



Full wwPDB X-ray Structure Validation Report

Aug 11, 2014 – 07:29 PM EDT

PDB ID : 4Q3D
Title : PylD cocrystallized with L-Ornithine-Nd-D-ornithineand NAD+
Authors : Quitterer, F.; Beck, P.; Bacher, A.; Groll, M.
Deposited on : 2014-04-11
Resolution : 2.20 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>

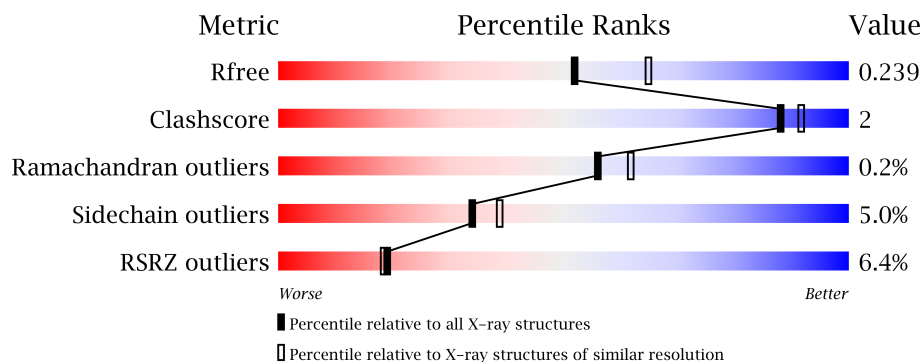
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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. 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
3	NA	C	902	-	X
3	NA	D	902	-	X
4	MG	D	903	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8198 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.

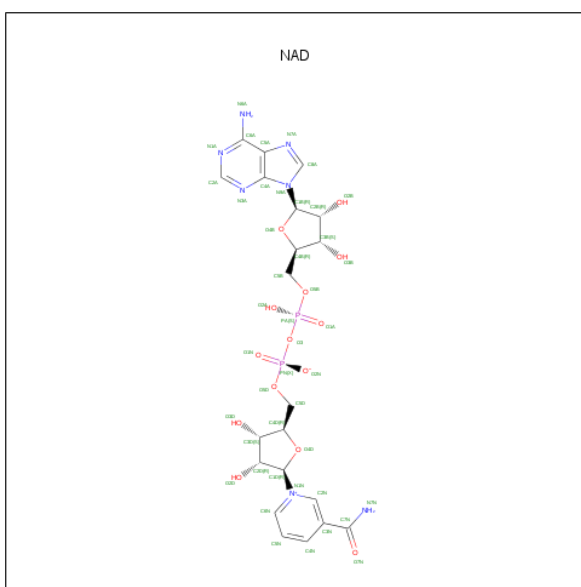
- Molecule 1 is a protein called PYLD, pyrrolysine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1948	1241	313	384	10			
1	B	258	Total	C	N	O	S	0	0	0
			1948	1241	313	384	10			
1	C	248	Total	C	N	O	S	0	0	0
			1772	1133	281	349	9			
1	D	256	Total	C	N	O	S	0	0	0
			1813	1159	284	361	9			

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).

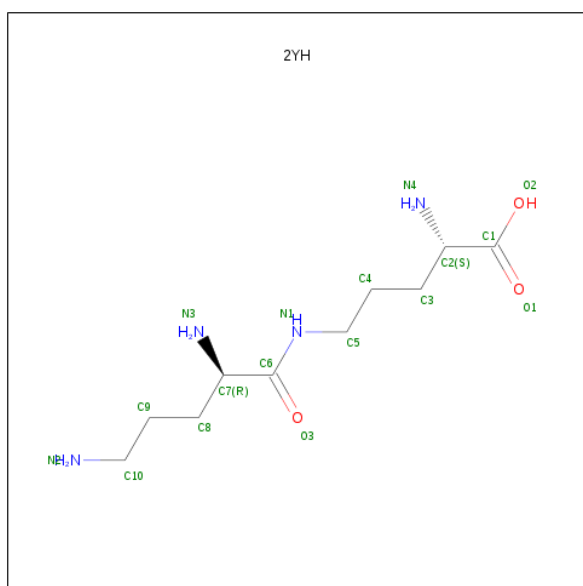
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

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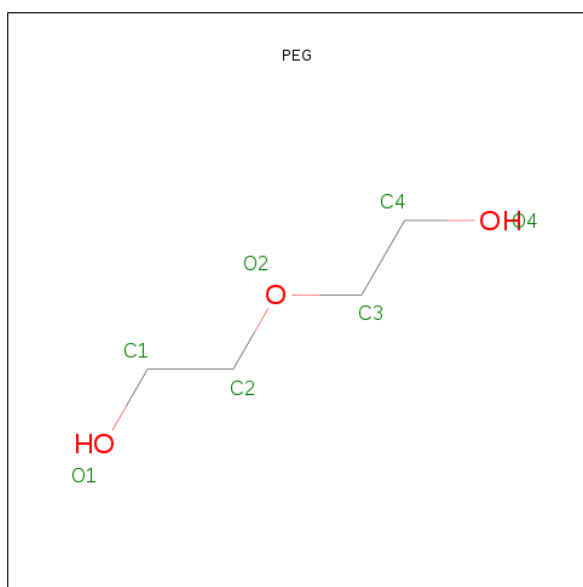
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is N 5 -D-ORNITHYL-L-ORNITHINE (three-letter code: 2YH) (formula: $C_{10}H_{22}N_4O_3$).



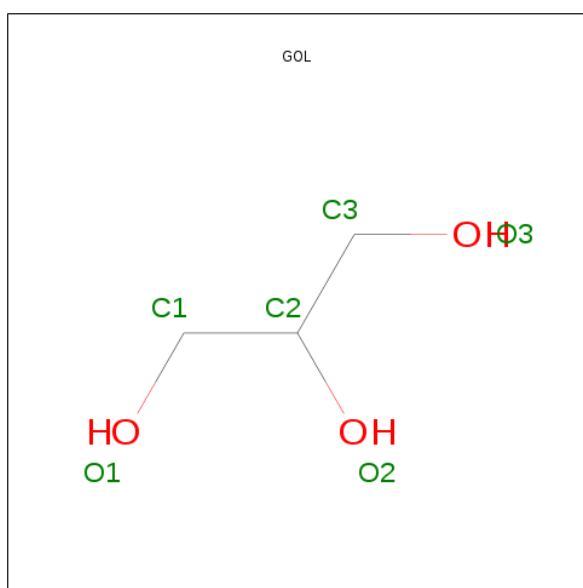
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			17	10	4	3		
5	B	1	Total	C	N	O	0	0
			17	10	4	3		
5	C	1	Total	C	N	O	0	0
			17	10	4	3		
5	D	1	Total	C	N	O	0	0
			17	10	4	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



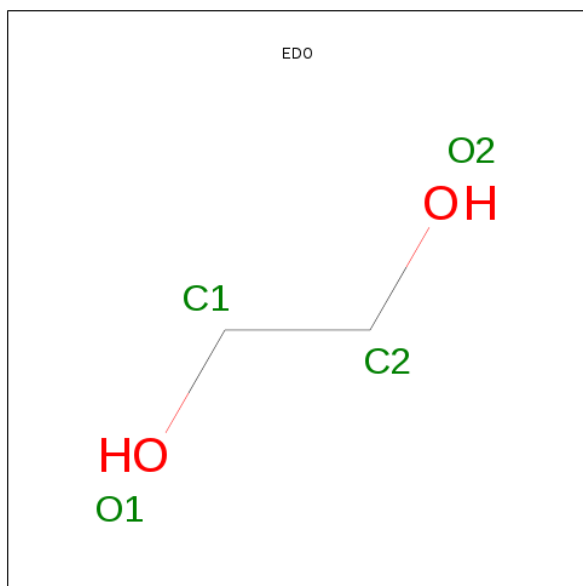
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

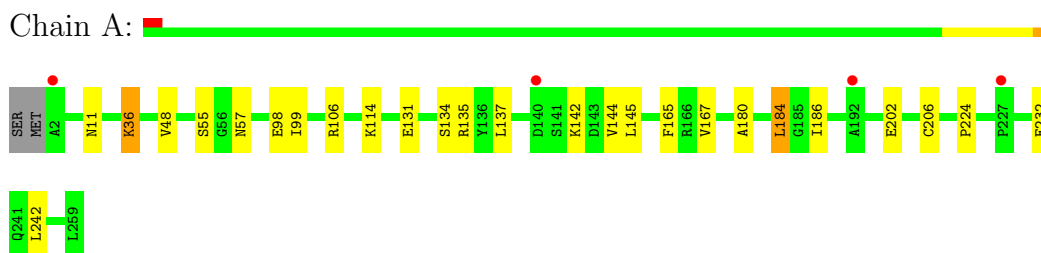
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	189	Total	O	0	0
			189	189		
9	B	169	Total	O	0	0
			169	169		
9	C	38	Total	O	0	0
			38	38		
9	D	35	Total	O	0	0
			35	35		

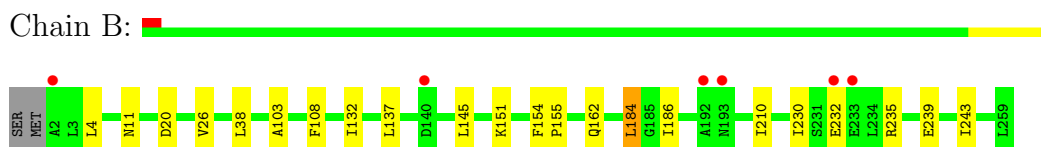
3 Residue-property plots

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.

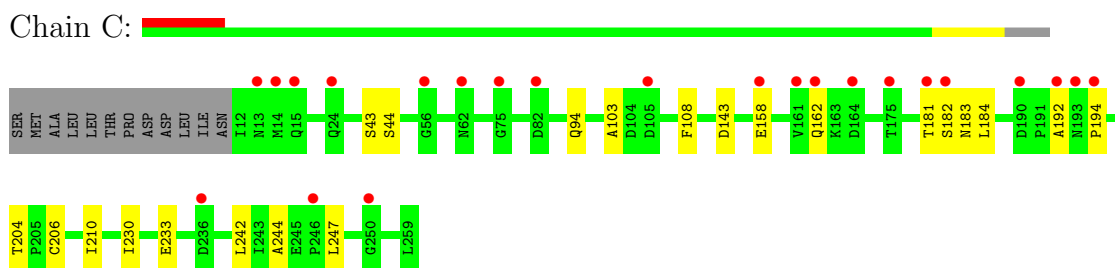
- Molecule 1: PYLD, pyrrolysine synthase



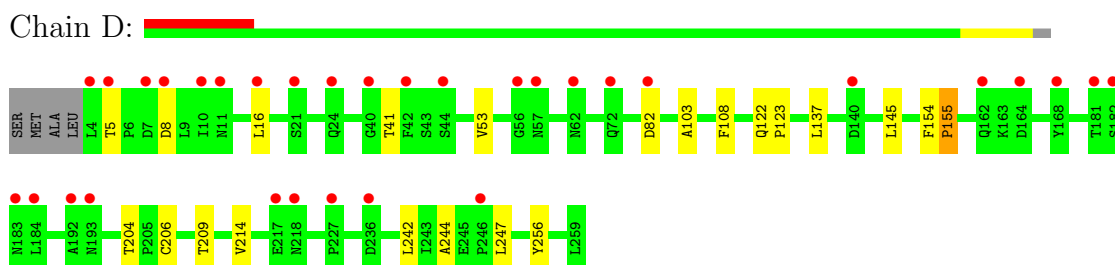
- Molecule 1: PYLD, pyrrolysine synthase



- Molecule 1: PYLD, pyrrolysine synthase



- Molecule 1: PYLD, pyrrolysine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	86.93Å 259.32Å 48.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 10.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (10.00-2.20) 99.4 (10.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.177 , 0.237 0.183 , 0.239	Depositor DCC
R_{free} test set	2812 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 52.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	4 of 56250 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8198	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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, 2YH, NA, EDO, 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	0.34	0/1984	0.58	0/2695
1	B	0.34	0/1984	0.57	0/2695
1	C	0.28	0/1807	0.48	0/2470
1	D	0.28	0/1849	0.47	0/2527
All	All	0.31	0/7624	0.53	0/10387

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	1948	0	1939	13	0
1	B	1948	0	1939	6	0
1	C	1772	0	1655	9	0
1	D	1813	0	1663	9	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	17	0	0	0	0
5	B	17	0	0	0	0
5	C	17	0	0	0	0
5	D	17	0	0	1	0
6	A	14	0	20	0	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	A	8	0	12	0	0
9	A	189	0	0	1	0
9	B	169	0	0	0	0
9	C	38	0	0	0	0
9	D	35	0	0	1	0
All	All	8198	0	7348	35	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 2.

All (35) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:206:CYS:HG	1:C:206:CYS:HG	1.38	0.67
1:A:98:GLU:OE1	1:A:114:LYS:HE2	1.97	0.65
1:D:41:THR:HG21	1:D:256:TYR:O	2.00	0.61
1:C:158:GLU:HG3	1:C:184:LEU:HD11	1.83	0.60
1:C:242:LEU:HD11	1:C:244:ALA:HB3	1.90	0.53
1:A:36:LYS:NZ	9:A:1061:HOH:O	2.41	0.52
1:C:210:ILE:HB	1:C:230:ILE:HG22	1.95	0.49
1:D:53:VAL:O	5:D:904:2YH:N4	2.47	0.48
1:D:204:THR:HG22	1:D:206:CYS:H	1.79	0.47
1:D:204:THR:HG21	1:D:209:THR:HG21	1.96	0.47
1:A:98:GLU:HB3	1:A:114:LYS:HE3	1.97	0.47
1:A:167:VAL:HB	1:A:186:ILE:HG22	1.96	0.47
1:A:98:GLU:OE1	1:A:114:LYS:CE	2.63	0.46
1:B:132:ILE:CG2	1:B:243:ILE:HD13	2.45	0.46
1:A:180:ALA:O	1:A:184:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:103:ALA:HB2	1:D:108:PHE:CD1	2.51	0.45
1:C:204:THR:HG23	2:C:901:NAD:C8A	2.47	0.45
1:B:210:ILE:HB	1:B:230:ILE:HG22	1.99	0.44
1:B:26:VAL:HG21	1:B:243:ILE:HD11	2.00	0.44
1:A:235:ARG:HG2	1:A:240:VAL:HB	2.00	0.43
1:B:154:PHE:HB3	1:B:155:PRO:HD3	2.00	0.43
1:A:202:GLU:O	1:A:224:PRO:HD2	2.19	0.43
1:B:184:LEU:HB3	1:B:186:ILE:HG23	2.01	0.42
1:D:122:GLN:HB2	1:D:123:PRO:CD	2.49	0.42
1:D:8:ASP:CB	9:D:1035:HOH:O	2.67	0.42
1:D:242:LEU:HD11	1:D:244:ALA:HB3	2.02	0.42
1:C:182:SER:O	1:C:183:ASN:CB	2.68	0.41
1:D:154:PHE:HB3	1:D:155:PRO:CD	2.51	0.41
1:A:131:GLU:OE1	1:A:135:ARG:HD2	2.21	0.41
1:C:103:ALA:HB2	1:C:108:PHE:CD1	2.56	0.41
1:B:103:ALA:HB2	1:B:108:PHE:CD1	2.56	0.41
1:A:134:SER:HB2	1:A:165:PHE:CZ	2.56	0.41
1:A:206:CYS:HG	1:C:206:CYS:CB	2.34	0.40
1:C:192:ALA:O	1:C:194:PRO:HD3	2.21	0.40
1:A:48:VAL:HG22	1:A:99:ILE:HB	2.03	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	256/260 (98%)	249 (97%)	7 (3%)	0	100	100
1	B	256/260 (98%)	247 (96%)	9 (4%)	0	100	100
1	C	246/260 (95%)	235 (96%)	10 (4%)	1 (0%)	43	45
1	D	254/260 (98%)	244 (96%)	9 (4%)	1 (0%)	43	45
All	All	1012/1040 (97%)	975 (96%)	35 (4%)	2 (0%)	56	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	247	LEU
1	D	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	213/215 (99%)	200 (94%)	13 (6%)	26	28
1	B	213/215 (99%)	201 (94%)	12 (6%)	30	33
1	C	174/215 (81%)	167 (96%)	7 (4%)	42	51
1	D	176/215 (82%)	169 (96%)	7 (4%)	42	51
All	All	776/860 (90%)	737 (95%)	39 (5%)	34	39

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	36	LYS
1	A	55	SER
1	A	57	ASN
1	A	106	ARG
1	A	137	LEU
1	A	142	LYS
1	A	144	VAL
1	A	145	LEU
1	A	184	LEU
1	A	232	GLU
1	A	235	ARG
1	A	242	LEU
1	B	4	LEU
1	B	11	ASN
1	B	20	ASP
1	B	38	LEU
1	B	137	LEU
1	B	145	LEU

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Mol	Chain	Res	Type
1	B	151	LYS
1	B	162	GLN
1	B	184	LEU
1	B	232	GLU
1	B	235	ARG
1	B	239	GLU
1	C	43	SER
1	C	44	SER
1	C	94	GLN
1	C	143	ASP
1	C	162	GLN
1	C	181	THR
1	C	233	GLU
1	D	5	THR
1	D	16	LEU
1	D	82	ASP
1	D	137	LEU
1	D	145	LEU
1	D	155	PRO
1	D	214	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	162	GLN
1	A	183	ASN
1	B	11	ASN
1	B	13	ASN
1	B	72	GLN
1	B	94	GLN
1	C	68	HIS
1	C	72	GLN
1	C	241	GLN
1	D	112	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 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 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	0.95	3 (6%)	73,73,73	1.76	12 (16%)
5	2YH	A	904	-	16,16,16	1.22	3 (18%)	19,19,19	1.61	3 (15%)
6	PEG	A	905	-	6,6,6	0.49	0	5,5,5	0.26	0
6	PEG	A	906	-	6,6,6	0.45	0	5,5,5	0.39	0
7	GOL	A	907	-	5,5,5	0.22	0	5,5,5	0.23	0
8	EDO	A	908	-	3,3,3	0.51	0	2,2,2	0.25	0
8	EDO	A	909	-	3,3,3	0.49	0	2,2,2	0.34	0
2	NAD	B	901	4	48,48,48	0.96	3 (6%)	73,73,73	1.71	12 (16%)
5	2YH	B	904	-	16,16,16	0.68	1 (6%)	19,19,19	1.64	2 (10%)
7	GOL	B	905	-	5,5,5	0.21	0	5,5,5	0.21	0
2	NAD	C	901	4	48,48,48	0.95	2 (4%)	73,73,73	1.76	11 (15%)
5	2YH	C	904	-	16,16,16	1.20	3 (18%)	19,19,19	1.72	3 (15%)
2	NAD	D	901	-	48,48,48	0.96	3 (6%)	73,73,73	1.79	12 (16%)
5	2YH	D	904	-	16,16,16	1.22	3 (18%)	19,19,19	1.54	1 (5%)

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	2YH	A	904	-	-	0/19/19/19	0/0/0/0
6	PEG	A	905	-	-	0/4/4/4	0/0/0/0
6	PEG	A	906	-	-	0/4/4/4	0/0/0/0
7	GOL	A	907	-	-	0/4/4/4	0/0/0/0
8	EDO	A	908	-	-	0/1/1/1	0/0/0/0
8	EDO	A	909	-	-	0/1/1/1	0/0/0/0
2	NAD	B	901	4	-	0/30/62/62	0/5/5/5
5	2YH	B	904	-	-	0/19/19/19	0/0/0/0
7	GOL	B	905	-	-	0/4/4/4	0/0/0/0
2	NAD	C	901	4	-	0/30/62/62	0/5/5/5
5	2YH	C	904	-	-	0/19/19/19	0/0/0/0
2	NAD	D	901	-	-	0/30/62/62	0/5/5/5
5	2YH	D	904	-	-	0/19/19/19	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	904	2YH	O1-C1	3.43	1.33	1.22
5	D	904	2YH	O1-C1	3.39	1.33	1.22
5	A	904	2YH	O1-C1	3.35	1.33	1.22
2	B	901	NAD	C4A-N9A	-3.23	1.33	1.37
2	A	901	NAD	C4A-N9A	-3.16	1.33	1.37
2	C	901	NAD	C4A-N9A	-3.15	1.33	1.37
2	D	901	NAD	C5A-C4A	3.02	1.47	1.40
2	B	901	NAD	C5A-C4A	2.92	1.47	1.40
2	C	901	NAD	C5A-C4A	2.91	1.47	1.40
2	A	901	NAD	C5A-C4A	2.90	1.47	1.40
2	D	901	NAD	C4A-N9A	-2.85	1.33	1.37
5	D	904	2YH	C6-N1	2.36	1.38	1.33
2	B	901	NAD	O4D-C1D	2.33	1.44	1.41
5	A	904	2YH	O2-C1	-2.28	1.22	1.30
5	A	904	2YH	C6-N1	2.24	1.38	1.33
5	C	904	2YH	C6-N1	2.18	1.38	1.33
2	D	901	NAD	O4D-C1D	2.17	1.44	1.41
5	C	904	2YH	O2-C1	-2.14	1.22	1.30
5	D	904	2YH	O2-C1	-2.10	1.22	1.30
5	B	904	2YH	C6-N1	2.02	1.37	1.33
2	A	901	NAD	O4D-C1D	2.00	1.43	1.41

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	NAD	N3A-C2A-N1A	-7.46	122.33	128.89
2	C	901	NAD	N3A-C2A-N1A	-7.26	122.50	128.89
2	A	901	NAD	N3A-C2A-N1A	-7.06	122.68	128.89
2	B	901	NAD	N3A-C2A-N1A	-6.95	122.78	128.89
2	D	901	NAD	C5A-C4A-N3A	-6.90	119.25	125.98
2	C	901	NAD	C5A-C4A-N3A	-6.70	119.45	125.98
2	A	901	NAD	C5A-C4A-N3A	-6.67	119.48	125.98
2	B	901	NAD	C5A-C4A-N3A	-6.34	119.80	125.98
5	C	904	2YH	C5-N1-C6	-5.96	110.81	122.58
5	B	904	2YH	C5-N1-C6	-5.50	111.72	122.58
5	D	904	2YH	C5-N1-C6	-5.31	112.09	122.58
2	B	901	NAD	N3A-C4A-N9A	5.18	134.28	125.39
2	A	901	NAD	N3A-C4A-N9A	5.09	134.12	125.39
2	D	901	NAD	N3A-C4A-N9A	5.07	134.08	125.39
5	A	904	2YH	C5-N1-C6	-5.06	112.58	122.58
2	C	901	NAD	N3A-C4A-N9A	4.73	133.51	125.39
2	C	901	NAD	C4A-C5A-N7A	-3.59	105.94	109.41
2	D	901	NAD	O4D-C1D-N1N	3.36	111.82	108.13
2	A	901	NAD	C3N-C7N-N7N	3.29	121.44	117.78
2	D	901	NAD	C4A-C5A-N7A	-3.25	106.27	109.41
2	A	901	NAD	C4A-C5A-N7A	-3.09	106.43	109.41
5	B	904	2YH	C8-C7-N3	3.01	115.70	109.59
2	C	901	NAD	PN-O3-PA	-2.94	121.34	133.17
2	B	901	NAD	C8A-N9A-C4A	2.88	109.30	106.96
2	C	901	NAD	C2A-N3A-C4A	2.87	121.52	113.27
2	D	901	NAD	C2A-N3A-C4A	2.86	121.50	113.27
2	A	901	NAD	C4B-O4B-C1B	-2.85	106.58	109.72
2	C	901	NAD	C1B-N9A-C4A	-2.83	121.74	126.64
2	C	901	NAD	O4D-C1D-N1N	2.83	111.24	108.13
2	D	901	NAD	PN-O3-PA	-2.83	121.80	133.17
2	B	901	NAD	O7N-C7N-N7N	-2.77	118.63	122.59
2	A	901	NAD	O4B-C1B-N9A	2.74	114.07	108.10
2	A	901	NAD	C2A-N3A-C4A	2.72	121.10	113.27
2	B	901	NAD	C4A-C5A-N7A	-2.72	106.78	109.41
2	C	901	NAD	C3N-C7N-N7N	2.68	120.77	117.78
2	A	901	NAD	C8A-N9A-C4A	2.63	109.09	106.96
2	D	901	NAD	C3N-C7N-N7N	2.57	120.64	117.78
2	A	901	NAD	C1B-N9A-C4A	-2.55	122.22	126.64
2	B	901	NAD	C3N-C7N-N7N	2.54	120.61	117.78
2	D	901	NAD	C1B-N9A-C4A	-2.54	122.25	126.64
2	B	901	NAD	C2A-N3A-C4A	2.53	120.54	113.27
2	D	901	NAD	O4B-C1B-N9A	2.48	113.50	108.10
2	A	901	NAD	PN-O3-PA	-2.43	123.41	133.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	NAD	PN-O3-PA	-2.39	123.56	133.17
2	C	901	NAD	C8A-N9A-C4A	2.35	108.87	106.96
2	D	901	NAD	C8A-N9A-C4A	2.29	108.81	106.96
5	A	904	2YH	O2-C1-O1	-2.23	119.05	124.05
2	B	901	NAD	C2A-N1A-C6A	2.21	122.70	118.76
5	C	904	2YH	O2-C1-O1	-2.21	119.09	124.05
2	C	901	NAD	C4B-O4B-C1B	-2.18	107.32	109.72
2	B	901	NAD	C1B-N9A-C4A	-2.14	122.93	126.64
5	C	904	2YH	O3-C6-N1	-2.14	118.76	123.07
2	B	901	NAD	C4B-O4B-C1B	-2.05	107.47	109.72
2	D	901	NAD	C2A-N1A-C6A	2.05	122.41	118.76
2	A	901	NAD	O7N-C7N-N7N	-2.03	119.69	122.59
5	A	904	2YH	C6-C7-N3	2.01	117.66	108.73

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	258/260 (99%)	-0.41	4 (1%) 68 69	15, 24, 42, 50	0
1	B	258/260 (99%)	-0.32	6 (2%) 57 58	16, 25, 49, 76	0
1	C	248/260 (95%)	0.63	23 (9%) 9 8	41, 66, 95, 114	0
1	D	256/260 (98%)	0.49	32 (12%) 5 4	40, 58, 87, 102	0
All	All	1020/1040 (98%)	0.09	65 (6%) 19 18	15, 44, 87, 114	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	192	ALA	7.4
1	B	192	ALA	7.4
1	C	75	GLY	6.2
1	D	182	SER	6.0
1	D	7	ASP	5.8
1	D	11	ASN	5.4
1	C	193	ASN	4.8
1	A	2	ALA	4.7
1	D	183	ASN	4.7
1	B	2	ALA	4.4
1	C	246	PRO	4.3
1	B	140	ASP	3.8
1	D	44	SER	3.6
1	C	162	GLN	3.6
1	C	14	MET	3.6
1	C	24	GLN	3.4
1	B	193	ASN	3.3
1	A	192	ALA	3.2
1	C	164	ASP	3.1
1	C	182	SER	3.0
1	D	162	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	4	LEU	3.0
1	D	192	ALA	2.9
1	D	72	GLN	2.9
1	D	40	GLY	2.9
1	D	217	GLU	2.8
1	D	164	ASP	2.8
1	D	8	ASP	2.7
1	D	140	ASP	2.7
1	D	246	PRO	2.7
1	A	140	ASP	2.7
1	D	24	GLN	2.7
1	D	181	THR	2.7
1	D	5	THR	2.6
1	C	194	PRO	2.6
1	D	10	ILE	2.5
1	C	56	GLY	2.5
1	C	15	GLN	2.5
1	D	193	ASN	2.5
1	D	236	ASP	2.5
1	C	181	THR	2.5
1	C	161	VAL	2.5
1	C	175	THR	2.4
1	C	190	ASP	2.4
1	B	233	GLU	2.4
1	C	82	ASP	2.4
1	D	227	PRO	2.4
1	A	227	PRO	2.4
1	C	13	ASN	2.4
1	D	168	TYR	2.3
1	C	236	ASP	2.3
1	D	16	LEU	2.3
1	D	184	LEU	2.2
1	B	232	GLU	2.2
1	C	62	ASN	2.2
1	D	42	PHE	2.1
1	C	105	ASP	2.1
1	D	62	ASN	2.1
1	D	21	SER	2.1
1	D	56	GLY	2.0
1	D	57	ASN	2.0
1	D	218	ASN	2.0
1	D	82	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	250	GLY	2.0
1	C	158	GLU	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
3	NA	C	902	1/1	0.28	4.76	59,59,59,59	0
4	MG	D	903	1/1	0.36	3.52	76,76,76,76	0
3	NA	D	902	1/1	0.29	2.62	66,66,66,66	0
4	MG	C	903	1/1	0.34	1.78	82,82,82,82	0
3	NA	B	902	1/1	0.17	1.50	42,42,42,42	0
5	2YH	D	904	17/17	0.20	1.31	32,41,48,52	0
5	2YH	C	904	17/17	0.23	1.14	27,41,51,51	0
6	PEG	A	905	7/7	0.11	1.11	28,31,38,40	0
8	EDO	A	908	4/4	0.13	0.99	50,50,53,56	0
7	GOL	B	905	6/6	0.14	0.51	41,60,67,69	0
5	2YH	A	904	17/17	0.11	0.31	19,23,32,33	0
6	PEG	A	906	7/7	0.15	0.30	52,71,82,83	0
5	2YH	B	904	17/17	0.12	0.25	22,25,31,31	0
2	NAD	D	901	44/44	0.14	0.11	44,56,68,69	0
4	MG	B	903	1/1	0.09	-0.17	31,31,31,31	0
2	NAD	C	901	44/44	0.13	-0.26	41,52,71,90	0
2	NAD	A	901	44/44	0.08	-0.41	21,26,33,40	0
8	EDO	A	909	4/4	0.10	-0.43	40,50,54,56	0
2	NAD	B	901	44/44	0.09	-0.45	20,29,37,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NA	A	902	1/1	0.07	-0.76	35,35,35,35	0
7	GOL	A	907	6/6	0.10	-0.93	44,53,57,62	0
4	MG	A	903	1/1	0.05	-3.70	29,29,29,29	0

6.5 Other polymers

There are no such residues in this entry.