



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:48 AM GMT

PDB ID : 3G1U
Title : Crystal structure of Leishmania major S-adenosylhomocysteine hydrolase
Authors : Siponen, M.I.; Welin, M.; Arrowsmith, C.H.; Berglund, H.; Bountra, C.; Collins, R.; Dahlgren, L.G.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, A.; Johansson, I.; Karlberg, T.; Kotenyova, T.; Lehtio, L.; Moche, M.; Nilsson, M.E.; Nordlund, P.; Nyman, T.; Persson, C.; Sagemark, J.; Schutz, P.; Thorsell, A.G.; Tresaugues, L.; Van Den Berg, S.; Weigelt, J.; Wisniewska, M.; Schueler, H.; Structural Genomics Consortium (SGC)
Deposited on : 2009-01-30
Resolution : 2.20 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

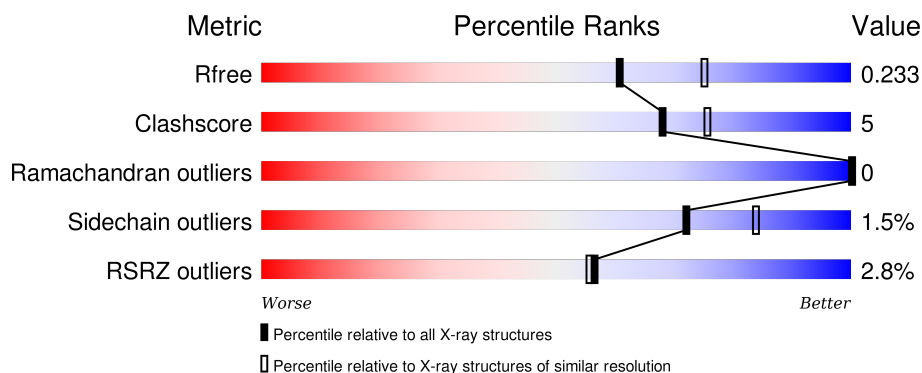
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	437	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>6%</div> </div> </div>
1	B	437	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
1	C	437	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>•</div> </div> </div>
1	D	437	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>•</div> </div> </div>

2 Entry composition [i](#)

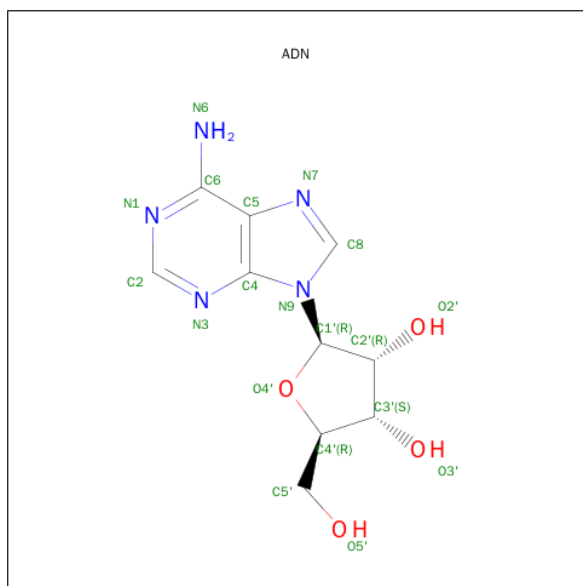
There are 4 unique types of molecules in this entry. The entry contains 13715 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3141	1981	539	601	20			
1	B	412	Total	C	N	O	S	0	2	0
			3154	1990	545	599	20			
1	C	424	Total	C	N	O	S	0	1	0
			3249	2055	561	612	21			
1	D	418	Total	C	N	O	S	0	5	0
			3221	2031	553	617	20			

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



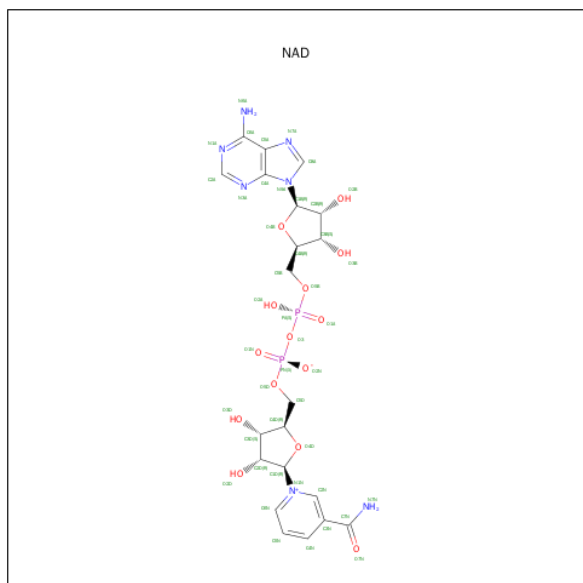
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	10	5	4		
2	B	1	Total	C	N	O	0	0
			19	10	5	4		

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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	206	Total	O	0	0
			206	206		
4	B	189	Total	O	0	0
			189	189		
4	C	150	Total	O	0	0
			150	150		

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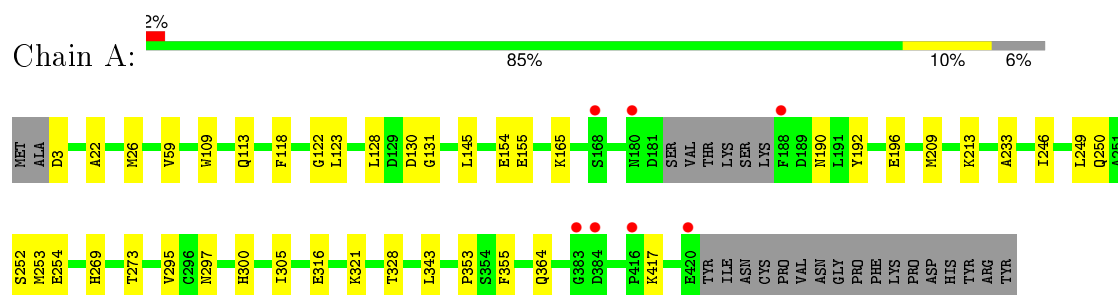
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	153	Total	O	0	0
			153	153		

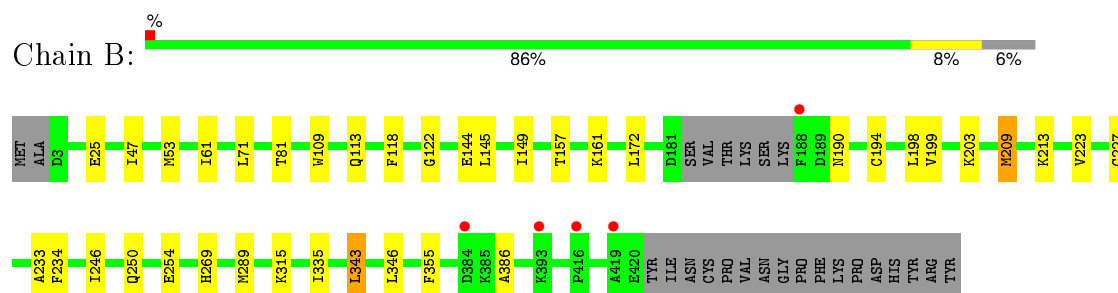
3 Residue-property plots

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.

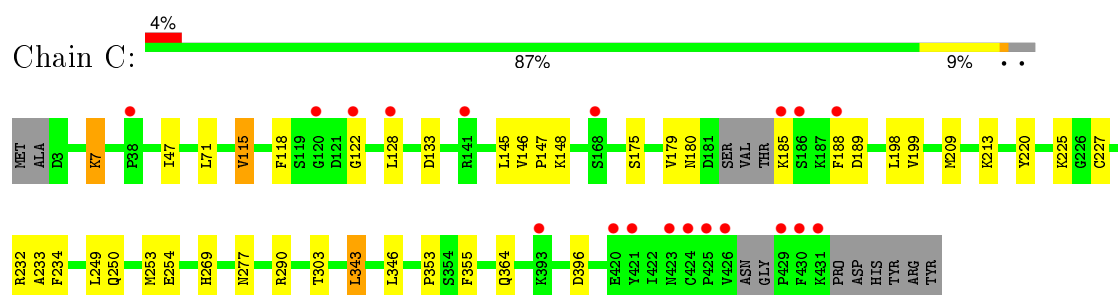
• Molecule 1: Adenosylhomocysteinase



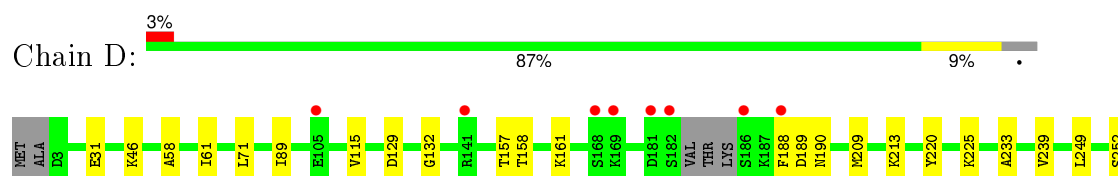
• Molecule 1: Adenosylhomocysteinase

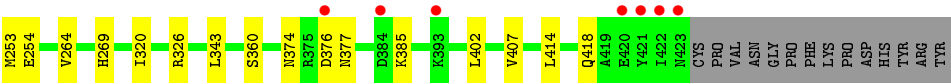


• Molecule 1: Adenosylhomocysteinase



• Molecule 1: Adenosylhomocysteinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.38Å 82.47Å 83.88Å 87.02° 71.41° 74.00°	Depositor
Resolution (Å)	22.87 – 2.20 22.65 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (22.87-2.20) 95.4 (22.65-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.5.0035	Depositor
R, R_{free}	0.181 , 0.232 0.182 , 0.233	Depositor DCC
R_{free} test set	4332 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.0	EDS
Estimated twinning fraction	0.016 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 86652 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13715	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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, NAD

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	0.54	0/3199	0.62	0/4336
1	B	0.56	0/3218	0.64	0/4360
1	C	0.54	0/3313	0.62	0/4485
1	D	0.53	0/3289	0.64	0/4454
All	All	0.54	0/13019	0.63	0/17635

There are no bond length outliers.

There are no bond angle outliers.

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	3141	0	3106	34	0
1	B	3154	0	3133	38	0
1	C	3249	0	3238	30	0
1	D	3221	0	3202	40	0
2	A	19	0	13	1	0
2	B	19	0	13	1	0
2	C	19	0	13	1	0
2	D	19	0	13	1	0
3	A	44	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	2	0
3	C	44	0	26	1	0
3	D	44	0	26	5	0
4	A	206	0	0	3	0
4	B	189	0	0	2	0
4	C	150	0	0	4	0
4	D	153	0	0	2	0
All	All	13715	0	12835	122	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 5.

All (122) 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:130:ASP:HB3	1:A:155:GLU:HB3	1.21	1.17
1:A:130:ASP:CB	1:A:155:GLU:HB3	1.94	0.95
1:A:22:ALA:HB1	1:A:26:MET:HE2	1.48	0.94
1:B:209:MET:HE1	1:D:253:MET:CE	2.09	0.83
1:A:130:ASP:HB3	1:A:155:GLU:CB	2.08	0.81
1:B:289:MET:HE3	1:B:335:ILE:HG12	1.64	0.80
1:B:209:MET:HE1	1:D:253:MET:HE1	1.65	0.79
1:A:252:SER:HB3	1:D:407:VAL:HG11	1.66	0.78
1:B:209:MET:CE	1:D:253:MET:CE	2.62	0.77
1:B:209:MET:CE	1:D:253:MET:HE1	2.16	0.75
1:A:233:ALA:HB1	1:B:233:ALA:HB1	1.67	0.75
1:C:180:ASN:HA	1:C:185:LYS:HD2	1.71	0.73
1:C:233:ALA:HB1	1:D:233:ALA:HB1	1.69	0.73
1:A:26:MET:CE	1:A:59:VAL:HG21	2.20	0.71
1:B:254:GLU:HG3	4:B:582:HOH:O	1.92	0.70
1:D:254:GLU:HG3	4:D:455:HOH:O	1.92	0.68
1:A:26:MET:HE3	1:A:59:VAL:HG21	1.74	0.67
1:B:289:MET:CE	1:B:335:ILE:HG12	2.25	0.67
1:B:250:GLN:O	1:B:254:GLU:HG2	1.97	0.64
1:B:209:MET:HE1	1:D:253:MET:HE3	1.79	0.64
1:D:31:GLU:HG2	1:D:402:LEU:HD22	1.79	0.64
1:B:213[A]:LYS:HD2	1:B:269:HIS:CG	2.33	0.63
1:D:158:THR:HG23	3:D:439:NAD:O3D	1.98	0.63
1:A:22:ALA:HB1	1:A:26:MET:CE	2.24	0.63
1:A:252:SER:CB	1:D:407:VAL:HG11	2.29	0.63
2:B:438:ADN:H3'	3:B:439:NAD:C4N	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:MET:CE	1:D:253:MET:HE3	2.30	0.60
1:C:353:PRO:HB2	1:D:209:MET:HB2	1.85	0.58
1:A:128:LEU:HD11	1:A:364:GLN:HG3	1.86	0.58
1:B:118:PHE:O	1:B:122:GLY:HA2	2.04	0.57
1:C:118:PHE:O	1:C:122:GLY:HA2	2.06	0.56
1:A:417:LYS:HB2	4:A:558:HOH:O	2.06	0.55
2:C:438:ADN:H3'	3:C:439:NAD:C4N	2.38	0.54
2:A:438:ADN:H3'	3:A:439:NAD:C4N	2.39	0.53
1:C:250:GLN:O	1:C:254:GLU:HG2	2.09	0.53
1:B:109:TRP:O	1:B:113:GLN:HG2	2.09	0.52
1:C:47:ILE:HB	1:C:71:LEU:HD23	1.91	0.52
1:A:130:ASP:HA	1:A:154:GLU:OE2	2.10	0.52
1:A:192:TYR:HE1	1:D:254:GLU:OE2	1.93	0.52
1:D:158:THR:CG2	3:D:439:NAD:O3D	2.58	0.52
1:D:320:ILE:HD11	1:D:326:ARG:HB2	1.92	0.52
1:D:31:GLU:HG2	1:D:402:LEU:CD2	2.41	0.51
1:B:213[B]:LYS:HD2	1:B:269:HIS:CG	2.45	0.51
1:A:316:GLU:HB3	1:A:328:THR:HB	1.91	0.51
1:D:254:GLU:CG	4:D:455:HOH:O	2.56	0.51
1:D:213:LYS:HD2	1:D:269:HIS:CG	2.45	0.51
1:A:355:PHE:HD2	1:B:209:MET:HE2	1.76	0.50
1:D:58:ALA:HB1	1:D:89:ILE:HD11	1.92	0.50
1:D:188:PHE:O	1:D:189:ASP:C	2.49	0.50
1:B:53:MET:HB3	1:B:81:THR:HG23	1.93	0.50
1:A:249:LEU:O	1:A:253:MET:HG2	2.11	0.49
1:C:199:VAL:HG11	1:C:234:PHE:CE2	2.47	0.49
1:A:246:ILE:O	1:A:250:GLN:HG3	2.13	0.49
1:C:198:LEU:HD22	1:C:227:CYS:HB3	1.94	0.49
1:D:61:ILE:HG23	1:D:71:LEU:HD13	1.94	0.49
1:B:199:VAL:HG11	1:B:234:PHE:CE2	2.48	0.49
1:B:61:ILE:HG23	1:B:71:LEU:HD13	1.95	0.49
1:A:353:PRO:HB2	1:B:209:MET:HB2	1.95	0.48
1:C:213:LYS:HD2	1:C:269:HIS:CG	2.48	0.48
1:A:213:LYS:HD2	1:A:269:HIS:CG	2.48	0.48
1:A:190:ASN:CG	3:A:439:NAD:H5N	2.34	0.48
1:A:26:MET:HE1	1:A:59:VAL:HG21	1.96	0.48
1:C:199:VAL:HG11	1:C:234:PHE:HE2	1.79	0.48
1:C:249:LEU:O	1:C:253:MET:HG2	2.14	0.48
1:A:3:ASP:N	4:A:595:HOH:O	2.47	0.48
1:D:157:THR:HG22	1:D:161:LYS:HD2	1.96	0.48
1:B:246:ILE:HD11	1:C:396:ASP:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:VAL:HG21	1:D:264:VAL:HG11	1.96	0.47
1:C:290:ARG:NH1	4:C:521:HOH:O	2.47	0.47
1:B:157:THR:HG22	1:B:161:LYS:HE2	1.96	0.47
2:D:438:ADN:H3'	3:D:439:NAD:C4N	2.44	0.47
1:B:144:GLU:HB2	4:B:454:HOH:O	2.15	0.47
1:D:249:LEU:O	1:D:253:MET:HG2	2.13	0.47
1:B:190:ASN:CG	3:B:439:NAD:H5N	2.35	0.47
1:B:145:LEU:HG	1:B:149:ILE:HD11	1.97	0.47
1:D:190:ASN:CG	3:D:439:NAD:H5N	2.35	0.47
1:A:295:VAL:HG12	1:A:305:ILE:HD13	1.96	0.47
1:C:355:PHE:HD2	1:D:209:MET:CE	2.28	0.47
1:B:199:VAL:HG11	1:B:234:PHE:HE2	1.80	0.46
1:C:220:TYR:CZ	1:C:225:LYS:HG2	2.50	0.46
1:C:7:LYS:HD3	4:C:584:HOH:O	2.14	0.46
1:A:321:LYS:NZ	4:A:548:HOH:O	2.49	0.46
1:C:148:LYS:HB3	4:C:481:HOH:O	2.16	0.46
1:D:158:THR:HG23	3:D:439:NAD:C3D	2.47	0.45
1:A:196:GLU:HB3	1:B:203:LYS:HE3	1.99	0.45
1:D:414:LEU:HD22	1:D:418:GLN:HB3	1.99	0.45
1:A:123:LEU:HD22	1:A:145:LEU:HD21	1.97	0.45
1:B:289:MET:CE	1:B:335:ILE:CD1	2.94	0.45
1:B:25:GLU:O	1:B:355:PHE:HA	2.17	0.45
1:D:115:VAL:O	1:D:115:VAL:CG1	2.65	0.44
1:C:343:LEU:HD22	1:C:346:LEU:HD12	2.00	0.44
1:A:233:ALA:HB1	1:B:233:ALA:CB	2.42	0.43
1:A:252:SER:HB3	1:D:407:VAL:CG1	2.44	0.43
1:C:128:LEU:HD11	1:C:364:GLN:HG3	1.99	0.43
1:C:133:ASP:HB2	4:C:486:HOH:O	2.17	0.43
1:D:220:TYR:CZ	1:D:225:LYS:HG2	2.53	0.43
1:B:343:LEU:HD22	1:B:346:LEU:HD12	2.00	0.43
1:B:47:ILE:HB	1:B:71:LEU:HD23	1.99	0.43
1:C:188:PHE:O	1:C:189:ASP:C	2.57	0.43
1:A:109:TRP:O	1:A:113:GLN:HG2	2.19	0.43
1:B:289:MET:CE	1:B:335:ILE:CG1	2.95	0.42
1:D:129:ASP:OD2	1:D:132:GLY:HA2	2.19	0.42
1:C:233:ALA:HB1	1:D:233:ALA:CB	2.45	0.42
1:B:198:LEU:HD22	1:B:227:CYS:HB3	2.01	0.42
1:B:172:LEU:O	1:B:386:ALA:HB3	2.20	0.42
1:C:220:TYR:CE2	1:C:225:LYS:HG2	2.55	0.42
1:A:118:PHE:O	1:A:122:GLY:HA2	2.20	0.42
1:A:233:ALA:CB	1:B:233:ALA:HB1	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:VAL:HB	1:C:147:PRO:HD3	2.01	0.42
1:C:115:VAL:O	1:C:115:VAL:HG13	2.20	0.42
1:C:145:LEU:HD12	1:C:148:LYS:HB2	2.03	0.41
1:D:220:TYR:CE2	1:D:225:LYS:HG2	2.55	0.41
1:C:233:ALA:CB	1:D:233:ALA:HB1	2.45	0.41
1:A:131:GLY:HA3	1:A:300:HIS:NE2	2.35	0.41
1:A:273:THR:OG1	1:A:297:ASN:HB2	2.19	0.41
1:C:115:VAL:O	1:C:115:VAL:CG1	2.68	0.41
1:B:194:CYS:SG	1:B:223:VAL:HG13	2.61	0.41
1:B:209:MET:HE3	1:D:253:MET:CE	2.47	0.41
1:D:374:ASN:OD1	1:D:377:ASN:ND2	2.52	0.40
1:C:232:ARG:NH2	1:C:254:GLU:O	2.33	0.40
1:C:355:PHE:HD2	1:D:209:MET:HE2	1.87	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	408/437 (93%)	399 (98%)	9 (2%)	0	100	100
1	B	410/437 (94%)	405 (99%)	5 (1%)	0	100	100
1	C	419/437 (96%)	403 (96%)	16 (4%)	0	100	100
1	D	419/437 (96%)	405 (97%)	14 (3%)	0	100	100
All	All	1656/1748 (95%)	1612 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	332/358 (93%)	328 (99%)	4 (1%)	78	88
1	B	334/358 (93%)	331 (99%)	3 (1%)	84	92
1	C	345/358 (96%)	337 (98%)	8 (2%)	58	71
1	D	345/358 (96%)	339 (98%)	6 (2%)	68	81
All	All	1356/1432 (95%)	1335 (98%)	21 (2%)	72	84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	LYS
1	A	209	MET
1	A	254	GLU
1	A	343	LEU
1	B	209	MET
1	B	315	LYS
1	B	343	LEU
1	C	7	LYS
1	C	115	VAL
1	C	175	SER
1	C	179	VAL
1	C	209	MET
1	C	277	ASN
1	C	303	THR
1	C	343	LEU
1	D	252	SER
1	D	343	LEU
1	D	360[A]	SER
1	D	360[B]	SER
1	D	376	ASP
1	D	385	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN

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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ADN	A	438	-	16,21,21	0.64	0	16,31,31	3.43	5 (31%)
3	NAD	A	439	-	38,48,48	1.61	3 (7%)	47,73,73	2.11	8 (17%)
2	ADN	B	438	-	16,21,21	0.77	0	16,31,31	3.30	6 (37%)
3	NAD	B	439	-	38,48,48	1.63	3 (7%)	47,73,73	1.96	4 (8%)
2	ADN	C	438	-	16,21,21	0.67	0	16,31,31	3.45	6 (37%)
3	NAD	C	439	-	38,48,48	1.66	4 (10%)	47,73,73	2.06	6 (12%)
2	ADN	D	438	-	16,21,21	0.60	0	16,31,31	3.18	4 (25%)
3	NAD	D	439	-	38,48,48	1.66	3 (7%)	47,73,73	2.17	6 (12%)

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	438	-	-	0/2/22/22	0/3/3/3
3	NAD	A	439	-	-	0/22/62/62	0/5/5/5
2	ADN	B	438	-	-	0/2/22/22	0/3/3/3
3	NAD	B	439	-	-	0/22/62/62	0/5/5/5
2	ADN	C	438	-	-	0/2/22/22	0/3/3/3
3	NAD	C	439	-	-	0/22/62/62	0/5/5/5
2	ADN	D	438	-	-	0/2/22/22	0/3/3/3
3	NAD	D	439	-	-	0/22/62/62	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	439	NAD	C2A-N1A	2.19	1.38	1.33
3	C	439	NAD	O4D-C1D	2.33	1.44	1.41
3	B	439	NAD	C2A-N1A	2.43	1.38	1.33
3	A	439	NAD	C2A-N1A	2.80	1.39	1.33
3	C	439	NAD	C2A-N1A	3.40	1.40	1.33
3	D	439	NAD	C2A-N3A	3.43	1.38	1.32
3	B	439	NAD	C2A-N3A	3.67	1.38	1.32
3	A	439	NAD	C2A-N3A	3.69	1.38	1.32
3	C	439	NAD	C2A-N3A	3.77	1.38	1.32
3	C	439	NAD	O7N-C7N	7.22	1.39	1.24
3	A	439	NAD	O7N-C7N	7.32	1.39	1.24
3	B	439	NAD	O7N-C7N	7.49	1.40	1.24
3	D	439	NAD	O7N-C7N	7.78	1.40	1.24

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	439	NAD	N3A-C2A-N1A	-12.65	119.21	128.89
3	A	439	NAD	N3A-C2A-N1A	-11.58	120.03	128.89
3	C	439	NAD	N3A-C2A-N1A	-11.49	120.10	128.89
3	B	439	NAD	N3A-C2A-N1A	-11.11	120.39	128.89
2	A	438	ADN	N3-C2-N1	-10.03	121.21	128.89
2	B	438	ADN	N3-C2-N1	-9.93	121.29	128.89
2	D	438	ADN	N3-C2-N1	-9.35	121.74	128.89
2	C	438	ADN	N3-C2-N1	-9.02	121.98	128.89
2	C	438	ADN	C4'-O4'-C1'	-5.64	103.52	109.72
2	A	438	ADN	C2'-C1'-N9	-4.91	106.78	114.29
2	D	438	ADN	C4'-O4'-C1'	-4.81	104.44	109.72
2	C	438	ADN	C5'-C4'-C3'	-4.61	104.18	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	438	ADN	C2'-C1'-N9	-4.45	107.50	114.29
2	B	438	ADN	C4'-O4'-C1'	-4.32	104.97	109.72
2	A	438	ADN	C4'-O4'-C1'	-4.14	105.17	109.72
2	B	438	ADN	C2'-C1'-N9	-3.74	108.58	114.29
3	A	439	NAD	O4D-C1D-N1N	-3.57	104.21	108.13
3	C	439	NAD	O4D-C1D-N1N	-3.56	104.22	108.13
2	C	438	ADN	C2'-C1'-N9	-3.41	109.09	114.29
2	B	438	ADN	C5'-C4'-C3'	-3.15	107.64	115.08
3	B	439	NAD	C1B-N9A-C4A	-3.00	122.41	126.94
3	B	439	NAD	C4A-C5A-N7A	-2.82	106.89	109.48
3	A	439	NAD	PN-O3-PA	-2.82	124.82	132.73
3	D	439	NAD	O3D-C3D-C4D	-2.67	103.04	111.05
2	A	438	ADN	C5'-C4'-C3'	-2.48	109.22	115.08
3	B	439	NAD	O3D-C3D-C4D	-2.44	103.74	111.05
3	A	439	NAD	C1B-N9A-C4A	-2.43	123.28	126.94
3	C	439	NAD	O3-PN-O5D	-2.39	96.61	102.94
2	B	438	ADN	C4-C5-N7	-2.34	107.32	109.48
3	D	439	NAD	C1B-N9A-C4A	-2.32	123.44	126.94
3	D	439	NAD	O4D-C1D-N1N	-2.26	105.65	108.13
2	C	438	ADN	C4-C5-N7	-2.24	107.42	109.48
3	A	439	NAD	C4A-C5A-N7A	-2.24	107.42	109.48
3	C	439	NAD	C4A-C5A-N7A	-2.19	107.47	109.48
3	C	439	NAD	O3D-C3D-C4D	-2.11	104.71	111.05
3	A	439	NAD	O3D-C3D-C4D	-2.08	104.80	111.05
3	D	439	NAD	PN-O3-PA	-2.05	126.98	132.73
3	D	439	NAD	C2B-C3B-C4B	2.13	106.99	102.61
3	A	439	NAD	C4D-O4D-C1D	2.28	112.22	109.72
3	A	439	NAD	C3N-C7N-N7N	2.31	120.34	117.82
3	C	439	NAD	C3N-C7N-N7N	2.67	120.73	117.82
2	D	438	ADN	O4'-C1'-N9	4.19	116.86	108.10
2	B	438	ADN	O4'-C1'-N9	4.63	117.79	108.10
2	A	438	ADN	O4'-C1'-N9	5.31	119.21	108.10
2	C	438	ADN	O4'-C1'-N9	5.86	120.37	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	438	ADN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	439	NAD	2	0
2	B	438	ADN	1	0
3	B	439	NAD	2	0
2	C	438	ADN	1	0
3	C	439	NAD	1	0
2	D	438	ADN	1	0
3	D	439	NAD	5	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	412/437 (94%)	-0.23	7 (1%) 73 72	15, 24, 40, 51	0
1	B	412/437 (94%)	-0.34	5 (1%) 81 80	13, 22, 38, 45	0
1	C	424/437 (97%)	-0.15	19 (4%) 37 36	15, 26, 44, 66	0
1	D	418/437 (95%)	-0.13	15 (3%) 46 45	16, 27, 45, 62	0
All	All	1666/1748 (95%)	-0.21	46 (2%) 56 55	13, 25, 42, 66	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	421	TYR	7.4
1	C	425	PRO	6.2
1	C	421	TYR	4.8
1	B	188	PHE	4.5
1	A	188	PHE	4.0
1	D	423	ASN	3.8
1	D	182	SER	3.7
1	C	429	PRO	3.7
1	D	422	ILE	3.6
1	C	426	VAL	3.5
1	D	168	SER	3.4
1	D	186	SER	3.4
1	B	384	ASP	3.4
1	C	186	SER	3.4
1	C	185	LYS	3.2
1	D	376	ASP	3.1
1	A	384	ASP	3.1
1	A	420	GLU	3.1
1	B	393	LYS	2.9
1	C	430	PHE	2.9
1	C	431	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	384	ASP	2.8
1	C	122	GLY	2.6
1	B	416	PRO	2.6
1	A	180	ASN	2.6
1	C	120	GLY	2.5
1	C	424	CYS	2.5
1	D	141	ARG	2.5
1	D	420	GLU	2.5
1	A	383	GLY	2.5
1	C	128	LEU	2.5
1	B	419	ALA	2.4
1	A	416	PRO	2.4
1	D	188	PHE	2.4
1	D	393	LYS	2.3
1	C	420	GLU	2.2
1	C	38	PRO	2.2
1	C	168	SER	2.2
1	C	188	PHE	2.2
1	C	141	ARG	2.1
1	D	105	GLU	2.1
1	C	393	LYS	2.1
1	C	423	ASN	2.1
1	D	169	LYS	2.0
1	A	168	SER	2.0
1	D	181	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
2	ADN	C	438	19/19	0.96	0.12	-0.36	24,27,30,30	0
2	ADN	A	438	19/19	0.95	0.11	-0.42	24,26,32,32	0
2	ADN	B	438	19/19	0.96	0.10	-0.43	17,21,27,29	0
2	ADN	D	438	19/19	0.95	0.10	-0.56	19,24,29,30	0
3	NAD	B	439	44/44	0.98	0.08	-0.76	13,18,19,21	0
3	NAD	C	439	44/44	0.98	0.08	-0.77	15,18,21,22	0
3	NAD	A	439	44/44	0.98	0.07	-0.91	13,19,21,23	0
3	NAD	D	439	44/44	0.98	0.08	-0.92	17,20,22,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.