



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:29 AM GMT

PDB ID : 3UNA
Title : Crystal Structure of Bovine Milk Xanthine Dehydrogenase with NAD Bound
Authors : Eger, B.T.; Okamoto, K.; Nishino, T.; Pai, E.F.
Deposited on : 2011-11-15
Resolution : 1.90 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>

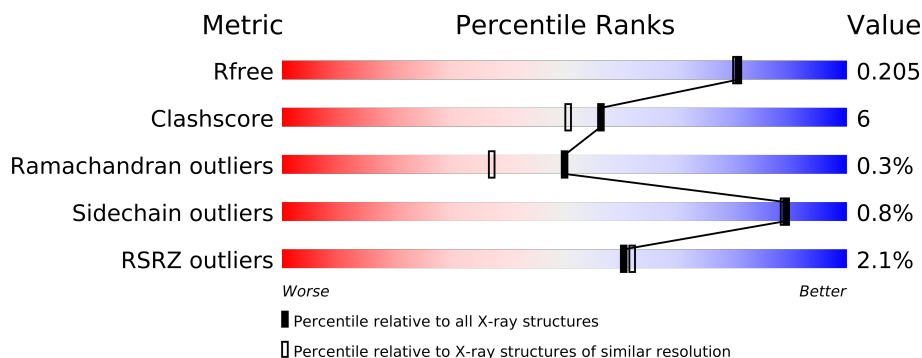
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.90 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	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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	1332	
1	B	1332	

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	MOS	A	1336	-	X
6	NAD	A	1338	-	X
6	NAD	B	1338	-	X
9	GOL	A	1341	-	X
9	GOL	A	1342	-	X
9	GOL	A	1343	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
9	GOL	A	1344	-	X
9	GOL	A	1347	-	X
9	GOL	A	1348	-	X
9	GOL	B	1341	-	X
9	GOL	B	1343	-	X
9	GOL	B	1345	-	X

2 Entry composition

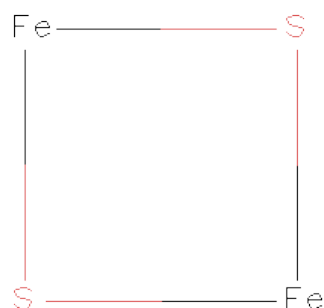
There are 11 unique types of molecules in this entry. The entry contains 21905 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Xanthine dehydrogenase/oxidase.

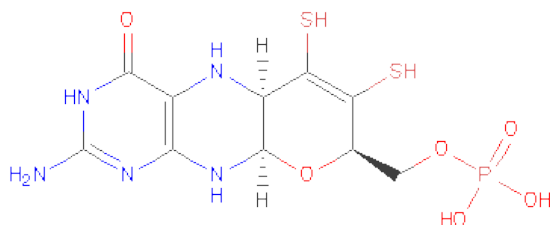
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1286	Total	C	N	O	S	0	7	0
			10036	6378	1717	1877	64			
1	B	1289	Total	C	N	O	S	0	4	0
			10035	6378	1717	1876	64			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



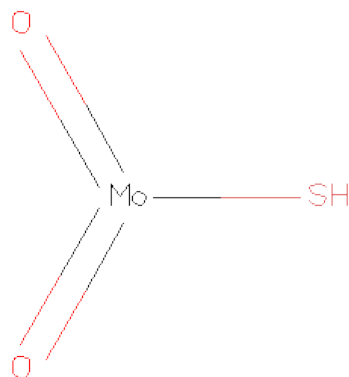
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



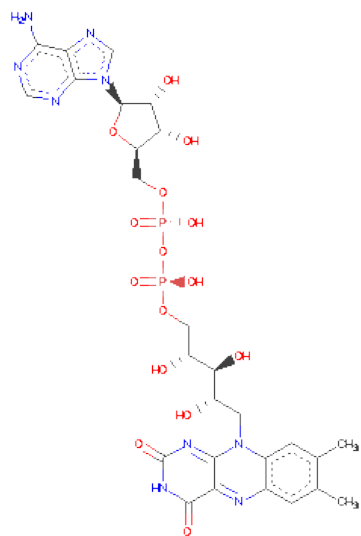
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 4 is DIOXOTHIOMOLYBDENUM(VI)ION (three-letter code: MOS) (formula: $HMoO_2S$).



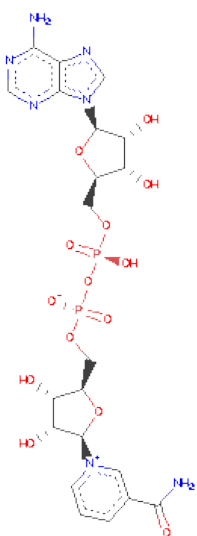
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
4	B	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



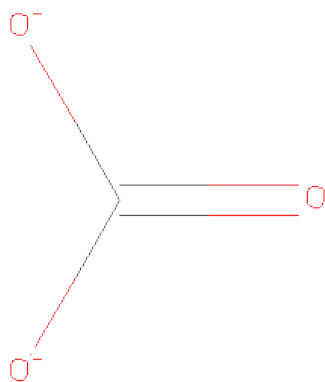
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



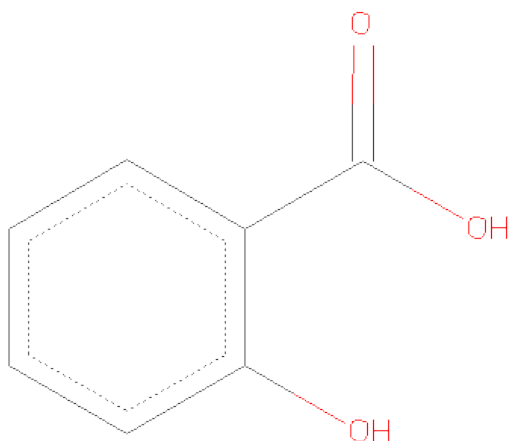
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
6	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 7 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



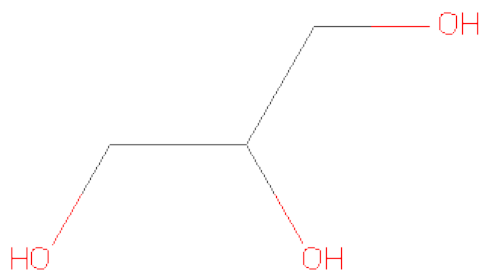
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	1	3		
7	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 8 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: $C_7H_6O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	7	3		
8	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Ca 1 1	0	0
10	A	1	Total Ca 1 1	0	0

- Molecule 11 is water.

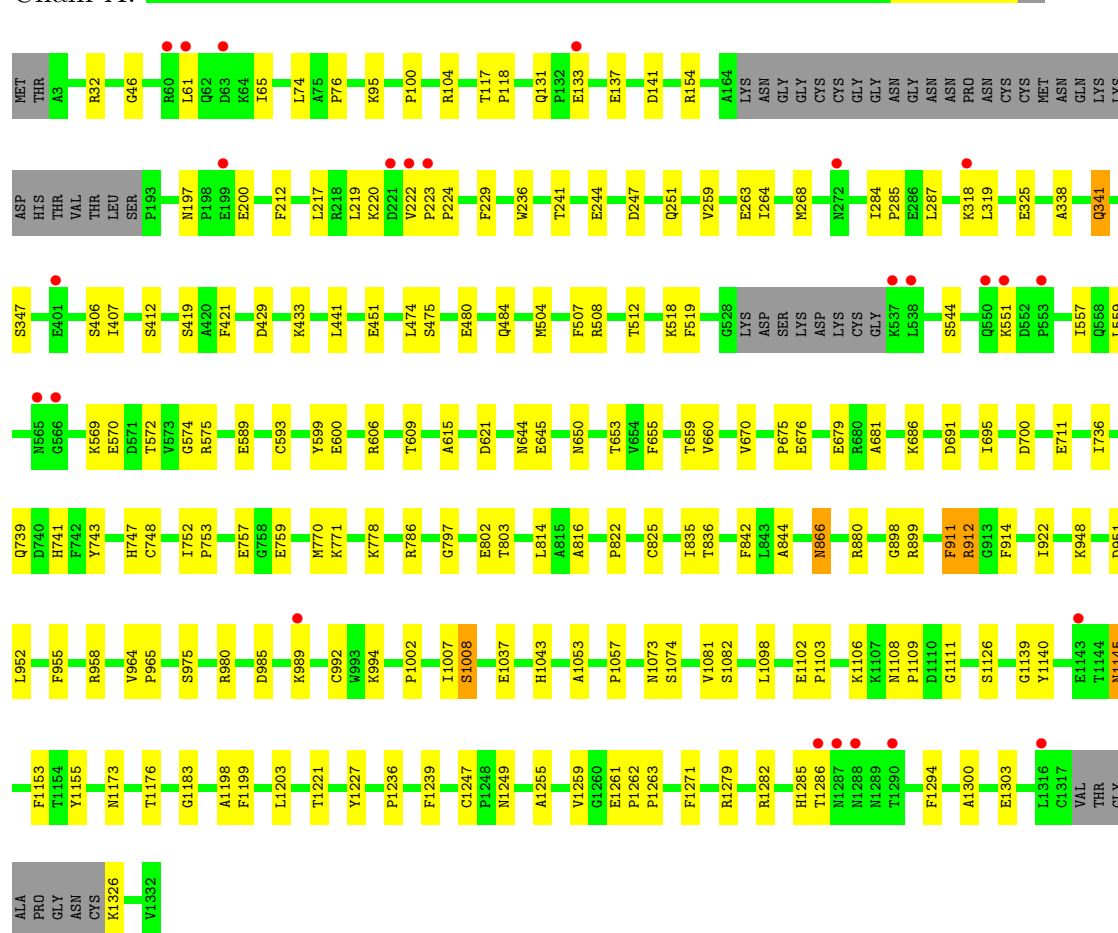
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	758	Total O 758 758	0	0
11	B	744	Total O 744 744	0	0

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.

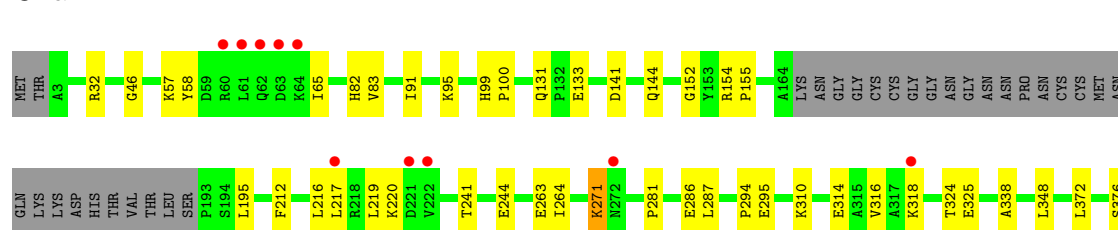
• Molecule 1: Xanthine dehydrogenase/oxidase

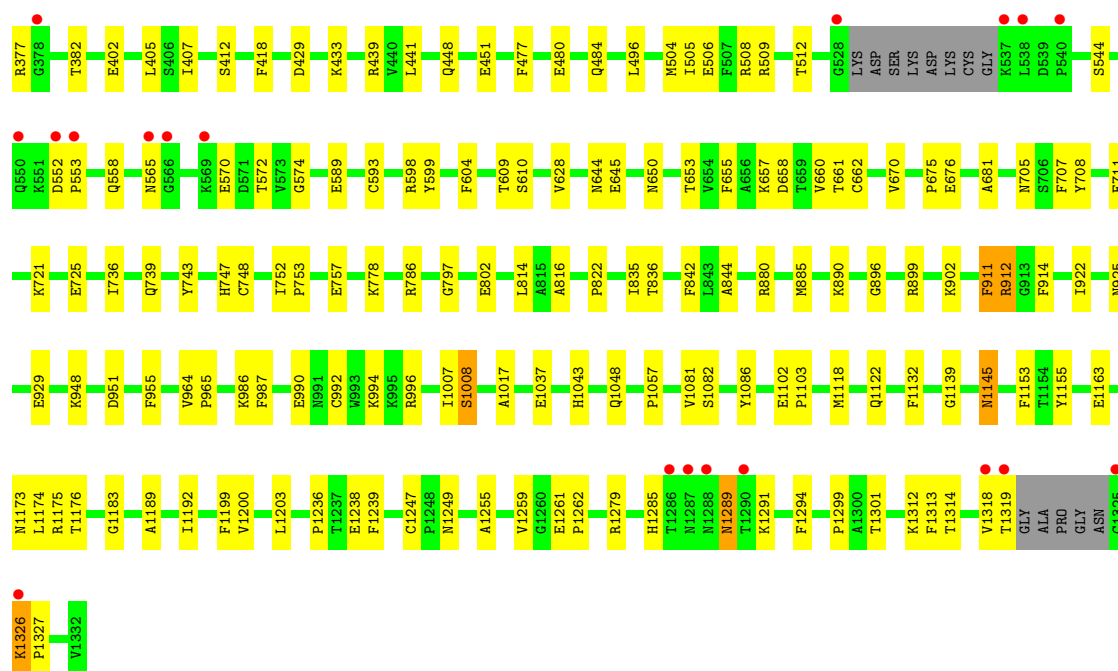
Chain A:



• Molecule 1: Xanthine dehydrogenase/oxidase

Chain B:





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.03Å 123.18Å 147.62Å 90.00° 91.02° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-1.90) 96.0 (19.95-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.181 , 0.214 0.175 , 0.205	Depositor DCC
R_{free} test set	2214 reflections (1.00%)	DCC
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 35.0	EDS
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 232449 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21905	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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, CO3, NAD, SAL, MOS, CA, FES, FAD, MTE

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	0.31	0/10254	0.61	0/13876
1	B	0.31	0/10253	0.61	0/13876
All	All	0.31	0/20507	0.61	0/27752

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	10036	0	10027	128	0
1	B	10035	0	10029	131	0
2	A	8	0	0	1	0
2	B	8	0	0	1	0
3	A	24	0	10	2	0
3	B	24	0	10	2	0
4	A	4	0	0	4	0
4	B	4	0	0	4	0
5	A	53	0	31	2	0
5	B	53	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	23	0	12	0	0
6	B	23	0	12	0	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
8	A	10	0	4	1	0
8	B	10	0	4	1	0
9	A	48	0	64	2	0
9	B	30	0	40	1	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	758	0	0	3	0
11	B	744	0	0	1	0
All	All	21905	0	20274	264	0

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 6.

All (264) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.28	0.95
1:A:341:GLN:H	1:A:341:GLN:HE21	1.09	0.92
1:B:131:GLN:HE21	1:B:133:GLU:H	1.16	0.90
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.38	0.87
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.38	0.85
1:A:131:GLN:HE21	1:A:133:GLU:H	1.25	0.84
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.42	0.84
1:A:948:LYS:HG2	1:A:951:ASP:OD2	1.85	0.76
1:A:518:LYS:HE2	11:A:2094:HOH:O	1.84	0.76
1:B:1279:ARG:HG2	1:B:1294:PHE:HE2	1.52	0.74
1:A:341:GLN:H	1:A:341:GLN:NE2	1.83	0.74
1:B:1326:LYS:HD3	1:B:1326:LYS:H	1.53	0.72
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.53	0.71
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.58	0.69
1:A:341:GLN:HE21	1:A:341:GLN:N	1.90	0.66
1:A:1221:THR:HG22	1:A:1227:TYR:HB2	1.78	0.65
4:B:1336:MOS:MO	4:B:1336:MOS:O2	1.67	0.65
4:A:1336:MOS:O2	4:A:1336:MOS:MO	1.67	0.64
1:B:948:LYS:HG2	1:B:951:ASP:OD2	1.97	0.63
1:B:241:THR:OG1	1:B:244:GLU:HG3	1.98	0.63
1:A:753:PRO:HD3	1:A:816:ALA:HB1	1.80	0.62
1:B:131:GLN:HE21	1:B:133:GLU:N	1.94	0.62
1:A:985:ASP:O	1:A:989:LYS:HG3	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:1336:MOS:MO	4:B:1336:MOS:S	2.11	0.61
1:A:1279:ARG:HG2	1:A:1294:PHE:HE2	1.65	0.61
1:A:433:LYS:HE2	1:A:504:MET:SD	2.40	0.60
1:A:217:LEU:O	1:A:220:LYS:HG2	2.01	0.60
4:A:1336:MOS:S	4:A:1336:MOS:MO	2.11	0.60
1:A:621:ASP:HB3	1:A:686:LYS:HE2	1.84	0.60
1:A:264:ILE:HD11	5:A:1337:FAD:H3B	1.82	0.60
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.84	0.59
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.03	0.59
1:B:32:ARG:HH12	1:B:676:GLU:CD	2.06	0.58
1:B:131:GLN:NE2	1:B:133:GLU:H	1.94	0.58
1:A:318:LYS:HE2	1:A:319:LEU:HD21	1.84	0.58
1:A:557:ILE:HG22	1:A:559:LEU:CD1	2.33	0.58
1:B:552:ASP:HB3	1:B:553:PRO:HD2	1.86	0.58
1:B:281:PRO:HB2	1:B:287:LEU:HD12	1.85	0.58
1:A:441:LEU:HB3	1:A:451:GLU:HB2	1.86	0.57
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.86	0.57
1:A:241:THR:OG1	1:A:244:GLU:HG3	2.05	0.57
1:A:593:CYS:HB3	1:A:748[B]:CYS:SG	2.44	0.57
1:A:559:LEU:HD13	11:A:1476:HOH:O	2.05	0.56
1:B:711:GLU:HA	1:B:899:ARG:HD2	1.87	0.56
1:B:1175:ARG:HG3	1:B:1238:GLU:HG2	1.86	0.56
1:B:570:GLU:OE2	1:B:1057:PRO:HG3	2.05	0.56
1:B:604:PHE:CD2	1:B:675:PRO:HG3	2.41	0.56
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.42	0.56
1:A:32:ARG:HH12	1:A:676:GLU:CD	2.08	0.55
1:A:1102:GLU:HB3	1:A:1103:PRO:HD3	1.88	0.55
1:A:407:ILE:N	1:A:407:ILE:HD12	2.22	0.55
1:B:310:LYS:O	1:B:314:GLU:HG3	2.07	0.55
1:B:433:LYS:HE3	1:B:433:LYS:HA	1.89	0.55
1:B:1008:SER:HA	1:B:1081:VAL:HG11	1.88	0.55
1:B:216:LEU:HD23	1:B:219:LEU:HD12	1.89	0.55
1:A:752:ILE:CD1	1:A:822:PRO:HB3	2.38	0.54
1:A:1008:SER:HA	1:A:1081:VAL:HG11	1.88	0.54
1:B:757:GLU:HB3	1:B:786:ARG:HE	1.70	0.54
1:B:377:ARG:HH11	1:B:377:ARG:HG3	1.71	0.54
1:B:318:LYS:N	1:B:318:LYS:HD2	2.22	0.54
1:B:1279:ARG:HG2	1:B:1294:PHE:CE2	2.39	0.54
1:A:474:LEU:O	1:A:475[A]:SER:HB2	2.07	0.53
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.09	0.53
1:A:615:ALA:O	1:A:659[A]:THR:HG23	2.09	0.52
1:B:281:PRO:HB2	1:B:287:LEU:CD1	2.39	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:141:ASP:OD1	1:A:551:LYS:NZ	2.42	0.52
1:B:752:ILE:CD1	1:B:822:PRO:HB3	2.39	0.52
1:A:406:SER:C	1:A:407:ILE:HD12	2.30	0.52
1:B:1326:LYS:N	1:B:1326:LYS:HD3	2.24	0.52
1:B:506:GLU:HG2	1:B:1319:THR:HG23	1.92	0.52
1:B:506:GLU:CG	1:B:1319:THR:HG23	2.40	0.51
1:A:1037:GLU:HB2	1:A:1043:HIS:CD2	2.46	0.51
1:A:421:PHE:CE2	1:A:518:LYS:NZ	2.79	0.51
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.92	0.51
1:B:91:ILE:O	1:B:99:HIS:HB2	2.11	0.51
1:B:264:ILE:HD11	5:B:1337:FAD:H3B	1.93	0.51
1:B:1314:THR:O	1:B:1318:VAL:HG13	2.11	0.51
3:B:1335:MTE:S1'	4:B:1336:MOS:S	3.09	0.50
1:A:544:SER:O	1:A:994:LYS:HE2	2.11	0.50
1:A:770[B]:MET:HE2	1:A:1073:ASN:C	2.31	0.50
1:A:247:ASP:O	1:A:251:GLN:HG3	2.12	0.50
1:B:711:GLU:HA	1:B:899:ARG:CD	2.41	0.50
1:A:747:HIS:CD2	1:A:836:THR:HG21	2.46	0.50
1:A:770[B]:MET:HE2	1:A:1074:SER:O	2.12	0.50
1:A:284:ILE:CG2	1:A:287:LEU:HD23	2.42	0.50
1:A:1007:ILE:O	1:A:1008:SER:CB	2.60	0.50
1:A:1153:PHE:HB2	1:A:1155:TYR:CZ	2.46	0.49
1:B:1007:ILE:O	1:B:1008:SER:CB	2.60	0.49
1:A:100:PRO:O	1:A:104:ARG:HG3	2.12	0.49
1:A:1082:SER:HB2	3:A:1335:MTE:O3P	2.12	0.49
1:A:911:PHE:O	1:A:912:ARG:C	2.50	0.49
1:B:572:THR:OG1	1:B:1048:GLN:HG2	2.12	0.49
1:B:1082:SER:HB2	3:B:1335:MTE:O3P	2.13	0.49
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.95	0.49
1:A:757:GLU:HB3	1:A:786:ARG:HE	1.78	0.49
1:B:82:HIS:NE2	1:B:219:LEU:HD13	2.27	0.48
1:B:217:LEU:O	1:B:220:LYS:HG2	2.13	0.48
1:A:32:ARG:NH1	1:A:676:GLU:OE2	2.43	0.48
1:B:348:LEU:HD13	1:B:407:ILE:CD1	2.43	0.48
1:A:1126:SER:HB2	1:B:1132:PHE:CD1	2.48	0.48
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.78	0.48
1:B:753:PRO:HD3	1:B:816:ALA:HB1	1.96	0.48
1:B:844:ALA:HB2	1:B:922:ILE:HD13	1.95	0.48
1:B:964:VAL:HB	1:B:965:PRO:HD3	1.96	0.48
1:A:338:ALA:HA	1:A:429:ASP:OD1	2.13	0.48
1:A:992[A]:CYS:SG	1:A:1285:HIS:CE1	3.07	0.48
1:B:992[A]:CYS:SG	1:B:1285:HIS:NE2	2.87	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:197:ASN:ND2	1:A:200:GLU:HG3	2.29	0.48
1:B:508:ARG:HD3	11:B:1385:HOH:O	2.14	0.47
1:A:219:LEU:O	1:A:222:VAL:HG12	2.13	0.47
1:A:263:GLU:HB2	5:A:1337:FAD:H52A	1.95	0.47
1:A:137:GLU:HG3	1:A:551:LYS:HD2	1.96	0.47
1:B:152:GLY:HA2	1:B:1200:VAL:HG21	1.96	0.47
1:A:770[B]:MET:HG3	1:A:1073:ASN:HA	1.96	0.47
1:B:911:PHE:O	1:B:912:ARG:C	2.53	0.47
1:B:736:ILE:CG2	1:B:842:PHE:HB2	2.43	0.47
1:B:376:SER:HB3	1:B:402:GLU:HG2	1.97	0.47
1:A:61:LEU:N	1:A:61:LEU:HD12	2.29	0.47
1:A:964:VAL:HB	1:A:965:PRO:HD3	1.95	0.47
1:A:480:GLU:O	1:A:484:GLN:HG3	2.14	0.47
1:B:721:LYS:O	1:B:725:GLU:HG3	2.15	0.47
1:A:606:ARG:CZ	1:A:679:GLU:HG3	2.45	0.47
1:A:569:LYS:NZ	1:A:569:LYS:HB3	2.29	0.47
1:B:433:LYS:HA	1:B:433:LYS:CE	2.46	0.46
1:B:593:CYS:HB3	1:B:748[B]:CYS:SG	2.55	0.46
1:B:348:LEU:HD13	1:B:407:ILE:HD11	1.95	0.46
1:B:441:LEU:HB3	1:B:451:GLU:HB2	1.96	0.46
1:B:263:GLU:HB2	5:B:1337:FAD:H52A	1.98	0.46
1:B:508:ARG:O	1:B:512:THR:HG23	2.16	0.46
1:B:1163:GLU:HB2	1:B:1174:LEU:HD11	1.98	0.46
1:A:992[A]:CYS:SG	1:A:1285:HIS:NE2	2.89	0.46
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.78	0.46
1:A:95:LYS:HG3	1:A:589:GLU:OE1	2.15	0.46
1:B:141:ASP:O	1:B:144:GLN:HG3	2.16	0.46
1:B:1153:PHE:HB2	1:B:1155:TYR:CZ	2.50	0.46
1:A:259:VAL:HG11	1:A:347:SER:HB3	1.97	0.46
1:B:338:ALA:HA	1:B:429:ASP:OD1	2.16	0.46
1:A:955:PHE:HA	1:A:1145:ASN:ND2	2.12	0.46
1:B:628:VAL:HG21	1:B:681:ALA:HA	1.98	0.46
1:A:1102:GLU:OE2	1:A:1106:LYS:HE3	2.16	0.46
1:A:1271:PHE:CE1	1:A:1300:ALA:HB2	2.51	0.45
1:B:377:ARG:HG3	1:B:377:ARG:NH1	2.29	0.45
1:B:992[A]:CYS:SG	1:B:1285:HIS:CE1	3.09	0.45
1:B:1183:GLY:HA2	1:B:1247:CYS:O	2.17	0.45
4:B:1336:MOS:O1	4:B:1336:MOS:S	2.75	0.45
3:A:1335:MTE:S1'	4:A:1336:MOS:S	3.13	0.45
1:B:1173:ASN:O	1:B:1236:PRO:HA	2.16	0.45
1:B:655:PHE:CE1	1:B:814:LEU:HD23	2.52	0.45
1:B:1312:LYS:HE3	1:B:1313:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:287:LEU:HD23	1:B:405:LEU:HD12	1.97	0.45
1:B:195:LEU:HD22	1:B:1189:ALA:HA	1.98	0.45
1:B:46:GLY:HA2	2:B:1334:FES:S1	2.57	0.45
1:A:599:TYR:HA	1:B:599:TYR:HA	1.97	0.45
1:A:1183:GLY:HA2	1:A:1247:CYS:O	2.16	0.45
1:B:58:TYR:CE2	1:B:220:LYS:HD2	2.52	0.45
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.80	0.45
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.80	0.45
1:A:1176:THR:HG21	1:A:1199:PHE:CZ	2.51	0.45
1:A:736:ILE:CG2	1:A:842:PHE:HB2	2.47	0.45
1:A:711:GLU:HA	1:A:899:ARG:CD	2.47	0.45
1:B:286:GLU:HB3	1:B:405:LEU:HD11	1.98	0.44
1:B:711:GLU:HB2	1:B:899:ARG:HD3	1.99	0.44
1:A:711:GLU:HA	1:A:899:ARG:HD2	1.99	0.44
1:B:509:ARG:HG2	1:B:509:ARG:HH11	1.83	0.44
1:B:1279:ARG:HB3	1:B:1279:ARG:NH1	2.32	0.44
1:A:644:ASN:O	1:A:653:THR:HA	2.17	0.44
1:B:271:LYS:N	1:B:271:LYS:HD2	2.33	0.44
1:A:1203:LEU:HD23	1:A:1203:LEU:C	2.36	0.44
1:A:325:GLU:HB2	1:A:412:SER:HB3	2.00	0.44
1:B:294:PRO:HG2	1:B:295:GLU:OE1	2.18	0.44
1:B:325:GLU:HB2	1:B:412:SER:HB3	1.98	0.44
1:B:65:ILE:HD13	1:B:212:PHE:CB	2.48	0.44
1:B:433:LYS:HD3	1:B:504:MET:SD	2.57	0.44
1:A:844:ALA:HB2	1:A:922:ILE:HD13	2.00	0.44
4:A:1336:MOS:S	4:A:1336:MOS:O1	2.76	0.44
1:A:229:PHE:HB2	1:A:236:TRP:HB3	2.00	0.44
1:A:609:THR:HG21	1:A:835:ILE:HD11	1.99	0.43
1:A:325:GLU:HB2	1:A:412:SER:CB	2.48	0.43
1:B:802:GLU:OE1	8:B:1340:SAL:H3	2.18	0.43
1:B:1289:ASN:ND2	1:B:1291:LYS:H	2.16	0.43
1:A:1102:GLU:HG3	1:A:1106:LYS:HE3	1.99	0.43
1:A:284:ILE:HA	1:A:285:PRO:HD3	1.90	0.43
1:A:975:SER:O	1:A:980:ARG:HD3	2.19	0.43
1:A:268[B]:MET:CE	11:A:1781:HOH:O	2.67	0.43
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.53	0.43
1:B:372:LEU:O	1:B:382:THR:HA	2.19	0.43
1:A:572:THR:HA	1:A:575:ARG:HD2	2.01	0.43
1:A:65:ILE:HD13	1:A:212:PHE:CB	2.49	0.43
1:B:986:LYS:HG2	1:B:990:GLU:OE2	2.19	0.43
1:B:1259:VAL:O	1:B:1259:VAL:HG22	2.19	0.43
1:A:1108:ASN:N	1:A:1109:PRO:HD3	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1118:MET:O	1:B:1122:GLN:HG2	2.18	0.43
1:A:739:GLN:HG2	1:A:911:PHE:CE1	2.54	0.43
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	2.01	0.42
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.82	0.42
1:A:508:ARG:O	1:A:512:THR:HG23	2.18	0.42
1:A:802:GLU:HG2	1:A:803:THR:HG23	2.01	0.42
1:B:955:PHE:HA	1:B:1145:ASN:ND2	2.20	0.42
1:A:621:ASP:CB	1:A:686:LYS:HE2	2.47	0.42
1:A:318:LYS:HG3	1:A:319:LEU:HG	2.02	0.42
1:A:284:ILE:HG21	1:A:287:LEU:HD23	2.02	0.42
1:B:1176:THR:HG21	1:B:1199:PHE:CZ	2.54	0.42
1:B:544:SER:O	1:B:994:LYS:HE2	2.19	0.42
1:A:1198:ALA:HB3	1:A:1263:PRO:HB2	2.00	0.42
1:A:771:LYS:HD3	1:A:771:LYS:HA	1.87	0.42
1:A:866:ASN:C	1:A:866:ASN:HD22	2.22	0.42
1:B:1326:LYS:HB2	1:B:1327:PRO:HD2	2.01	0.42
1:B:890:LYS:HE2	1:B:951:ASP:CG	2.40	0.42
1:A:898:GLY:O	1:A:899:ARG:HD2	2.19	0.42
1:A:46:GLY:HA2	2:A:1334:FES:S1	2.60	0.42
1:B:609:THR:HG21	1:B:835:ILE:HD11	2.01	0.42
1:B:657:LYS:O	1:B:658:ASP:HB2	2.18	0.42
1:A:1259:VAL:O	1:A:1259:VAL:HG22	2.19	0.42
1:B:57:LYS:HE2	1:B:83:VAL:HG22	2.01	0.42
1:B:407:ILE:HG13	1:B:407:ILE:O	2.19	0.42
1:A:74:LEU:O	1:A:76:PRO:HD3	2.20	0.42
1:A:759:GLU:OE1	9:A:1348:GOL:H12	2.20	0.42
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.20	0.42
1:A:419:SER:HB2	1:A:519:PHE:CD1	2.55	0.42
1:A:655:PHE:CE1	1:A:814:LEU:HD23	2.54	0.42
1:B:574:GLY:CA	9:B:1344:GOL:H12	2.50	0.42
1:B:418:PHE:CD1	1:B:439:ARG:HB2	2.54	0.42
1:A:574:GLY:CA	9:A:1345:GOL:H12	2.49	0.42
1:B:661:THR:O	1:B:662:CYS:HB3	2.20	0.42
1:B:95:LYS:HG3	1:B:589:GLU:OE1	2.20	0.42
1:B:448:GLN:HB2	1:B:477:PHE:CE2	2.55	0.41
1:B:1299:PRO:HG2	1:B:1301:THR:HG23	2.01	0.41
1:B:885:MET:SD	1:B:896:GLY:HA3	2.59	0.41
1:B:480:GLU:HG3	1:B:484:GLN:HE21	1.85	0.41
1:B:644:ASN:O	1:B:653:THR:HA	2.21	0.41
1:B:890:LYS:HE2	1:B:951:ASP:OD2	2.19	0.41
1:A:600:GLU:OE2	1:B:598:ARG:HG2	2.20	0.41
1:B:752:ILE:HD13	1:B:822:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:987:PHE:CD2	1:B:996:ARG:HG3	2.56	0.41
1:B:316:VAL:HA	1:B:324:THR:HG21	2.02	0.41
1:A:675:PRO:HG2	1:A:676:GLU:OE1	2.20	0.41
1:B:65:ILE:HD13	1:B:212:PHE:HB2	2.03	0.41
1:A:1108:ASN:ND2	1:A:1111:GLY:HA3	2.36	0.41
1:A:154:ARG:HD2	1:A:154:ARG:C	2.41	0.41
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.54	0.41
1:A:570:GLU:CD	1:A:1057:PRO:HG3	2.41	0.41
1:A:659[A]:THR:HG22	1:A:660:VAL:N	2.35	0.41
1:A:802:GLU:OE1	8:A:1340:SAL:H3	2.20	0.41
1:B:610:SER:HB2	1:B:660:VAL:HG11	2.03	0.41
1:B:705:ASN:HA	1:B:707:PHE:CE1	2.55	0.41
1:A:1282:ARG:O	1:A:1286:THR:HB	2.21	0.41
1:B:1102:GLU:HB3	1:B:1103:PRO:HD3	2.02	0.41
1:A:1173:ASN:O	1:A:1236:PRO:HA	2.21	0.41
1:A:318:LYS:HG3	1:A:319:LEU:N	2.36	0.41
1:A:748[B]:CYS:HA	1:A:825:CYS:O	2.21	0.41
1:B:925:ASN:O	1:B:929:GLU:HG3	2.21	0.41
1:B:496:LEU:HB2	1:B:505:ILE:HG23	2.02	0.41
1:B:154:ARG:N	1:B:155:PRO:HD2	2.35	0.41
1:A:952:LEU:HD23	1:A:958:ARG:HA	2.02	0.41
1:A:507:PHE:HB2	1:A:1303:GLU:HG3	2.03	0.41
1:A:695:ILE:HG23	1:A:700:ASP:HB3	2.04	0.40
1:A:955:PHE:HB2	1:A:1140:TYR:CE1	2.56	0.40
1:A:615:ALA:HB2	1:A:691:ASP:HA	2.02	0.40
1:B:325:GLU:HB2	1:B:412:SER:CB	2.51	0.40
1:A:117:THR:HB	1:A:118:PRO:HD3	2.03	0.40
1:B:1203:LEU:HD23	1:B:1203:LEU:C	2.42	0.40
1:B:739:GLN:HG2	1:B:911:PHE:CE1	2.56	0.40
1:B:708:TYR:CE2	1:B:902:LYS:HD3	2.57	0.40
1:A:741:HIS:HA	1:A:911:PHE:CE1	2.56	0.40

There are no symmetry-related clashes.

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	1285/1332 (96%)	1241 (97%)	40 (3%)	4 (0%)	50	37
1	B	1285/1332 (96%)	1248 (97%)	33 (3%)	4 (0%)	50	37
All	All	2570/2664 (96%)	2489 (97%)	73 (3%)	8 (0%)	50	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	1008	SER
1	A	912	ARG
1	B	912	ARG
1	A	797	GLY
1	B	797	GLY
1	B	1139	GLY
1	A	1139	GLY

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	1098/1128 (97%)	1090 (99%)	8 (1%)	91	90
1	B	1098/1128 (97%)	1089 (99%)	9 (1%)	89	89
All	All	2196/2256 (97%)	2179 (99%)	17 (1%)	89	89

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	GLN
1	A	743	TYR
1	A	866	ASN
1	A	911	PHE
1	A	1002	PRO
1	A	1145	ASN
1	A	1239	PHE
1	A	1326	LYS
1	B	100	PRO

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Mol	Chain	Res	Type
1	B	271	LYS
1	B	565	ASN
1	B	743	TYR
1	B	911	PHE
1	B	1145	ASN
1	B	1239	PHE
1	B	1289	ASN
1	B	1326	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	251	GLN
1	A	272	ASN
1	A	341	GLN
1	A	471	GLN
1	A	473	GLN
1	A	650	ASN
1	A	683	HIS
1	A	866	ASN
1	A	1088	GLN
1	A	1145	ASN
1	A	1289	ASN
1	B	131	GLN
1	B	251	GLN
1	B	473	GLN
1	B	484	GLN
1	B	565	ASN
1	B	626	GLN
1	B	650	ASN
1	B	875	HIS
1	B	1088	GLN
1	B	1108	ASN
1	B	1145	ASN
1	B	1288	ASN
1	B	1289	ASN

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 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 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	FES	A	1333	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	A	1334	1	0,4,4	0.00	-	0,4,4	0.00	-
3	MTE	A	1335	4	26,26,26	2.65	9 (34%)	34,40,40	2.54	14 (41%)
4	MOS	A	1336	3	0,3,3	0.00	-	0,3,3	0.00	-
5	FAD	A	1337	-	58,58,58	2.53	19 (32%)	85,89,89	2.58	24 (28%)
6	NAD	A	1338	-	25,25,48	2.73	9 (36%)	38,38,73	2.21	9 (23%)
7	CO3	A	1339	-	0,3,3	0.00	-	0,3,3	0.00	-
8	SAL	A	1340	-	10,10,10	1.81	5 (50%)	13,13,13	1.92	4 (30%)
9	GOL	A	1341	-	5,5,5	0.57	0	5,5,5	0.37	0
9	GOL	A	1342	-	5,5,5	0.50	0	5,5,5	0.36	0
9	GOL	A	1343	-	5,5,5	0.57	0	5,5,5	0.30	0
9	GOL	A	1344	-	5,5,5	0.61	0	5,5,5	0.30	0
9	GOL	A	1345	-	5,5,5	0.57	0	5,5,5	0.33	0
9	GOL	A	1346	-	5,5,5	0.59	0	5,5,5	0.30	0
9	GOL	A	1347	-	5,5,5	0.54	0	5,5,5	0.31	0
9	GOL	A	1348	-	5,5,5	0.49	0	5,5,5	0.35	0
2	FES	B	1333	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	B	1334	1	0,4,4	0.00	-	0,4,4	0.00	-
3	MTE	B	1335	4	26,26,26	2.62	9 (34%)	34,40,40	2.51	13 (38%)
4	MOS	B	1336	3	0,3,3	0.00	-	0,3,3	0.00	-
5	FAD	B	1337	-	58,58,58	2.47	19 (32%)	85,89,89	2.56	24 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAD	B	1338	-	25,25,48	2.73	9 (36%)	38,38,73	2.15	9 (23%)
7	CO3	B	1339	-	0,3,3	0.00	-	0,3,3	0.00	-
8	SAL	B	1340	-	10,10,10	1.81	5 (50%)	13,13,13	1.90	4 (30%)
9	GOL	B	1341	-	5,5,5	0.53	0	5,5,5	0.37	0
9	GOL	B	1342	-	5,5,5	0.55	0	5,5,5	0.31	0
9	GOL	B	1343	-	5,5,5	0.60	0	5,5,5	0.31	0
9	GOL	B	1344	-	5,5,5	0.57	0	5,5,5	0.33	0
9	GOL	B	1345	-	5,5,5	0.52	0	5,5,5	0.27	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
2	FES	A	1333	1	-	0/0/4/4	0/0/1/1
2	FES	A	1334	1	-	0/0/4/4	0/0/1/1
3	MTE	A	1335	4	-	0/6/34/34	0/0/3/3
4	MOS	A	1336	3	-	0/0/0/0	0/0/0/0
5	FAD	A	1337	-	-	0/34/50/50	0/1/6/6
6	NAD	A	1338	-	-	0/10/26/62	0/1/3/5
7	CO3	A	1339	-	-	0/0/0/0	0/0/0/0
8	SAL	A	1340	-	-	0/4/4/4	0/1/1/1
9	GOL	A	1341	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1342	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1343	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1344	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1345	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1346	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1347	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1348	-	-	0/4/4/4	0/0/0/0
2	FES	B	1333	1	-	0/0/4/4	0/0/1/1
2	FES	B	1334	1	-	0/0/4/4	0/0/1/1
3	MTE	B	1335	4	-	0/6/34/34	0/0/3/3
4	MOS	B	1336	3	-	0/0/0/0	0/0/0/0
5	FAD	B	1337	-	-	0/34/50/50	0/1/6/6
6	NAD	B	1338	-	-	0/10/26/62	0/1/3/5
7	CO3	B	1339	-	-	0/0/0/0	0/0/0/0
8	SAL	B	1340	-	-	0/4/4/4	0/1/1/1
9	GOL	B	1341	-	-	0/4/4/4	0/0/0/0
9	GOL	B	1342	-	-	0/4/4/4	0/0/0/0
9	GOL	B	1343	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	B	1344	-	-	0/4/4/4	0/0/0/0
9	GOL	B	1345	-	-	0/4/4/4	0/0/0/0

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1337	FAD	C9A-N10	8.42	1.51	1.38
5	B	1337	FAD	C9A-N10	8.06	1.50	1.38
5	A	1337	FAD	O4B-C1B	6.62	1.51	1.41
5	B	1337	FAD	O4B-C1B	6.57	1.51	1.41
6	B	1338	NAD	C4A-N3A	6.47	1.45	1.35
6	A	1338	NAD	C4A-N3A	6.46	1.45	1.35
3	A	1335	MTE	C10-N8	6.39	1.47	1.35
3	B	1335	MTE	C10-N8	6.32	1.47	1.35
5	A	1337	FAD	C4X-C10	5.93	1.51	1.40
5	B	1337	FAD	C4X-C10	5.80	1.51	1.40
6	B	1338	NAD	C2A-N3A	5.58	1.43	1.32
6	A	1338	NAD	C2A-N3A	5.55	1.43	1.32
3	A	1335	MTE	O4-C4	5.24	1.34	1.24
6	B	1338	NAD	C4A-N9A	5.12	1.45	1.37
3	B	1335	MTE	O4-C4	5.07	1.34	1.24
6	A	1338	NAD	C4A-N9A	5.00	1.45	1.37
6	B	1338	NAD	C2A-N1A	4.86	1.43	1.33
6	A	1338	NAD	C2A-N1A	4.83	1.43	1.33
3	A	1335	MTE	C2-N1	4.81	1.39	1.33
3	B	1335	MTE	C2-N1	4.59	1.39	1.33
5	A	1337	FAD	C4A-N3A	4.58	1.42	1.35
3	B	1335	MTE	O3'-C3'	4.54	1.50	1.43
3	A	1335	MTE	O3'-C3'	4.49	1.50	1.43
3	A	1335	MTE	C9-C10	4.40	1.47	1.41
5	B	1337	FAD	C4A-N3A	4.36	1.42	1.35
5	B	1337	FAD	C2-N3	4.28	1.45	1.37
5	A	1337	FAD	C2-N3	4.28	1.45	1.37
3	B	1335	MTE	C9-C10	4.26	1.47	1.41
6	A	1338	NAD	C8A-N7A	4.20	1.42	1.34
6	B	1338	NAD	C8A-N7A	4.18	1.42	1.34
5	A	1337	FAD	C5X-N5	4.06	1.41	1.35
3	B	1335	MTE	O3'-C7	4.02	1.49	1.44
5	B	1337	FAD	C5X-N5	3.97	1.41	1.35
5	B	1337	FAD	C2A-N1A	3.96	1.41	1.33
5	A	1337	FAD	C2A-N1A	3.88	1.41	1.33
5	B	1337	FAD	C9A-C5X	3.86	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1337	FAD	C6-C5X	3.86	1.46	1.41
5	A	1337	FAD	C2A-N3A	3.85	1.39	1.32
3	A	1335	MTE	O3'-C7	3.78	1.49	1.44
5	A	1337	FAD	C9A-C5X	3.71	1.50	1.42
5	B	1337	FAD	C2A-N3A	3.65	1.39	1.32
5	A	1337	FAD	O4B-C4B	3.57	1.53	1.45
5	B	1337	FAD	C4-C4X	3.54	1.47	1.41
5	A	1337	FAD	C4-C4X	3.51	1.47	1.41
5	B	1337	FAD	C6-C5X	3.50	1.45	1.41
6	B	1338	NAD	O4B-C1B	3.47	1.46	1.41
5	B	1337	FAD	O4B-C4B	3.46	1.53	1.45
5	A	1337	FAD	C9-C9A	3.40	1.47	1.40
6	A	1338	NAD	O4B-C1B	3.38	1.46	1.41
5	A	1337	FAD	C8-C7	3.34	1.50	1.40
5	B	1337	FAD	C8-C7	3.33	1.50	1.40
5	B	1337	FAD	C9-C9A	3.13	1.46	1.40
3	A	1335	MTE	C9-N5	3.00	1.48	1.38
3	B	1335	MTE	C9-N5	2.99	1.48	1.38
6	A	1338	NAD	PA-O5B	-2.94	1.51	1.60
6	B	1338	NAD	PA-O5B	-2.92	1.51	1.60
5	A	1337	FAD	C4-N3	2.88	1.42	1.37
8	A	1340	SAL	C1-C1'	-2.88	1.43	1.49
5	B	1337	FAD	C2B-C1B	-2.83	1.49	1.53
8	B	1340	SAL	C1-C1'	-2.83	1.43	1.49
5	B	1337	FAD	C4-N3	2.82	1.41	1.37
5	B	1337	FAD	C5A-C4A	2.79	1.46	1.40
5	A	1337	FAD	C5A-C4A	2.77	1.46	1.40
5	A	1337	FAD	C2B-C1B	-2.71	1.49	1.53
6	A	1338	NAD	C6A-N6A	2.66	1.43	1.35
3	A	1335	MTE	C2'-S2'	2.65	1.84	1.74
6	B	1338	NAD	C6A-N6A	2.57	1.43	1.35
5	A	1337	FAD	C10-N1	2.56	1.40	1.35
5	A	1337	FAD	C8A-N9A	2.55	1.40	1.36
3	B	1335	MTE	C2'-S2'	2.49	1.83	1.74
5	B	1337	FAD	C8A-N9A	2.47	1.40	1.36
8	B	1340	SAL	C5-C6	2.45	1.44	1.39
8	A	1340	SAL	C5-C6	2.41	1.44	1.39
8	A	1340	SAL	O2'-C1'	-2.41	1.22	1.30
8	B	1340	SAL	O2'-C1'	-2.39	1.22	1.30
8	A	1340	SAL	C6-C1	2.38	1.43	1.39
5	B	1337	FAD	C10-N1	2.36	1.39	1.35
8	B	1340	SAL	C6-C1	2.32	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1338	NAD	O3B-C3B	2.17	1.48	1.43
3	B	1335	MTE	C1'-S1'	2.14	1.82	1.74
6	B	1338	NAD	O3B-C3B	2.11	1.48	1.43
8	B	1340	SAL	C3-C2	2.07	1.43	1.39
3	A	1335	MTE	C1'-S1'	2.03	1.82	1.74
8	A	1340	SAL	C3-C2	2.01	1.43	1.39

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1337	FAD	C2-N1-C10	9.57	124.63	114.98
5	A	1337	FAD	C2-N1-C10	9.46	124.51	114.98
5	A	1337	FAD	O4B-C1B-N9A	-8.97	100.10	108.44
5	B	1337	FAD	O4B-C1B-N9A	-8.75	100.30	108.44
5	A	1337	FAD	N3A-C2A-N1A	-8.73	121.41	128.71
5	B	1337	FAD	N3A-C2A-N1A	-8.46	121.64	128.71
6	B	1338	NAD	O5B-C5B-C4B	7.47	136.37	108.94
6	A	1338	NAD	O5B-C5B-C4B	7.44	136.26	108.94
5	A	1337	FAD	C4X-C10-N10	-7.24	116.90	120.51
5	B	1337	FAD	C4X-C10-N10	-7.10	116.97	120.51
3	A	1335	MTE	N2-C2-N3	6.45	124.96	117.86
3	B	1335	MTE	N2-C2-N3	6.31	124.80	117.86
3	A	1335	MTE	C2-N1-C10	5.60	125.57	117.61
3	B	1335	MTE	C4-C9-N5	5.56	127.19	119.10
3	A	1335	MTE	C4-C9-N5	5.54	127.15	119.10
3	B	1335	MTE	C2-N1-C10	5.48	125.40	117.61
5	A	1337	FAD	C5X-C9A-N10	-5.14	111.75	116.80
5	B	1337	FAD	C5X-C9A-N10	-5.12	111.77	116.80
6	A	1338	NAD	C1B-N9A-C4A	-5.02	117.96	126.64
5	B	1337	FAD	C2'-C1'-N10	5.00	119.08	112.45
5	A	1337	FAD	C2'-C1'-N10	5.00	119.08	112.45
6	B	1338	NAD	C1B-N9A-C4A	-4.87	118.21	126.64
5	A	1337	FAD	C4X-N5-C5X	4.75	122.02	116.69
3	A	1335	MTE	N8-C10-N1	4.73	123.93	116.51
3	B	1335	MTE	N8-C10-N1	4.73	123.93	116.51
5	B	1337	FAD	C4X-N5-C5X	4.65	121.92	116.69
5	B	1337	FAD	C9-C9A-N10	4.43	131.12	121.59
5	A	1337	FAD	C9-C9A-N10	4.42	131.12	121.59
6	A	1338	NAD	C8A-N9A-C1B	4.38	135.02	126.38
6	B	1338	NAD	C8A-N9A-C1B	4.28	134.80	126.38
5	B	1337	FAD	C9A-N10-C10	4.20	125.89	121.77
5	A	1337	FAD	C9A-N10-C10	4.05	125.74	121.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1338	NAD	C4B-O4B-C1B	4.04	114.14	109.75
8	A	1340	SAL	O2'-C1'-O1'	-3.84	114.64	123.35
8	B	1340	SAL	O2'-C1'-O1'	-3.83	114.67	123.35
6	A	1338	NAD	C3B-C2B-C1B	3.66	106.63	100.91
6	A	1338	NAD	N3A-C2A-N1A	-3.64	125.67	128.71
6	B	1338	NAD	N3A-C2A-N1A	-3.63	125.68	128.71
6	B	1338	NAD	C4B-O4B-C1B	3.52	113.57	109.75
6	A	1338	NAD	O4B-C1B-C2B	-3.51	101.39	106.77
6	B	1338	NAD	C3B-C2B-C1B	3.47	106.35	100.91
3	A	1335	MTE	N3-C2-N1	-3.44	116.96	121.78
3	B	1335	MTE	N3-C2-N1	-3.39	117.03	121.78
6	B	1338	NAD	O4B-C1B-C2B	-3.36	101.63	106.77
5	A	1337	FAD	C8A-N9A-C4A	-3.33	104.36	106.90
3	B	1335	MTE	C4'-C3'-C2'	-3.18	107.22	110.98
5	A	1337	FAD	N3A-C4A-N9A	3.13	131.08	125.43
5	B	1337	FAD	C8A-N9A-C4A	-3.11	104.52	106.90
8	B	1340	SAL	C3-C2-C1	3.11	123.65	119.89
5	B	1337	FAD	C8M-C8-C7	3.09	127.88	120.74
8	A	1340	SAL	C3-C2-C1	3.09	123.62	119.89
5	A	1337	FAD	C8M-C8-C7	3.09	127.88	120.74
3	A	1335	MTE	C7-C6-N5	3.05	112.31	108.44
6	A	1338	NAD	O4B-C1B-N9A	3.01	111.24	108.44
5	B	1337	FAD	N3A-C4A-N9A	3.01	130.86	125.43
3	A	1335	MTE	C9-C10-N1	-2.96	116.76	121.50
3	A	1335	MTE	C9-C4-N3	2.92	121.55	114.06
5	A	1337	FAD	C1'-N10-C9A	-2.87	116.08	118.87
3	B	1335	MTE	C9-C10-N1	-2.87	116.92	121.50
3	B	1335	MTE	C9-C4-N3	2.85	121.36	114.06
5	B	1337	FAD	C1'-N10-C9A	-2.83	116.12	118.87
3	A	1335	MTE	C4'-C3'-C2'	-2.75	107.73	110.98
3	B	1335	MTE	O3'-C7-C6	-2.75	105.76	109.50
8	A	1340	SAL	C2-C1-C1'	2.73	123.10	120.03
5	A	1337	FAD	C4A-C5A-N7A	2.66	111.80	109.52
3	B	1335	MTE	C7-C6-N5	2.64	111.80	108.44
5	B	1337	FAD	C8M-C8-C9	-2.63	114.03	120.38
3	A	1335	MTE	O3'-C7-C6	-2.63	105.92	109.50
5	A	1337	FAD	C8M-C8-C9	-2.62	114.05	120.38
3	B	1335	MTE	O4'-C4'-C3'	2.57	115.19	108.53
5	B	1337	FAD	O3B-C3B-C4B	-2.56	103.53	111.08
6	B	1338	NAD	O4B-C1B-N9A	2.54	110.80	108.44
5	B	1337	FAD	C4'-C3'-C2'	-2.52	107.55	113.25
3	A	1335	MTE	O4'-C4'-C3'	2.51	115.02	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1337	FAD	O3B-C3B-C4B	-2.51	103.69	111.08
8	B	1340	SAL	C2-C1-C1'	2.50	122.84	120.03
5	B	1337	FAD	C4A-C5A-N7A	2.48	111.65	109.52
5	B	1337	FAD	O3'-C3'-C4'	2.42	114.85	108.74
5	A	1337	FAD	C4'-C3'-C2'	-2.42	107.78	113.25
5	A	1337	FAD	O3'-C3'-C4'	2.41	114.84	108.74
8	B	1340	SAL	O2'-C1'-C1	2.35	122.49	115.47
5	A	1337	FAD	N1-C10-N10	2.35	122.14	115.97
8	A	1340	SAL	O2'-C1'-C1	2.34	122.45	115.47
5	B	1337	FAD	N3-C2-N1	-2.34	116.22	121.19
5	A	1337	FAD	N3-C2-N1	-2.33	116.24	121.19
5	B	1337	FAD	N1-C10-N10	2.30	122.03	115.97
3	A	1335	MTE	C4-C9-C10	2.26	116.66	114.56
5	B	1337	FAD	P-O3P-PA	2.25	138.29	131.68
5	B	1337	FAD	C4B-O4B-C1B	-2.24	107.32	109.75
5	B	1337	FAD	C8A-N9A-C1B	2.23	130.77	126.38
5	A	1337	FAD	P-O3P-PA	2.23	138.21	131.68
3	A	1335	MTE	C3'-C2'-C1'	2.15	124.66	117.86
3	B	1335	MTE	C3'-C2'-C1'	2.14	124.63	117.86
6	B	1338	NAD	C4A-C5A-N7A	2.12	111.34	109.52
3	B	1335	MTE	C4-C9-C10	2.11	116.52	114.56
5	A	1337	FAD	O2'-C2'-C3'	2.08	114.22	109.05
3	A	1335	MTE	C7-O3'-C3'	2.07	116.07	112.03
5	A	1337	FAD	C4B-O4B-C1B	-2.06	107.51	109.75
5	A	1337	FAD	C8A-N9A-C1B	2.03	130.38	126.38
5	B	1337	FAD	O2'-C2'-C3'	2.03	114.09	109.05
6	A	1338	NAD	C4A-C5A-N7A	2.01	111.25	109.52

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	1286/1332 (96%)	-0.11	25 (1%) 64 65	9, 18, 33, 53	0
1	B	1289/1332 (96%)	-0.07	29 (2%) 59 60	9, 18, 33, 52	0
All	All	2575/2664 (96%)	-0.09	54 (2%) 60 62	9, 18, 33, 53	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1288	ASN	6.7
1	B	1325	CYS	6.2
1	B	1288	ASN	6.0
1	A	61	LEU	5.4
1	B	537	LYS	5.2
1	B	1318	VAL	5.1
1	B	61	LEU	4.5
1	B	1319	THR	4.2
1	A	221	ASP	4.0
1	B	528	GLY	4.0
1	A	565	ASN	3.8
1	B	565	ASN	3.8
1	B	566	GLY	3.8
1	A	537	LYS	3.6
1	B	222	VAL	3.6
1	B	221	ASP	3.5
1	A	553	PRO	3.3
1	B	63	ASP	3.1
1	A	566	GLY	3.1
1	A	1290	THR	3.1
1	A	551	LYS	3.0
1	B	1326	LYS	3.0
1	A	223	PRO	3.0
1	A	63	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	552	ASP	2.9
1	A	1286	THR	2.9
1	B	378	GLY	2.8
1	A	222	VAL	2.8
1	B	272	ASN	2.8
1	B	553	PRO	2.7
1	A	272	ASN	2.7
1	A	1287	ASN	2.6
1	B	1290	THR	2.6
1	A	60	ARG	2.5
1	A	199	GLU	2.4
1	B	540	PRO	2.4
1	B	60	ARG	2.4
1	A	1316	LEU	2.3
1	B	62	GLN	2.3
1	B	1287	ASN	2.3
1	B	1286	THR	2.3
1	B	217	LEU	2.3
1	B	318	LYS	2.3
1	A	401	GLU	2.2
1	A	1143	GLU	2.2
1	A	133	GLU	2.2
1	A	318	LYS	2.2
1	B	569	LYS	2.2
1	A	550	GLN	2.2
1	B	64	LYS	2.1
1	A	538	LEU	2.1
1	A	989	LYS	2.1
1	B	550	GLN	2.1
1	B	538	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, 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
9	GOL	B	1343	6/6	0.28	27.45	50,52,53,54	0
9	GOL	A	1347	6/6	0.25	14.61	40,43,44,47	0
9	GOL	A	1342	6/6	0.32	11.96	44,46,47,49	0
9	GOL	A	1348	6/6	0.22	9.59	28,29,32,34	0
9	GOL	A	1343	6/6	0.20	7.45	35,39,40,41	0
9	GOL	B	1345	6/6	0.17	7.21	21,24,24,26	0
4	MOS	A	1336	4/4	0.12	3.74	21,23,24,30	0
9	GOL	B	1341	6/6	0.14	3.74	17,21,23,24	0
6	NAD	A	1338	23/44	0.19	3.51	45,50,59,59	0
6	NAD	B	1338	23/44	0.20	3.46	46,50,59,61	0
9	GOL	A	1341	6/6	0.12	2.52	16,18,18,19	0
9	GOL	A	1344	6/6	0.15	2.29	35,38,39,39	0
4	MOS	B	1336	4/4	0.10	1.81	20,22,23,28	0
9	GOL	B	1342	6/6	0.13	1.30	18,25,26,31	0
8	SAL	B	1340	10/10	0.11	1.26	23,25,27,27	0
9	GOL	A	1345	6/6	0.15	1.16	30,33,34,35	0
9	GOL	A	1346	6/6	0.14	0.85	25,30,30,31	0
9	GOL	B	1344	6/6	0.15	0.42	28,30,32,33	0
3	MTE	B	1335	24/24	0.09	0.40	13,17,19,20	0
8	SAL	A	1340	10/10	0.10	0.38	19,22,25,26	0
5	FAD	A	1337	53/53	0.09	-0.21	13,16,19,19	0
5	FAD	B	1337	53/53	0.09	-0.27	12,15,18,19	0
3	MTE	A	1335	24/24	0.08	-0.41	14,17,19,20	0
7	CO3	A	1339	4/4	0.07	-1.30	11,12,13,14	0
2	FES	A	1334	4/4	0.05	-1.86	11,12,12,13	0
7	CO3	B	1339	4/4	0.07	-1.87	15,15,16,16	0
2	FES	B	1333	4/4	0.04	-1.97	12,12,12,12	0
2	FES	A	1333	4/4	0.04	-2.28	12,12,12,13	0
10	CA	A	1349	1/1	0.05	-2.36	14,14,14,14	0
2	FES	B	1334	4/4	0.05	-2.51	11,11,11,12	0
10	CA	B	1346	1/1	0.03	-4.58	15,15,15,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.