



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:32 PM GMT

PDB ID : 4LVC
Title : Crystal structure of S-adenosyl-L-homocysteine hydrolase from *Bradyrhizobium elkanii* in complex with adenosine
Authors : Manszewski, T.; Singh, K.; Imiolczyk, B.; Jaskolski, M.
Deposited on : 2013-07-26
Resolution : 1.74 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

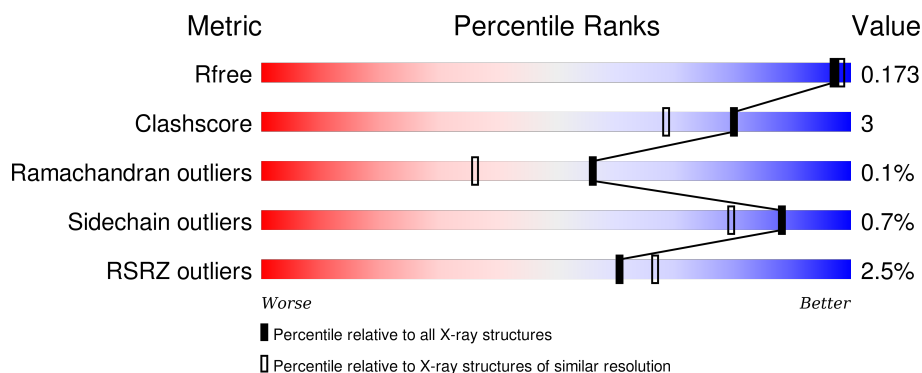
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	2417 (1.76-1.72)
Clashscore	102246	2570 (1.76-1.72)
Ramachandran outliers	100387	2544 (1.76-1.72)
Sidechain outliers	100360	2544 (1.76-1.72)
RSRZ outliers	91569	2420 (1.76-1.72)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	479	<div> <div>2%</div> <div>92%</div> <div>5%</div> <div>.</div> </div>
1	B	479	<div> <div>3%</div> <div>92%</div> <div>5%</div> <div>.</div> </div>
1	C	479	<div> <div>%</div> <div>94%</div> <div>.</div> <div>.</div> </div>
1	D	479	<div> <div>3%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>

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	ADN	A	501	-	-	-	X
2	ADN	B	501	-	-	-	X
2	ADN	C	501	-	-	-	X
3	NH4	B	502	-	-	-	X
3	NH4	C	502	-	-	-	X
5	GOL	A	504	-	-	-	X
5	GOL	A	506	-	-	-	X
5	GOL	B	504	-	-	-	X
5	GOL	C	504	-	-	-	X
5	GOL	C	505	-	-	-	X
5	GOL	C	506	-	-	-	X
5	GOL	C	507	-	-	-	X
5	GOL	D	502	-	-	-	X
5	GOL	D	505	-	-	-	X
6	ACT	B	509	-	-	-	X
6	ACT	C	508	-	-	-	X

2 Entry composition [i](#)

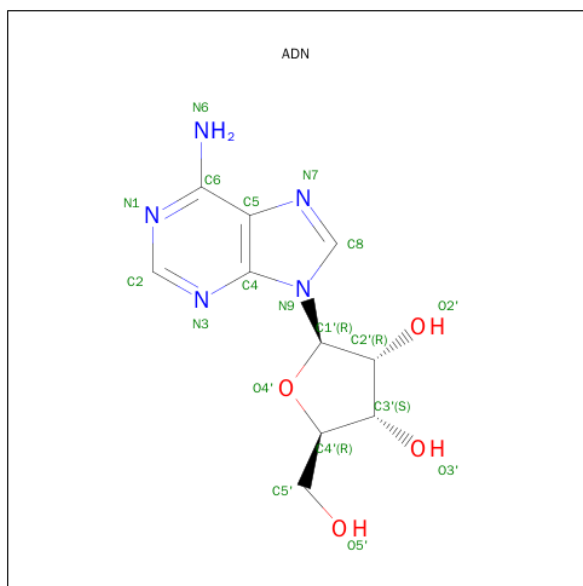
There are 7 unique types of molecules in this entry. The entry contains 16686 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 S-adenosyl-L-homocysteine hydrolase (SAHase).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	3	0
			3637	2302	627	687	21			
1	B	468	Total	C	N	O	S	0	5	0
			3660	2317	629	693	21			
1	C	468	Total	C	N	O	S	0	5	0
			3655	2312	631	691	21			
1	D	468	Total	C	N	O	S	0	10	0
			3691	2332	635	703	21			

- Molecule 2 is ADENOSINE (three-letter code: ADN) (formula: C₁₀H₁₃N₅O₄).



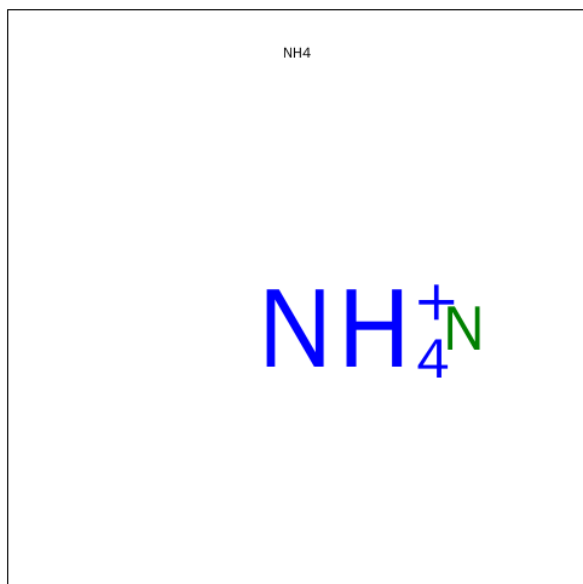
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	10	5	4		
2	B	1	Total	C	N	O	0	0
			19	10	5	4		

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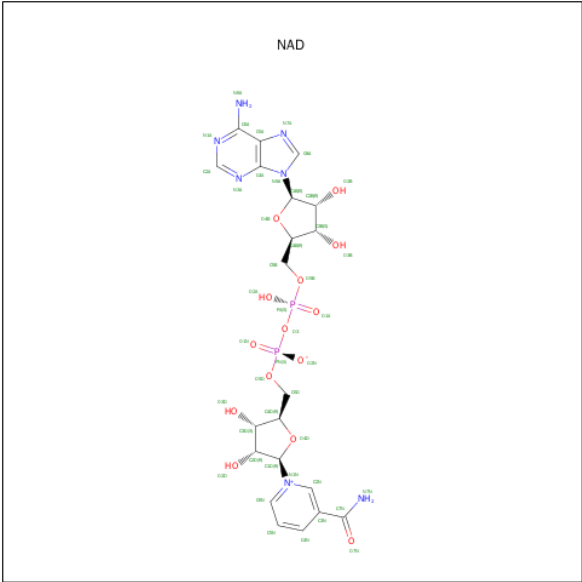
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 3 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).



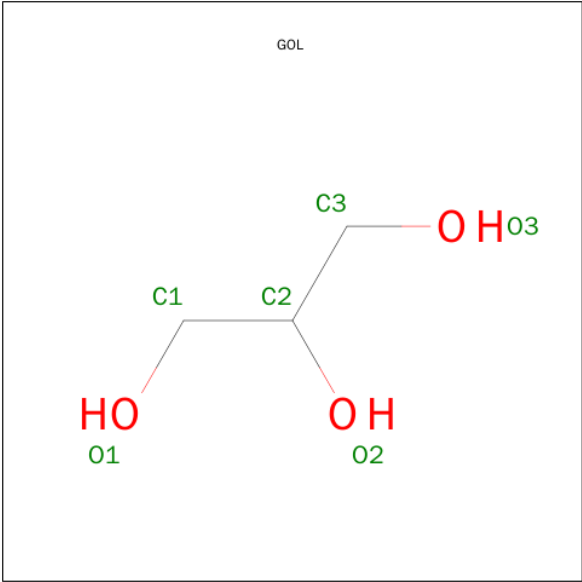
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	N	0	0
			1	1		
3	B	1	Total	N	0	0
			1	1		
3	C	1	Total	N	0	0
			1	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



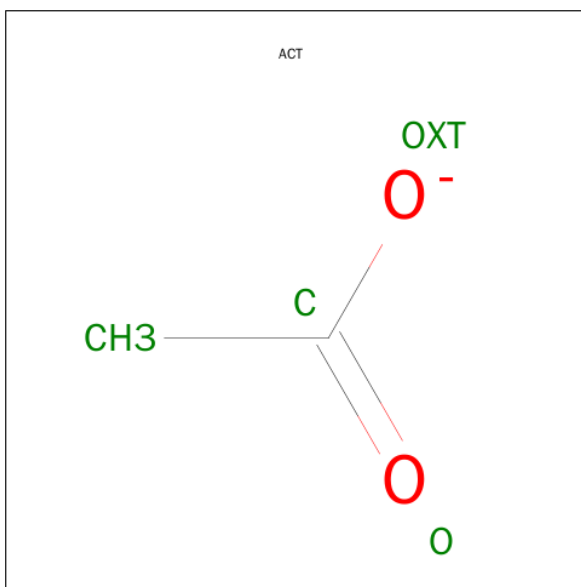
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

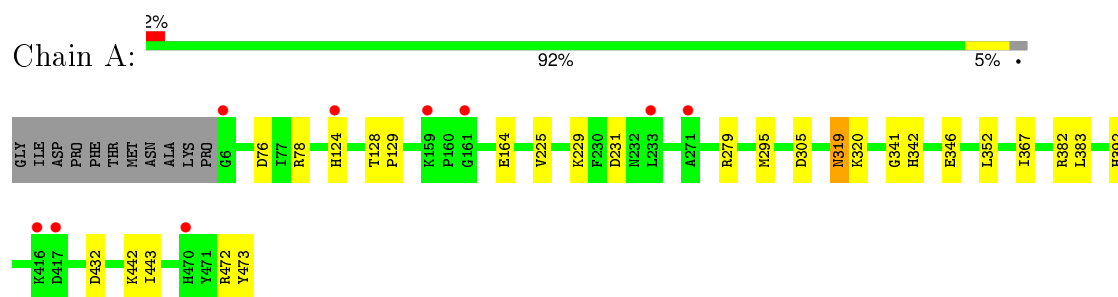
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	458	Total	O	0	0
			458	458		
7	B	411	Total	O	0	0
			411	411		
7	C	405	Total	O	0	1
			406	406		
7	D	430	Total	O	0	0
			430	430		

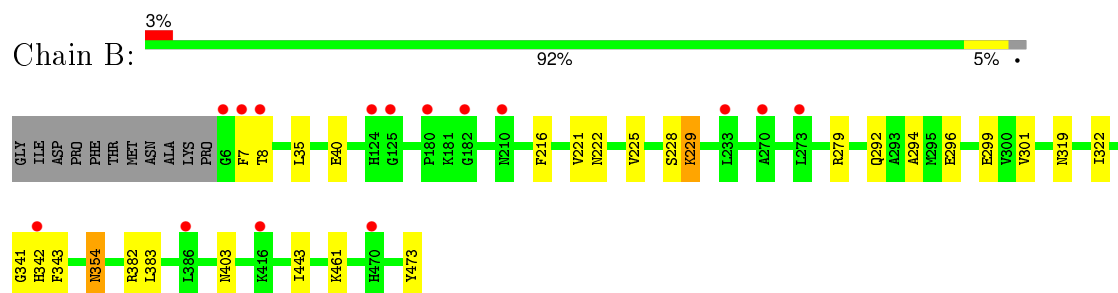
3 Residue-property plots [i](#)

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.

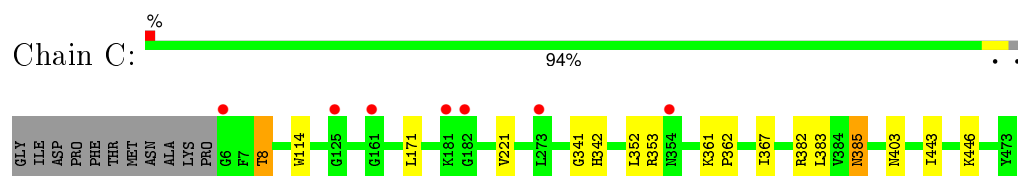
- Molecule 1: S-adenosyl-L-homocysteine hydrolase (SAHase)



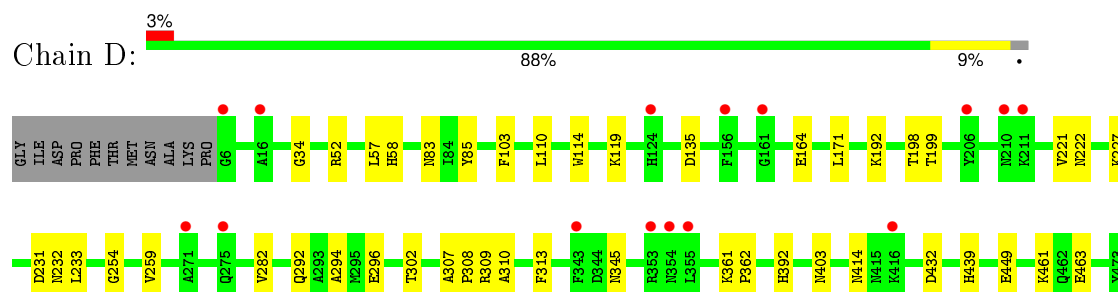
- Molecule 1: S-adenosyl-L-homocysteine hydrolase (SAHase)



- Molecule 1: S-adenosyl-L-homocysteine hydrolase (SAHase)



- Molecule 1: S-adenosyl-L-homocysteine hydrolase (SAHase)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.72Å 176.47Å 104.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.85 – 1.74 46.93 – 1.74	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.85-1.74) 98.7 (46.93-1.74)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.148 , 0.172 0.154 , 0.173	Depositor DCC
R_{free} test set	1011 reflections (0.51%)	DCC
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.2	EDS
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 200548 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16686	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADN, GOL, ACT, NAD, NH4

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	0.81	0/3714	0.76	2/5015 (0.0%)
1	B	0.84	0/3729	0.80	1/5034 (0.0%)
1	C	0.83	1/3730 (0.0%)	0.78	1/5036 (0.0%)
1	D	0.81	0/3764	0.76	3/5083 (0.1%)
All	All	0.82	1/14937 (0.0%)	0.78	7/20168 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	382	ARG	CG-CD	-5.26	1.38	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	ASP	CB-CG-OD1	5.64	123.38	118.30
1	C	382	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	279	ARG	NE-CZ-NH1	-5.37	117.62	120.30
1	D	432	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	382	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	52	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	D	432	ASP	CB-CG-OD2	-5.05	113.75	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3637	0	3645	32	0
1	B	3660	0	3654	32	0
1	C	3655	0	3652	15	0
1	D	3691	0	3685	34	0
2	A	19	0	13	1	0
2	B	19	0	13	1	0
2	C	19	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
3	C	1	0	0	0	0
4	A	44	0	26	2	0
4	B	44	0	26	2	0
4	C	44	0	26	1	0
4	D	44	0	26	1	0
5	A	18	0	24	0	0
5	B	24	0	32	1	0
5	C	24	0	32	1	0
5	D	24	0	31	5	0
6	B	8	0	6	0	0
6	C	4	0	3	1	0
7	A	458	0	0	4	0
7	B	411	0	0	2	0
7	C	406	0	0	2	0
7	D	430	0	0	5	0
All	All	16686	0	14907	103	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (103) 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:124[B]:HIS:NE2	7:A:1057:HOH:O	1.62	1.32
1:A:124[B]:HIS:CE1	7:A:1057:HOH:O	1.99	1.04
1:C:8:THR:HG22	7:C:868:HOH:O	1.60	1.00
1:A:295:MET:CE	1:B:443:ILE:CD1	2.46	0.92
1:A:295:MET:HE3	1:B:443:ILE:HD12	1.53	0.91
1:B:341[A]:GLY:O	1:B:383:LEU:CD2	2.23	0.86
1:A:295:MET:HE3	1:B:443:ILE:CD1	2.08	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:MET:CE	1:B:443:ILE:HD11	2.12	0.80
1:B:461:LYS:NZ	7:B:1010:HOH:O	2.22	0.71
2:C:501:ADN:H3'	4:C:503:NAD:C4N	2.21	0.70
1:A:319:ASN:HD22	1:A:320:LYS:H	1.39	0.69
1:C:353:ARG:HE	6:C:508:ACT:H1	1.58	0.68
2:B:501:ADN:H3'	4:B:503:NAD:C4N	2.25	0.67
1:B:354:ASN:H	1:B:354:ASN:HD22	1.42	0.67
1:B:341[A]:GLY:O	1:B:383:LEU:HD21	1.95	0.67
1:D:192:LYS:NZ	7:D:995:HOH:O	2.28	0.66
1:D:231:ASP:O	1:D:392:HIS:HE1	1.79	0.65
1:C:341:GLY:O	1:C:383:LEU:CD2	2.45	0.65
1:B:342[B]:HIS:CD2	1:B:343[B]:PHE:CD2	2.85	0.65
1:D:232:ASN:HD22	4:D:501:NAD:H5N	1.62	0.65
1:C:341:GLY:O	1:C:383:LEU:HD23	1.97	0.64
1:B:342[A]:HIS:HA	1:B:383:LEU:HD21	1.78	0.64
1:B:443:ILE:HD11	1:D:254[A]:GLY:HA3	1.81	0.64
1:A:231:ASP:OD2	1:A:231:ASP:C	2.36	0.63
1:D:233[B]:LEU:HD23	1:D:233[B]:LEU:C	2.20	0.62
1:A:319:ASN:ND2	1:A:320:LYS:H	1.99	0.61
2:A:501:ADN:H3'	4:A:503:NAD:C4N	2.30	0.60
1:B:341[A]:GLY:O	1:B:383:LEU:HD23	2.00	0.60
1:A:319:ASN:HD22	1:A:320:LYS:N	2.02	0.57
1:A:295:MET:HE1	1:B:443:ILE:HD11	1.86	0.57
1:A:124[B]:HIS:CD2	1:A:124[B]:HIS:H	2.20	0.56
1:A:352:LEU:HD13	1:A:367:ILE:HD13	1.87	0.56
1:D:199[B]:THR:HG23	7:D:916:HOH:O	2.04	0.56
1:A:231:ASP:OD2	1:A:392:HIS:CE1	2.59	0.56
1:D:392:HIS:HD2	7:D:746:HOH:O	1.90	0.54
1:D:164:GLU:OE2	5:D:503:GOL:C3	2.56	0.54
1:C:385:ASN:HD22	1:C:385:ASN:H	1.56	0.54
1:A:78:ARG:HH11	1:A:124[B]:HIS:HD2	1.54	0.54
1:C:446:LYS:HG2	1:D:302:THR:HG23	1.90	0.54
1:B:7:PHE:HD2	1:B:8:THR:HG23	1.74	0.53
1:C:385:ASN:N	1:C:385:ASN:HD22	2.06	0.53
1:A:229:LYS:NZ	1:B:229:LYS:NZ	2.57	0.53
1:C:342:HIS:HA	1:C:383:LEU:HD21	1.91	0.52
1:C:446:LYS:HE2	1:D:302:THR:HG23	1.90	0.52
1:A:295:MET:HE2	1:B:443:ILE:CD1	2.37	0.52
1:A:229:LYS:NZ	1:B:229:LYS:HZ3	2.08	0.51
1:D:221:VAL:HG13	1:D:403:ASN:HB3	1.92	0.50
1:A:231:ASP:OD2	1:A:231:ASP:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLY:O	1:A:383:LEU:CD2	2.60	0.50
1:A:341:GLY:O	1:A:383:LEU:HD23	2.12	0.50
1:A:342:HIS:HA	1:A:383:LEU:HD21	1.94	0.50
1:B:342[B]:HIS:O	1:B:343[B]:PHE:C	2.50	0.49
1:D:361:LYS:HB2	1:D:362:PRO:CD	2.42	0.49
1:D:114:TRP:HB3	1:D:171:LEU:HD22	1.95	0.49
1:D:164:GLU:OE2	5:D:503:GOL:H32	2.13	0.49
1:B:342[B]:HIS:HB3	4:B:503:NAD:O3D	2.13	0.49
1:C:341:GLY:O	1:C:383:LEU:HD21	2.13	0.48
1:D:461:LYS:HE2	1:D:463:GLU:OE2	2.14	0.48
1:D:83:ASN:ND2	1:D:85:TYR:H	2.12	0.48
1:D:254[B]:GLY:N	7:D:795:HOH:O	2.46	0.47
1:D:103:PHE:CE1	1:D:119:LYS:HE3	2.49	0.47
1:D:233[B]:LEU:HD21	5:D:504:GOL:H32	1.97	0.46
1:D:231:ASP:O	1:D:392:HIS:CE1	2.64	0.46
1:B:225:VAL:HG21	1:B:473:TYR:CE1	2.51	0.46
1:D:135:ASP:OD1	1:D:198:THR:HG21	2.16	0.46
1:B:221:VAL:HG13	1:B:403:ASN:HB3	1.98	0.46
1:B:222:ASN:O	1:B:228:SER:HB3	2.16	0.45
1:B:342[B]:HIS:HD2	1:B:343[B]:PHE:CD2	2.33	0.45
1:A:383:LEU:HD22	4:A:503:NAD:N7N	2.31	0.45
1:A:442:LYS:HE2	7:A:856:HOH:O	2.16	0.45
5:C:506:GOL:H2	7:C:820:HOH:O	2.16	0.45
1:C:352:LEU:HD13	1:C:367:ILE:HD13	1.99	0.45
1:A:128:THR:HB	1:A:129:PRO:HD2	1.99	0.44
1:D:233[B]:LEU:HD11	5:D:504:GOL:H11	2.00	0.44
1:C:443:ILE:HD12	1:D:294:ALA:HB1	2.00	0.44
1:A:76:ASP:OD1	1:A:124[B]:HIS:HE1	2.00	0.44
1:D:307:ALA:HB3	1:D:308:PRO:HD3	2.00	0.44
1:A:279[A]:ARG:NH1	7:A:716:HOH:O	2.50	0.44
1:B:40:GLU:OE1	5:B:505:GOL:H12	2.17	0.44
1:A:443:ILE:HD12	1:B:294:ALA:HB1	2.00	0.44
3:B:502:NH4:N	7:B:756:HOH:O	2.37	0.43
1:C:221:VAL:HG13	1:C:403:ASN:HB3	1.99	0.43
1:D:414:ASN:HB2	7:D:1018:HOH:O	2.18	0.43
1:C:361:LYS:HB2	1:C:362:PRO:CD	2.48	0.43
1:C:114:TRP:HB3	1:C:171:LEU:HD22	2.01	0.43
1:A:225:VAL:HG21	1:A:473:TYR:CE1	2.54	0.43
1:D:222:ASN:HD22	1:D:227:LYS:NZ	2.17	0.43
1:B:382:ARG:O	1:B:383:LEU:C	2.58	0.42
1:D:361:LYS:HB2	1:D:362:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:ILE:HD11	1:D:254[B]:GLY:HA3	2.01	0.42
1:D:292:GLN:O	1:D:296:GLU:HG2	2.20	0.41
1:A:472:ARG:CZ	1:B:225:VAL:HG22	2.50	0.41
1:D:310:ALA:HB3	1:D:313:PHE:CZ	2.56	0.41
1:D:34:GLY:HA3	1:D:439:HIS:CE1	2.56	0.41
1:B:35:LEU:HA	1:B:35:LEU:HD23	1.90	0.40
1:A:341:GLY:HA3	1:A:346:GLU:OE2	2.21	0.40
1:D:259:VAL:O	1:D:282:VAL:HA	2.21	0.40
1:B:319:ASN:HB3	1:B:322:ILE:HD11	2.03	0.40
1:B:299:GLU:HG2	1:B:301:VAL:HG13	2.04	0.40
1:D:233[B]:LEU:HD11	5:D:504:GOL:C1	2.51	0.40
1:A:225:VAL:N	1:A:432:ASP:OD2	2.48	0.40
1:B:292:GLN:O	1:B:296:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

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	469/479 (98%)	457 (97%)	12 (3%)	0	100	100
1	B	471/479 (98%)	456 (97%)	15 (3%)	0	100	100
1	C	471/479 (98%)	457 (97%)	14 (3%)	0	100	100
1	D	476/479 (99%)	469 (98%)	6 (1%)	1 (0%)	52	32
All	All	1887/1916 (98%)	1839 (98%)	47 (2%)	1 (0%)	56	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	58	HIS

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	381/387 (98%)	379 (100%)	2 (0%)	92	87
1	B	382/387 (99%)	379 (99%)	3 (1%)	86	77
1	C	382/387 (99%)	380 (100%)	2 (0%)	92	87
1	D	387/387 (100%)	382 (99%)	5 (1%)	76	60
All	All	1532/1548 (99%)	1520 (99%)	12 (1%)	88	77

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	GLU
1	A	319	ASN
1	B	216	PHE
1	B	229	LYS
1	B	354	ASN
1	C	8	THR
1	C	385	ASN
1	D	57	LEU
1	D	110	LEU
1	D	309	ARG
1	D	449[A]	GLU
1	D	449[B]	GLU

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

Mol	Chain	Res	Type
1	A	203	HIS
1	A	319	ASN
1	A	392	HIS
1	A	408	GLN
1	B	210	ASN
1	B	354	ASN
1	D	83	ASN

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Mol	Chain	Res	Type
1	D	190	ASN
1	D	222	ASN
1	D	232	ASN
1	D	388	ASN
1	D	392	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 3 are modelled with single atom - leaving 25 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	ADN	A	501	-	16,21,21	1.42	2 (12%)	16,31,31	2.39	6 (37%)
4	NAD	A	503	-	38,48,48	1.36	5 (13%)	47,73,73	1.89	7 (14%)
5	GOL	A	504	-	5,5,5	0.26	0	5,5,5	0.21	0
5	GOL	A	505	-	5,5,5	0.61	0	5,5,5	0.69	0
5	GOL	A	506	-	5,5,5	0.45	0	5,5,5	0.36	0
2	ADN	B	501	-	16,21,21	1.35	2 (12%)	16,31,31	2.14	4 (25%)
4	NAD	B	503	-	38,48,48	1.52	7 (18%)	47,73,73	1.58	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	B	504	-	5,5,5	0.39	0	5,5,5	0.98	0
5	GOL	B	505	-	5,5,5	0.81	0	5,5,5	1.21	0
5	GOL	B	506	-	5,5,5	0.34	0	5,5,5	0.75	0
5	GOL	B	507	-	5,5,5	0.57	0	5,5,5	0.78	0
6	ACT	B	508	-	1,3,3	0.83	0	0,3,3	0.00	-
6	ACT	B	509	-	1,3,3	1.15	0	0,3,3	0.00	-
2	ADN	C	501	-	16,21,21	1.47	2 (12%)	16,31,31	2.56	5 (31%)
4	NAD	C	503	-	38,48,48	1.36	6 (15%)	47,73,73	1.79	8 (17%)
5	GOL	C	504	-	5,5,5	0.20	0	5,5,5	0.54	0
5	GOL	C	505	-	5,5,5	0.35	0	5,5,5	0.44	0
5	GOL	C	506	-	5,5,5	0.28	0	5,5,5	0.68	0
5	GOL	C	507	-	5,5,5	0.37	0	5,5,5	0.29	0
6	ACT	C	508	-	1,3,3	0.61	0	0,3,3	0.00	-
4	NAD	D	501	-	38,48,48	1.29	4 (10%)	47,73,73	1.80	8 (17%)
5	GOL	D	502	-	5,5,5	0.38	0	5,5,5	0.51	0
5	GOL	D	503	-	5,5,5	0.52	0	5,5,5	0.63	0
5	GOL	D	504	-	5,5,5	0.80	0	5,5,5	1.41	1 (20%)
5	GOL	D	505	-	5,5,5	0.44	0	5,5,5	0.64	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	ADN	A	501	-	-	0/2/22/22	0/3/3/3
4	NAD	A	503	-	-	0/22/62/62	0/5/5/5
5	GOL	A	504	-	-	0/4/4/4	0/0/0/0
5	GOL	A	505	-	-	0/4/4/4	0/0/0/0
5	GOL	A	506	-	-	0/4/4/4	0/0/0/0
2	ADN	B	501	-	-	0/2/22/22	0/3/3/3
4	NAD	B	503	-	-	0/22/62/62	0/5/5/5
5	GOL	B	504	-	-	0/4/4/4	0/0/0/0
5	GOL	B	505	-	-	0/4/4/4	0/0/0/0
5	GOL	B	506	-	-	0/4/4/4	0/0/0/0
5	GOL	B	507	-	-	0/4/4/4	0/0/0/0
6	ACT	B	508	-	-	0/0/0/0	0/0/0/0
6	ACT	B	509	-	-	0/0/0/0	0/0/0/0
2	ADN	C	501	-	-	0/2/22/22	0/3/3/3
4	NAD	C	503	-	-	0/22/62/62	0/5/5/5
5	GOL	C	504	-	-	0/4/4/4	0/0/0/0
5	GOL	C	505	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	506	-	-	0/4/4/4	0/0/0/0
5	GOL	C	507	-	-	0/4/4/4	0/0/0/0
6	ACT	C	508	-	-	0/0/0/0	0/0/0/0
4	NAD	D	501	-	-	0/22/62/62	0/5/5/5
5	GOL	D	502	-	-	0/4/4/4	0/0/0/0
5	GOL	D	503	-	-	0/4/4/4	0/0/0/0
5	GOL	D	504	-	-	0/4/4/4	0/0/0/0
5	GOL	D	505	-	-	0/4/4/4	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	NAD	C2B-C3B	-3.76	1.43	1.53
4	A	503	NAD	C2B-C3B	-3.23	1.44	1.53
4	C	503	NAD	C2B-C3B	-3.19	1.44	1.53
4	B	503	NAD	O4B-C1B	-3.08	1.37	1.41
4	D	501	NAD	C2B-C3B	-2.47	1.46	1.53
4	C	503	NAD	O3D-C3D	-2.44	1.37	1.43
4	D	501	NAD	O3D-C3D	-2.37	1.37	1.43
4	B	503	NAD	O2D-C2D	-2.16	1.37	1.43
4	A	503	NAD	O4B-C4B	-2.12	1.40	1.45
2	A	501	ADN	C5-N7	-2.09	1.32	1.39
4	B	503	NAD	C5A-C4A	2.04	1.45	1.40
2	B	501	ADN	C2-N3	2.10	1.35	1.32
4	C	503	NAD	O4D-C1D	2.18	1.44	1.41
4	A	503	NAD	O4D-C1D	2.18	1.44	1.41
4	C	503	NAD	C5N-C4N	2.32	1.43	1.38
2	C	501	ADN	C2-N3	2.45	1.36	1.32
4	B	503	NAD	O4D-C1D	2.63	1.44	1.41
4	D	501	NAD	C6A-N6A	2.75	1.43	1.34
4	B	503	NAD	C6A-N6A	2.89	1.43	1.34
4	C	503	NAD	C6A-N6A	2.90	1.43	1.34
4	A	503	NAD	C6A-N6A	2.97	1.44	1.34
4	C	503	NAD	C7N-N7N	2.99	1.39	1.33
4	A	503	NAD	C7N-N7N	3.63	1.40	1.33
2	B	501	ADN	C5-C4	3.78	1.49	1.40
2	C	501	ADN	C5-C4	3.98	1.49	1.40
4	B	503	NAD	C7N-N7N	4.10	1.41	1.33
4	D	501	NAD	C7N-N7N	4.22	1.41	1.33
2	A	501	ADN	C5-C4	4.44	1.50	1.40

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	NAD	N3A-C2A-N1A	-9.43	121.67	128.89
4	D	501	NAD	N3A-C2A-N1A	-7.49	123.16	128.89
4	B	503	NAD	N3A-C2A-N1A	-5.58	124.62	128.89
4	C	503	NAD	N3A-C2A-N1A	-5.22	124.89	128.89
4	B	503	NAD	C4B-O4B-C1B	-5.15	104.06	109.72
2	C	501	ADN	C4-C5-N7	-5.11	104.78	109.48
4	C	503	NAD	C4B-O4B-C1B	-5.00	104.22	109.72
2	A	501	ADN	C4-C5-N7	-4.83	105.04	109.48
2	B	501	ADN	C4-C5-N7	-4.70	105.15	109.48
2	C	501	ADN	C4'-O4'-C1'	-4.60	104.66	109.72
2	A	501	ADN	N3-C2-N1	-4.51	125.44	128.89
2	C	501	ADN	N3-C2-N1	-4.36	125.56	128.89
4	D	501	NAD	C4B-O4B-C1B	-4.00	105.33	109.72
4	A	503	NAD	C4B-O4B-C1B	-3.46	105.92	109.72
4	C	503	NAD	O7N-C7N-N7N	-3.43	117.77	122.59
4	C	503	NAD	PN-O3-PA	-3.41	123.15	132.73
4	A	503	NAD	C5N-C4N-C3N	-3.38	116.09	120.33
2	B	501	ADN	C1'-N9-C4	-3.18	122.14	126.94
4	D	501	NAD	C5N-C4N-C3N	-2.98	116.58	120.33
2	A	501	ADN	C4'-O4'-C1'	-2.94	106.49	109.72
4	D	501	NAD	C4A-C5A-N7A	-2.92	106.79	109.48
4	D	501	NAD	O7N-C7N-N7N	-2.91	118.50	122.59
4	D	501	NAD	PN-O3-PA	-2.81	124.83	132.73
5	D	504	GOL	C3-C2-C1	-2.60	100.92	111.12
4	A	503	NAD	C1B-N9A-C4A	-2.58	123.05	126.94
4	A	503	NAD	O4D-C1D-N1N	-2.55	105.33	108.13
4	B	503	NAD	O7N-C7N-N7N	-2.50	119.08	122.59
4	B	503	NAD	PN-O3-PA	-2.41	125.95	132.73
4	D	501	NAD	C1B-N9A-C4A	-2.17	123.66	126.94
4	B	503	NAD	C5N-C4N-C3N	-2.16	117.62	120.33
2	A	501	ADN	C1'-N9-C4	-2.10	123.78	126.94
4	C	503	NAD	O4D-C1D-N1N	-2.08	105.85	108.13
4	B	503	NAD	C1B-N9A-C4A	-2.07	123.82	126.94
4	C	503	NAD	C4A-C5A-N7A	-2.07	107.58	109.48
4	B	503	NAD	C4A-C5A-N7A	-2.06	107.58	109.48
2	B	501	ADN	N3-C2-N1	-2.05	127.32	128.89
4	A	503	NAD	O7N-C7N-N7N	-2.03	119.73	122.59
2	A	501	ADN	C2-N1-C6	2.15	122.60	118.77
4	B	503	NAD	C2B-C1B-N9A	2.28	117.77	114.29
4	A	503	NAD	O7N-C7N-C3N	2.32	122.12	119.59
4	C	503	NAD	C2B-C1B-N9A	2.34	117.87	114.29
2	C	501	ADN	C5'-C4'-C3'	2.37	120.69	115.08
4	D	501	NAD	O7N-C7N-C3N	3.28	123.16	119.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	ADN	O4'-C1'-N9	3.88	116.23	108.10
2	A	501	ADN	O4'-C1'-N9	4.17	116.84	108.10
2	B	501	ADN	O4'-C1'-N9	5.29	119.18	108.10
4	C	503	NAD	O7N-C7N-C3N	5.67	125.78	119.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ADN	1	0
4	A	503	NAD	2	0
2	B	501	ADN	1	0
4	B	503	NAD	2	0
5	B	505	GOL	1	0
2	C	501	ADN	1	0
4	C	503	NAD	1	0
5	C	506	GOL	1	0
6	C	508	ACT	1	0
4	D	501	NAD	1	0
5	D	503	GOL	2	0
5	D	504	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	468/479 (97%)	-0.15	9 (1%) 70 76	16, 25, 41, 55	2 (0%)
1	B	468/479 (97%)	-0.04	15 (3%) 51 57	16, 25, 40, 65	2 (0%)
1	C	468/479 (97%)	-0.13	7 (1%) 76 82	16, 24, 44, 64	1 (0%)
1	D	468/479 (97%)	-0.09	15 (3%) 51 57	17, 26, 41, 55	3 (0%)
All	All	1872/1916 (97%)	-0.10	46 (2%) 61 67	16, 25, 41, 65	8 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	343	PHE	6.0
1	B	7	PHE	5.1
1	C	161	GLY	4.4
1	D	6	GLY	4.4
1	B	342[A]	HIS	3.7
1	D	210	ASN	3.6
1	A	6	GLY	3.6
1	D	206	TYR	3.6
1	B	8	THR	3.6
1	D	161	GLY	3.2
1	B	124	HIS	3.1
1	D	416	LYS	3.1
1	B	6	GLY	2.8
1	A	233	LEU	2.8
1	C	181	LYS	2.8
1	C	125	GLY	2.7
1	A	470	HIS	2.7
1	D	354	ASN	2.7
1	A	159	LYS	2.5
1	C	6	GLY	2.5
1	D	211	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	470	HIS	2.4
1	D	271	ALA	2.4
1	D	124	HIS	2.3
1	A	416	LYS	2.3
1	A	417	ASP	2.3
1	A	271	ALA	2.2
1	A	161	GLY	2.2
1	D	355	LEU	2.2
1	D	16	ALA	2.2
1	C	273	LEU	2.2
1	B	416	LYS	2.2
1	B	270	ALA	2.2
1	B	210	ASN	2.2
1	C	354	ASN	2.2
1	D	353	ARG	2.1
1	B	182	GLY	2.1
1	B	386	LEU	2.1
1	D	156	PHE	2.1
1	A	124[A]	HIS	2.1
1	B	180	PRO	2.1
1	B	125	GLY	2.1
1	B	233	LEU	2.1
1	B	273	LEU	2.1
1	D	275[A]	GLN	2.1
1	C	182	GLY	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	A	506	6/6	0.94	0.20	10.73	19,30,31,33	6
5	GOL	C	506	6/6	0.79	0.34	9.36	32,34,36,37	6
5	GOL	A	504	6/6	0.86	0.20	7.92	34,36,37,37	6
3	NH4	B	502	1/1	0.96	0.29	7.31	31,31,31,31	0
5	GOL	C	505	6/6	0.95	0.22	6.76	22,26,29,30	6
6	ACT	B	509	4/4	0.76	0.13	6.25	67,67,67,67	0
2	ADN	C	501	19/19	0.85	0.22	6.11	17,26,37,38	19
6	ACT	C	508	4/4	0.60	0.26	4.71	48,50,51,52	0
2	ADN	A	501	19/19	0.86	0.23	4.63	19,26,38,38	19
5	GOL	C	507	6/6	0.56	0.26	4.52	48,49,50,51	6
5	GOL	D	505	6/6	0.84	0.26	3.90	44,46,47,48	6
5	GOL	C	504	6/6	0.93	0.14	3.78	25,33,33,35	6
3	NH4	C	502	1/1	0.98	0.12	3.37	25,25,25,25	0
5	GOL	D	502	6/6	0.90	0.16	2.55	23,26,26,28	6
5	GOL	B	504	6/6	0.90	0.14	2.16	21,32,36,39	6
2	ADN	B	501	19/19	0.90	0.21	2.08	17,27,36,37	19
5	GOL	A	505	6/6	0.92	0.13	1.72	29,38,39,39	6
5	GOL	D	504	6/6	0.86	0.20	1.20	30,40,45,46	0
5	GOL	B	505	6/6	0.91	0.13	1.08	25,28,29,32	6
3	NH4	A	502	1/1	0.98	0.10	0.63	24,24,24,24	0
5	GOL	D	503	6/6	0.91	0.10	0.42	26,32,33,34	6
5	GOL	B	506	6/6	0.92	0.12	0.39	28,38,38,39	0
5	GOL	B	507	6/6	0.93	0.10	-0.15	29,32,35,37	0
4	NAD	A	503	44/44	0.98	0.09	-0.22	17,21,24,26	0
4	NAD	D	501	44/44	0.99	0.07	-0.29	16,21,27,33	0
4	NAD	C	503	44/44	0.98	0.09	-0.31	16,19,24,26	0
4	NAD	B	503	44/44	0.98	0.09	-0.52	17,21,24,25	0
6	ACT	B	508	4/4	0.74	0.26	-	59,60,60,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.