



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:24 AM UTC

PDB ID : 4I8C / pdb_00004i8c
Title : X-ray structure of NikA in complex with Ni-(L-His)₂
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

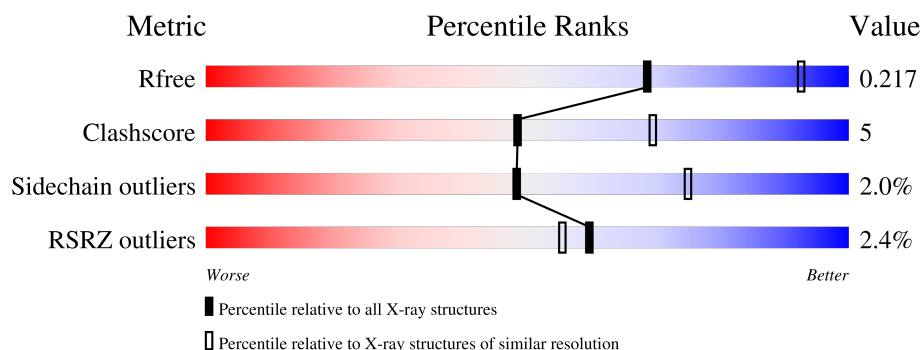
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	 86% 12% ..
1	B	502	 85% 15% .
1	C	502	 84% 14% ..

2 Entry composition [i](#)

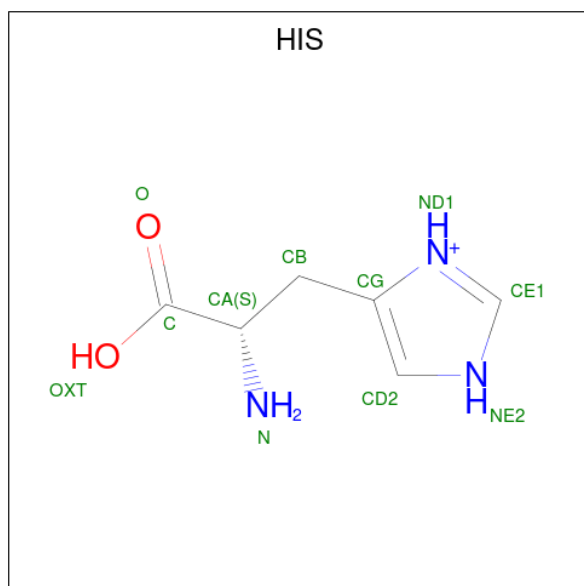
There are 8 unique types of molecules in this entry. The entry contains 12432 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: HIS) (formula: C₆H₁₀N₃O₂).



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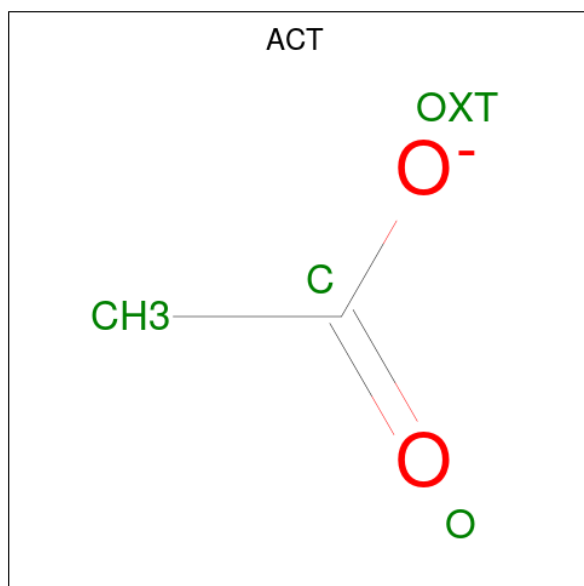
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			11	6	3	2		
2	C	1	Total	C	N	O	0	0
			11	6	3	2		
2	C	1	Total	C	N	O	0	0
			11	6	3	2		

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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 (CCD ID: GOL) (formula: $C_3H_8O_3$).

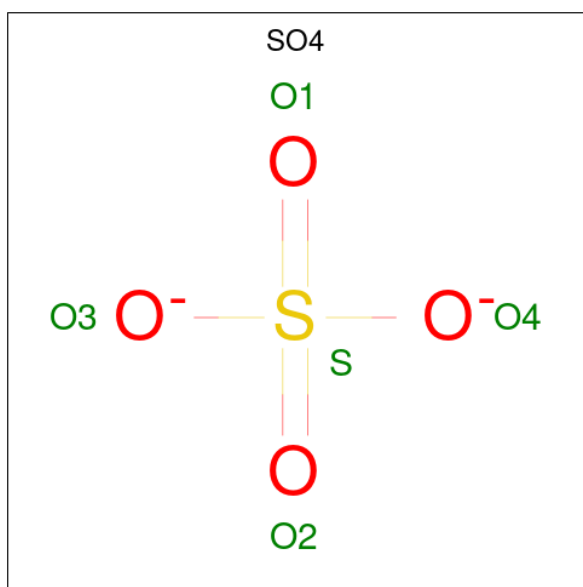


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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		

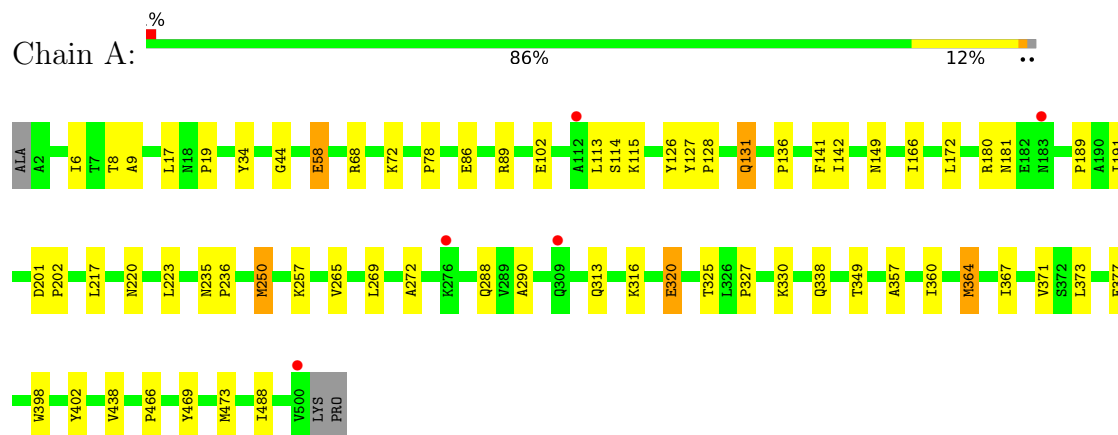
- Molecule 8 is water.

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		

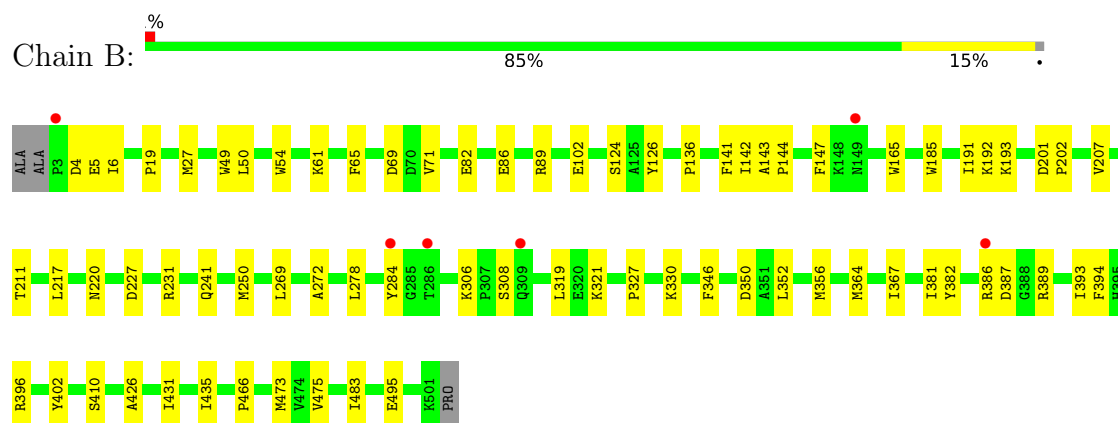
3 Residue-property plots

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.

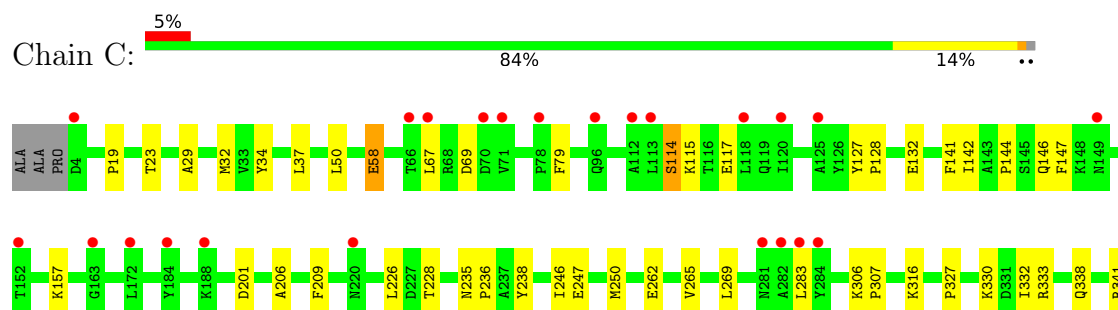
• Molecule 1: Nickel-binding periplasmic protein

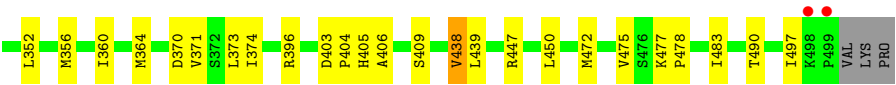


• Molecule 1: Nickel-binding periplasmic protein



• Molecule 1: Nickel-binding periplasmic protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	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) 99.5 (48.50-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.189 , 0.234 (Not available) , 0.217	Depositor DCC
R_{free} test set	3327 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SO4, ACT, CL, NI, GOL

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	0.53	0/4089	0.84	1/5570 (0.0%)
1	B	0.55	0/4086	0.81	1/5564 (0.0%)
1	C	0.47	0/4050	0.82	3/5517 (0.1%)
All	All	0.52	0/12225	0.82	5/16651 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	201	ASP	CA-C-N	6.08	125.80	119.05
1	C	201	ASP	C-N-CA	6.08	125.80	119.05
1	A	141	PHE	N-CA-C	6.01	118.53	108.02
1	B	141	PHE	N-CA-C	5.45	117.55	108.02
1	C	141	PHE	N-CA-C	5.11	116.74	108.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	40	0
1	B	3982	0	3933	47	0
1	C	3947	0	3891	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	131	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 (131) 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:223:LEU:HB3	1:A:473:MET:HE3	1.61	0.83
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:352:LEU:HG	1:B:356:MET:HE2	1.72	0.71
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:86:GLU:OE1	1:A:89:ARG:NH2	2.24	0.60
1:A:327:PRO:HG2	1:A:330:LYS:HB2	1.81	0.60
1:B:86:GLU:OE1	1:B:89:ARG:NH2	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:377[B]:GLU:H	1:A:377[B]:GLU:CD	2.17	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:386[A]:ARG:HH21	2:B:602:HIS:C	2.20	0.49
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:C:58:GLU:CD	1:C:58:GLU:H	2.20	0.48
1:A:58:GLU:H	1:A:58:GLU:CD	2.20	0.48
1:A:272:ALA:HB2	1:A:367:ILE:HD13	1.95	0.48
1:C:29:ALA:HA	1:C:32:MET:HE3	1.94	0.48
1:A:349:THR:HG23	8:A:838:HOH:O	2.12	0.48
1:B:27:MET:HE1	1:B:402:TYR:OH	2.13	0.48
2:B:601:HIS:CE1	2:B:602:HIS:CE1	3.01	0.48
1:A:320:GLU:OE1	1:A:325:THR:HG22	2.14	0.47
1:C:209:PHE:CZ	1:C:475:VAL:HG12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LEU:HD22	1:B:364:MET:HE2	1.96	0.47
2:C:601:HIS:CE1	2:C:602:HIS:CE1	3.02	0.47
1:C:69:ASP:OD1	1:C:69:ASP:N	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:495[B]:GLU:H	1:B:495[B]:GLU:CD	2.24	0.46
1:B:346:PHE:HB3	1:B:394:PHE:CD2	2.50	0.45
1:B:71:VAL:HG22	1:B:185:TRP:CG	2.51	0.45
1:B:426:ALA:O	1:C:338:GLN:HG2	2.16	0.45
5:C:608:GOL:H12	8:C:738:HOH:O	2.16	0.45
1:B:356:MET:HE3	1:B:394:PHE:HE1	1.81	0.45
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: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: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:356:MET:HE3	1:B:394:PHE:CE1	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	1:B:319:LEU:HA	1.87	0.41
1:C:37:LEU:HA	1:C:50:LEU:HB2	2.02	0.41
1:C:373:LEU:O	1:C:374:ILE:HD13	2.19	0.41
1:A:357:ALA:HB1	1:A:373:LEU:HD22	2.02	0.41
1:C:352:LEU:HD11	1:C:356:MET:HE3	2.02	0.41
1:A:257:LYS:HE2	1:A:257:LYS:HB2	1.84	0.41
1:A:313[A]:GLN:OE1	1:A:316:LYS:HE2	2.20	0.41
1:B:27:MET:HE2	1:B:136:PRO:HG2	2.02	0.41
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: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:C:472:MET:HE2	1:C:472:MET:HB2	1.92	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
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
2:C:601:HIS:CE1	2:C:602:HIS:HE1	2.39	0.41
1:A:398:TRP:HB2	1:A:402:TYR:HB2	2.02	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:A:17:LEU:O	1:A:34:TYR:OH	2.33	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

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

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%)	416 (98%)	10 (2%)	44	72
1	B	426/425 (100%)	420 (99%)	6 (1%)	59	81
1	C	422/425 (99%)	415 (98%)	7 (2%)	53	78
All	All	1274/1275 (100%)	1251 (98%)	23 (2%)	48	77

All (23) 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	320	GLU
1	A	338	GLN
1	A	364	MET
1	A	438	VAL
1	B	82	GLU
1	B	231	ARG
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

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Mol	Chain	Res	Type
1	C	250	MET
1	C	341	ARG
1	C	438	VAL
1	C	490	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	288	GLN
1	A	416	HIS
1	B	220	ASN
1	B	241	GLN
1	B	244	GLN
1	B	287	GLN
1	B	288	GLN
1	C	41	GLN
1	C	239	HIS
1	C	287	GLN
1	C	361	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 oligosaccharides 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
4	ACT	A	608	-	3,3,3	0.85	0	3,3,3	1.23	0
5	GOL	A	611	-	5,5,5	0.39	0	5,5,5	0.56	0
5	GOL	C	608	-	5,5,5	0.41	0	5,5,5	0.39	0
4	ACT	B	606	-	3,3,3	0.80	0	3,3,3	1.46	0
2	HIS	C	601	3	10,11,11	0.77	1 (10%)	10,14,14	1.30	1 (10%)
4	ACT	A	610	-	3,3,3	0.82	0	3,3,3	1.41	0
2	HIS	A	601	3	10,11,11	0.84	1 (10%)	10,14,14	1.22	1 (10%)
4	ACT	C	605	-	3,3,3	0.76	0	3,3,3	1.52	0
5	GOL	A	612	-	5,5,5	0.31	0	5,5,5	0.57	0
5	GOL	C	607	-	5,5,5	0.39	0	5,5,5	0.48	0
4	ACT	A	604	-	3,3,3	0.79	0	3,3,3	1.41	0
4	ACT	A	605	-	3,3,3	0.76	0	3,3,3	1.23	0
4	ACT	A	606	-	3,3,3	0.81	0	3,3,3	1.38	0
4	ACT	C	604	-	3,3,3	0.77	0	3,3,3	1.43	0
4	ACT	B	608	-	3,3,3	0.81	0	3,3,3	1.57	0
2	HIS	B	601	3	10,11,11	0.87	1 (10%)	10,14,14	1.35	2 (20%)
4	ACT	A	607	-	3,3,3	0.82	0	3,3,3	1.32	0
2	HIS	C	602	3	10,11,11	0.75	1 (10%)	10,14,14	1.16	1 (10%)
4	ACT	B	614	-	3,3,3	0.80	0	3,3,3	1.47	0
4	ACT	C	606	-	3,3,3	0.89	0	3,3,3	1.44	0
7	SO4	C	609	-	4,4,4	0.24	0	6,6,6	0.11	0
2	HIS	B	602	3	10,11,11	0.76	1 (10%)	10,14,14	1.18	1 (10%)
5	GOL	B	612	-	5,5,5	0.38	0	5,5,5	0.36	0
4	ACT	B	609	-	3,3,3	0.83	0	3,3,3	1.44	0
4	ACT	B	605	-	3,3,3	0.80	0	3,3,3	1.44	0
4	ACT	A	609	-	3,3,3	0.79	0	3,3,3	1.51	0
5	GOL	B	610	-	5,5,5	0.44	0	5,5,5	0.44	0
7	SO4	B	613	-	4,4,4	0.23	0	6,6,6	0.10	0
2	HIS	A	602	3	10,11,11	0.71	0	10,14,14	1.27	1 (10%)
5	GOL	B	611	-	5,5,5	0.37	0	5,5,5	0.20	0
5	GOL	A	613	-	5,5,5	0.43	0	5,5,5	0.55	0
4	ACT	B	607	-	3,3,3	0.85	0	3,3,3	1.27	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
5	GOL	A	611	-	-	4/4/4/4	-
5	GOL	C	607	-	-	2/4/4/4	-
2	HIS	C	602	3	-	1/8/8/8	0/1/1/1
5	GOL	B	610	-	-	2/4/4/4	-
5	GOL	C	608	-	-	3/4/4/4	-
2	HIS	A	602	3	-	3/8/8/8	0/1/1/1
2	HIS	C	601	3	-	2/8/8/8	0/1/1/1
5	GOL	B	611	-	-	0/4/4/4	-
2	HIS	A	601	3	-	2/8/8/8	0/1/1/1
2	HIS	B	602	3	-	0/8/8/8	0/1/1/1
5	GOL	A	613	-	-	2/4/4/4	-
5	GOL	B	612	-	-	4/4/4/4	-
5	GOL	A	612	-	-	2/4/4/4	-
2	HIS	B	601	3	-	2/8/8/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HIS	OXT-C	-2.32	1.23	1.30
2	B	601	HIS	OXT-C	-2.10	1.24	1.30
2	B	602	HIS	OXT-C	-2.08	1.24	1.30
2	C	602	HIS	OXT-C	-2.08	1.24	1.30
2	C	601	HIS	OXT-C	-2.07	1.24	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	HIS	OXT-C-O	-2.90	117.49	124.08
2	A	602	HIS	OXT-C-O	-2.78	117.77	124.08
2	B	602	HIS	OXT-C-O	-2.50	118.40	124.08
2	A	601	HIS	OXT-C-O	-2.36	118.72	124.08
2	C	602	HIS	OXT-C-O	-2.25	118.97	124.08
2	B	601	HIS	CD2-CG-ND1	-2.15	104.51	108.86
2	B	601	HIS	OXT-C-O	-2.06	119.40	124.08

There are no chirality outliers.

All (29) torsion outliers are listed below:

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

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	611	GOL	2	0
5	C	608	GOL	2	0
2	C	601	HIS	2	0
4	A	610	ACT	1	0
5	A	612	GOL	1	0
5	C	607	GOL	1	0
2	B	601	HIS	1	0
2	C	602	HIS	2	0
4	C	606	ACT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	HIS	4	0
4	A	609	ACT	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, 95th 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 ²)	Q<0.9
1	A	499/502 (99%)	0.00	5 (1%) 79 76	26, 47, 67, 83	4 (0%)
1	B	499/502 (99%)	-0.05	6 (1%) 76 73	24, 46, 66, 82	3 (0%)
1	C	496/502 (98%)	0.54	25 (5%) 34 30	28, 60, 93, 114	7 (1%)
All	All	1494/1506 (99%)	0.17	36 (2%) 59 55	24, 50, 83, 114	14 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	500	VAL	3.6
1	B	3	PRO	3.6
1	C	113	LEU	3.4
1	C	220[A]	ASN	3.4
1	C	499	PRO	3.1
1	C	284	TYR	2.9
1	C	96	GLN	2.9
1	C	66	THR	2.8
1	B	284	TYR	2.8
1	C	498	LYS	2.8
1	B	149	ASN	2.8
1	C	152	THR	2.7
1	B	309	GLN	2.6
1	C	281	ASN	2.6
1	C	78	PRO	2.5
1	C	163	GLY	2.5
1	C	282	ALA	2.5
1	C	125	ALA	2.5
1	B	286	THR	2.5
1	C	112	ALA	2.4
1	B	386[A]	ARG	2.3
1	C	67	LEU	2.3
1	A	183	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	112	ALA	2.3
1	C	283	LEU	2.3
1	C	70	ASP	2.3
1	C	188	LYS	2.3
1	C	118	LEU	2.3
1	C	4	ASP	2.3
1	C	149	ASN	2.2
1	A	276	LYS	2.2
1	A	309	GLN	2.1
1	C	71	VAL	2.1
1	C	184	TYR	2.1
1	C	172	LEU	2.0
1	C	120	ILE	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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(Å ²)	Q<0.9
4	ACT	B	608	4/4	0.62	0.19	60,70,78,83	0
5	GOL	A	613	6/6	0.63	0.23	67,73,88,97	0
5	GOL	B	611	6/6	0.67	0.14	73,78,80,88	0
4	ACT	A	609	4/4	0.70	0.15	64,64,77,78	0
4	ACT	B	606	4/4	0.71	0.21	64,64,70,77	0
7	SO4	C	609	5/5	0.71	0.10	82,83,101,106	0
5	GOL	B	610	6/6	0.75	0.20	56,63,71,74	0
4	ACT	B	614	4/4	0.75	0.15	57,64,66,66	0
4	ACT	B	605	4/4	0.75	0.15	63,70,72,76	0
4	ACT	B	609	4/4	0.77	0.18	52,64,67,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HIS	A	602	11/11	0.78	0.24	54,63,73,73	11
4	ACT	A	606	4/4	0.78	0.17	68,68,73,78	0
5	GOL	C	607	6/6	0.79	0.15	52,65,71,76	0
4	ACT	C	604	4/4	0.79	0.19	66,69,71,75	0
4	ACT	A	607	4/4	0.80	0.14	55,63,67,69	0
4	ACT	A	604	4/4	0.82	0.17	69,72,72,75	0
4	ACT	A	610	4/4	0.83	0.15	65,66,72,75	0
5	GOL	C	608	6/6	0.83	0.19	53,60,63,71	0
4	ACT	A	605	4/4	0.83	0.14	56,59,59,60	0
4	ACT	B	607	4/4	0.84	0.11	50,54,57,59	0
4	ACT	C	605	4/4	0.84	0.13	57,60,60,61	0
5	GOL	A	611	6/6	0.86	0.15	51,51,61,62	0
5	GOL	A	612	6/6	0.86	0.11	44,56,59,63	0
5	GOL	B	612	6/6	0.87	0.18	52,54,57,57	0
4	ACT	C	606	4/4	0.88	0.13	55,61,61,69	0
4	ACT	A	608	4/4	0.88	0.14	65,72,74,74	0
2	HIS	B	602	11/11	0.92	0.14	39,49,58,61	11
2	HIS	C	602	11/11	0.93	0.17	56,63,72,78	11
7	SO4	B	613	5/5	0.93	0.21	60,69,74,82	0
2	HIS	A	601	11/11	0.93	0.10	38,44,48,49	0
2	HIS	C	601	11/11	0.94	0.09	46,53,57,59	0
2	HIS	B	601	11/11	0.98	0.05	34,38,42,44	0
3	NI	C	603	1/1	0.99	0.04	56,56,56,56	0
6	CL	B	604	1/1	0.99	0.03	49,49,49,49	0
3	NI	A	603	1/1	1.00	0.04	55,55,55,55	0
3	NI	B	603	1/1	1.00	0.03	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.