



Full wwPDB X-ray Structure Validation Report

Aug 11, 2014 – 07:27 PM EDT

PDB ID : 4Q3C
Title : PylD cocrystallized with L-Lysine-Ne-L-lysine and NAD+
Authors : Quitterer, F.; Beck, P.; Bacher, A.; Groll, M.
Deposited on : 2014-04-11
Resolution : 2.10 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>

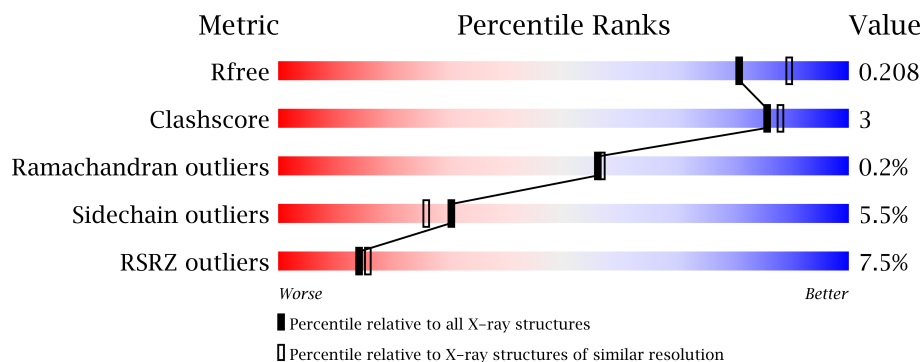
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
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) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.10 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	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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	260	
1	B	260	
1	C	260	
1	D	260	

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	MG	C	903	-	X
4	MG	D	903	-	X
6	GOL	A	905	-	X
6	GOL	A	907	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	GOL	B	905	-	X
8	PEG	B	906	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8384 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.

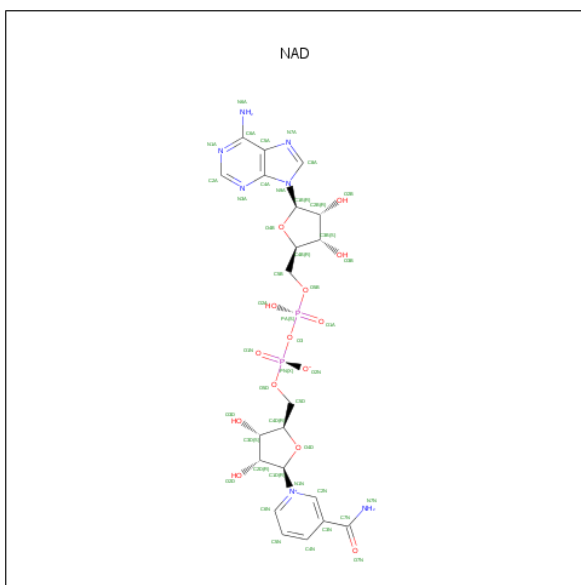
- Molecule 1 is a protein called PylD, pyrrolysine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1956	1246	314	385	11			
1	B	259	Total	C	N	O	S	0	0	0
			1956	1246	314	385	11			
1	C	259	Total	C	N	O	S	0	0	0
			1956	1246	314	385	11			
1	D	258	Total	C	N	O	S	0	0	0
			1948	1241	313	384	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q46E80
B	0	SER	-	EXPRESSION TAG	UNP Q46E80
C	0	SER	-	EXPRESSION TAG	UNP Q46E80
D	0	SER	-	EXPRESSION TAG	UNP Q46E80

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

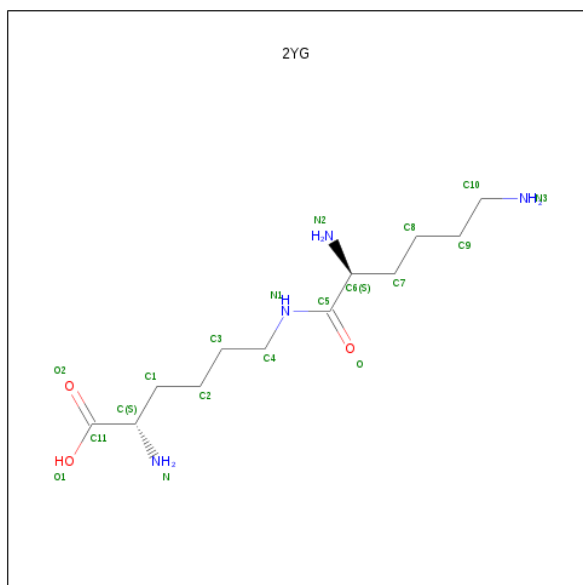
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

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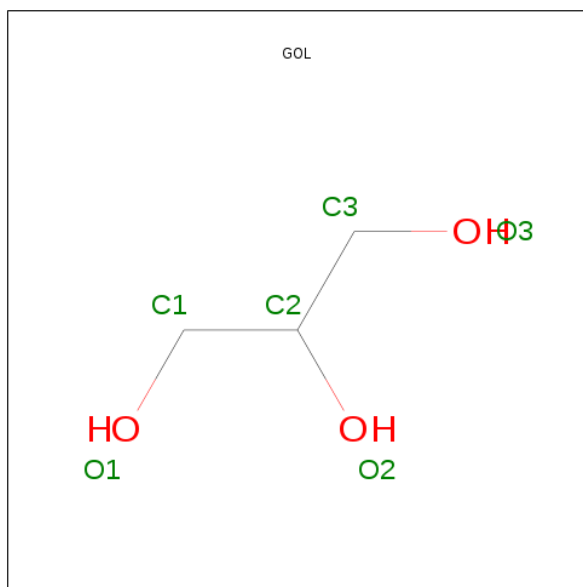
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is N 6 -L-LYSYL-L-LYSINE (three-letter code: 2YG) (formula: $C_{12}H_{26}N_4O_3$).



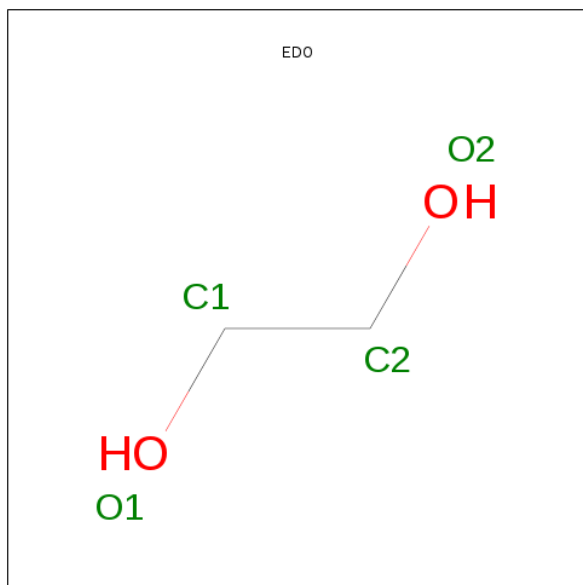
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			19	12	4	3		
5	B	1	Total	C	N	O	0	0
			19	12	4	3		
5	C	1	Total	C	N	O	0	0
			15	9	3	3		
5	D	1	Total	C	N	O	0	0
			15	9	3	3		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



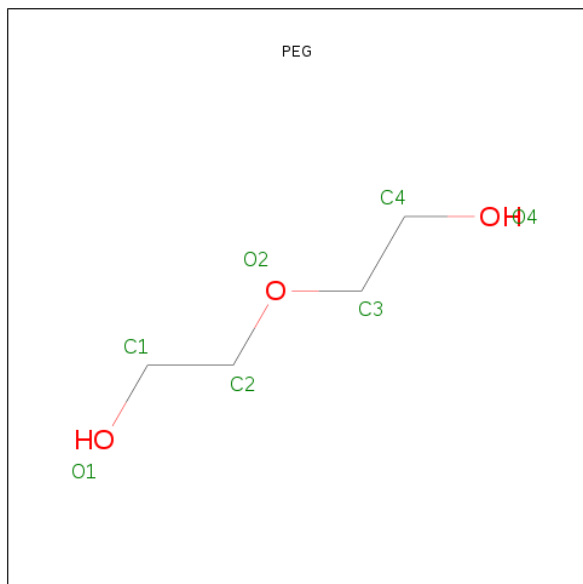
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 9 is water.

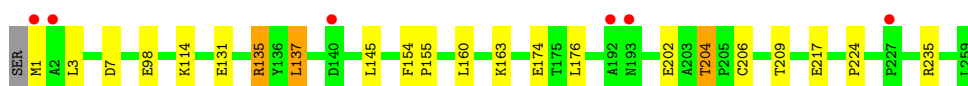
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	133	Total	O	0	0
			133	133		
9	B	111	Total	O	0	0
			111	111		
9	C	16	Total	O	0	0
			16	16		
9	D	13	Total	O	0	0
			13	13		

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: PylD, pyrrolysine synthase

Chain A: 



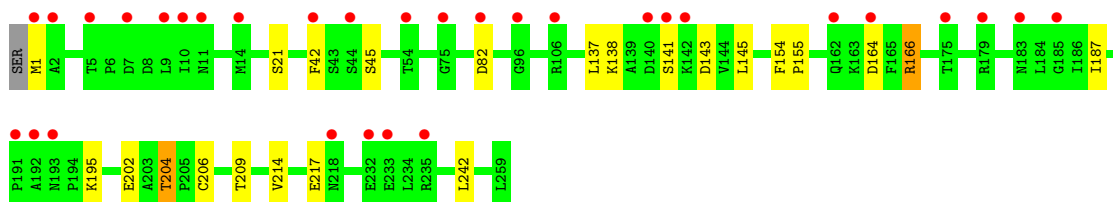
- Molecule 1: PylD, pyrrolysine synthase

Chain B: 



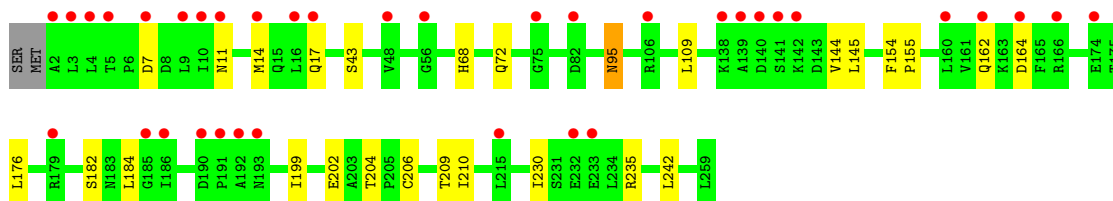
- Molecule 1: PylD, pyrrolysine synthase

Chain C: 



- Molecule 1: PylD, pyrrolysine synthase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.25Å 259.77Å 48.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.10 14.93 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.00-2.10) 99.9 (14.93-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.169 , 0.198 0.180 , 0.208	Depositor DCC
R_{free} test set	3380 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.987	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 127075 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8384	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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, MG, NAD, 2YG, EDO, NA, PEG

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	0.68	0/1992	0.84	3/2705 (0.1%)
1	B	0.67	0/1992	0.81	1/2705 (0.0%)
1	C	0.34	0/1992	0.58	0/2705
1	D	0.33	0/1984	0.56	0/2695
All	All	0.53	0/7960	0.71	4/10810 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ARG	NE-CZ-NH1	-11.29	114.66	120.30
1	A	135	ARG	NE-CZ-NH2	8.42	124.51	120.30
1	B	166	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	135	ARG	CG-CD-NE	-5.10	101.08	111.80

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	1956	0	1950	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1956	0	1950	10	0
1	C	1956	0	1950	6	0
1	D	1948	0	1938	9	0
2	A	44	0	26	1	0
2	B	44	0	26	3	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	19	0	0	1	0
5	B	19	0	0	2	0
5	C	15	0	0	0	0
5	D	15	0	0	0	0
6	A	18	0	24	0	0
6	B	6	0	8	0	0
7	A	12	0	18	6	0
8	B	7	0	10	0	0
9	A	133	0	0	1	0
9	B	111	0	0	2	0
9	C	16	0	0	0	0
9	D	13	0	0	0	0
All	All	8384	0	7952	44	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 3.

All (44) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:204:THR:HG21	1:A:209:THR:HG21	1.64	0.79
1:D:204:THR:HG21	1:D:209:THR:HG21	1.70	0.74
1:A:204:THR:HG22	1:A:206:CYS:H	1.50	0.73
1:D:204:THR:HG22	1:D:206:CYS:H	1.58	0.68
1:A:202:GLU:OE1	1:A:204:THR:HB	1.99	0.62
1:C:204:THR:HG21	1:C:209:THR:HG21	1.82	0.62
1:C:204:THR:HG22	1:C:206:CYS:H	1.66	0.60
1:A:163:LYS:HD2	7:A:909:EDO:H22	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:95:ASN:N	1:D:95:ASN:HD22	2.04	0.56
1:A:135:ARG:HB3	7:A:910:EDO:H11	1.89	0.55
1:A:131:GLU:OE1	1:A:135:ARG:HD2	2.07	0.54
2:B:901:NAD:C4N	5:B:904:2YG:C10	2.86	0.54
1:A:163:LYS:HD2	7:A:909:EDO:C2	2.40	0.52
1:B:109:LEU:C	1:B:109:LEU:HD12	2.30	0.52
1:B:2:ALA:HB3	9:B:1111:HOH:O	2.10	0.51
1:A:137:LEU:HD13	7:A:910:EDO:H12	1.93	0.51
2:B:901:NAD:C3N	5:B:904:2YG:C10	2.90	0.50
1:B:36:LYS:NZ	9:B:1095:HOH:O	2.45	0.50
9:A:1094:HOH:O	1:B:36:LYS:HE2	2.12	0.49
1:A:204:THR:CG2	1:A:206:CYS:H	2.24	0.49
1:D:68:HIS:O	1:D:72:GLN:HG2	2.11	0.49
1:D:202:GLU:OE1	1:D:204:THR:HB	2.14	0.48
1:A:98:GLU:OE1	1:A:114:LYS:HD3	2.13	0.48
1:A:154:PHE:HB3	1:A:155:PRO:HD3	1.96	0.47
2:A:901:NAD:C4N	5:A:904:2YG:C9	2.93	0.47
1:A:135:ARG:CB	7:A:910:EDO:H11	2.45	0.46
1:D:154:PHE:HB3	1:D:155:PRO:HD3	1.96	0.46
1:A:137:LEU:CD1	7:A:910:EDO:H12	2.46	0.45
1:C:202:GLU:OE1	1:C:204:THR:HB	2.17	0.45
1:C:143:ASP:OD2	1:C:195:LYS:NZ	2.38	0.45
1:A:202:GLU:O	1:A:224:PRO:HD2	2.17	0.44
1:B:61:GLY:O	1:B:62:ASN:HB2	2.17	0.43
1:C:154:PHE:HB3	1:C:155:PRO:HD3	2.01	0.43
1:B:224:PRO:O	2:B:901:NAD:H2N	2.19	0.43
1:B:71:THR:HG22	1:B:255:LEU:HD11	2.01	0.42
1:C:166:ARG:HD3	1:C:187:ILE:HD13	2.00	0.42
1:A:202:GLU:CD	1:A:204:THR:HB	2.40	0.42
1:B:167:VAL:HB	1:B:186:ILE:HG22	2.01	0.42
1:D:210:ILE:HB	1:D:230:ILE:HG22	2.02	0.41
1:A:98:GLU:OE1	1:A:114:LYS:CD	2.67	0.41
1:D:144:VAL:HG23	1:D:199:ILE:HG22	2.03	0.41
1:B:145:LEU:HD12	1:B:214:VAL:HG11	2.02	0.41
1:D:109:LEU:C	1:D:109:LEU:HD12	2.41	0.41
1:B:202:GLU:O	1:B:224:PRO:HD2	2.20	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	257/260 (99%)	247 (96%)	10 (4%)	0	100	100
1	B	257/260 (99%)	245 (95%)	11 (4%)	1 (0%)	43	39
1	C	257/260 (99%)	246 (96%)	10 (4%)	1 (0%)	43	39
1	D	256/260 (98%)	246 (96%)	10 (4%)	0	100	100
All	All	1027/1040 (99%)	984 (96%)	41 (4%)	2 (0%)	56	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	141	SER
1	B	247	LEU

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	214/215 (100%)	203 (95%)	11 (5%)	33	29
1	B	214/215 (100%)	206 (96%)	8 (4%)	45	45
1	C	214/215 (100%)	200 (94%)	14 (6%)	24	20
1	D	213/215 (99%)	199 (93%)	14 (7%)	24	19
All	All	855/860 (99%)	808 (94%)	47 (6%)	30	26

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	LEU
1	A	7	ASP
1	A	137	LEU
1	A	145	LEU
1	A	160	LEU
1	A	174	GLU
1	A	176	LEU
1	A	204	THR
1	A	217	GLU
1	A	235	ARG
1	B	106	ARG
1	B	137	LEU
1	B	145	LEU
1	B	166	ARG
1	B	178	GLU
1	B	233	GLU
1	B	235	ARG
1	B	242	LEU
1	C	1	MET
1	C	21	SER
1	C	42	PHE
1	C	45	SER
1	C	82	ASP
1	C	137	LEU
1	C	138	LYS
1	C	145	LEU
1	C	164	ASP
1	C	166	ARG
1	C	204	THR
1	C	214	VAL
1	C	217	GLU
1	C	242	LEU
1	D	7	ASP
1	D	11	ASN
1	D	14	MET
1	D	17	GLN
1	D	43	SER
1	D	95	ASN
1	D	145	LEU
1	D	162	GLN
1	D	164	ASP
1	D	176	LEU

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Mol	Chain	Res	Type
1	D	182	SER
1	D	184	LEU
1	D	235	ARG
1	D	242	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	162	GLN
1	A	208	ASN
1	A	218	ASN
1	B	13	ASN
1	B	72	GLN
1	B	162	GLN
1	B	218	ASN
1	C	17	GLN
1	D	11	ASN
1	D	72	GLN
1	D	95	ASN
1	D	162	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	NAD	A	901	4	48,48,48	1.51	5 (10%)	73,73,73	2.13	16 (21%)
5	2YG	A	904	-	18,18,18	0.56	0	21,21,21	0.85	0
6	GOL	A	905	-	5,5,5	0.16	0	5,5,5	0.28	0
6	GOL	A	906	-	5,5,5	0.23	0	5,5,5	0.49	0
6	GOL	A	907	-	5,5,5	0.39	0	5,5,5	0.27	0
7	EDO	A	908	-	3,3,3	0.41	0	2,2,2	0.62	0
7	EDO	A	909	-	3,3,3	0.49	0	2,2,2	0.52	0
7	EDO	A	910	-	3,3,3	0.44	0	2,2,2	0.59	0
2	NAD	B	901	4	48,48,48	1.12	4 (8%)	73,73,73	2.00	17 (23%)
5	2YG	B	904	-	18,18,18	0.53	0	21,21,21	1.00	0
6	GOL	B	905	-	5,5,5	0.40	0	5,5,5	0.60	0
8	PEG	B	906	-	6,6,6	0.38	0	5,5,5	0.91	0
2	NAD	C	901	4	48,48,48	1.00	3 (6%)	73,73,73	1.89	12 (16%)
5	2YG	C	904	-	13,14,18	1.25	1 (7%)	15,17,21	1.13	2 (13%)
2	NAD	D	901	-	48,48,48	0.96	2 (4%)	73,73,73	1.90	14 (19%)
5	2YG	D	904	-	13,14,18	0.55	0	15,17,21	1.22	2 (13%)

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	NAD	A	901	4	-	0/30/62/62	0/5/5/5
5	2YG	A	904	-	-	0/21/21/21	0/0/0/0
6	GOL	A	905	-	-	0/4/4/4	0/0/0/0
6	GOL	A	906	-	-	0/4/4/4	0/0/0/0
6	GOL	A	907	-	-	0/4/4/4	0/0/0/0
7	EDO	A	908	-	-	0/1/1/1	0/0/0/0
7	EDO	A	909	-	-	0/1/1/1	0/0/0/0
7	EDO	A	910	-	-	0/1/1/1	0/0/0/0
2	NAD	B	901	4	-	0/30/62/62	0/5/5/5
5	2YG	B	904	-	-	0/21/21/21	0/0/0/0
6	GOL	B	905	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEG	B	906	-	-	0/4/4/4	0/0/0/0
2	NAD	C	901	4	-	0/30/62/62	0/5/5/5
5	2YG	C	904	-	-	0/16/16/21	0/0/0/0
2	NAD	D	901	-	-	0/30/62/62	0/5/5/5
5	2YG	D	904	-	-	0/16/16/21	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	NAD	C4N-C3N	6.60	1.50	1.39
5	C	904	2YG	O2-C11	3.68	1.34	1.22
2	A	901	NAD	C4A-N9A	-3.65	1.32	1.37
2	C	901	NAD	C4A-N9A	-3.60	1.32	1.37
2	B	901	NAD	C4A-N9A	-3.45	1.32	1.37
2	A	901	NAD	C5N-C4N	3.06	1.45	1.38
2	D	901	NAD	C4A-N9A	-2.80	1.33	1.37
2	A	901	NAD	O4D-C1D	2.79	1.44	1.41
2	C	901	NAD	C5A-C4A	2.68	1.46	1.40
2	A	901	NAD	C5A-C4A	2.67	1.46	1.40
2	D	901	NAD	C5A-C4A	2.65	1.46	1.40
2	B	901	NAD	O4D-C1D	2.61	1.44	1.41
2	B	901	NAD	C5A-C4A	2.49	1.46	1.40
2	C	901	NAD	O4D-C1D	2.24	1.44	1.41
2	B	901	NAD	C3N-C7N	2.10	1.54	1.50

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	NAD	N3A-C2A-N1A	-8.16	121.71	128.89
2	A	901	NAD	N3A-C2A-N1A	-8.05	121.81	128.89
2	C	901	NAD	N3A-C2A-N1A	-7.42	122.36	128.89
2	D	901	NAD	C5A-C4A-N3A	-7.28	118.88	125.98
2	D	901	NAD	N3A-C2A-N1A	-7.03	122.70	128.89
2	A	901	NAD	C5A-C4A-N3A	-6.32	119.82	125.98
2	C	901	NAD	C5A-C4A-N3A	-6.20	119.93	125.98
2	A	901	NAD	C5N-C4N-C3N	-6.20	112.61	120.34
2	B	901	NAD	C5A-C4A-N3A	-6.10	120.03	125.98
2	D	901	NAD	N3A-C4A-N9A	5.53	134.87	125.39
2	C	901	NAD	O4D-C1D-N1N	5.47	114.14	108.13
2	D	901	NAD	O4D-C1D-N1N	5.19	113.84	108.13
2	B	901	NAD	N3A-C4A-N9A	4.81	133.64	125.39
2	C	901	NAD	N3A-C4A-N9A	4.70	133.45	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	NAD	N3A-C4A-N9A	4.66	133.38	125.39
2	B	901	NAD	C3N-C7N-N7N	3.96	122.19	117.78
2	A	901	NAD	C4B-O4B-C1B	-3.75	105.60	109.72
2	B	901	NAD	C8A-N9A-C4A	3.70	109.96	106.96
2	A	901	NAD	C4A-C5A-N7A	-3.70	105.84	109.41
2	A	901	NAD	C1B-N9A-C4A	-3.53	120.53	126.64
2	B	901	NAD	C1B-N9A-C4A	-3.51	120.58	126.64
2	A	901	NAD	PN-O3-PA	-3.49	119.14	133.17
2	A	901	NAD	C2D-C1D-N1N	3.42	120.32	113.48
2	A	901	NAD	C8A-N9A-C4A	3.31	109.64	106.96
2	C	901	NAD	C1B-N9A-C4A	-3.30	120.93	126.64
2	C	901	NAD	PN-O3-PA	-3.20	120.30	133.17
2	B	901	NAD	C4B-O4B-C1B	-3.20	106.21	109.72
2	C	901	NAD	C3N-C7N-N7N	3.18	121.33	117.78
2	B	901	NAD	C4A-C5A-N7A	-3.18	106.34	109.41
2	D	901	NAD	C4B-O4B-C1B	-3.13	106.28	109.72
2	B	901	NAD	PN-O3-PA	-3.04	120.95	133.17
2	D	901	NAD	C3N-C7N-N7N	3.03	121.16	117.78
2	C	901	NAD	C4A-C5A-N7A	-2.97	106.54	109.41
2	B	901	NAD	C2A-N3A-C4A	2.94	121.75	113.27
2	D	901	NAD	C2A-N3A-C4A	2.91	121.64	113.27
2	A	901	NAD	C2A-N3A-C4A	2.83	121.42	113.27
2	C	901	NAD	C2A-N3A-C4A	2.74	121.17	113.27
2	C	901	NAD	C8A-N9A-C4A	2.73	109.17	106.96
2	B	901	NAD	O7N-C7N-N7N	-2.73	118.69	122.59
5	C	904	2YG	O1-C11-O2	-2.71	117.96	124.05
2	A	901	NAD	C2A-N1A-C6A	2.66	123.50	118.76
2	A	901	NAD	C6N-C5N-C4N	2.62	123.51	119.44
2	D	901	NAD	C8A-N9A-C4A	2.51	109.00	106.96
2	B	901	NAD	O3-PN-O1N	2.51	114.84	108.77
2	D	901	NAD	C4A-C5A-N7A	-2.49	107.00	109.41
2	D	901	NAD	PN-O3-PA	-2.45	123.33	133.17
2	C	901	NAD	O7N-C7N-N7N	-2.43	119.12	122.59
2	A	901	NAD	C3N-C7N-N7N	2.43	120.48	117.78
2	A	901	NAD	O7N-C7N-N7N	-2.39	119.17	122.59
5	D	904	2YG	O1-C11-O2	-2.34	118.80	124.05
2	D	901	NAD	C1B-N9A-C4A	-2.33	122.61	126.64
2	D	901	NAD	O7N-C7N-N7N	-2.33	119.26	122.59
2	B	901	NAD	C2N-C3N-C4N	-2.33	115.70	118.31
2	C	901	NAD	O4D-C1D-C2D	-2.30	103.35	106.69
2	B	901	NAD	O2A-PA-O1A	2.23	124.50	112.14
5	C	904	2YG	O1-C11-C	2.19	121.89	116.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	NAD	O4B-C1B-N9A	2.19	112.86	108.10
5	D	904	2YG	C6-C5-N1	2.13	119.00	115.69
2	D	901	NAD	O4B-C1B-N9A	2.13	112.73	108.10
2	B	901	NAD	C2A-N1A-C6A	2.08	122.47	118.76
2	D	901	NAD	C6N-N1N-C1D	2.06	124.44	119.33
2	A	901	NAD	C6A-C5A-C4A	-2.02	115.28	117.55
2	B	901	NAD	C2D-C1D-N1N	2.00	117.48	113.48

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	259/260 (99%)	-0.07	6 (2%) 57 62	19, 24, 49, 94	0
1	B	259/260 (99%)	-0.02	5 (1%) 64 68	19, 25, 52, 96	0
1	C	259/260 (99%)	0.62	31 (11%) 5 6	42, 58, 81, 95	0
1	D	258/260 (99%)	0.80	36 (13%) 3 4	40, 65, 95, 119	0
All	All	1035/1040 (99%)	0.33	78 (7%) 14 16	19, 48, 86, 119	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	ILE	7.2
1	D	2	ALA	7.0
1	D	192	ALA	6.8
1	C	2	ALA	5.4
1	A	1	MET	5.0
1	D	7	ASP	5.0
1	C	140	ASP	4.6
1	D	14	MET	4.5
1	D	140	ASP	4.5
1	C	1	MET	4.4
1	C	192	ALA	4.3
1	B	192	ALA	4.1
1	C	193	ASN	4.0
1	C	42	PHE	3.9
1	B	1	MET	3.8
1	D	106	ARG	3.6
1	B	193	ASN	3.5
1	C	7	ASP	3.4
1	D	164	ASP	3.4
1	D	142	LYS	3.3
1	C	14	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	9	LEU	3.1
1	D	75	GLY	3.1
1	D	141	SER	3.1
1	C	75	GLY	2.9
1	A	2	ALA	2.9
1	C	183	ASN	2.9
1	D	162	GLN	2.9
1	D	3	LEU	2.9
1	C	179	ARG	2.8
1	C	82	ASP	2.8
1	C	232	GLU	2.8
1	D	11	ASN	2.7
1	D	166	ARG	2.7
1	D	193	ASN	2.7
1	D	185	GLY	2.7
1	C	175	THR	2.7
1	D	9	LEU	2.6
1	C	141	SER	2.6
1	D	5	THR	2.6
1	D	186	ILE	2.5
1	A	140	ASP	2.5
1	B	191	PRO	2.5
1	B	179	ARG	2.5
1	C	162	GLN	2.5
1	D	48	VAL	2.5
1	C	235	ARG	2.5
1	D	174	GLU	2.4
1	C	10	ILE	2.4
1	A	193	ASN	2.4
1	D	190	ASP	2.3
1	C	54	THR	2.3
1	D	17	GLN	2.3
1	C	44	SER	2.3
1	D	139	ALA	2.3
1	D	232	GLU	2.2
1	C	106	ARG	2.2
1	C	96	GLY	2.2
1	C	11	ASN	2.2
1	D	191	PRO	2.2
1	C	191	PRO	2.2
1	A	192	ALA	2.2
1	D	138	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	227	PRO	2.1
1	C	142	LYS	2.1
1	C	185	GLY	2.1
1	D	4	LEU	2.1
1	D	82	ASP	2.1
1	C	233	GLU	2.1
1	D	233	GLU	2.1
1	D	56	GLY	2.1
1	D	179	ARG	2.1
1	C	218	ASN	2.1
1	D	215	LEU	2.1
1	C	164	ASP	2.1
1	D	160	LEU	2.0
1	C	5	THR	2.0
1	D	16	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
4	MG	C	903	1/1	0.33	10.52	82,82,82,82	0
4	MG	D	903	1/1	0.23	5.97	85,85,85,85	0
6	GOL	B	905	6/6	0.13	2.64	33,37,46,46	0
6	GOL	A	905	6/6	0.21	2.59	50,64,70,78	0
8	PEG	B	906	7/7	0.19	2.56	30,39,45,48	0
6	GOL	A	907	6/6	0.19	2.53	46,59,60,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NA	C	902	1/1	0.21	1.86	60,60,60,60	0
7	EDO	A	908	4/4	0.15	1.84	44,44,48,53	0
6	GOL	A	906	6/6	0.15	1.48	49,55,61,66	0
7	EDO	A	909	4/4	0.15	1.09	29,35,41,50	0
7	EDO	A	910	4/4	0.14	0.96	32,41,51,59	0
5	2YG	B	904	19/19	0.14	0.89	22,27,45,49	0
5	2YG	A	904	19/19	0.15	0.83	26,33,46,52	0
5	2YG	C	904	15/19	0.17	0.32	46,61,66,70	0
3	NA	D	902	1/1	0.11	-0.07	51,51,51,51	0
3	NA	A	902	1/1	0.10	-0.08	39,39,39,39	0
5	2YG	D	904	15/19	0.16	-0.16	49,54,68,70	0
2	NAD	C	901	44/44	0.11	-0.33	45,53,64,68	0
2	NAD	D	901	44/44	0.11	-0.33	40,48,70,95	0
2	NAD	B	901	44/44	0.09	-0.64	23,31,37,45	0
3	NA	B	902	1/1	0.08	-0.67	43,43,43,43	0
2	NAD	A	901	44/44	0.08	-0.73	21,25,33,35	0
4	MG	A	903	1/1	0.09	-0.87	39,39,39,39	0
4	MG	B	903	1/1	0.07	-2.88	38,38,38,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.