



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:35 PM GMT

PDB ID : 3MVW
Title : X-ray structure of a "NikA+Iron complex" hybrid, NikA/1
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Deposited on : 2010-05-05
Resolution : 1.79 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

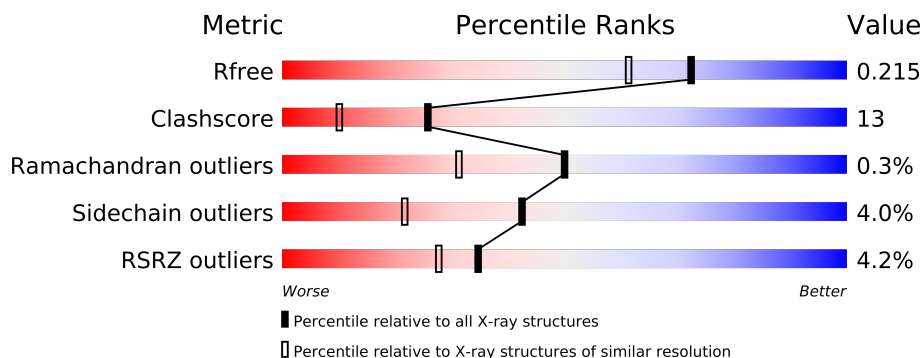
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.79 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}	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	502	
1	B	502	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	ACT	A	505	-	X
4	ACT	A	506	-	X
4	ACT	A	507	-	X
4	ACT	B	505	-	X
4	ACT	B	511	-	X
5	SO4	A	508	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	GOL	A	509	-	X
6	GOL	A	510	-	X
6	GOL	A	512	-	X
6	GOL	B	506	-	X

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 9006 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

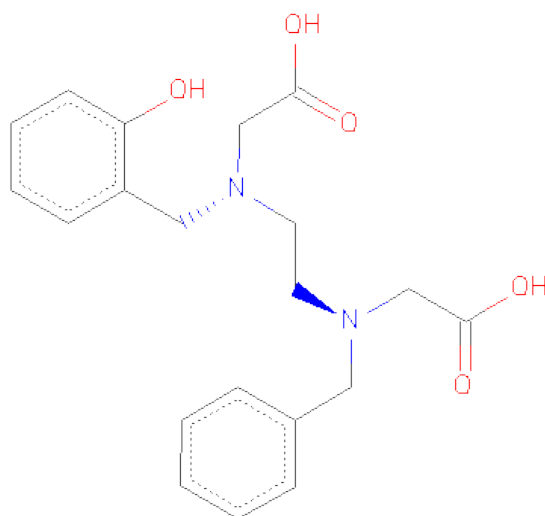
- Molecule 1 is a protein called Nickel-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	4	10	0
			3998	2563	672	753	10			
1	B	498	Total	C	N	O	S	0	5	0
			3970	2546	668	745	11			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

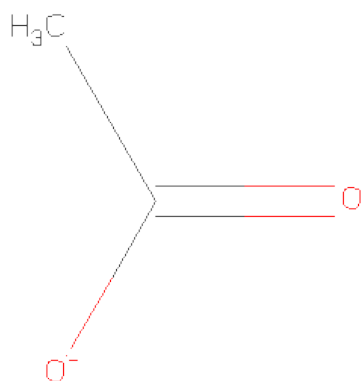
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 2-[2-[CARBOXYMETHYL(PHENYLMETHYL)AMINO]ETHYL-[(2-HYDROXYPHENYL)METHYL]AMINO]ETHANOICACID (three-letter code: BHZ) (formula: C₂₀H₂₄N₂O₅).



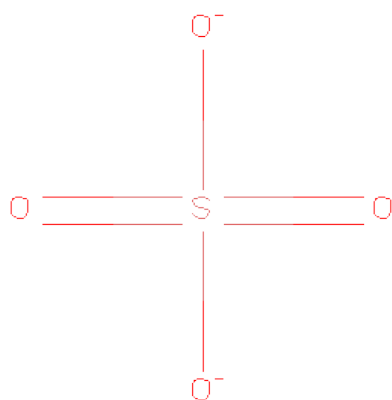
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	20	2	5		
3	B	1	Total	C	N	O	0	0
			27	20	2	5		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



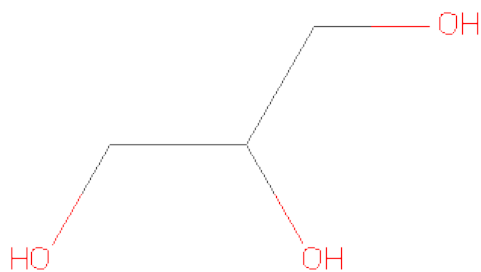
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

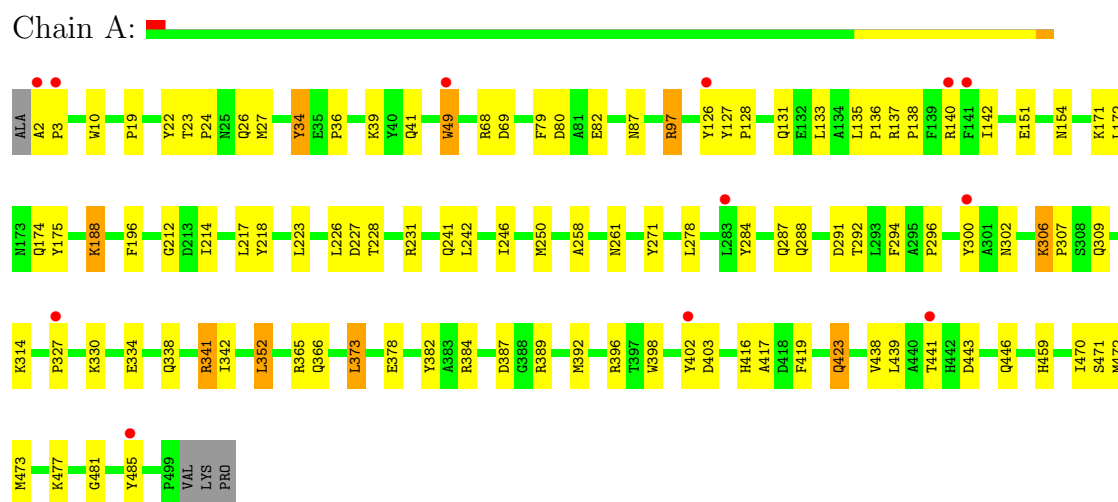
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	483	Total	O	0	0
			483	483		
8	B	416	Total	O	0	0
			416	416		

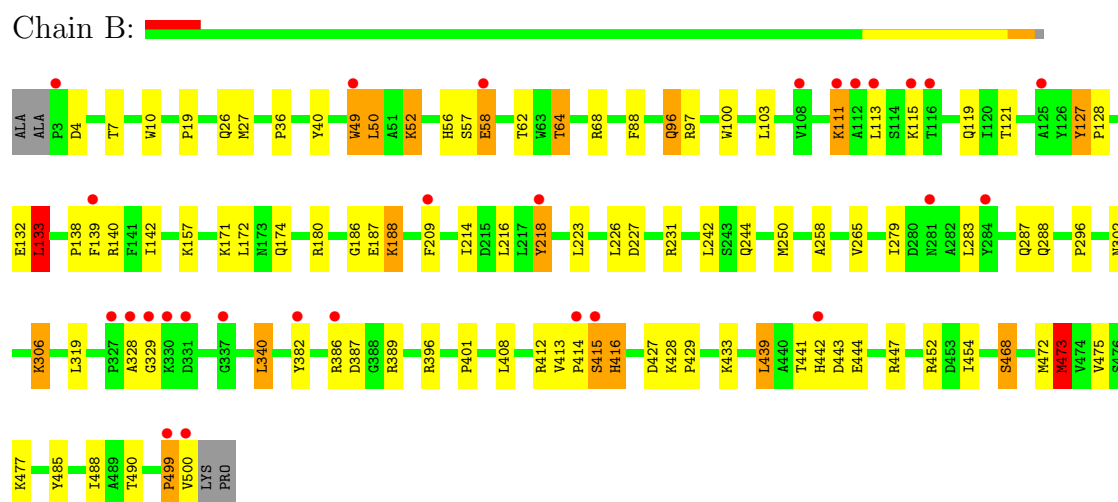
3 Residue-property plots

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



- Molecule 1: Nickel-binding periplasmic protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.97Å 94.58Å 124.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.29 – 1.79 47.29 – 1.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.29-1.79) 99.6 (47.29-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.47 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.159 , 0.204 0.175 , 0.215	Depositor DCC
R_{free} test set	4853 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 34.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 97054 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9006	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, BHZ, SO4, ACT, FE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.21	2/4123 (0.0%)	1.02	13/5620 (0.2%)
1	B	1.19	6/4086 (0.1%)	1.01	8/5565 (0.1%)
All	All	1.20	8/8209 (0.1%)	1.02	21/11185 (0.2%)

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
1	B	0	3
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	40	TYR	CD2-CE2	6.00	1.48	1.39
1	B	258	ALA	CA-CB	5.41	1.63	1.52
1	B	216	LEU	C-O	-5.25	1.13	1.23
1	A	34	TYR	CG-CD2	5.23	1.46	1.39
1	B	132	GLU	CB-CG	5.19	1.62	1.52
1	B	88	PHE	CE2-CZ	5.10	1.47	1.37
1	A	417	ALA	CA-CB	5.10	1.63	1.52
1	B	265	VAL	CB-CG1	5.09	1.63	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	439	LEU	CB-CG-CD2	5.99	121.19	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	LEU	CB-CG-CD2	5.90	121.03	111.00
1	A	365	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	140	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	396	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	B	231	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	B	396	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	226	LEU	CA-CB-CG	-5.46	102.74	115.30
1	A	97	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	340	LEU	CB-CG-CD2	5.44	120.25	111.00
1	A	373	LEU	CB-CG-CD1	5.43	120.24	111.00
1	A	403	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	133	LEU	CB-CG-CD1	-5.36	101.88	111.00
1	A	384	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	242	LEU	CB-CG-CD1	-5.30	101.99	111.00
1	B	133	LEU	CB-CG-CD1	5.26	119.95	111.00
1	B	50	LEU	CB-CG-CD1	5.21	119.85	111.00
1	A	443	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	294	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	B	443	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	419	PHE	CB-CG-CD1	-5.02	117.29	120.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	288[A]	GLN	Mainchain
1	B	244[A]	GLN	Mainchain
1	B	468[A]	SER	Mainchain
1	B	473[A]	MET	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3998	0	3947	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3970	0	3923	104	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	21	6	0
3	B	27	0	21	1	0
4	A	12	0	9	0	0
4	B	8	0	6	4	1
5	A	5	0	0	0	0
6	A	36	0	48	21	0
6	B	18	0	23	2	0
7	A	2	0	0	3	0
7	B	2	0	0	0	0
8	A	483	0	0	25	1
8	B	416	0	0	21	0
All	All	9006	0	7998	217	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (217) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:209:PHE:CZ	1:B:475:VAL:HG12	1.62	1.34
1:B:306:LYS:HD3	1:B:306:LYS:N	1.55	1.16
1:B:306:LYS:H	1:B:306:LYS:CD	1.53	1.14
1:A:477:LYS:HE2	6:A:509:GOL:C3	1.80	1.11
1:A:387[B]:ASP:OD2	1:A:389:ARG:HG3	1.51	1.10
1:A:341:ARG:HH11	1:A:341:ARG:HG3	0.97	1.10
1:B:209:PHE:CZ	1:B:475:VAL:CG1	2.37	1.07
1:A:69:ASP:HA	6:A:512:GOL:H12	1.34	1.05
1:B:209:PHE:CE2	1:B:475:VAL:CG1	2.40	1.04
1:A:477:LYS:HE2	6:A:509:GOL:H31	1.04	1.03
1:B:442:HIS:H	1:B:442:HIS:CD2	1.76	1.02
1:B:414:PRO:O	8:B:943:HOH:O	1.79	1.00
1:A:27:MET:HG3	8:A:600:HOH:O	1.61	1.00
6:A:509:GOL:H12	8:A:536:HOH:O	1.62	0.99
1:B:64:THR:HG23	8:B:1063:HOH:O	1.62	0.98
1:B:306:LYS:HD3	1:B:306:LYS:H	0.84	0.97
1:A:341:ARG:NH1	1:A:341:ARG:HG3	1.68	0.97
1:A:477:LYS:CE	6:A:509:GOL:H31	1.96	0.95
1:B:287:GLN:HE22	1:B:473[B]:MET:CE	1.79	0.94
1:A:188:LYS:H	1:A:188:LYS:HD2	1.32	0.94
1:A:135:LEU:HD22	1:A:402:TYR:CZ	2.03	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:A:509:GOL:C1	8:A:536:HOH:O	2.15	0.92
1:B:414:PRO:O	1:B:415:SER:HB2	1.67	0.91
1:A:341:ARG:HH11	1:A:341:ARG:CG	1.84	0.91
1:B:209:PHE:CE1	1:B:475:VAL:HG12	2.07	0.88
1:B:485:TYR:HB3	6:B:506:GOL:H11	1.54	0.88
6:A:510:GOL:H12	8:A:860:HOH:O	1.72	0.87
1:B:427:ASP:HB3	8:B:675:HOH:O	1.73	0.87
1:B:287:GLN:HE22	1:B:473[B]:MET:HE3	1.39	0.87
1:B:477:LYS:HE3	8:B:1050:HOH:O	1.76	0.86
1:B:180:ARG:HD2	1:B:188:LYS:HG2	1.59	0.83
1:A:172:LEU:HD11	8:A:878:HOH:O	1.78	0.83
1:B:209:PHE:CE2	1:B:475:VAL:HG11	2.14	0.83
1:B:287:GLN:HG3	8:B:795:HOH:O	1.77	0.82
1:B:64:THR:CG2	8:B:1063:HOH:O	2.20	0.81
1:A:23[A]:THR:HG22	7:A:516:CL:CL	2.21	0.78
6:A:510:GOL:C1	8:A:860:HOH:O	2.27	0.78
1:A:151[B]:GLU:OE2	1:A:154:ASN:ND2	2.17	0.78
1:B:414:PRO:O	1:B:415:SER:CB	2.32	0.78
1:B:171:LYS:HG2	1:B:174:GLN:HG3	1.66	0.77
1:A:23[A]:THR:HG23	8:A:1037:HOH:O	1.86	0.76
1:B:287:GLN:NE2	1:B:473[B]:MET:HE3	2.01	0.75
1:A:171:LYS:HG3	1:A:175:TYR:CZ	2.20	0.75
1:A:387[B]:ASP:CG	1:A:389:ARG:HG3	2.05	0.75
1:B:287:GLN:NE2	1:B:473[B]:MET:CE	2.49	0.74
1:A:10:TRP:HE1	1:A:26:GLN:HE21	1.36	0.74
1:A:23[A]:THR:CG2	7:A:516:CL:CL	2.72	0.73
1:B:386:ARG:HA	1:B:415:SER:O	1.89	0.73
1:B:52:LYS:HG3	1:B:68:ARG:HG2	1.69	0.72
1:B:242:LEU:CD1	1:B:473[B]:MET:SD	2.78	0.72
1:B:27:MET:HG3	8:B:602:HOH:O	1.88	0.72
1:A:23[B]:THR:CG2	1:A:24:PRO:HA	2.20	0.71
1:A:23[B]:THR:HG23	1:A:24:PRO:HA	1.71	0.70
1:A:87:ASN:HD21	1:A:142:ILE:H	1.38	0.70
1:A:97:ARG:HH11	3:A:504:BHZ:C16	2.04	0.70
1:B:10:TRP:HE1	1:B:26:GLN:HE21	1.40	0.70
6:A:512:GOL:H31	8:A:794:HOH:O	1.89	0.70
1:B:58:GLU:CD	1:B:58:GLU:H	1.94	0.70
1:A:223:LEU:HB3	1:A:473:MET:HE3	1.74	0.69
1:A:416:HIS:HB2	8:A:1023:HOH:O	1.91	0.69
1:A:378:GLU:HG2	1:A:382:TYR:CE2	2.28	0.69
1:A:126:TYR:CE1	1:A:439:LEU:HB3	2.29	0.68
1:A:39:LYS:HE2	8:A:904:HOH:O	1.94	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:36:PRO:HD2	1:A:49:TRP:CD1	2.30	0.67
1:A:287:GLN:HE22	1:A:471:SER:H	1.43	0.67
1:B:64:THR:HG21	8:B:598:HOH:O	1.94	0.67
1:A:97:ARG:CZ	8:A:552:HOH:O	2.42	0.66
1:A:126:TYR:CE2	1:A:128:PRO:HD2	2.31	0.66
1:B:36:PRO:HD2	1:B:49:TRP:CD1	2.30	0.65
1:A:438:VAL:O	1:A:441:THR:HG22	1.98	0.64
1:A:79:PHE:O	6:A:512:GOL:H11	1.97	0.64
1:B:218:TYR:CZ	1:B:472:MET:HG2	2.33	0.64
1:A:126:TYR:CD2	1:A:128:PRO:HD2	2.34	0.63
1:B:416:HIS:HB2	8:B:812:HOH:O	1.98	0.63
1:A:416:HIS:HE1	8:A:882:HOH:O	1.81	0.63
1:A:140:ARG:HG3	8:A:659:HOH:O	1.99	0.62
1:A:135:LEU:HD22	1:A:402:TYR:CE2	2.35	0.62
1:B:4:ASP:N	1:B:4:ASP:OD1	2.29	0.61
1:A:212:GLY:HA2	6:A:509:GOL:O3	1.99	0.61
1:B:287:GLN:OE1	1:B:473[B]:MET:HE1	2.01	0.61
4:B:511:ACT:H1	8:B:688:HOH:O	2.01	0.60
6:A:512:GOL:C3	8:A:794:HOH:O	2.48	0.60
1:B:442:HIS:CD2	1:B:442:HIS:N	2.60	0.60
1:A:34:TYR:HB3	1:A:140:ARG:HB3	1.84	0.59
1:A:136:PRO:HD2	1:A:402:TYR:OH	2.03	0.59
1:B:58:GLU:CD	1:B:58:GLU:N	2.55	0.58
1:B:490:THR:HG22	6:B:508:GOL:O2	2.04	0.58
1:B:96:GLN:HG2	8:B:629:HOH:O	2.03	0.57
1:B:96:GLN:H	1:B:96:GLN:NE2	2.03	0.57
1:B:444[A]:GLU:HA	1:B:447:ARG:NH1	2.20	0.57
1:A:481:GLY:HA2	1:B:444[B]:GLU:HG2	1.86	0.57
1:A:231[B]:ARG:HH21	6:A:515:GOL:HO3	1.52	0.57
1:A:287:GLN:HE21	1:A:470:ILE:HA	1.69	0.57
1:B:121:THR:HG23	8:B:612:HOH:O	2.05	0.56
1:A:97:ARG:NH1	3:A:504:BHZ:C16	2.69	0.56
1:B:227:ASP:OD2	4:B:505:ACT:H2	2.05	0.56
1:B:62:THR:HG23	1:B:121:THR:HG22	1.88	0.56
1:B:444[A]:GLU:HA	1:B:447:ARG:HH11	1.71	0.56
1:B:209:PHE:CE2	1:B:475:VAL:HG12	2.10	0.55
1:A:446:GLN:HE21	1:A:446:GLN:HA	1.71	0.55
1:B:283:LEU:HD13	8:B:795:HOH:O	2.06	0.55
1:B:10:TRP:HE1	1:B:26:GLN:NE2	2.03	0.55
1:B:444[B]:GLU:HA	1:B:447:ARG:HH11	1.72	0.55
6:A:509:GOL:H11	8:A:536:HOH:O	1.91	0.55
1:A:23[A]:THR:HG21	7:A:516:CL:CL	2.44	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:444[B]:GLU:HA	1:B:447:ARG:NH1	2.21	0.55
1:A:416:HIS:CE1	8:A:882:HOH:O	2.59	0.54
1:A:97:ARG:HH11	3:A:504:BHZ:C15	2.19	0.54
1:B:218:TYR:CD2	1:B:218:TYR:C	2.81	0.54
1:B:242:LEU:HD12	1:B:473[B]:MET:SD	2.47	0.54
1:B:499:PRO:O	1:B:500:VAL:CB	2.55	0.54
1:A:271:TYR:CZ	1:A:314:LYS:HD3	2.43	0.54
1:B:382:TYR:CZ	1:B:386:ARG:HD2	2.42	0.53
1:A:49:TRP:HA	1:A:49:TRP:CE3	2.42	0.53
1:A:172:LEU:CD1	8:A:878:HOH:O	2.45	0.53
1:A:300:TYR:OH	8:A:775:HOH:O	2.13	0.53
1:B:287:GLN:NE2	1:B:473[B]:MET:HE1	2.21	0.53
1:B:296:PRO:HB3	1:B:302:ASN:HD22	1.73	0.53
1:A:241:GLN:HB3	1:A:485:TYR:OH	2.08	0.52
1:A:231[B]:ARG:NH2	6:A:515:GOL:O3	2.35	0.52
1:B:100:TRP:HA	1:B:413:VAL:HG21	1.92	0.52
1:B:242:LEU:HD11	1:B:473[B]:MET:SD	2.49	0.52
1:A:287:GLN:NE2	1:A:471:SER:H	2.08	0.52
1:A:296:PRO:HB3	1:A:302:ASN:HD22	1.75	0.52
1:B:416:HIS:CB	8:B:812:HOH:O	2.57	0.51
1:B:288:GLN:O	1:B:468[B]:SER:HB2	2.10	0.51
1:A:10:TRP:HE1	1:A:26:GLN:NE2	2.07	0.51
1:A:387[B]:ASP:OD2	1:A:389:ARG:CG	2.42	0.51
1:A:292:THR:HG22	1:A:459:HIS:CE1	2.45	0.51
1:B:171:LYS:CG	1:B:174:GLN:HG3	2.40	0.50
1:A:68:ARG:O	6:A:512:GOL:H12	2.11	0.50
1:B:127:TYR:N	1:B:128:PRO:HD3	2.27	0.50
1:A:41:GLN:NE2	8:A:917:HOH:O	2.44	0.50
1:B:387:ASP:OD2	1:B:389:ARG:NH1	2.41	0.50
1:B:226:LEU:HD12	1:B:283:LEU:HA	1.92	0.50
1:B:103:LEU:HD21	1:B:133:LEU:HD13	1.93	0.50
1:A:241:GLN:CB	1:A:485:TYR:OH	2.60	0.50
1:A:416:HIS:HD2	8:A:827:HOH:O	1.94	0.50
1:B:49:TRP:CE3	1:B:49:TRP:HA	2.46	0.49
1:A:126:TYR:HE1	1:A:439:LEU:HB3	1.76	0.49
1:B:412:ARG:O	1:B:414:PRO:HD3	2.12	0.49
1:B:52:LYS:HE3	1:B:68:ARG:HG2	1.93	0.49
1:B:452:ARG:HD2	8:B:735:HOH:O	2.12	0.49
1:B:7:THR:HG22	1:B:214:ILE:HG22	1.95	0.49
1:B:227:ASP:OD1	4:B:505:ACT:H2	2.12	0.49
1:A:366:GLN:NE2	8:A:809:HOH:O	2.35	0.48
1:A:473:MET:HG2	8:A:578:HOH:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:127:TYR:N	1:B:128:PRO:CD	2.77	0.47
1:A:477:LYS:HE2	6:A:509:GOL:O3	2.14	0.47
1:B:227:ASP:CG	4:B:505:ACT:H2	2.34	0.47
1:A:477:LYS:CE	6:A:509:GOL:C3	2.72	0.47
1:A:398:TRP:HB3	3:A:504:BHZ:C2	2.45	0.47
1:A:80:ASP:HB3	6:A:512:GOL:H2	1.97	0.47
1:A:241:GLN:NE2	1:A:485:TYR:OH	2.32	0.47
1:A:423:GLN:NE2	8:A:943:HOH:O	2.48	0.47
1:B:19:PRO:HG3	1:B:142:ILE:HB	1.97	0.47
1:A:477:LYS:CG	6:A:509:GOL:H31	2.45	0.47
1:B:209:PHE:CD2	1:B:475:VAL:HG11	2.48	0.47
1:A:481:GLY:HA2	1:B:444[B]:GLU:CG	2.44	0.47
1:A:416:HIS:CB	8:A:1023:HOH:O	2.56	0.46
1:B:433:LYS:HE3	8:B:600:HOH:O	2.16	0.46
1:A:171:LYS:HG3	1:A:175:TYR:CE2	2.51	0.45
1:A:227:ASP:OD1	1:A:228:THR:N	2.48	0.45
1:A:137:ARG:HB2	1:A:138:PRO:HA	1.98	0.45
1:A:39:LYS:HD2	1:A:49:TRP:CZ2	2.52	0.45
1:B:287:GLN:CD	1:B:473[B]:MET:HE1	2.37	0.45
1:A:477:LYS:HG2	6:A:509:GOL:H31	1.99	0.45
1:B:306:LYS:CD	1:B:306:LYS:N	2.33	0.44
1:A:97:ARG:O	3:A:504:BHZ:H15	2.16	0.44
1:B:226:LEU:CD1	1:B:283:LEU:HA	2.47	0.44
1:A:342:ILE:HG21	1:A:392:MET:HG3	1.99	0.44
1:A:438:VAL:HA	1:A:441:THR:HG22	2.00	0.44
1:B:386:ARG:HD3	8:B:527:HOH:O	2.16	0.44
1:A:171:LYS:HB2	1:A:174:GLN:HB2	1.99	0.44
1:B:499:PRO:HG2	1:B:500:VAL:H	1.83	0.44
1:A:327:PRO:HG2	1:A:330:LYS:HB2	2.00	0.43
1:B:401:PRO:HD3	1:B:488:ILE:HG12	2.00	0.43
1:A:82:GLU:HB2	8:A:717:HOH:O	2.18	0.43
1:B:328:ALA:HA	1:B:329:GLY:HA2	1.81	0.43
1:A:423:GLN:HE21	1:A:423:GLN:HB3	1.73	0.43
1:A:258:ALA:HA	1:A:261:ASN:OD1	2.17	0.43
1:A:218:TYR:CE2	1:A:472:MET:HE2	2.53	0.43
1:B:103:LEU:HD23	1:B:139:PHE:CE2	2.54	0.43
1:A:19:PRO:HG3	1:A:142:ILE:HB	2.01	0.43
1:A:291:ASP:HB3	1:A:307:PRO:HB3	2.00	0.43
1:B:287:GLN:HE22	1:B:473[B]:MET:HE1	1.70	0.42
1:B:389:ARG:NH2	8:B:628:HOH:O	2.51	0.42
1:A:481:GLY:CA	1:B:444[B]:GLU:HG2	2.48	0.42
1:B:56:HIS:HD2	1:B:57:SER:O	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:119:GLN:NE2	8:B:598:HOH:O	2.23	0.42
1:A:175:TYR:C	1:A:175:TYR:CD2	2.92	0.42
1:B:4:ASP:HA	1:B:499:PRO:HB3	2.02	0.42
1:A:342:ILE:CG2	1:A:392:MET:HG3	2.49	0.42
1:A:334:GLU:HA	1:A:338:GLN:O	2.20	0.42
1:A:188:LYS:H	1:A:188:LYS:CD	2.13	0.42
1:A:246:ILE:HD13	1:A:472:MET:HG2	2.00	0.42
1:B:223:LEU:HD23	1:B:473[A]:MET:HG3	2.02	0.41
1:B:111:LYS:HD2	1:B:113:LEU:HD23	2.02	0.41
1:A:214:ILE:CD1	1:A:217:LEU:HD21	2.50	0.41
1:A:175:TYR:HA	1:A:196:PHE:O	2.20	0.41
1:B:186:GLY:HA3	8:B:847:HOH:O	2.21	0.41
1:A:306:LYS:HE3	1:A:306:LYS:HB2	1.49	0.41
1:A:23[B]:THR:HG22	1:A:24:PRO:HA	2.02	0.41
1:A:398:TRP:HB3	3:A:504:BHZ:H2	2.02	0.41
1:B:441:THR:O	1:B:447:ARG:NH2	2.53	0.41
1:B:389:ARG:NE	8:B:840:HOH:O	2.47	0.41
1:B:408:LEU:HD13	1:B:454:ILE:HG21	2.03	0.41
1:A:22:TYR:O	1:A:23[A]:THR:C	2.58	0.41
1:B:442:HIS:H	1:B:442:HIS:HD2	1.51	0.41
1:B:428:LYS:N	1:B:429:PRO:CD	2.85	0.40
1:A:278:LEU:HD23	1:A:278:LEU:C	2.42	0.40
1:B:96:GLN:H	1:B:96:GLN:CD	2.25	0.40
1:B:97:ARG:O	3:B:504:BHZ:H15	2.21	0.40
1:B:279:ILE:HA	1:B:283:LEU:HD12	2.03	0.40
1:A:126:TYR:CZ	1:A:128:PRO:HD2	2.56	0.40
1:A:2:ALA:N	1:A:3:PRO:HD3	2.36	0.40

All (1) 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	Distance(Å)	Clash(Å)
4:B:505:ACT:CH3	8:A:592:HOH:O[2_554]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	506/502 (101%)	488 (96%)	18 (4%)	0	100	100
1	B	500/502 (100%)	486 (97%)	11 (2%)	3 (1%)	33	15
All	All	1006/1004 (100%)	974 (97%)	29 (3%)	3 (0%)	50	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	499	PRO
1	B	415	SER
1	B	157	LYS

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	429/425 (101%)	417 (97%)	12 (3%)	56	38
1	B	426/425 (100%)	403 (95%)	23 (5%)	31	12
All	All	855/850 (101%)	820 (96%)	35 (4%)	42	21

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	TRP
1	A	127	TYR
1	A	131	GLN
1	A	188	LYS
1	A	250	MET
1	A	284	TYR
1	A	306	LYS
1	A	309	GLN
1	A	341	ARG
1	A	352	LEU
1	A	373	LEU
1	A	423	GLN
1	B	49	TRP
1	B	50	LEU

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Mol	Chain	Res	Type
1	B	52	LYS
1	B	58	GLU
1	B	64	THR
1	B	96	GLN
1	B	111	LYS
1	B	115	LYS
1	B	127	TYR
1	B	133	LEU
1	B	138	PRO
1	B	172	LEU
1	B	187	GLU
1	B	188	LYS
1	B	218	TYR
1	B	250	MET
1	B	306	LYS
1	B	319	LEU
1	B	340	LEU
1	B	416	HIS
1	B	439	LEU
1	B	473[A]	MET
1	B	473[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	41	GLN
1	A	87	ASN
1	A	131	GLN
1	A	154	ASN
1	A	197	ASN
1	A	287	GLN
1	A	302	ASN
1	A	416	HIS
1	A	423	GLN
1	A	446	GLN
1	B	25	ASN
1	B	26	GLN
1	B	56	HIS
1	B	96	GLN
1	B	234	GLN
1	B	287	GLN

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Mol	Chain	Res	Type
1	B	288	GLN
1	B	336	ASN
1	B	385	GLN
1	B	442	HIS
1	B	482	ASN
1	B	496	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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	$\# Z > 2$
3	BHZ	A	504	2	28,28,28	1.59	4 (14%)	36,36,36	1.70	7 (19%)
4	ACT	A	505	-	1,3,3	0.79	0	0,3,3	0.00	-
4	ACT	A	506	-	1,3,3	2.96	1 (100%)	0,3,3	0.00	-
4	ACT	A	507	-	1,3,3	1.48	0	0,3,3	0.00	-
5	SO4	A	508	-	4,4,4	0.13	0	6,6,6	0.19	0
6	GOL	A	509	-	5,5,5	0.35	0	5,5,5	0.25	0
6	GOL	A	510	-	5,5,5	0.34	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	A	512	-	5,5,5	0.48	0	5,5,5	1.18	0
6	GOL	A	513	-	5,5,5	0.67	0	5,5,5	0.53	0
6	GOL	A	514	-	5,5,5	0.39	0	5,5,5	1.21	1 (20%)
6	GOL	A	515	-	5,5,5	0.34	0	5,5,5	0.78	0
3	BHZ	B	504	2	28,28,28	1.70	4 (14%)	36,36,36	1.24	3 (8%)
4	ACT	B	505	-	1,3,3	1.22	0	0,3,3	0.00	-
6	GOL	B	506	-	5,5,5	1.07	0	5,5,5	0.80	0
6	GOL	B	507	-	5,5,5	0.34	0	5,5,5	0.25	0
6	GOL	B	508	-	5,5,5	0.34	0	5,5,5	0.25	0
4	ACT	B	511	-	1,3,3	0.49	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
3	BHZ	A	504	2	-	0/21/21/21	0/2/2/2
4	ACT	A	505	-	-	0/0/0/0	0/0/0/0
4	ACT	A	506	-	-	0/0/0/0	0/0/0/0
4	ACT	A	507	-	-	0/0/0/0	0/0/0/0
5	SO4	A	508	-	-	0/0/0/0	0/0/0/0
6	GOL	A	509	-	-	0/4/4/4	0/0/0/0
6	GOL	A	510	-	-	0/4/4/4	0/0/0/0
6	GOL	A	512	-	-	0/4/4/4	0/0/0/0
6	GOL	A	513	-	-	0/4/4/4	0/0/0/0
6	GOL	A	514	-	-	0/4/4/4	0/0/0/0
6	GOL	A	515	-	-	0/4/4/4	0/0/0/0
3	BHZ	B	504	2	-	0/21/21/21	0/2/2/2
4	ACT	B	505	-	-	0/0/0/0	0/0/0/0
6	GOL	B	506	-	-	0/4/4/4	0/0/0/0
6	GOL	B	507	-	-	0/4/4/4	0/0/0/0
6	GOL	B	508	-	-	0/4/4/4	0/0/0/0
4	ACT	B	511	-	-	0/0/0/0	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	504	BHZ	C12-C13	4.27	1.59	1.51
3	B	504	BHZ	C12-N11	4.14	1.55	1.47
3	B	504	BHZ	C12-C13	3.66	1.58	1.51
3	A	504	BHZ	C21-N11	3.59	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	504	BHZ	C21-C22	3.28	1.59	1.51
4	A	506	ACT	CH3-C	2.96	1.53	1.48
3	B	504	BHZ	C19-C20	2.62	1.57	1.51
3	A	504	BHZ	C19-C20	2.47	1.57	1.51
3	A	504	BHZ	C7-C1	2.35	1.55	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	504	BHZ	C12-N11-C10	4.31	120.45	111.20
3	A	504	BHZ	C7-N8-C19	-4.19	103.86	112.58
3	A	504	BHZ	C21-N11-C10	-3.52	103.52	112.34
3	B	504	BHZ	C7-C1-C6	3.13	123.69	120.47
3	B	504	BHZ	C7-N8-C19	-3.06	106.22	112.58
3	A	504	BHZ	C7-C1-C6	3.05	123.60	120.47
3	B	504	BHZ	C13-C12-N11	-2.74	107.79	113.20
3	A	504	BHZ	C7-N8-C9	-2.59	105.64	111.20
6	A	514	GOL	O3-C3-C2	-2.31	98.44	109.71
3	A	504	BHZ	C4-C5-C6	2.07	122.80	120.05
3	A	504	BHZ	C16-C15-C14	-2.05	116.76	120.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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%)	-0.09	12 (2%) 56 49	6, 13, 26, 45	1 (0%)
1	B	498/502 (99%)	0.12	28 (5%) 24 18	6, 17, 39, 51	0
All	All	996/1004 (99%)	0.02	40 (4%) 35 29	6, 15, 35, 51	1 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	6.5
1	B	499	PRO	6.3
1	B	209	PHE	5.8
1	B	328	ALA	5.4
1	A	49	TRP	5.2
1	A	485	TYR	5.2
1	B	218	TYR	4.8
1	A	141	PHE	4.7
1	B	49	TRP	4.5
1	A	300	TYR	4.3
1	A	402	TYR	3.8
1	B	3	PRO	3.5
1	B	125	ALA	3.4
1	B	327	PRO	3.4
1	B	500	VAL	3.4
1	A	3	PRO	3.3
1	B	382	TYR	3.3
1	B	58	GLU	3.2
1	B	329	GLY	3.1
1	B	139	PHE	3.1
1	A	126	TYR	3.1
1	A	283[A]	LEU	3.1
1	B	442	HIS	3.0
1	A	140	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	414	PRO	2.9
1	B	330	LYS	2.8
1	B	112	ALA	2.7
1	B	415	SER	2.7
1	B	108	VAL	2.7
1	B	284	TYR	2.6
1	A	327	PRO	2.4
1	B	113	LEU	2.4
1	B	281	ASN	2.4
1	B	116	THR	2.3
1	B	386	ARG	2.3
1	A	441	THR	2.2
1	B	331	ASP	2.2
1	B	337	GLY	2.1
1	B	111	LYS	2.0
1	B	115	LYS	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	GOL	A	512	6/6	0.38	25.99	21,37,39,45	0
6	GOL	A	509	6/6	0.45	14.16	20,20,20,20	0
4	ACT	B	511	4/4	0.45	13.21	20,20,20,20	0
4	ACT	B	505	4/4	0.22	12.30	55,55,56,56	0
4	ACT	A	505	4/4	0.22	7.48	37,39,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	SO4	A	508	5/5	0.26	4.78	92,93,94,95	0
6	GOL	B	506	6/6	0.34	3.97	55,56,56,61	0
4	ACT	A	507	4/4	0.16	3.79	31,35,36,36	0
6	GOL	A	510	6/6	0.31	3.17	40,49,51,51	0
4	ACT	A	506	4/4	0.12	2.37	37,38,38,40	0
6	GOL	A	514	6/6	0.11	1.91	19,28,32,36	0
6	GOL	B	508	6/6	0.11	1.71	14,17,20,23	0
7	CL	B	509	1/1	0.12	1.48	40,40,40,40	0
6	GOL	A	515	6/6	0.14	1.37	27,29,34,37	0
6	GOL	B	507	6/6	0.15	0.78	18,22,28,34	0
3	BHZ	B	504	27/27	0.10	0.20	12,17,25,29	0
3	BHZ	A	504	27/27	0.10	-0.80	11,16,26,28	0
7	CL	A	516	1/1	0.10	-0.86	51,51,51,51	0
6	GOL	A	513	6/6	0.07	-1.35	12,20,22,24	0
7	CL	B	510	1/1	0.08	-1.50	41,41,41,41	0
7	CL	A	517	1/1	0.05	-1.70	46,46,46,46	0
2	FE	A	503	1/1	0.07	-	14,14,14,14	0
2	FE	B	503	1/1	0.06	-	15,15,15,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.