.41
1:C:37:LEU:HA	1:C:50:LEU:HB2	2.02	0.41
1:A:357:ALA:HB1	1:A:373:LEU:HD22	2.02	0.41
1:A:257:LYS:HB2	1:A:257:LYS:HE2	1.84	0.41
1:A:313[A]:GLN:OE1	1:A:316:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:LEU:HD23	1:C:79:PHE:CE2	2.56	0.41
1:B:346:PHE:HB3	1:B:394:PHE:HD2	1.85	0.41
1:B:431:ILE:O	1:B:435:ILE:HG13	2.21	0.41
1:C:128:PRO:O	1:C:132:GLU:HG3	2.20	0.41
1:A:166:ILE:HG13	1:A:181:ASN:HB2	2.02	0.41
1:B:495[B]:GLU:H	1:B:495[B]:GLU:CD	2.24	0.41
1:B:49:TRP:HB3	1:B:50:LEU:H	1.75	0.41
1:C:235:ASN:HA	1:C:236:PRO:HD2	1.94	0.41
1:A:127:TYR:CG	1:A:128:PRO:HD3	2.55	0.41
1:A:235:ASN:HA	1:A:236:PRO:HD2	1.86	0.41
2:C:601:HIS:CE1	2:C:602:HIS:HE1	2.39	0.41
1:B:201:ASP:HA	1:B:202:PRO:HD3	1.92	0.41
1:C:114:SER:HB3	1:C:117:GLU:HB2	2.03	0.41
1:C:396:ARG:HG2	4:C:606:ACT:H3	2.03	0.41
1:A:398:TRP:HB2	1:A:402:TYR:HB2	2.02	0.41
1:A:223:LEU:HB3	1:A:473:MET:CE	2.51	0.41
1:B:143:ALA:HA	1:B:144:PRO:HD3	1.95	0.40
1:C:477:LYS:HA	1:C:478:PRO:HD3	1.92	0.40
1:C:306:LYS:HA	1:C:307:PRO:HD3	1.96	0.40
1:C:19:PRO:HG3	1:C:34:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

## 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	500/502 (100%)	484 (97%)	16 (3%)	0	100	100
1	B	499/502 (99%)	483 (97%)	15 (3%)	1 (0%)	47	68
1	C	495/502 (99%)	478 (97%)	17 (3%)	0	100	100
All	All	1494/1506 (99%)	1445 (97%)	48 (3%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	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	426/425 (100%)	417 (98%)	9 (2%)	53	78
1	B	426/425 (100%)	421 (99%)	5 (1%)	71	88
1	C	422/425 (99%)	415 (98%)	7 (2%)	60	82
All	All	1274/1275 (100%)	1253 (98%)	21 (2%)	59	84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	113	LEU
1	A	131	GLN
1	A	172	LEU
1	A	250	MET
1	A	288	GLN
1	A	338	GLN
1	A	364	MET
1	A	438	VAL
1	B	250	MET
1	B	306	LYS
1	B	308	SER
1	B	410	SER
1	B	473	MET
1	C	23	THR
1	C	58	GLU
1	C	114	SER
1	C	250	MET
1	C	438	VAL
1	C	473	MET

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Mol	Chain	Res	Type
1	C	490	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	220	ASN
1	B	288	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 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	$\# Z  > 2$
5	GOL	B	610	-	5,5,5	0.42	0	5,5,5	0.42	0
4	ACT	C	606	-	1,3,3	1.87	0	0,3,3	0.00	-
4	ACT	A	606	-	1,3,3	1.38	0	0,3,3	0.00	-
2	HIS	A	602	3	4,11,11	0.45	0	3,14,14	1.33	1 (33%)
4	ACT	A	608	-	1,3,3	1.49	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	C	608	-	5,5,5	0.40	0	5,5,5	0.36	0
4	ACT	B	614	-	1,3,3	1.46	0	0,3,3	0.00	-
5	GOL	A	612	-	5,5,5	0.30	0	5,5,5	0.53	0
7	SO4	C	609	-	4,4,4	0.12	0	6,6,6	0.09	0
5	GOL	C	607	-	5,5,5	0.38	0	5,5,5	0.44	0
2	HIS	A	601	3	4,11,11	0.47	0	3,14,14	1.37	1 (33%)
4	ACT	A	605	-	1,3,3	1.16	0	0,3,3	0.00	-
2	HIS	C	601	3	4,11,11	0.52	0	3,14,14	1.53	1 (33%)
5	GOL	A	611	-	5,5,5	0.39	0	5,5,5	0.52	0
4	ACT	B	607	-	1,3,3	1.40	0	0,3,3	0.00	-
4	ACT	A	607	-	1,3,3	1.52	0	0,3,3	0.00	-
2	HIS	B	601	3	4,11,11	0.42	0	3,14,14	0.90	0
4	ACT	A	609	-	1,3,3	1.67	0	0,3,3	0.00	-
4	ACT	A	604	-	1,3,3	1.35	0	0,3,3	0.00	-
4	ACT	A	610	-	1,3,3	1.49	0	0,3,3	0.00	-
4	ACT	B	608	-	1,3,3	1.82	0	0,3,3	0.00	-
5	GOL	A	613	-	5,5,5	0.41	0	5,5,5	0.53	0
4	ACT	B	605	-	1,3,3	1.50	0	0,3,3	0.00	-
2	HIS	B	602	3	4,11,11	0.61	0	3,14,14	1.16	0
5	GOL	B	611	-	5,5,5	0.37	0	5,5,5	0.18	0
7	SO4	B	613	-	4,4,4	0.14	0	6,6,6	0.08	0
5	GOL	B	612	-	5,5,5	0.37	0	5,5,5	0.34	0
4	ACT	B	609	-	1,3,3	1.43	0	0,3,3	0.00	-
2	HIS	C	602	3	4,11,11	0.59	0	3,14,14	1.20	0
4	ACT	C	604	-	1,3,3	1.63	0	0,3,3	0.00	-
4	ACT	C	605	-	1,3,3	1.58	0	0,3,3	0.00	-
4	ACT	B	606	-	1,3,3	1.52	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
5	GOL	B	610	-	-	2/4/4/4	-
5	GOL	A	612	-	-	2/4/4/4	-
5	GOL	A	611	-	-	4/4/4/4	-
2	HIS	B	602	3	-	1/4/8/8	0/1/1/1
5	GOL	C	607	-	-	2/4/4/4	-
2	HIS	B	601	3	-	2/4/8/8	0/1/1/1
5	GOL	B	612	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	611	-	-	0/4/4/4	-
2	HIS	A	601	3	-	1/4/8/8	0/1/1/1
2	HIS	C	602	3	-	1/4/8/8	0/1/1/1
2	HIS	A	602	3	-	1/4/8/8	0/1/1/1
2	HIS	C	601	3	-	2/4/8/8	0/1/1/1
5	GOL	A	613	-	-	2/4/4/4	-
5	GOL	C	608	-	-	3/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	HIS	CD2-NE2-CE1	2.27	109.32	105.78
2	A	602	HIS	CD2-NE2-CE1	2.10	109.06	105.78
2	A	601	HIS	CD2-NE2-CE1	2.01	108.91	105.78

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	610	GOL	O1-C1-C2-C3
2	A	602	HIS	CA-CB-CG-ND1
5	C	608	GOL	O1-C1-C2-C3
5	A	612	GOL	O1-C1-C2-C3
2	A	601	HIS	CA-CB-CG-ND1
2	C	601	HIS	CA-CB-CG-ND1
2	C	601	HIS	CA-CB-CG-CD2
5	A	611	GOL	O1-C1-C2-O2
5	A	611	GOL	O1-C1-C2-C3
5	A	611	GOL	C1-C2-C3-O3
5	A	611	GOL	O2-C2-C3-O3
2	B	601	HIS	CA-CB-CG-ND1
2	B	601	HIS	CA-CB-CG-CD2
2	B	602	HIS	CA-CB-CG-ND1
5	B	612	GOL	C1-C2-C3-O3
5	C	607	GOL	O1-C1-C2-C3
5	A	613	GOL	O1-C1-C2-C3
5	B	612	GOL	O1-C1-C2-C3
5	C	608	GOL	O1-C1-C2-O2
5	C	607	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	612	GOL	O1-C1-C2-O2
5	B	610	GOL	O1-C1-C2-O2
5	A	612	GOL	O1-C1-C2-O2
5	A	613	GOL	O2-C2-C3-O3
5	B	612	GOL	O2-C2-C3-O3
2	C	602	HIS	CA-CB-CG-ND1
5	C	608	GOL	C1-C2-C3-O3

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	606	ACT	1	0
5	C	608	GOL	2	0
5	A	612	GOL	1	0
5	C	607	GOL	1	0
2	C	601	HIS	2	0
5	A	611	GOL	2	0
2	B	601	HIS	1	0
4	A	609	ACT	1	0
4	A	610	ACT	1	0
2	B	602	HIS	4	0
2	C	602	HIS	2	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%)	-0.16	2 (0%) 92 93	30, 47, 67, 83	1 (0%)
1	B	499/502 (99%)	-0.02	7 (1%) 75 77	31, 47, 67, 82	1 (0%)
1	C	496/502 (98%)	0.31	35 (7%) 16 16	38, 61, 94, 114	6 (1%)
All	All	1494/1506 (99%)	0.04	44 (2%) 51 55	30, 50, 84, 114	8 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	149	ASN	5.7
1	C	70	ASP	4.3
1	C	71	VAL	4.1
1	C	175	TYR	4.1
1	C	67	LEU	4.0
1	C	148	LYS	3.8
1	B	149	ASN	3.8
1	C	152	THR	3.5
1	C	151	GLU	3.5
1	C	73	PHE	3.3
1	C	163	GLY	3.2
1	C	76	GLY	3.1
1	C	150	HIS	3.1
1	A	500	VAL	2.9
1	C	183	ASN	2.8
1	C	153	MET	2.8
1	C	116	THR	2.7
1	C	147	PHE	2.7
1	B	108	VAL	2.7
1	C	74	SER	2.7
1	C	281	ASN	2.6
1	B	147	PHE	2.6
1	C	166	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	113	LEU	2.5
1	C	174	GLN	2.4
1	C	155	GLY	2.4
1	C	60	GLY	2.4
1	C	72	LYS	2.4
1	C	157	LYS	2.4
1	C	69	ASP	2.3
1	B	58	GLU	2.3
1	C	83	ALA	2.3
1	C	171	LYS	2.3
1	C	80	ASP	2.2
1	C	79	PHE	2.2
1	C	75	ASN	2.2
1	C	184	TYR	2.2
1	C	143	ALA	2.2
1	C	284	TYR	2.2
1	B	150	HIS	2.1
1	C	158	ALA	2.1
1	B	309	GLN	2.1
1	C	145	SER	2.1
1	A	58	GLU	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 monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	B	610	6/6	0.77	0.22	56,63,71,74	0
2	HIS	A	602	11/11	0.79	0.39	54,63,73,73	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	C	608	6/6	0.79	0.32	53,60,63,71	0
5	GOL	A	613	6/6	0.80	0.31	67,73,88,97	0
5	GOL	B	611	6/6	0.80	0.20	73,78,80,88	0
4	ACT	C	604	4/4	0.82	0.38	66,69,71,75	0
4	ACT	B	609	4/4	0.83	0.17	52,64,67,70	0
5	GOL	C	607	6/6	0.83	0.25	52,65,71,76	0
4	ACT	A	607	4/4	0.86	0.23	55,63,67,69	0
4	ACT	B	614	4/4	0.87	0.16	57,64,66,66	0
7	SO4	C	609	5/5	0.88	0.24	82,83,101,106	0
5	GOL	B	612	6/6	0.88	0.20	52,54,57,57	0
4	ACT	A	608	4/4	0.89	0.29	65,72,74,74	0
5	GOL	A	611	6/6	0.89	0.21	51,51,61,62	0
4	ACT	B	606	4/4	0.90	0.14	64,64,70,77	0
4	ACT	C	606	4/4	0.90	0.17	55,61,61,69	0
4	ACT	A	606	4/4	0.90	0.26	68,68,73,78	0
4	ACT	A	609	4/4	0.90	0.10	64,64,77,78	0
4	ACT	B	608	4/4	0.90	0.18	60,70,78,83	0
4	ACT	A	605	4/4	0.91	0.15	56,59,59,60	0
2	HIS	C	602	11/11	0.91	0.25	56,63,72,78	11
5	GOL	A	612	6/6	0.91	0.10	44,56,59,63	0
4	ACT	B	605	4/4	0.93	0.41	63,70,72,76	0
4	ACT	A	604	4/4	0.93	0.13	69,72,72,75	0
4	ACT	B	607	4/4	0.94	0.16	50,54,57,59	0
4	ACT	A	610	4/4	0.94	0.15	65,66,72,75	0
2	HIS	B	602	11/11	0.97	0.22	39,49,58,61	11
2	HIS	A	601	11/11	0.97	0.16	38,44,48,49	0
7	SO4	B	613	5/5	0.97	0.13	60,69,74,82	0
4	ACT	C	605	4/4	0.97	0.12	57,60,60,61	0
2	HIS	C	601	11/11	0.98	0.15	46,53,57,59	0
3	NI	C	603	1/1	0.98	0.16	56,56,56,56	0
3	NI	A	603	1/1	0.99	0.15	55,55,55,55	0
2	HIS	B	601	11/11	0.99	0.14	34,38,42,44	0
6	CL	B	604	1/1	0.99	0.14	49,49,49,49	0
3	NI	B	603	1/1	1.00	0.15	39,39,39,39	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.