Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 11:21 AM EDT

PDB ID	:	3QIM
Title	:	Histidine 416 of the periplamsic binding protein NikA is essential for nickel uptake in Escherichia coli
Authors	:	Cavazza, C.; Martin, L.; Laffly, E.; Lebrette, H.; Cherrier, M.V.; Zeppieri, L.; Richaud, P.; Carriere, M.; Fontecilla-Camps, J.C.
Deposited on	:	2011-01-27
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

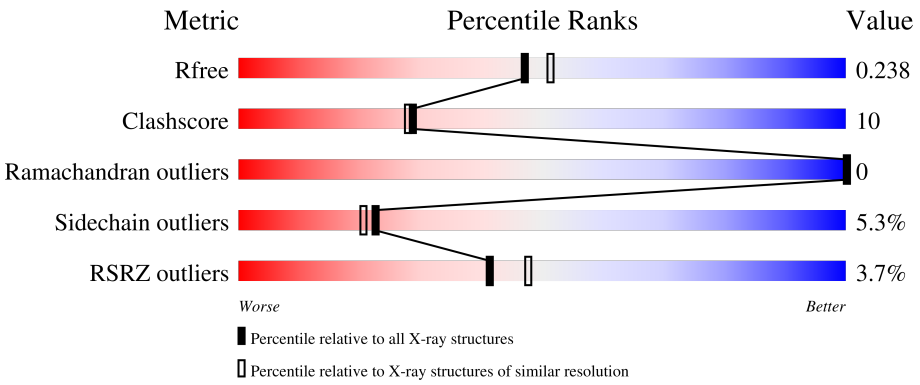
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	3% 84% 13% • •
1	B	502	5% 79% 17% • •

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	GOL	A	515	-	-	X	-
3	ACT	A	511	-	-	X	-
3	ACT	A	514	-	-	X	-
3	ACT	B	505	-	-	X	-
3	ACT	B	508	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8617 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.

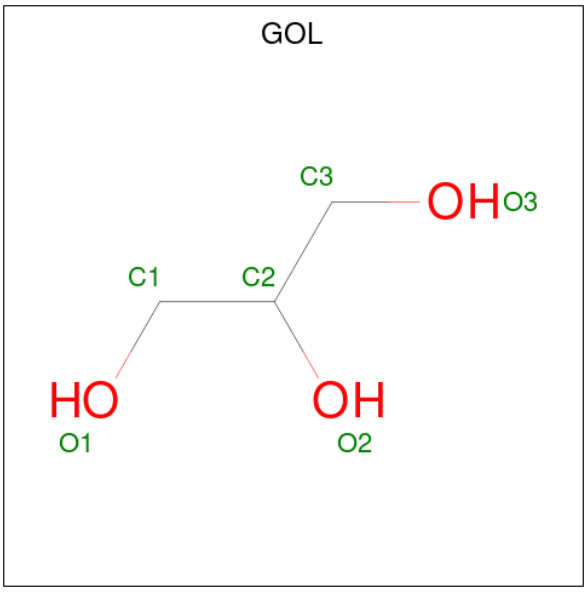
- Molecule 1 is a protein called Nickel-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	498	3995	2562	671	751	11	0	9	0
1	B	498	3996	2565	669	752	10	0	10	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	416	ILE	HIS	engineered mutation	UNP P33590
B	416	ILE	HIS	engineered mutation	UNP P33590

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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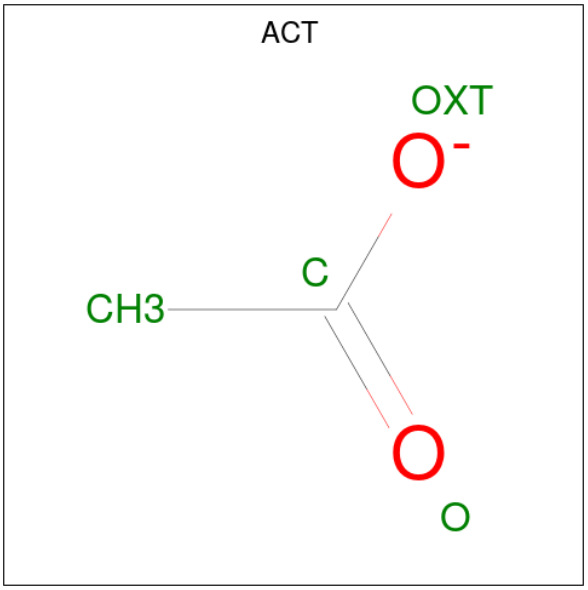
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
			Total	C	O		
2	A	1	6	3	3	0	0
			Total	C	O		
2	A	1	6	3	3	0	0
			Total	C	O		
2	A	1	6	3	3	0	0
			Total	C	O		
2	A	1	6	3	3	0	0
			Total	C	O		
2	A	1	6	3	3	0	0
			Total	C	O		
2	B	1	6	3	3	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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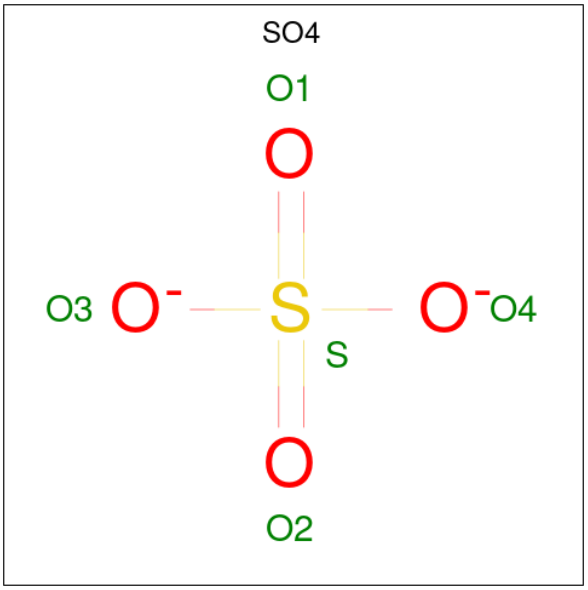
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 5 is water.

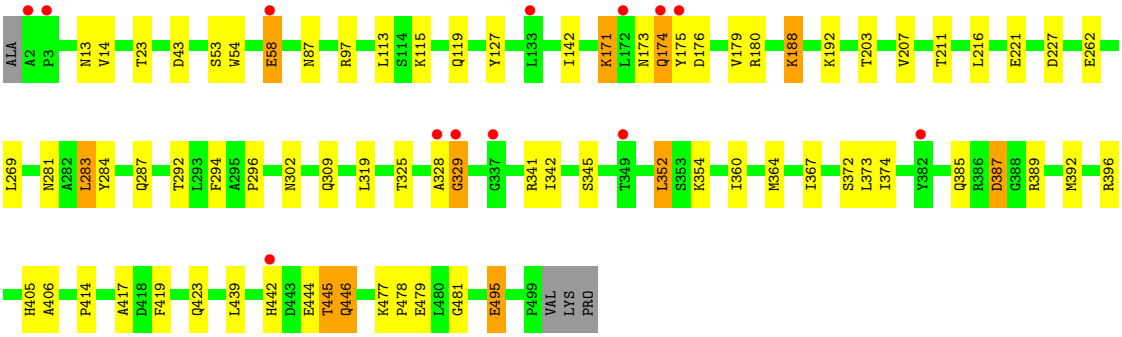
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	276	276	276	0	0
			Total	O		
5	B	230	230	230	0	0

3 Residue-property plots (i)

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.

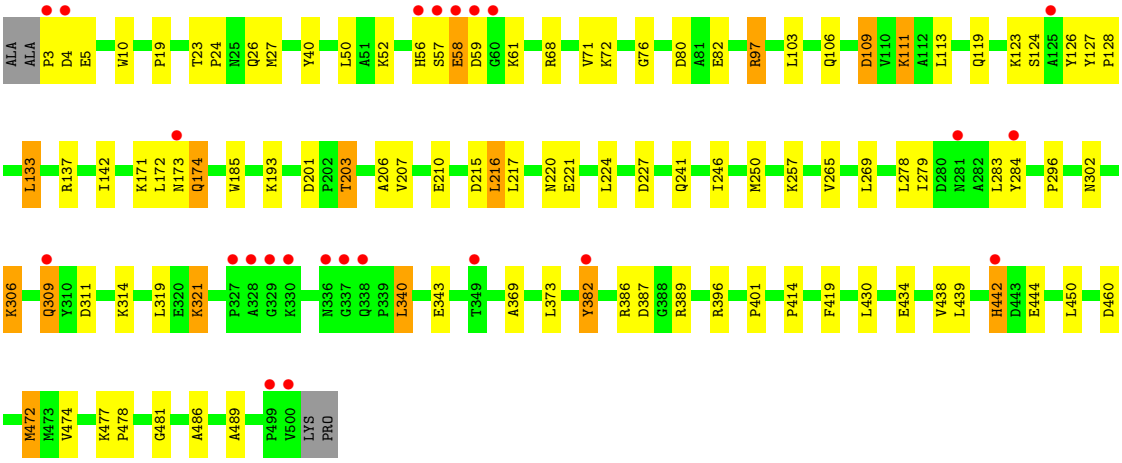
• Molecule 1: Nickel-binding periplasmic protein

Chain A:



• Molecule 1: Nickel-binding periplasmic protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.73Å 94.00Å 124.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.84 – 2.10 24.84 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.84-2.10) 99.4 (24.84-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.24 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.176 , 0.237 0.178 , 0.238	Depositor DCC
R_{free} test set	2981 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8617	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, 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	0.77	0/4120	0.77	3/5612 (0.1%)
1	B	0.70	0/4119	0.73	1/5611 (0.0%)
All	All	0.74	0/8239	0.75	4/11223 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	389	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	B	216	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	329	GLY	N-CA-C	-5.70	98.86	113.10
1	A	387	ASP	CB-CG-OD2	-5.18	113.64	118.30

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	3995	0	3963	79	1
1	B	3996	0	3951	81	1
2	A	42	0	56	8	1
2	B	6	0	8	0	0
3	A	28	0	21	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	18	6	0
4	A	15	0	0	1	0
4	B	5	0	0	0	0
5	A	276	0	0	14	0
5	B	230	0	0	15	1
All	All	8617	0	8017	156	2

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 10.

All (156) 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:287[A]:GLN:HG3	5:A:654:HOH:O	1.37	1.21
1:A:423:GLN:HG2	5:A:765:HOH:O	1.58	1.03
1:A:58:GLU:HG2	5:A:716:HOH:O	1.62	0.99
1:B:442[A]:HIS:CD2	1:B:442[A]:HIS:H	1.73	0.94
1:A:97:ARG:HE	2:A:515:GOL:H11	1.31	0.93
1:A:364[B]:MET:HE3	1:A:364[B]:MET:HA	1.49	0.92
1:B:97:ARG:HH22	3:B:505:ACT:H3	1.38	0.89
1:A:174:GLN:HE21	1:A:174:GLN:HA	1.38	0.88
1:B:396:ARG:HG2	3:B:508:ACT:H1	1.61	0.82
1:B:442[B]:HIS:HE1	5:B:592:HOH:O	1.63	0.81
1:B:5:GLU:HG2	1:B:193:LYS:HB3	1.65	0.79
1:A:360:ILE:O	1:A:364[B]:MET:HG2	1.83	0.78
1:B:382:TYR:CZ	1:B:386:ARG:HD2	2.18	0.78
1:A:292[B]:THR:HG21	5:A:522:HOH:O	1.83	0.77
1:A:221:GLU:OE2	1:A:396:ARG:NH2	2.17	0.76
1:B:52:LYS:HE3	1:B:68:ARG:HG2	1.67	0.76
1:B:10:TRP:HE1	1:B:26:GLN:HE21	1.32	0.76
1:A:442:HIS:H	1:A:442:HIS:CD2	2.01	0.76
1:A:97:ARG:NE	2:A:515:GOL:H11	2.02	0.74
1:A:283:LEU:HD12	1:A:352:LEU:HD21	1.69	0.73
1:B:442[A]:HIS:H	1:B:442[A]:HIS:HD2	1.31	0.72
1:B:442[B]:HIS:CE1	5:B:592:HOH:O	2.39	0.72
2:A:515:GOL:H12	5:A:666:HOH:O	1.88	0.72
1:B:201:ASP:OD1	1:B:203:THR:HB	1.90	0.72
1:B:438:VAL:HG12	1:B:450:LEU:HB3	1.72	0.71
1:A:444:GLU:HG2	1:B:481:GLY:HA2	1.73	0.71
1:B:489:ALA:HB3	5:B:583:HOH:O	1.89	0.71
1:A:87:ASN:HD21	1:A:142:ILE:H	1.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ASN:HA	1:B:472:MET:HE2	1.72	0.70
1:A:227:ASP:HB3	1:A:284:TYR:CZ	2.27	0.70
1:A:325:THR:CG2	5:A:756:HOH:O	2.39	0.69
1:B:321:LYS:HD3	5:B:648:HOH:O	1.93	0.68
1:A:292[B]:THR:HG22	1:A:294:PHE:O	1.94	0.67
3:A:511:ACT:H2	5:A:620:HOH:O	1.95	0.67
1:B:206:ALA:O	1:B:210:GLU:HG3	1.95	0.67
1:A:174:GLN:HA	1:A:174:GLN:NE2	2.08	0.67
1:B:434:GLU:O	1:B:438:VAL:HG13	1.95	0.66
1:A:292[A]:THR:HG23	1:A:294:PHE:O	1.96	0.66
3:B:508:ACT:CH3	5:B:554:HOH:O	2.43	0.66
1:A:444:GLU:HG2	1:B:481:GLY:CA	2.26	0.66
1:A:444:GLU:CG	1:B:481:GLY:HA2	2.26	0.65
1:B:10:TRP:HE1	1:B:26:GLN:NE2	1.93	0.65
1:A:364[B]:MET:HA	1:A:364[B]:MET:CE	2.24	0.65
1:A:174:GLN:HE21	1:A:174:GLN:CA	2.10	0.64
1:B:284:TYR:HB3	5:B:555:HOH:O	1.98	0.64
1:B:309:GLN:HE22	1:B:314:LYS:NZ	1.96	0.63
1:B:306:LYS:HE3	5:B:641:HOH:O	1.98	0.62
1:A:446:GLN:HE21	1:A:446:GLN:HA	1.65	0.62
1:A:14:VAL:HG13	1:A:176:ASP:OD2	2.00	0.62
1:A:97:ARG:HE	2:A:515:GOL:C1	2.08	0.61
1:A:58:GLU:CG	5:A:716:HOH:O	2.33	0.61
1:B:296:PRO:HB3	1:B:302:ASN:HD22	1.66	0.61
1:A:13:ASN:OD1	1:A:173:ASN:N	2.34	0.60
1:A:445:THR:HB	1:B:478:PRO:HB2	1.83	0.60
1:A:23:THR:HG23	2:A:515:GOL:O3	2.01	0.60
1:B:414:PRO:HA	1:B:419:PHE:CD1	2.38	0.59
1:B:340:LEU:HD13	1:B:369:ALA:HB2	1.85	0.59
1:A:54:TRP:H	2:A:506:GOL:H12	1.68	0.58
1:B:97:ARG:O	1:B:97:ARG:HD3	2.03	0.58
1:A:445:THR:HG21	5:B:700:HOH:O	2.02	0.58
1:A:385:GLN:HB3	1:A:417:ALA:HB2	1.84	0.58
1:A:325:THR:HG22	5:A:756:HOH:O	2.00	0.58
1:A:269:LEU:HD23	1:A:364[B]:MET:HE1	1.85	0.57
1:B:311:ASP:OD2	1:B:314:LYS:HD2	2.04	0.57
1:A:171:LYS:HB2	1:A:174:GLN:HB2	1.85	0.57
1:B:227:ASP:HB3	1:B:284:TYR:CE1	2.40	0.57
1:B:207:VAL:HA	1:B:210:GLU:HG3	1.87	0.57
1:A:281:ASN:HD21	3:A:514:ACT:H2	1.71	0.56
1:A:477:LYS:HB3	1:A:479[A]:GLU:OE1	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:GLU:HA	3:A:511:ACT:H1	1.87	0.55
1:B:109:ASP:HB3	1:B:111:LYS:HE2	1.89	0.55
1:B:97:ARG:NH2	3:B:505:ACT:H3	2.15	0.55
1:B:220:ASN:CA	1:B:472:MET:HE2	2.38	0.54
1:A:227:ASP:HB3	1:A:284:TYR:CE1	2.42	0.54
1:B:56:HIS:CD2	1:B:57:SER:O	2.61	0.53
1:A:481:GLY:HA2	1:B:444[B]:GLU:CG	2.39	0.53
1:A:283:LEU:CD1	1:A:352:LEU:HD21	2.39	0.53
1:A:292[B]:THR:CG2	1:A:294:PHE:O	2.56	0.53
1:A:481:GLY:CA	1:B:444[B]:GLU:HG2	2.40	0.52
1:A:341:ARG:HD3	5:A:770:HOH:O	2.10	0.52
1:A:481:GLY:HA2	1:B:444[B]:GLU:HG2	1.91	0.52
1:A:174:GLN:O	1:A:175:TYR:HB3	2.09	0.52
1:A:296:PRO:HB3	1:A:302:ASN:HD22	1.74	0.52
1:A:442:HIS:CD2	1:A:442:HIS:N	2.77	0.52
1:A:207:VAL:O	1:A:211:THR:HG23	2.10	0.51
1:A:495[B]:GLU:CD	1:A:495[B]:GLU:H	2.14	0.51
1:B:382:TYR:CE2	1:B:386:ARG:CD	2.93	0.50
1:B:265:VAL:O	1:B:269:LEU:HG	2.11	0.50
1:B:382:TYR:HB2	5:B:605:HOH:O	2.12	0.50
1:B:382:TYR:CE2	1:B:386:ARG:HD2	2.46	0.50
1:A:478:PRO:O	1:B:444[B]:GLU:HG3	2.11	0.50
1:B:171:LYS:HG2	1:B:174:GLN:HG3	1.94	0.49
1:B:126:TYR:CZ	1:B:128:PRO:HG2	2.48	0.49
1:B:309:GLN:HE22	1:B:314:LYS:HZ3	1.61	0.49
1:A:113:LEU:HD11	1:A:119:GLN:NE2	2.27	0.49
1:B:309:GLN:HB2	5:B:677:HOH:O	2.13	0.48
1:B:486:ALA:HB1	5:B:525:HOH:O	2.12	0.48
1:A:53:SER:HA	2:A:506:GOL:H31	1.95	0.48
1:A:292[A]:THR:CG2	1:A:294:PHE:O	2.62	0.48
1:B:278:LEU:C	1:B:278:LEU:HD23	2.34	0.48
1:A:269:LEU:CD2	1:A:364[B]:MET:CE	2.91	0.48
1:A:364[B]:MET:HE3	1:A:364[B]:MET:CA	2.26	0.48
3:B:508:ACT:H3	5:B:554:HOH:O	2.08	0.48
1:B:438:VAL:HG12	1:B:450:LEU:CB	2.41	0.48
1:B:279:ILE:HG12	1:B:283:LEU:HD12	1.96	0.48
1:A:442:HIS:HB3	5:A:790:HOH:O	2.14	0.47
1:B:257:LYS:HE2	5:B:643:HOH:O	2.14	0.47
1:B:382:TYR:C	1:B:382:TYR:CD2	2.88	0.47
1:B:171:LYS:HE3	1:B:174:GLN:HE21	1.79	0.47
1:A:345:SER:HA	1:A:374:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASN:O	1:A:174:GLN:NE2	2.46	0.47
1:B:430:LEU:C	1:B:430:LEU:HD23	2.35	0.47
1:A:479[A]:GLU:H	1:A:479[A]:GLU:CD	2.19	0.46
1:B:19:PRO:HG3	1:B:142:ILE:HB	1.98	0.46
1:B:279:ILE:HA	1:B:283:LEU:HD12	1.97	0.46
1:B:103:LEU:HD21	1:B:133:LEU:HD13	1.97	0.46
1:A:97:ARG:NE	2:A:515:GOL:O2	2.49	0.46
1:B:396:ARG:CD	5:B:557:HOH:O	2.64	0.45
1:B:40:TYR:CE1	1:B:401:PRO:HB3	2.52	0.45
1:B:387:ASP:OD2	1:B:389:ARG:NH1	2.49	0.45
1:B:106:GLN:OE1	1:B:124:SER:HB3	2.17	0.45
1:A:87:ASN:ND2	1:A:142:ILE:H	2.11	0.45
1:A:414:PRO:HA	1:A:419:PHE:CD1	2.52	0.44
1:A:495[A]:GLU:HG3	5:A:644:HOH:O	2.17	0.44
1:B:113:LEU:HD11	1:B:119:GLN:HE21	1.81	0.44
3:B:508:ACT:H2	5:B:554:HOH:O	2.11	0.44
1:A:341:ARG:CD	5:A:770:HOH:O	2.64	0.44
1:A:405:HIS:CG	1:A:406:ALA:N	2.86	0.43
1:B:61:LYS:HE3	1:B:123:LYS:O	2.18	0.43
1:B:309:GLN:N	1:B:309:GLN:OE1	2.51	0.43
1:A:188:LYS:H	1:A:188:LYS:CD	2.31	0.43
1:A:354:LYS:HG3	5:A:676:HOH:O	2.18	0.43
1:A:445:THR:HB	1:B:478:PRO:CB	2.48	0.43
1:B:382:TYR:CE2	1:B:386:ARG:HD3	2.53	0.43
1:B:241:GLN:HB2	1:B:474:VAL:HB	2.01	0.43
1:B:221:GLU:OE1	1:B:396:ARG:NH1	2.38	0.43
1:A:269:LEU:HD23	1:A:364[B]:MET:CE	2.48	0.42
1:B:3:PRO:HB2	1:B:4:ASP:H	1.68	0.42
1:A:23:THR:HB	4:A:517:SO4:O1	2.18	0.42
1:A:296:PRO:HB3	1:A:302:ASN:ND2	2.34	0.42
1:B:72:LYS:HD3	1:B:76:GLY:O	2.19	0.42
1:A:342:ILE:CG2	1:A:392:MET:HG3	2.49	0.42
1:A:281:ASN:HD21	3:A:514:ACT:CH3	2.30	0.42
1:A:328:ALA:HA	1:A:329:GLY:HA2	1.88	0.42
1:A:180:ARG:HH22	1:A:192:LYS:CE	2.33	0.41
1:B:27:MET:HG2	1:B:137:ARG:CZ	2.50	0.41
1:A:364[B]:MET:HE1	1:A:367:ILE:HD11	2.02	0.41
1:B:58:GLU:OE1	1:B:59:ASP:N	2.53	0.41
1:B:246:ILE:HD11	1:B:472:MET:HE3	2.02	0.41
1:B:71:VAL:HG22	1:B:185:TRP:CG	2.55	0.41
1:B:173:ASN:C	1:B:174:GLN:HG2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:PHE:CD1	1:A:419:PHE:C	2.95	0.40
1:B:215:ASP:OD1	1:B:477:LYS:NZ	2.49	0.40
1:B:217:LEU:HD13	1:B:224:LEU:HD13	2.03	0.40
1:B:23[A]:THR:OG1	1:B:24:PRO:HA	2.21	0.40

All (2) 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)
2:A:503:GOL:O2	5:B:624:HOH:O[2_555]	1.96	0.24
1:A:387:ASP:OD2	1:B:460:ASP:OD2[3_545]	2.16	0.04

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	504/502 (100%)	489 (97%)	15 (3%)	0	100	100
1	B	504/502 (100%)	485 (96%)	19 (4%)	0	100	100
All	All	1008/1004 (100%)	974 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	430/425 (101%)	408 (95%)	22 (5%)	24	22
1	B	430/425 (101%)	403 (94%)	27 (6%)	18	15
All	All	860/850 (101%)	811 (94%)	49 (6%)	22	18

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	A	58	GLU
1	A	115	LYS
1	A	127	TYR
1	A	171	LYS
1	A	174	GLN
1	A	179	VAL
1	A	188	LYS
1	A	203	THR
1	A	216	LEU
1	A	283	LEU
1	A	309[A]	GLN
1	A	309[B]	GLN
1	A	319	LEU
1	A	352	LEU
1	A	372	SER
1	A	373	LEU
1	A	439	LEU
1	A	445	THR
1	A	446	GLN
1	A	495[A]	GLU
1	A	495[B]	GLU
1	B	50	LEU
1	B	58	GLU
1	B	80[A]	ASP
1	B	80[B]	ASP
1	B	82	GLU
1	B	97	ARG
1	B	109	ASP
1	B	111	LYS
1	B	127	TYR
1	B	133	LEU
1	B	172	LEU
1	B	174	GLN
1	B	203	THR

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Mol	Chain	Res	Type
1	B	216	LEU
1	B	250	MET
1	B	306	LYS
1	B	309	GLN
1	B	319	LEU
1	B	321	LYS
1	B	340	LEU
1	B	343	GLU
1	B	373	LEU
1	B	382	TYR
1	B	439	LEU
1	B	442[A]	HIS
1	B	442[B]	HIS
1	B	472	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	87	ASN
1	A	119	GLN
1	A	131	GLN
1	A	174	GLN
1	A	197	ASN
1	A	281	ASN
1	A	288	GLN
1	A	302	ASN
1	A	385	GLN
1	A	442	HIS
1	A	446	GLN
1	B	25	ASN
1	B	26	GLN
1	B	56	HIS
1	B	174	GLN
1	B	234	GLN
1	B	302	ASN
1	B	309	GLN
1	B	385	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)

25 ligands are modelled in this entry.

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	GOL	A	504	-	5,5,5	0.28	0	5,5,5	0.84	0
4	SO4	A	518	-	4,4,4	0.28	0	6,6,6	0.21	0
4	SO4	B	510	-	4,4,4	0.17	0	6,6,6	0.24	0
3	ACT	B	506	-	3,3,3	0.97	0	3,3,3	1.54	1 (33%)
3	ACT	A	514	-	3,3,3	0.68	0	3,3,3	1.07	0
2	GOL	A	510	-	5,5,5	0.39	0	5,5,5	0.41	0
3	ACT	B	504	-	3,3,3	0.79	0	3,3,3	1.54	1 (33%)
4	SO4	A	517	-	4,4,4	0.22	0	6,6,6	0.32	0
2	GOL	A	503	-	5,5,5	0.41	0	5,5,5	0.97	0
3	ACT	A	511	-	3,3,3	0.94	0	3,3,3	1.64	1 (33%)
3	ACT	A	513	-	3,3,3	0.83	0	3,3,3	1.35	0
2	GOL	A	505	-	5,5,5	0.59	0	5,5,5	0.89	0
3	ACT	A	512	-	3,3,3	0.87	0	3,3,3	1.15	0
3	ACT	B	507	-	3,3,3	0.77	0	3,3,3	1.57	0
3	ACT	B	508	-	3,3,3	0.78	0	3,3,3	1.07	0
3	ACT	A	516	-	3,3,3	0.74	0	3,3,3	1.34	0
3	ACT	A	507	-	3,3,3	0.82	0	3,3,3	1.72	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	B	503	-	5,5,5	0.27	0	5,5,5	1.09	0
3	ACT	B	509	-	3,3,3	0.80	0	3,3,3	1.31	0
2	GOL	A	508	-	5,5,5	0.34	0	5,5,5	0.51	0
3	ACT	B	505	-	3,3,3	0.91	0	3,3,3	1.46	0
4	SO4	A	519	-	4,4,4	0.14	0	6,6,6	0.28	0
2	GOL	A	515	-	5,5,5	0.55	0	5,5,5	0.45	0
3	ACT	A	509	-	3,3,3	0.88	0	3,3,3	1.31	0
2	GOL	A	506	-	5,5,5	0.38	0	5,5,5	0.74	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	GOL	A	504	-	-	0/4/4/4	-
2	GOL	B	503	-	-	3/4/4/4	-
2	GOL	A	508	-	-	2/4/4/4	-
2	GOL	A	510	-	-	4/4/4/4	-
2	GOL	A	503	-	-	1/4/4/4	-
2	GOL	A	515	-	-	4/4/4/4	-
2	GOL	A	505	-	-	2/4/4/4	-
2	GOL	A	506	-	-	0/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	507	ACT	OXT-C-O	-2.21	113.91	122.05
3	A	511	ACT	OXT-C-O	-2.20	113.94	122.05
3	B	506	ACT	OXT-C-O	-2.19	113.99	122.05
3	B	504	ACT	OXT-C-O	-2.01	114.64	122.05
3	A	507	ACT	OXT-C-CH3	2.01	123.47	115.18

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	505	GOL	O1-C1-C2-C3
2	A	508	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	510	GOL	O1-C1-C2-C3
2	A	510	GOL	C1-C2-C3-O3
2	A	515	GOL	O1-C1-C2-O2
2	A	515	GOL	O1-C1-C2-C3
2	A	503	GOL	C1-C2-C3-O3
2	A	508	GOL	C1-C2-C3-O3
2	A	515	GOL	C1-C2-C3-O3
2	B	503	GOL	O1-C1-C2-C3
2	A	505	GOL	O1-C1-C2-O2
2	A	510	GOL	O1-C1-C2-O2
2	A	510	GOL	O2-C2-C3-O3
2	A	515	GOL	O2-C2-C3-O3
2	B	503	GOL	O1-C1-C2-O2
2	B	503	GOL	O2-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	514	ACT	2	0
4	A	517	SO4	1	0
2	A	503	GOL	0	1
3	A	511	ACT	2	0
3	B	508	ACT	4	0
3	B	505	ACT	2	0
2	A	515	GOL	6	0
2	A	506	GOL	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	498/502 (99%)	-0.22	13 (2%)	56	61	13, 22, 38, 50	0
1	B	498/502 (99%)	0.01	24 (4%)	30	36	13, 27, 49, 61	1 (0%)
All	All	996/1004 (99%)	-0.10	37 (3%)	41	48	13, 25, 44, 61	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	5.3
1	B	329	GLY	5.3
1	B	58	GLU	5.0
1	B	500	VAL	5.0
1	A	58	GLU	4.5
1	B	382	TYR	4.5
1	B	499	PRO	3.9
1	B	328	ALA	3.8
1	B	330	LYS	3.6
1	A	3	PRO	3.5
1	A	329	GLY	3.4
1	B	3	PRO	3.3
1	A	382	TYR	3.3
1	A	442	HIS	3.2
1	B	284	TYR	3.1
1	B	336	ASN	2.9
1	B	327	PRO	2.8
1	A	328	ALA	2.6
1	A	172	LEU	2.6
1	A	174	GLN	2.6
1	B	442[A]	HIS	2.5
1	B	338	GLN	2.5
1	B	57	SER	2.5
1	A	337	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	60	GLY	2.4
1	B	337	GLY	2.3
1	A	133	LEU	2.3
1	B	125	ALA	2.3
1	A	349	THR	2.3
1	B	349	THR	2.2
1	B	173	ASN	2.2
1	B	309	GLN	2.2
1	A	175	TYR	2.2
1	B	56	HIS	2.1
1	B	281	ASN	2.1
1	B	4	ASP	2.1
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 monosaccharides 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
3	ACT	A	509	4/4	0.72	0.22	64,64,64,64	0
2	GOL	A	510	6/6	0.73	0.27	49,51,52,52	0
2	GOL	A	515	6/6	0.74	0.19	64,67,68,70	0
2	GOL	A	508	6/6	0.74	0.20	52,53,53,54	0
2	GOL	A	506	6/6	0.79	0.31	54,57,57,57	0
3	ACT	A	512	4/4	0.80	0.17	44,46,46,46	0
3	ACT	A	513	4/4	0.82	0.17	45,46,46,46	0
3	ACT	A	514	4/4	0.83	0.29	41,43,43,43	0
2	GOL	A	503	6/6	0.84	0.19	37,43,46,47	0
2	GOL	A	505	6/6	0.85	0.18	37,39,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	B	503	6/6	0.85	0.14	34,37,39,41	0
3	ACT	A	516	4/4	0.85	0.14	56,56,56,56	0
3	ACT	B	509	4/4	0.85	0.21	46,46,47,47	0
3	ACT	B	505	4/4	0.87	0.14	62,62,62,63	0
3	ACT	A	507	4/4	0.87	0.22	57,57,57,57	0
2	GOL	A	504	6/6	0.88	0.16	25,34,35,38	0
3	ACT	B	507	4/4	0.89	0.18	48,48,48,49	0
3	ACT	A	511	4/4	0.92	0.18	40,40,41,41	0
3	ACT	B	508	4/4	0.95	0.12	44,44,45,45	0
4	SO4	A	517	5/5	0.95	0.12	39,40,40,41	5
4	SO4	A	518	5/5	0.95	0.15	40,41,43,43	5
4	SO4	A	519	5/5	0.96	0.14	50,51,51,54	0
3	ACT	B	504	4/4	0.97	0.08	40,40,41,41	0
3	ACT	B	506	4/4	0.98	0.07	27,28,28,28	0
4	SO4	B	510	5/5	0.99	0.11	41,42,43,45	0

6.5 Other polymers (i)

There are no such residues in this entry.