Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:42 AM GMT

PDB ID	:	3MVY
Title	:	X-ray structure of the diatomic oxo-intermediate NikA/1-Int', prior hydroxylation
Authors	:	Cavazza, C.; Bochot, C.; Rousselot-Pailley, P.; Carpentier, P.; Cherrier, M.V.; Martin, L.; Marchi-Delapierre, C.; Fontecilla-Camps, J.C.; Menage, S.
Deposited on	:	2010-05-05
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

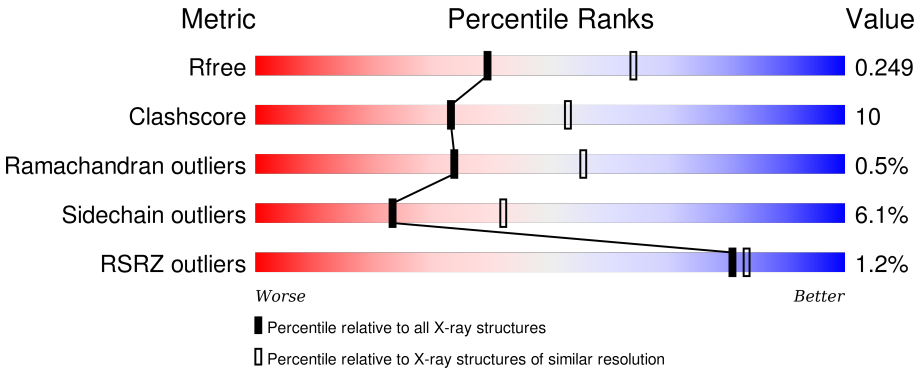
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 >=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 <=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	78% 18%
1	B	502	75% 20%

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	505	-	-	-	X
2	ACT	A	517	-	-	-	X
2	ACT	B	504	-	-	-	X
2	ACT	B	509	-	-	X	X
3	SO4	A	506	-	-	-	X
4	GOL	A	507	-	-	-	X
4	GOL	A	509	-	-	-	X
4	GOL	A	516	-	-	-	X
4	GOL	A	518	-	-	-	X
4	GOL	B	505	-	-	-	X
4	GOL	B	510	-	-	-	X

2 Entry composition

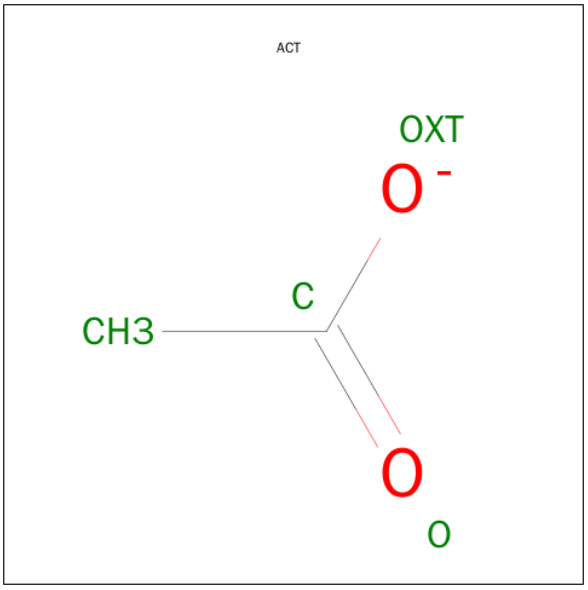
There are 9 unique types of molecules in this entry. The entry contains 8373 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	4	2	0
			3955	2535	670	740	10			
1	B	497	Total	C	N	O	S	0	0	0
			3925	2516	662	737	10			

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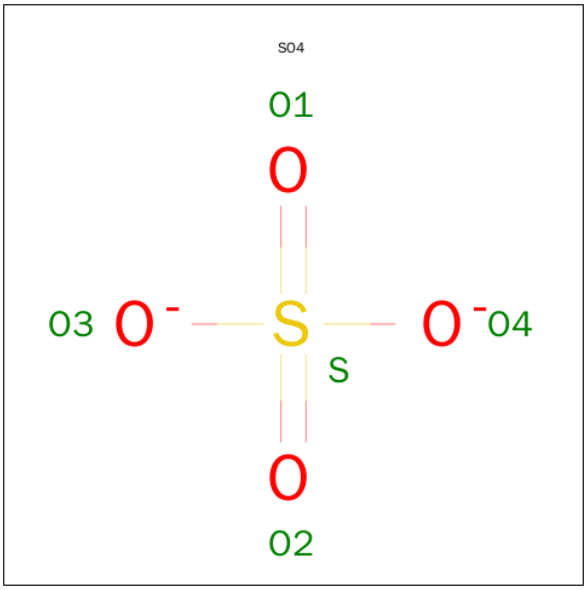
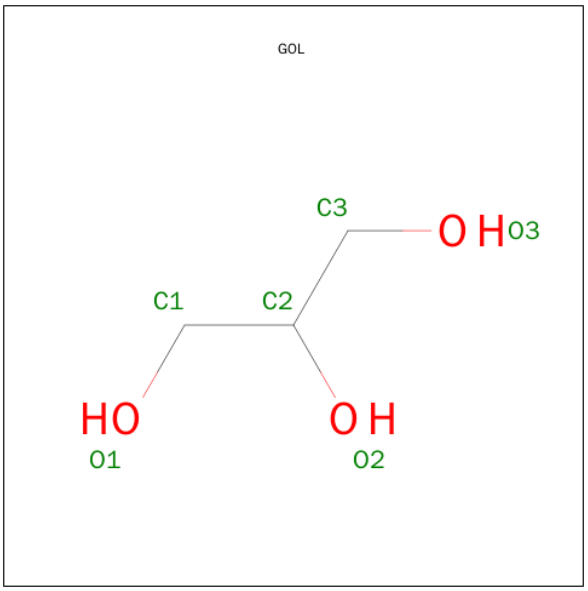
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

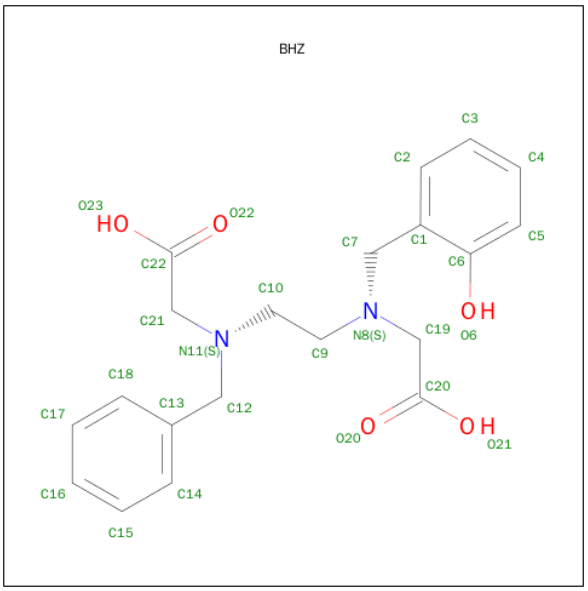


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

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

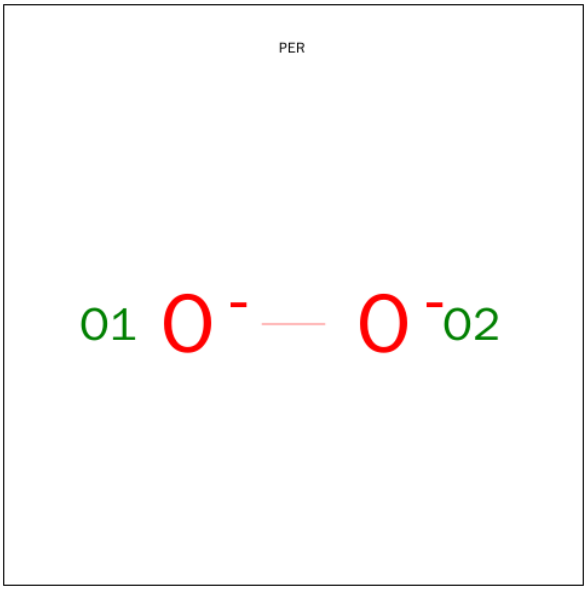
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Fe 1 1	0	0
5	A	1	Total Fe 1 1	0	0

- Molecule 6 is 2-[2-[CARBOXYMETHYL(PHENYLMETHYL)AMINO]ETHYL-[(2-HYDROXYPHENYL)METHYL]AMINO]ETHANOIC ACID (three-letter code: BHZ) (formula: $C_{20}H_{24}N_2O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 27 20 2 5	0	0
6	B	1	Total C N O 27 20 2 5	0	0

- Molecule 7 is PEROXIDE ION (three-letter code: PER) (formula: O_2).



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

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

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

- Molecule 9 is water.

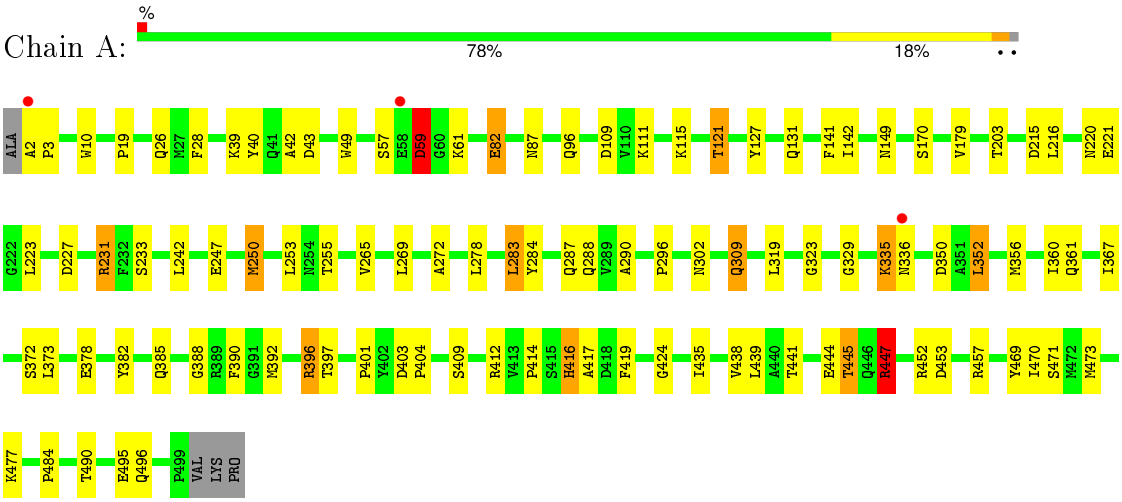
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	193	Total O 193 193	0	0
9	B	157	Total O 157 157	0	0

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 (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.

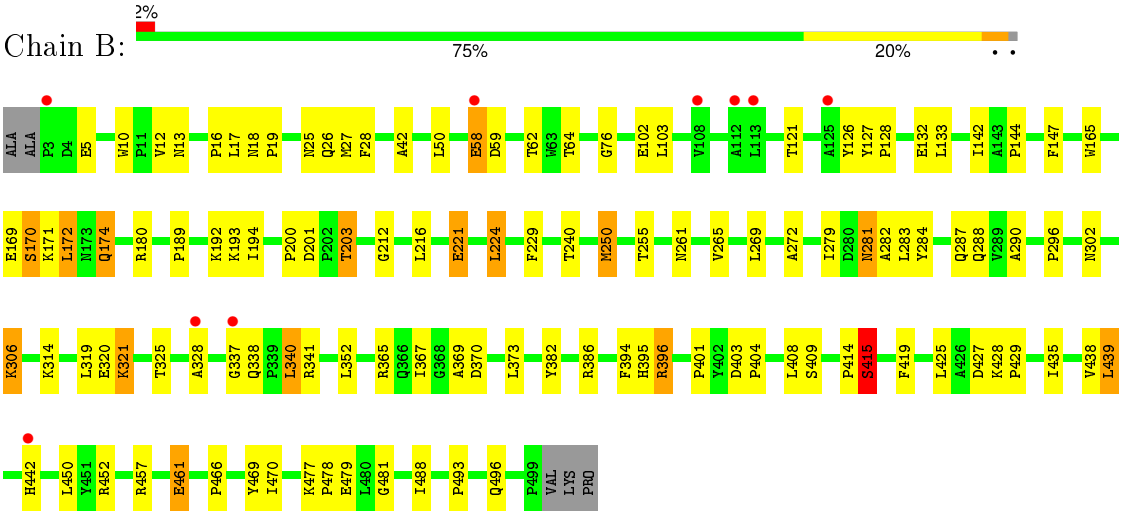
- Molecule 1: Nickel-binding periplasmic protein

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	86.98Å 95.17Å 125.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.49 – 2.50 43.49 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.49-2.50) 99.6 (43.49-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.88 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.173 , 0.249 0.177 , 0.249	Depositor DCC
R_{free} test set	1823 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 36448 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8373	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, PER, BHZ, FE, ACT, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.75	0/4065	0.79	3/5540 (0.1%)
1	B	0.73	0/4029	0.78	3/5492 (0.1%)
All	All	0.74	0/8094	0.78	6/11032 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	224	LEU	CA-CB-CG	5.99	129.08	115.30
1	B	396	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	B	396	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	227	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	329	GLY	N-CA-C	-5.38	99.66	113.10
1	A	447	ARG	NE-CZ-NH2	-5.27	117.67	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	59	ASP	Peptide

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	3955	0	3895	81	0
1	B	3925	0	3846	89	3
2	A	16	0	12	0	0
2	B	12	0	9	3	0
3	A	5	0	0	0	0
4	A	36	0	48	6	0
4	B	12	0	16	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	27	0	21	1	0
6	B	27	0	21	2	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	A	2	0	0	0	0
9	A	193	0	0	9	3
9	B	157	0	0	9	0
All	All	8373	0	7868	164	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (164) 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:59:ASP:HB3	1:A:61:LYS:H	1.02	1.14
1:A:149:ASN:H	4:A:508:GOL:H11	1.07	1.10
1:A:59:ASP:HB3	1:A:61:LYS:N	1.80	0.97
1:A:335:LYS:O	1:A:336:ASN:CB	2.13	0.93
1:A:220:ASN:HB3	4:A:515:GOL:H11	1.50	0.91
1:A:57:SER:OG	1:A:59:ASP:HB2	1.71	0.90
1:A:453:ASP:O	1:A:457:ARG:HG3	1.71	0.90
1:B:250:MET:CE	1:B:396:ARG:HA	2.02	0.90
1:B:414:PRO:O	1:B:415:SER:HB2	1.70	0.89
1:B:425:LEU:HD22	1:B:461:GLU:HG3	1.54	0.88
1:A:87:ASN:HD21	1:A:142:ILE:H	1.23	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:MET:HE1	1:B:396:ARG:HA	1.57	0.87
1:A:323:GLY:O	1:A:335:LYS:HB2	1.77	0.85
1:B:314:LYS:NZ	2:B:509:ACT:H2	1.93	0.84
1:B:337:GLY:O	1:B:338:GLN:HG2	1.82	0.80
1:B:337:GLY:C	1:B:338:GLN:HG2	2.01	0.80
1:B:10:TRP:HE1	1:B:26:GLN:HE21	1.29	0.80
1:A:335:LYS:O	1:A:336:ASN:HB3	1.83	0.78
1:A:149:ASN:N	4:A:508:GOL:H11	1.93	0.78
1:A:335:LYS:O	1:A:335:LYS:HG2	1.83	0.78
1:B:425:LEU:CD2	1:B:461:GLU:HG3	2.13	0.77
1:B:314:LYS:HZ1	2:B:509:ACT:H2	1.50	0.77
1:A:10:TRP:HE1	1:A:26:GLN:HE21	1.33	0.76
1:B:180:ARG:HD3	1:B:192:LYS:HA	1.69	0.74
1:A:444:GLU:HG3	9:A:619:HOH:O	1.86	0.74
1:B:180:ARG:NH1	1:B:189:PRO:O	2.21	0.73
1:A:378:GLU:HG2	1:A:382:TYR:CE2	2.24	0.72
1:A:445:THR:HB	1:B:478:PRO:HB2	1.73	0.71
1:B:320:GLU:OE1	1:B:325:THR:HG22	1.89	0.71
1:B:27:MET:HG3	9:B:518:HOH:O	1.91	0.70
1:A:43:ASP:HB3	9:B:517:HOH:O	1.90	0.70
1:B:10:TRP:HE1	1:B:26:GLN:NE2	1.88	0.70
1:B:382:TYR:CE2	1:B:386:ARG:HD2	2.27	0.70
1:A:335:LYS:O	1:A:336:ASN:HB2	1.91	0.69
1:A:444:GLU:HG2	1:B:481:GLY:CA	2.21	0.69
1:B:457:ARG:O	1:B:461:GLU:HB2	1.95	0.66
1:A:444:GLU:HG2	1:B:481:GLY:HA2	1.79	0.65
1:B:496:GLN:HG2	9:B:653:HOH:O	1.96	0.65
1:B:19:PRO:HG3	1:B:142:ILE:HB	1.79	0.65
1:A:82:GLU:HB2	9:A:712:HOH:O	1.97	0.64
1:A:253:LEU:HD22	1:A:392:MET:HG2	1.79	0.64
1:B:58:GLU:HG2	1:B:59:ASP:N	2.12	0.64
1:A:416:HIS:HE1	9:A:622:HOH:O	1.81	0.64
1:A:131:GLN:HG3	9:A:685:HOH:O	1.97	0.64
1:A:231[A]:ARG:HG3	9:A:569:HOH:O	1.97	0.64
1:A:356:MET:O	1:A:360:ILE:HG12	1.98	0.63
1:A:59:ASP:CB	1:A:61:LYS:H	1.94	0.62
1:B:306:LYS:HD3	9:B:586:HOH:O	1.98	0.62
1:A:444:GLU:CG	1:B:481:GLY:HA2	2.29	0.61
1:A:361:GLN:HE22	4:A:509:GOL:H2	1.64	0.61
1:A:253:LEU:CD2	1:A:392:MET:HG2	2.32	0.60
1:A:385:GLN:HG2	1:A:417:ALA:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:THR:HA	4:A:515:GOL:H31	1.84	0.59
1:B:144:PRO:HA	1:B:147:PHE:CE2	2.39	0.58
1:B:250:MET:HE1	1:B:396:ARG:CA	2.30	0.58
1:B:409:SER:HB2	1:B:439:LEU:HD21	1.85	0.57
1:B:414:PRO:O	1:B:415:SER:CB	2.44	0.57
1:B:341:ARG:HH11	1:B:341:ARG:HG3	1.69	0.57
1:A:233:SER:O	1:B:452:ARG:NH2	2.37	0.57
1:A:287:GLN:HE21	1:A:470:ILE:HA	1.69	0.57
1:A:296:PRO:HB3	1:A:302:ASN:HD22	1.70	0.56
1:B:283:LEU:CD2	1:B:352:LEU:HD11	2.36	0.56
1:B:180:ARG:HD3	1:B:192:LYS:HD2	1.88	0.56
1:B:314:LYS:HZ2	2:B:509:ACT:H2	1.69	0.56
1:A:87:ASN:ND2	1:A:141:PHE:HA	2.21	0.54
1:B:250:MET:HE3	1:B:396:ARG:HA	1.88	0.54
6:A:511:BHZ:O6	6:A:511:BHZ:H18	2.07	0.54
1:B:201:ASP:OD1	1:B:203:THR:HB	2.08	0.54
1:A:109:ASP:HB3	1:A:121:THR:HG23	1.91	0.53
1:B:341:ARG:HG3	1:B:370:ASP:HB3	1.91	0.53
1:A:10:TRP:HE1	1:A:26:GLN:NE2	2.04	0.53
1:A:278:LEU:C	1:A:278:LEU:HD23	2.29	0.52
1:B:171:LYS:O	1:B:172:LEU:O	2.27	0.52
1:A:221:GLU:OE2	1:A:396:ARG:NH2	2.40	0.52
1:A:309:GLN:H	1:A:309:GLN:CD	2.10	0.52
1:A:115:LYS:HA	9:A:676:HOH:O	2.09	0.51
1:A:414:PRO:HA	1:A:419:PHE:CD1	2.45	0.51
1:B:250:MET:HB2	1:B:466:PRO:HA	1.91	0.51
1:B:5:GLU:HG2	1:B:193:LYS:HB3	1.93	0.51
1:A:477:LYS:HE2	9:A:574:HOH:O	2.11	0.50
1:B:221:GLU:HG3	1:B:470:ILE:HG21	1.92	0.50
1:B:18:ASN:H	1:B:25:ASN:HD21	1.59	0.50
1:A:42:ALA:HB3	1:B:42:ALA:HB3	1.94	0.50
1:B:470:ILE:C	1:B:470:ILE:HD12	2.32	0.50
1:A:42:ALA:CB	1:B:42:ALA:HB3	2.41	0.50
1:B:62:THR:HG23	1:B:121:THR:HG22	1.94	0.50
1:B:272:ALA:HB2	1:B:367:ILE:HD13	1.94	0.50
1:A:272:ALA:HB2	1:A:367:ILE:HD13	1.94	0.49
1:B:17:LEU:H	1:B:25:ASN:ND2	2.09	0.49
1:B:102:GLU:HB3	1:B:126:TYR:OH	2.13	0.49
1:A:396:ARG:HG2	1:A:397:THR:O	2.13	0.49
1:B:428:LYS:HB3	1:B:429:PRO:HD3	1.94	0.49
1:A:350:ASP:OD1	1:A:350:ASP:C	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ASP:OD2	1:A:457:ARG:HD2	2.14	0.48
1:B:126:TYR:CZ	1:B:128:PRO:HG2	2.49	0.48
1:A:215:ASP:OD2	1:A:477:LYS:HE3	2.14	0.48
1:B:493:PRO:HB2	1:B:496:GLN:HE21	1.79	0.47
1:B:200:PRO:HD2	9:B:553:HOH:O	2.14	0.47
1:A:290:ALA:HA	1:A:469:TYR:CE2	2.49	0.47
1:B:403:ASP:HA	1:B:404:PRO:HA	1.74	0.47
1:A:2:ALA:N	1:A:3:PRO:HD3	2.30	0.47
1:B:438:VAL:HG12	1:B:450:LEU:HB2	1.97	0.47
1:B:408:LEU:O	1:B:435:ILE:HD13	2.15	0.46
1:A:250:MET:HE1	1:A:397:THR:HG23	1.98	0.46
1:B:296:PRO:HB3	1:B:302:ASN:HD22	1.80	0.46
1:B:427:ASP:HA	9:B:564:HOH:O	2.15	0.46
1:A:409:SER:O	1:A:412[B]:ARG:HB2	2.15	0.46
1:B:103:LEU:HB2	1:B:132:GLU:OE2	2.15	0.46
6:B:507:BHZ:O20	9:B:669:HOH:O	2.21	0.46
1:A:265:VAL:O	1:A:269:LEU:HG	2.15	0.46
1:A:484:PRO:HG2	1:A:496:GLN:HB2	1.98	0.46
1:B:282:ALA:C	1:B:283:LEU:HD23	2.35	0.46
1:B:401:PRO:HD3	1:B:488:ILE:HG12	1.98	0.46
1:A:2:ALA:N	1:A:3:PRO:CD	2.79	0.46
1:A:388:GLY:HA2	1:A:390:PHE:CE2	2.51	0.46
1:B:172:LEU:O	1:B:174:GLN:N	2.45	0.45
1:A:42:ALA:HB3	1:B:42:ALA:CB	2.47	0.45
1:A:283:LEU:HD12	1:A:352:LEU:HD21	1.98	0.45
1:B:365:ARG:HH11	1:B:365:ARG:HG3	1.81	0.45
1:A:87:ASN:ND2	1:A:142:ILE:H	2.03	0.45
1:A:111:LYS:HE3	1:A:111:LYS:HB2	1.80	0.44
1:A:287:GLN:HE22	1:A:471:SER:H	1.66	0.44
1:B:394:PHE:HB3	4:B:510:GOL:H2	1.99	0.44
1:B:425:LEU:HD22	1:B:461:GLU:CG	2.38	0.44
1:B:203:THR:CG2	9:B:546:HOH:O	2.65	0.44
1:B:27:MET:HE3	6:B:507:BHZ:O23	2.18	0.44
1:A:121:THR:HG22	9:A:650:HOH:O	2.17	0.44
1:B:283:LEU:HD13	1:B:287:GLN:HG3	1.99	0.44
1:B:283:LEU:CD1	1:B:287:GLN:HG3	2.48	0.43
1:A:378:GLU:HG2	1:A:382:TYR:CZ	2.53	0.43
1:B:144:PRO:HA	1:B:147:PHE:CD2	2.53	0.43
1:B:212:GLY:HA2	1:B:477:LYS:HZ1	1.82	0.43
1:B:10:TRP:CE2	1:B:28:PHE:HE1	2.37	0.43
1:B:169:GLU:HG2	1:B:170:SER:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:MET:HE3	1:B:395:HIS:C	2.38	0.43
1:A:247:GLU:OE2	9:A:602:HOH:O	2.21	0.43
1:B:229:PHE:CE1	1:B:240:THR:HB	2.53	0.43
1:B:290:ALA:HA	1:B:469:TYR:CE2	2.54	0.43
1:A:255:THR:O	1:A:424:GLY:HA3	2.19	0.43
1:A:223:LEU:HB3	1:A:473:MET:HE2	2.01	0.42
1:B:165:TRP:CH2	1:B:194:ILE:HD11	2.54	0.42
1:B:16:PRO:O	1:B:17:LEU:HB2	2.19	0.42
1:B:281:ASN:HA	1:B:281:ASN:HD22	1.63	0.42
1:A:242:LEU:HD12	1:A:473:MET:HB3	2.02	0.42
1:A:441:THR:O	1:A:447:ARG:NH1	2.47	0.42
1:A:57:SER:HG	1:A:59:ASP:HB2	1.79	0.42
1:B:203:THR:HG22	9:B:546:HOH:O	2.19	0.42
1:A:435:ILE:O	1:A:438:VAL:HG12	2.20	0.42
1:B:265:VAL:O	1:B:269:LEU:HG	2.19	0.42
1:B:425:LEU:HD21	1:B:461:GLU:HG3	1.98	0.42
1:B:180:ARG:CD	1:B:192:LYS:HA	2.45	0.42
1:A:149:ASN:H	4:A:508:GOL:C1	2.00	0.41
1:A:470:ILE:HD12	1:A:470:ILE:C	2.40	0.41
1:A:39:LYS:HD2	1:A:49:TRP:CZ3	2.55	0.41
1:B:171:LYS:HB3	1:B:174:GLN:HG3	2.03	0.41
1:A:403:ASP:HA	1:A:404:PRO:HA	1.81	0.41
1:B:340:LEU:HD13	1:B:369:ALA:HB2	2.03	0.41
1:A:19:PRO:HG3	1:A:142:ILE:HB	2.03	0.40
1:B:255:THR:O	1:B:261:ASN:HA	2.21	0.40
1:B:12:VAL:HG23	1:B:13:ASN:O	2.22	0.40
1:A:40:TYR:CE1	1:A:401:PRO:HB3	2.56	0.40
1:A:28:PHE:C	1:A:28:PHE:CD2	2.94	0.40
1:A:495:GLU:CD	1:A:495:GLU:H	2.24	0.40
1:B:414:PRO:HA	1:B:419:PHE:CD1	2.56	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:LYS:CE	9:A:617:HOH:O[3_555]	0.76	1.44
1:B:321:LYS:NZ	9:A:617:HOH:O[3_555]	0.84	1.36
1:B:321:LYS:CD	9:A:617:HOH:O[3_555]	1.70	0.50

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	498/502 (99%)	477 (96%)	20 (4%)	1 (0%)	52 75
1	B	495/502 (99%)	473 (96%)	18 (4%)	4 (1%)	24 41
All	All	993/1004 (99%)	950 (96%)	38 (4%)	5 (0%)	34 55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	B	172	LEU
1	B	415	SER
1	B	328	ALA
1	B	76	GLY

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	420/425 (99%)	394 (94%)	26 (6%)	23 41
1	B	416/425 (98%)	390 (94%)	26 (6%)	22 40
All	All	836/850 (98%)	784 (94%)	52 (6%)	23 41

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	GLU

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Mol	Chain	Res	Type
1	A	96	GLN
1	A	121	THR
1	A	127	TYR
1	A	170	SER
1	A	179	VAL
1	A	203	THR
1	A	216	LEU
1	A	231[A]	ARG
1	A	231[B]	ARG
1	A	250	MET
1	A	283	LEU
1	A	284	TYR
1	A	288	GLN
1	A	309	GLN
1	A	319	LEU
1	A	335	LYS
1	A	352	LEU
1	A	372	SER
1	A	373	LEU
1	A	396	ARG
1	A	416	HIS
1	A	439	LEU
1	A	445	THR
1	A	447	ARG
1	A	452	ARG
1	B	50	LEU
1	B	58	GLU
1	B	64	THR
1	B	127	TYR
1	B	133	LEU
1	B	170	SER
1	B	174	GLN
1	B	203	THR
1	B	216	LEU
1	B	221	GLU
1	B	224	LEU
1	B	250	MET
1	B	279	ILE
1	B	281	ASN
1	B	284	TYR
1	B	288	GLN
1	B	306	LYS

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Mol	Chain	Res	Type
1	B	319	LEU
1	B	321	LYS
1	B	340	LEU
1	B	373	LEU
1	B	415	SER
1	B	439	LEU
1	B	442	HIS
1	B	461	GLU
1	B	479	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	87	ASN
1	A	197	ASN
1	A	287	GLN
1	A	302	ASN
1	A	361	GLN
1	A	366	GLN
1	A	385	GLN
1	A	416	HIS
1	A	446	GLN
1	B	25	ASN
1	B	26	GLN
1	B	173	ASN
1	B	234	GLN
1	B	244	GLN
1	B	281	ASN
1	B	302	ASN
1	B	336	ASN
1	B	385	GLN
1	B	416	HIS
1	B	442	HIS
1	B	496	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	503	-	1,3,3	1.03	0	0,3,3	0.00	-
2	ACT	A	504	-	1,3,3	2.01	1 (100%)	0,3,3	0.00	-
2	ACT	A	505	-	1,3,3	2.23	1 (100%)	0,3,3	0.00	-
3	SO4	A	506	-	4,4,4	0.17	0	6,6,6	0.24	0
4	GOL	A	507	-	5,5,5	0.44	0	5,5,5	0.45	0
4	GOL	A	508	-	5,5,5	0.48	0	5,5,5	0.77	0
4	GOL	A	509	-	5,5,5	0.35	0	5,5,5	0.24	0
6	BHZ	A	511	5	22,28,28	0.77	0	30,36,36	1.49	5 (16%)
7	PER	A	512	5	0,1,1	0.00	-	0,0,0	0.00	-
4	GOL	A	515	-	5,5,5	0.50	0	5,5,5	1.44	0
4	GOL	A	516	-	5,5,5	0.36	0	5,5,5	0.38	0
2	ACT	A	517	-	1,3,3	0.53	0	0,3,3	0.00	-
4	GOL	A	518	-	5,5,5	0.48	0	5,5,5	0.77	0
2	ACT	B	503	-	1,3,3	1.49	0	0,3,3	0.00	-
2	ACT	B	504	-	1,3,3	1.66	0	0,3,3	0.00	-
4	GOL	B	505	-	5,5,5	0.31	0	5,5,5	0.47	0
6	BHZ	B	507	5	22,28,28	1.11	2 (9%)	30,36,36	1.46	5 (16%)
7	PER	B	508	5	0,1,1	0.00	-	0,0,0	0.00	-
2	ACT	B	509	-	1,3,3	1.58	0	0,3,3	0.00	-
4	GOL	B	510	-	5,5,5	0.45	0	5,5,5	0.86	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	503	-	-	0/0/0/0	0/0/0/0
2	ACT	A	504	-	-	0/0/0/0	0/0/0/0
2	ACT	A	505	-	-	0/0/0/0	0/0/0/0
3	SO4	A	506	-	-	0/0/0/0	0/0/0/0
4	GOL	A	507	-	-	0/4/4/4	0/0/0/0
4	GOL	A	508	-	-	0/4/4/4	0/0/0/0
4	GOL	A	509	-	-	0/4/4/4	0/0/0/0
6	BHZ	A	511	5	-	0/17/21/21	0/2/2/2
7	PER	A	512	5	-	0/0/0/0	0/0/0/0
4	GOL	A	515	-	-	0/4/4/4	0/0/0/0
4	GOL	A	516	-	-	0/4/4/4	0/0/0/0
2	ACT	A	517	-	-	0/0/0/0	0/0/0/0
4	GOL	A	518	-	-	0/4/4/4	0/0/0/0
2	ACT	B	503	-	-	0/0/0/0	0/0/0/0
2	ACT	B	504	-	-	0/0/0/0	0/0/0/0
4	GOL	B	505	-	-	0/4/4/4	0/0/0/0
6	BHZ	B	507	5	-	0/17/21/21	0/2/2/2
7	PER	B	508	5	-	0/0/0/0	0/0/0/0
2	ACT	B	509	-	-	0/0/0/0	0/0/0/0
4	GOL	B	510	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	504	ACT	CH3-C	2.01	1.51	1.48
2	A	505	ACT	CH3-C	2.23	1.51	1.48
6	B	507	BHZ	C12-C13	2.64	1.56	1.51
6	B	507	BHZ	C7-C1	2.65	1.56	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	507	BHZ	C20-C19-N8	-3.86	107.82	113.53
6	A	511	BHZ	C12-N11-C10	-3.52	103.93	111.28
6	A	511	BHZ	C20-C19-N8	-3.00	109.09	113.53
6	B	507	BHZ	C21-N11-C12	-2.30	106.80	110.73
6	B	507	BHZ	C19-N8-C9	-2.23	106.61	111.28
6	B	507	BHZ	C21-N11-C10	-2.22	106.64	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	511	BHZ	C1-C7-N8	-2.21	108.93	112.79
6	A	511	BHZ	C18-C13-C14	2.06	121.43	118.13
6	A	511	BHZ	C7-C1-C6	2.59	123.08	120.48
6	B	507	BHZ	C7-C1-C6	4.03	124.53	120.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	508	GOL	3	0
4	A	509	GOL	1	0
6	A	511	BHZ	1	0
4	A	515	GOL	2	0
6	B	507	BHZ	2	0
2	B	509	ACT	3	0
4	B	510	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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%)	-0.60	3 (0%)	90	91	8, 16, 30, 43	1 (0%)
1	B	497/502 (99%)	-0.34	9 (1%)	71	75	10, 24, 46, 53	1 (0%)
All	All	995/1004 (99%)	-0.47	12 (1%)	81	83	8, 20, 42, 53	2 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	336	ASN	3.4
1	B	108	VAL	3.4
1	A	2	ALA	2.9
1	B	58	GLU	2.9
1	B	112	ALA	2.5
1	A	58	GLU	2.5
1	B	125	ALA	2.4
1	B	328	ALA	2.3
1	B	3	PRO	2.2
1	B	337	GLY	2.1
1	B	442	HIS	2.1
1	B	113	LEU	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 carbohydrates 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. 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^{th} 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^2)	Q<0.9
4	GOL	A	518	6/6	0.70	0.37	12.30	20,20,20,20	0
3	SO4	A	506	5/5	0.76	0.27	10.45	90,90,90,90	0
2	ACT	A	517	4/4	0.79	0.23	7.44	20,20,20,20	0
4	GOL	A	507	6/6	0.83	0.19	5.55	40,42,42,42	0
2	ACT	B	504	4/4	0.81	0.32	4.53	73,73,73,73	0
4	GOL	A	509	6/6	0.73	0.31	4.33	3,11,13,14	0
2	ACT	B	509	4/4	0.96	0.17	4.29	37,37,37,37	0
4	GOL	B	510	6/6	0.87	0.18	4.08	49,51,52,52	0
4	GOL	B	505	6/6	0.89	0.17	2.94	33,34,35,36	0
4	GOL	A	516	6/6	0.96	0.14	2.29	28,31,31,32	0
2	ACT	A	505	4/4	0.91	0.18	2.06	39,39,39,39	0
4	GOL	A	515	6/6	0.91	0.18	1.22	18,24,26,29	0
6	BHZ	B	507	27/27	0.96	0.12	0.91	14,22,31,32	0
6	BHZ	A	511	27/27	0.97	0.14	0.74	16,18,31,32	0
5	FE	A	510	1/1	1.00	0.09	-	14,14,14,14	0
2	ACT	A	503	4/4	0.88	0.18	-	53,54,54,54	0
2	ACT	B	503	4/4	0.93	0.17	-	53,54,54,54	0
8	CL	A	513	1/1	0.99	0.06	-	27,27,27,27	0
2	ACT	A	504	4/4	0.95	0.11	-	45,45,45,45	0
7	PER	A	512	2/2	0.98	0.12	-	20,20,20,22	0
7	PER	B	508	2/2	0.97	0.08	-	25,25,25,30	0
5	FE	B	506	1/1	1.00	0.06	-	20,20,20,20	0
4	GOL	A	508	6/6	0.83	0.19	-	50,51,52,52	0
8	CL	A	514	1/1	0.95	0.08	-	42,42,42,42	0

6.5 Other polymers

There are no such residues in this entry.