



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2017 – 10:25 PM EDT

PDB ID : 3KB6
Title : Crystal structure of D-Lactate dehydrogenase from aquifex aeolicus complexed with NAD and Lactic acid
Authors : Antonyuk, S.V.; Strange, R.W.; Ellis, M.J.; Bessho, Y.; Kuramitsu, S.; Yokoyama, S.; Hasnain, S.S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : unknown
Resolution : 2.12 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

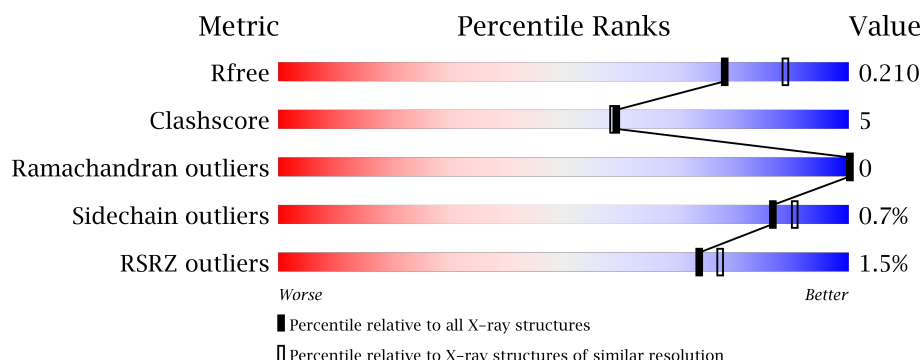
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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}	100719	4988 (2.14-2.10)
Clashscore	112137	5557 (2.14-2.10)
Ramachandran outliers	110173	5504 (2.14-2.10)
Sidechain outliers	110143	5505 (2.14-2.10)
RSRZ outliers	101464	5021 (2.14-2.10)

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. 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	334	<div> <div>0.1%</div> <div>94%</div> <div>6%</div> </div>
1	B	334	<div> <div>0.1%</div> <div>85%</div> <div>15%</div> </div>
1	C	334	<div> <div>4%</div> <div>90%</div> <div>10%</div> </div>
1	D	334	<div> <div>86%</div> <div>13%</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.

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PPI	A	398	-	-	-	X
2	PPI	A	453	-	-	-	X
2	PPI	B	398	-	-	-	X
2	PPI	C	398	-	-	-	X
2	PPI	D	398	-	-	-	X
5	PEG	A	403	-	-	-	X
5	PEG	A	555	-	-	-	X
5	PEG	A	701	-	-	X	X
5	PEG	A	772	-	-	-	X
5	PEG	A	803	-	-	-	X
5	PEG	C	771	-	-	-	X
6	1PE	A	335	-	-	-	X
6	1PE	A	404	-	-	-	X
6	1PE	A	444	-	-	-	X
6	1PE	B	404	-	-	-	X
6	1PE	B	407	-	-	-	X
6	1PE	B	804	-	-	-	X
6	1PE	C	404	-	-	-	X
7	GOL	A	800	-	-	-	X
7	GOL	B	711	-	-	-	X
7	GOL	B	770	-	-	-	X
7	GOL	B	777	-	-	-	X
7	GOL	B	800	-	-	-	X
7	GOL	B	801	-	-	-	X
7	GOL	C	401	-	-	-	X

2 Entry composition [i](#)

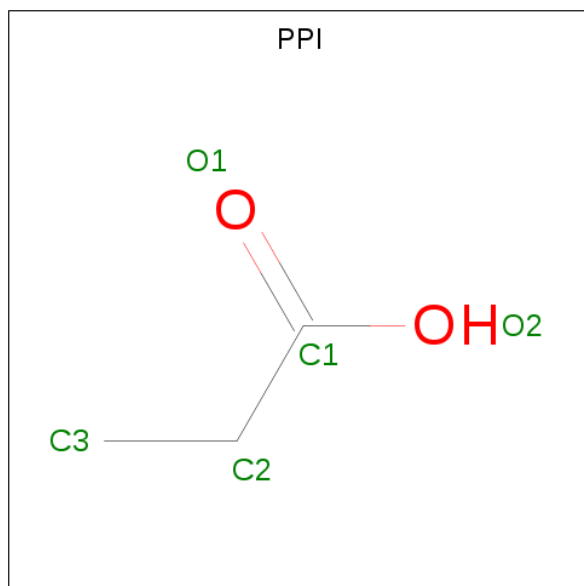
There are 8 unique types of molecules in this entry. The entry contains 12114 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-lactate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	Se	0	5	0
			2689	1730	446	501	5	7			
1	B	334	Total	C	N	O	S	Se	6	8	0
			2718	1749	450	505	5	9			
1	C	334	Total	C	N	O	S	Se	0	4	0
			2696	1730	453	501	4	8			
1	D	334	Total	C	N	O	S	Se	0	6	0
			2701	1736	447	504	5	9			

- Molecule 2 is PROPANOIC ACID (three-letter code: PPI) (formula: C₃H₆O₂).



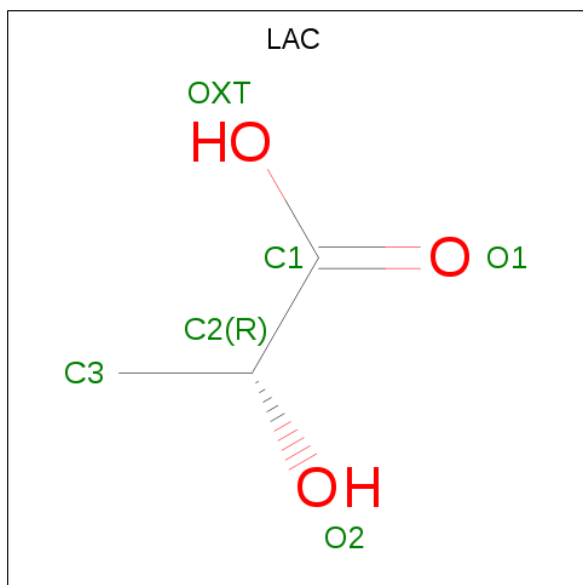
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			5	3	2		
2	A	1	Total	C	O	0	0
			5	3	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			5	3	2		
2	C	1	Total	C	O	0	0
			5	3	2		
2	D	1	Total	C	O	0	0
			5	3	2		

- Molecule 3 is LACTIC ACID (three-letter code: LAC) (formula: $C_3H_6O_3$).



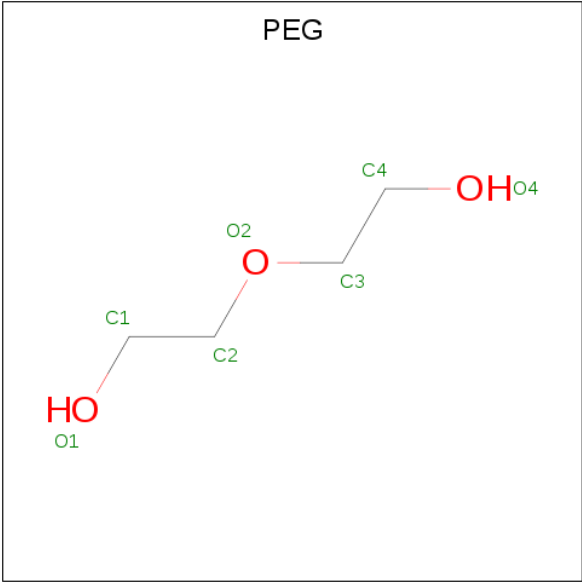
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



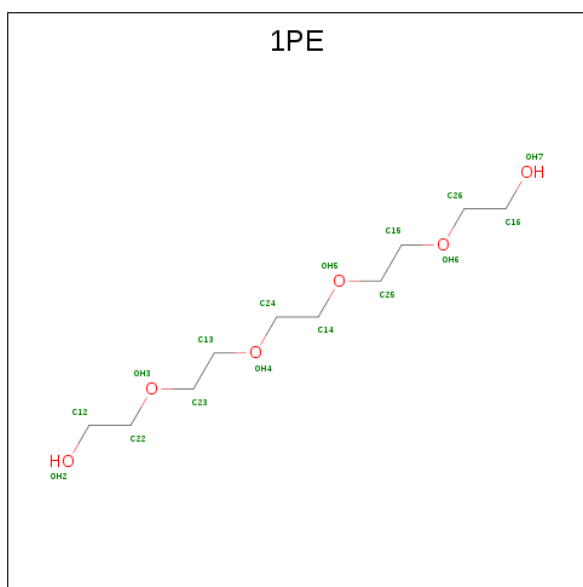
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 6 4 2	0	0
5	A	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



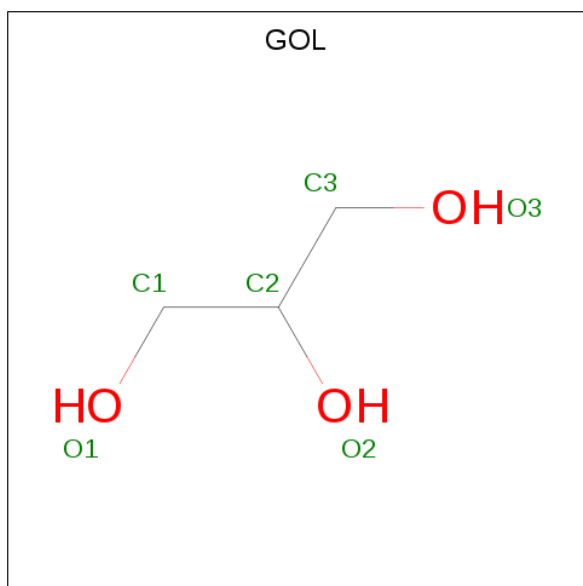
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 8 5	0	0
6	A	1	Total C O 13 8 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	5	3		
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			15	10	5		
6	B	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		

- 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	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

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

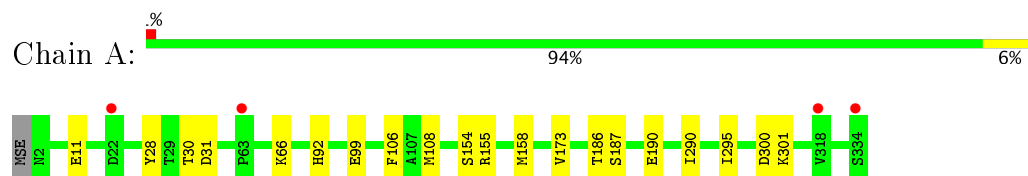
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	206	Total 207	O 207	0	1
8	B	235	Total 235	O 235	0	6
8	C	194	Total 197	O 197	0	6
8	D	218	Total 219	O 219	0	2

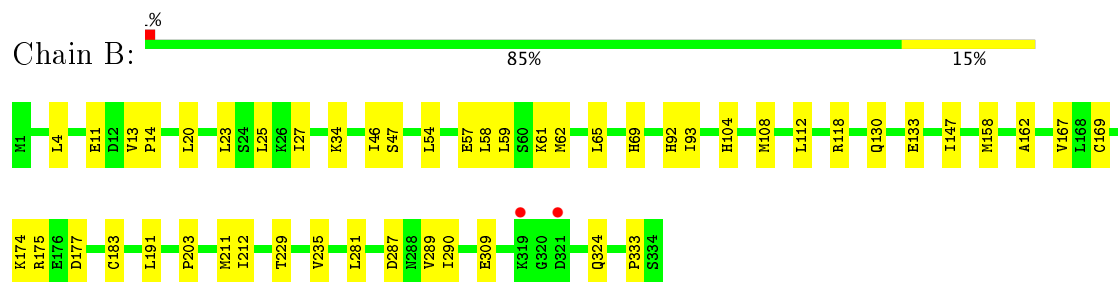
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

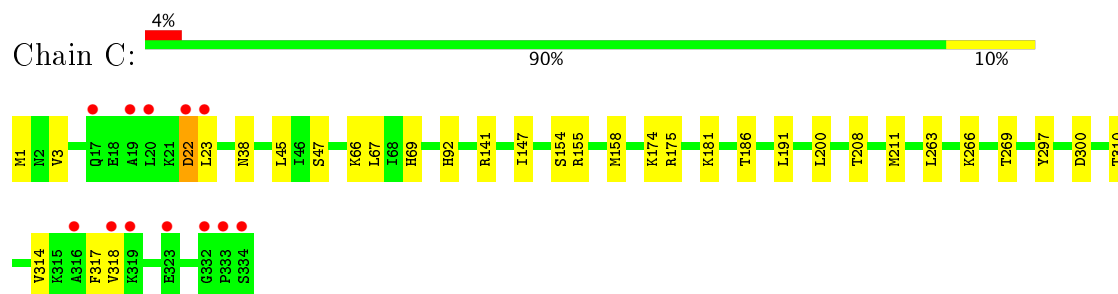
- Molecule 1: D-lactate dehydrogenase



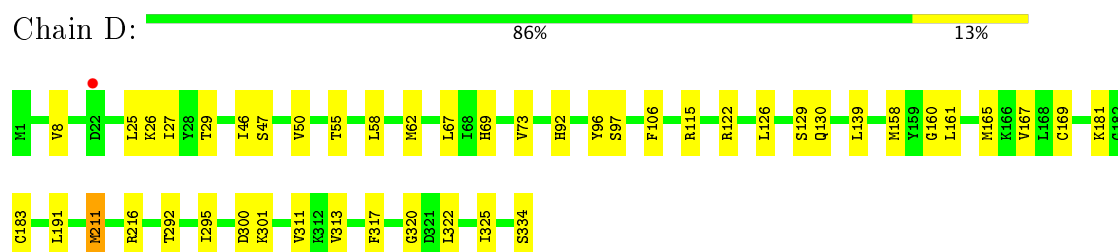
- Molecule 1: D-lactate dehydrogenase



- Molecule 1: D-lactate dehydrogenase



- Molecule 1: D-lactate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.94Å 94.43Å 188.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.00 – 2.12 38.30 – 2.12	Depositor EDS
% Data completeness (in resolution range)	95.3 (38.00-2.12) 95.1 (38.30-2.12)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.20 (at 2.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.164 , 0.212 0.168 , 0.210	Depositor DCC
R_{free} test set	4440 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.840	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12114	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, NAD, PPI, LAC, 1PE, 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	0.75	0/2740	0.75	3/3682 (0.1%)
1	B	0.75	0/2778	0.74	1/3731 (0.0%)
1	C	0.73	0/2742	0.70	1/3681 (0.0%)
1	D	0.72	0/2752	0.72	4/3694 (0.1%)
All	All	0.74	0/11012	0.73	9/14788 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	D	211	MSE	CG-SE-CE	-6.11	85.47	98.90
1	A	155	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	C	300	ASP	CB-CG-OD1	5.41	123.16	118.30
1	B	287	ASP	CB-CG-OD1	5.30	123.07	118.30
1	D	300	ASP	CB-CG-OD1	5.30	123.07	118.30
1	D	122	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	D	115	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	300	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	333	PRO	Mainchain

5.2 Too-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 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	2689	0	2811	19	0
1	B	2718	0	2848	44	0
1	C	2696	0	2807	26	0
1	D	2701	0	2814	34	0
2	A	10	0	10	1	0
2	B	5	0	5	1	0
2	C	5	0	5	1	0
2	D	5	0	5	0	0
3	A	6	0	5	1	0
3	B	6	0	5	1	0
3	C	6	0	5	1	0
3	D	6	0	5	1	0
4	A	44	0	26	1	0
4	B	44	0	26	2	0
4	C	44	0	26	1	0
4	D	44	0	26	0	0
5	A	48	0	67	7	0
5	C	14	0	20	0	0
5	D	7	0	10	0	0
6	A	44	0	56	0	0
6	B	38	0	49	10	0
6	C	10	0	13	2	0
7	A	12	0	16	0	0
7	B	30	0	40	0	0
7	C	12	0	16	0	0
7	D	12	0	16	0	0
8	A	207	0	0	2	0
8	B	235	0	0	5	0
8	C	197	0	0	5	0
8	D	219	0	0	2	0
All	All	12114	0	11732	125	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 (125) 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:D:158[B]:MSE:SE	1:D:181:LYS:HD3	1.99	1.11
1:A:186[B]:THR:HG23	1:A:190:GLU:HB3	1.49	0.94
1:A:186[B]:THR:HG22	1:A:187:SER:O	1.68	0.93
3:C:399:LAC:H2	4:C:400:NAD:C4N	2.09	0.82
1:A:173:VAL:HB	5:A:701:PEG:H11	1.62	0.81
3:B:399:LAC:H2	4:B:400:NAD:C4N	2.10	0.80
1:D:160:GLY:HA2	1:D:165[A]:MSE:HE3	1.63	0.78
3:A:399:LAC:H2	4:A:400:NAD:C4N	2.13	0.78
1:B:162:ALA:HB2	6:B:804:IPE:H251	1.71	0.71
1:A:186[A]:THR:HG23	1:A:187:SER:O	1.90	0.71
1:A:186[B]:THR:CG2	1:A:190:GLU:HB3	2.21	0.70
1:B:62[A]:MSE:HE3	1:B:65:LEU:HD22	1.71	0.70
1:B:147:ILE:HG21	1:B:211:MSE:HE1	1.74	0.68
2:A:453:PPI:H32	8:A:533:HOH:O	1.94	0.66
1:A:108:MSE:HE2	1:A:290[B]:ILE:HG12	1.77	0.65
1:B:59:LEU:HD23	1:B:62[A]:MSE:CE	2.26	0.65
1:B:61:LYS:NZ	6:B:407:IPE:H241	2.11	0.65
1:B:61:LYS:HZ2	6:B:407:IPE:H241	1.64	0.63
1:C:147:ILE:HG21	1:C:211:MSE:HE1	1.81	0.62
1:D:320:GLY:O	1:D:322:LEU:HD13	1.99	0.61
1:C:263:LEU:HD22	1:D:126[B]:LEU:HD21	1.82	0.60
1:B:108:MSE:HE1	1:B:229:THR:CG2	2.31	0.60
1:B:118[B]:ARG:NH1	1:B:133[B]:GLU:OE1	2.35	0.59
1:C:158[B]:MSE:SE	1:C:181:LYS:HD3	2.52	0.59
1:D:167:VAL:HG12	1:D:183[B]:CYS:SG	2.42	0.59
1:B:108:MSE:HE1	1:B:229:THR:HG22	1.82	0.59
1:D:161:LEU:HD11	1:D:183[A]:CYS:SG	2.42	0.59
1:C:186:THR:HG22	8:C:459:HOH:O	2.02	0.59
2:B:398:PPI:H33	8:B:522:HOH:O	2.01	0.58
1:A:173:VAL:CB	5:A:701:PEG:H11	2.33	0.57
1:D:158[B]:MSE:SE	1:D:181:LYS:CD	2.90	0.57
1:B:167:VAL:HG12	1:B:183[B]:CYS:SG	2.44	0.57
1:B:54:LEU:HD23	1:B:58:LEU:HD23	1.86	0.56
1:D:191:LEU:C	1:D:191:LEU:HD23	2.26	0.56
1:C:158[B]:MSE:SE	1:C:181:LYS:CD	3.04	0.55
1:C:47:SER:HA	1:C:69:HIS:O	2.07	0.55
1:A:66:LYS:NZ	8:A:597:HOH:O	2.40	0.55
1:B:62[A]:MSE:CE	1:B:65:LEU:HD22	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:LEU:HD13	1:C:317:PHE:CD1	2.42	0.54
1:B:147:ILE:CG2	1:B:211:MSE:HE1	2.37	0.54
1:D:8:VAL:HG21	1:D:27:ILE:HG23	1.88	0.54
1:B:158[B]:MSE:HE3	6:B:804:1PE:C25	2.38	0.53
1:C:174:LYS:HZ1	6:C:404:1PE:H142	1.74	0.53
1:D:47:SER:HA	1:D:69:HIS:O	2.10	0.52
1:C:266:LYS:O	1:C:269:THR:HB	2.09	0.52
1:B:324:GLN:NE2	8:B:487:HOH:O	2.26	0.52
1:D:160:GLY:HA2	1:D:165[A]:MSE:CE	2.38	0.51
1:D:55:THR:CG2	1:D:58:LEU:H	2.23	0.51
1:B:61:LYS:NZ	6:B:407:1PE:C24	2.73	0.51
1:D:158[B]:MSE:CE	1:D:181:LYS:HD3	2.40	0.51
1:D:169:CYS:SG	1:D:183[A]:CYS:HB3	2.51	0.51
1:B:59:LEU:HD23	1:B:62[A]:MSE:HE2	1.91	0.51
1:A:173:VAL:HG12	5:A:701:PEG:H12	1.93	0.50
1:D:311:VAL:HG22	8:D:481:HOH:O	2.13	0.49
1:A:173:VAL:CG1	5:A:701:PEG:H11	2.44	0.48
1:A:154:SER:O	1:A:158[B]:MSE:HG3	2.14	0.48
1:C:141[A]:ARG:HE	1:D:301:LYS:HD2	1.79	0.48
1:B:112:LEU:HD21	1:B:290[A]:ILE:HG12	1.95	0.48
1:C:1:MSE:HE3	1:C:66:LYS:HD2	1.95	0.48
1:C:154:SER:O	1:C:158[A]:MSE:HG3	2.13	0.47
8:C:538:HOH:O	1:D:129:SER:HB3	2.13	0.47
8:C:491:HOH:O	1:D:130:GLN:CG	2.63	0.47
1:D:55:THR:HG23	1:D:58:LEU:H	1.77	0.47
1:B:61:LYS:HZ1	6:B:407:1PE:C23	2.26	0.47
1:D:139:LEU:O	1:D:165[A]:MSE:HG2	2.15	0.47
1:B:175:ARG:HB3	1:B:177:ASP:OD1	2.15	0.46
8:C:491:HOH:O	1:D:130:GLN:HG3	2.15	0.46
5:A:772:PEG:H11	1:B:281:LEU:HD22	1.97	0.46
1:D:160:GLY:CA	1:D:165[A]:MSE:HE3	2.40	0.46
1:D:211:MSE:O	1:D:216:ARG:HD2	2.16	0.45
1:C:314:VAL:O	1:C:318:VAL:HG13	2.17	0.45
1:B:212:ILE:HB	1:B:235[A]:VAL:HG12	1.98	0.45
1:C:174:LYS:HZ1	6:C:404:1PE:C14	2.30	0.45
1:A:186[B]:THR:CG2	1:A:187:SER:O	2.51	0.45
1:A:173:VAL:CG1	5:A:701:PEG:C1	2.93	0.45
1:B:203:PRO:HD3	4:B:400:NAD:H52A	1.99	0.45
1:B:61:LYS:HZ2	6:B:407:1PE:C24	2.29	0.45
1:D:292:THR:HB	1:D:295:ILE:HD11	1.98	0.45
1:B:54:LEU:HD23	1:B:58:LEU:CD2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:THR:O	1:C:211:MSE:HB2	2.17	0.44
1:B:174:LYS:HE3	6:B:404:1PE:H242	1.99	0.44
1:B:20:LEU:HB3	1:B:23:LEU:HD12	1.99	0.44
1:D:73:VAL:HG23	1:D:96:TYR:CE2	2.52	0.44
1:A:28:TYR:HB3	1:A:30:THR:HG22	2.00	0.44
1:B:57:GLU:OE2	6:B:407:1PE:OH4	2.36	0.44
1:C:154:SER:O	1:C:158[B]:MSE:HG2	2.19	0.43
1:D:8:VAL:O	1:D:29:THR:HG22	2.18	0.43
1:A:99:GLU:OE1	1:A:301:LYS:NZ	2.50	0.43
1:C:1:MSE:HE1	1:C:317:PHE:CE2	2.54	0.43
1:B:108:MSE:CE	1:B:229:THR:CG2	2.95	0.43
1:B:25:LEU:HD21	1:B:27:ILE:HD11	2.01	0.43
1:B:47:SER:HA	1:B:69:HIS:O	2.17	0.43
1:C:22:ASP:O	1:C:23:LEU:HD23	2.19	0.43
1:D:50:VAL:HG11	3:D:399:LAC:H32	2.01	0.43
1:A:295:ILE:CG2	1:B:130:GLN:HG2	2.49	0.43
1:A:173:VAL:HG21	5:A:701:PEG:H42	2.01	0.43
1:C:175:ARG:NH1	8:C:481:HOH:O	2.39	0.42
1:D:106:PHE:CZ	1:D:165[A]:MSE:HE1	2.53	0.42
1:A:295:ILE:C	1:A:295:ILE:HD12	2.39	0.42
1:B:169:CYS:SG	1:B:183[A]:CYS:HB3	2.60	0.42
1:B:235[A]:VAL:HG23	8:B:421:HOH:O	2.20	0.42
1:C:155:ARG:HA	1:C:158[A]:MSE:HE3	2.02	0.42
1:D:313:VAL:HA	1:D:325:ILE:HG21	2.02	0.42
1:C:147:ILE:CG2	1:C:211:MSE:HE1	2.48	0.42
1:D:46:ILE:HD12	1:D:62:MSE:HE1	2.01	0.42
1:A:11:GLU:H	1:A:11:GLU:CD	2.23	0.42
1:B:289:VAL:O	1:B:290[A]:ILE:HD13	2.19	0.42
1:D:25:LEU:HD12	1:D:26:LYS:N	2.35	0.42
1:C:3:VAL:HG13	1:C:45:LEU:HD22	2.01	0.41
1:B:104:HIS:ND1	1:B:108:MSE:HE2	2.35	0.41
1:D:334:SER:HA	8:D:575:HOH:O	2.20	0.41
1:D:97:SER:HB2	1:D:301:LYS:HE2	2.03	0.41
1:B:93:ILE:HG23	1:B:309[B]:GLU:HG2	2.02	0.41
1:B:11:GLU:CD	1:B:11:GLU:H	2.24	0.41
1:B:13:VAL:N	1:B:14:PRO:CD	2.84	0.41
1:C:69:HIS:CD2	1:C:310:THR:HG23	2.55	0.41
1:B:158[A]:MSE:SE	8:B:587:HOH:O	2.89	0.41
1:C:191:LEU:HD23	1:C:191:LEU:C	2.41	0.41
1:D:67:LEU:CD1	1:D:317:PHE:CD1	3.04	0.41
1:B:174:LYS:HE3	6:B:404:1PE:C24	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:TYR:OH	2:C:398:PPI:H31	2.21	0.41
1:B:4:LEU:O	1:B:46:ILE:HA	2.21	0.41
1:C:147:ILE:HD12	1:C:200:LEU:CD2	2.51	0.41
1:B:235[A]:VAL:HG21	8:B:415:HOH:O	2.21	0.40
1:B:191:LEU:HD23	1:B:191:LEU:C	2.41	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	336/334 (101%)	327 (97%)	9 (3%)	0	100	100
1	B	340/334 (102%)	331 (97%)	9 (3%)	0	100	100
1	C	335/334 (100%)	327 (98%)	8 (2%)	0	100	100
1	D	337/334 (101%)	328 (97%)	9 (3%)	0	100	100
All	All	1348/1336 (101%)	1313 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	305/294 (104%)	302 (99%)	3 (1%)	80	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	309/294 (105%)	307 (99%)	2 (1%)	89	92
1	C	304/294 (103%)	301 (99%)	3 (1%)	80	84
1	D	306/294 (104%)	305 (100%)	1 (0%)	94	96
All	All	1224/1176 (104%)	1215 (99%)	9 (1%)	87	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASP
1	A	92	HIS
1	A	106	PHE
1	B	34	LYS
1	B	92	HIS
1	C	22	ASP
1	C	38	ASN
1	C	92	HIS
1	D	92	HIS

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	2	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

42 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
6	1PE	A	335	-	9,9,15	0.49	0	8,8,14	0.20	0
2	PPI	A	398	-	1,4,4	0.47	0	1,4,4	2.71	1 (100%)
3	LAC	A	399	-	2,5,5	0.53	0	1,6,6	1.27	0
4	NAD	A	400	-	41,48,48	1.37	3 (7%)	43,73,73	2.12	5 (11%)
5	PEG	A	403	-	6,6,6	0.46	0	5,5,5	0.27	0
6	1PE	A	404	-	12,12,15	0.60	0	11,11,14	0.47	0
6	1PE	A	444	-	12,12,15	0.56	0	11,11,14	0.25	0
2	PPI	A	453	-	1,4,4	0.54	0	1,4,4	0.76	0
5	PEG	A	454	-	6,6,6	0.52	0	5,5,5	0.20	0
5	PEG	A	555	-	6,6,6	0.70	0	5,5,5	0.72	0
6	1PE	A	700	-	7,7,15	0.47	0	6,6,14	0.21	0
5	PEG	A	701	-	6,6,6	0.63	0	5,5,5	1.09	0
7	GOL	A	710	-	5,5,5	0.34	0	5,5,5	0.30	0
5	PEG	A	772	-	6,6,6	0.44	0	5,5,5	0.32	0
7	GOL	A	800	-	5,5,5	0.27	0	5,5,5	0.18	0
5	PEG	A	802	-	6,6,6	0.49	0	5,5,5	0.21	0
5	PEG	A	803	-	5,5,6	0.61	0	4,4,5	0.55	0
2	PPI	B	398	-	1,4,4	0.73	0	1,4,4	3.80	1 (100%)
3	LAC	B	399	-	2,5,5	0.34	0	1,6,6	0.25	0
4	NAD	B	400	-	41,48,48	1.56	5 (12%)	43,73,73	2.09	4 (9%)
6	1PE	B	404	-	14,14,15	0.56	0	13,13,14	0.45	0
6	1PE	B	407	-	12,12,15	0.47	0	11,11,14	0.45	0
7	GOL	B	711	-	5,5,5	0.31	0	5,5,5	0.22	0
7	GOL	B	770	-	5,5,5	0.48	0	5,5,5	0.30	0
7	GOL	B	777	-	5,5,5	0.30	0	5,5,5	0.72	0
7	GOL	B	800	-	5,5,5	0.25	0	5,5,5	0.32	0
7	GOL	B	801	-	5,5,5	0.41	0	5,5,5	0.61	0
6	1PE	B	804	-	9,9,15	0.50	0	8,8,14	0.75	0
2	PPI	C	398	-	1,4,4	0.49	0	1,4,4	0.21	0
3	LAC	C	399	-	2,5,5	0.20	0	1,6,6	0.29	0
4	NAD	C	400	-	41,48,48	1.43	4 (9%)	43,73,73	1.87	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	C	401	-	5,5,5	0.42	0	5,5,5	0.22	0
6	1PE	C	404	-	9,9,15	0.49	0	8,8,14	0.26	0
7	GOL	C	650	-	5,5,5	0.35	0	5,5,5	0.41	0
5	PEG	C	702	-	6,6,6	0.69	0	5,5,5	0.51	0
5	PEG	C	771	-	6,6,6	0.57	0	5,5,5	0.40	0
2	PPI	D	398	-	1,4,4	0.54	0	1,4,4	1.26	0
3	LAC	D	399	-	2,5,5	0.43	0	1,6,6	0.80	0
4	NAD	D	400	-	41,48,48	1.45	3 (7%)	43,73,73	2.12	5 (11%)
7	GOL	D	401	-	5,5,5	0.40	0	5,5,5	0.69	0
5	PEG	D	405	-	6,6,6	0.46	0	5,5,5	0.55	0
7	GOL	D	777	-	5,5,5	0.35	0	5,5,5	0.42	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
6	1PE	A	335	-	-	0/7/7/13	0/0/0/0
2	PPI	A	398	-	-	0/0/2/2	0/0/0/0
3	LAC	A	399	-	-	0/0/4/4	0/0/0/0
4	NAD	A	400	-	-	0/22/62/62	0/5/5/5
5	PEG	A	403	-	-	0/4/4/4	0/0/0/0
6	1PE	A	404	-	-	0/10/10/13	0/0/0/0
6	1PE	A	444	-	-	0/10/10/13	0/0/0/0
2	PPI	A	453	-	-	0/0/2/2	0/0/0/0
5	PEG	A	454	-	-	0/4/4/4	0/0/0/0
5	PEG	A	555	-	-	0/4/4/4	0/0/0/0
6	1PE	A	700	-	-	0/5/5/13	0/0/0/0
5	PEG	A	701	-	-	0/4/4/4	0/0/0/0
7	GOL	A	710	-	-	0/4/4/4	0/0/0/0
5	PEG	A	772	-	-	0/4/4/4	0/0/0/0
7	GOL	A	800	-	-	0/4/4/4	0/0/0/0
5	PEG	A	802	-	-	0/4/4/4	0/0/0/0
5	PEG	A	803	-	-	0/3/3/4	0/0/0/0
2	PPI	B	398	-	-	0/0/2/2	0/0/0/0
3	LAC	B	399	-	-	0/0/4/4	0/0/0/0
4	NAD	B	400	-	-	0/22/62/62	0/5/5/5
6	1PE	B	404	-	-	0/12/12/13	0/0/0/0
6	1PE	B	407	-	-	0/10/10/13	0/0/0/0
7	GOL	B	711	-	-	0/4/4/4	0/0/0/0
7	GOL	B	770	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	777	-	-	0/4/4/4	0/0/0/0
7	GOL	B	800	-	-	0/4/4/4	0/0/0/0
7	GOL	B	801	-	-	0/4/4/4	0/0/0/0
6	1PE	B	804	-	-	0/7/7/13	0/0/0/0
2	PPI	C	398	-	-	0/0/2/2	0/0/0/0
3	LAC	C	399	-	-	0/0/4/4	0/0/0/0
4	NAD	C	400	-	-	0/22/62/62	0/5/5/5
7	GOL	C	401	-	-	0/4/4/4	0/0/0/0
6	1PE	C	404	-	-	0/7/7/13	0/0/0/0
7	GOL	C	650	-	-	0/4/4/4	0/0/0/0
5	PEG	C	702	-	-	0/4/4/4	0/0/0/0
5	PEG	C	771	-	-	0/4/4/4	0/0/0/0
2	PPI	D	398	-	-	0/0/2/2	0/0/0/0
3	LAC	D	399	-	-	0/0/4/4	0/0/0/0
4	NAD	D	400	-	-	0/22/62/62	0/5/5/5
7	GOL	D	401	-	-	0/4/4/4	0/0/0/0
5	PEG	D	405	-	-	0/4/4/4	0/0/0/0
7	GOL	D	777	-	-	0/4/4/4	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	400	NAD	O4B-C4B	-2.07	1.40	1.45
4	C	400	NAD	O4B-C4B	-2.04	1.40	1.45
4	A	400	NAD	C2A-N1A	2.11	1.37	1.33
4	B	400	NAD	C4N-C3N	2.22	1.43	1.39
4	C	400	NAD	C2A-N1A	2.83	1.39	1.33
4	B	400	NAD	C2A-N1A	2.88	1.39	1.33
4	D	400	NAD	C2A-N1A	3.29	1.40	1.33
4	A	400	NAD	C2A-N3A	3.68	1.38	1.32
4	D	400	NAD	C2A-N3A	3.91	1.38	1.32
4	B	400	NAD	C2A-N3A	3.98	1.38	1.32
4	C	400	NAD	C2A-N3A	4.06	1.38	1.32
4	A	400	NAD	O7N-C7N	5.19	1.34	1.24
4	D	400	NAD	O7N-C7N	5.94	1.36	1.24
4	C	400	NAD	O7N-C7N	6.07	1.36	1.24
4	B	400	NAD	O7N-C7N	6.80	1.38	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	400	NAD	N3A-C2A-N1A	-10.73	119.51	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	400	NAD	N3A-C2A-N1A	-10.24	119.94	128.86
4	D	400	NAD	N3A-C2A-N1A	-9.92	120.22	128.86
4	C	400	NAD	N3A-C2A-N1A	-9.31	120.75	128.86
4	B	400	NAD	O7N-C7N-C3N	-3.53	115.50	119.62
4	D	400	NAD	O7N-C7N-C3N	-3.37	115.69	119.62
4	A	400	NAD	O7N-C7N-C3N	-3.08	116.03	119.62
4	B	400	NAD	C4D-O4D-C1D	-3.04	106.53	109.77
4	D	400	NAD	O7N-C7N-N7N	-2.41	119.15	122.58
4	C	400	NAD	O7N-C7N-N7N	-2.28	119.34	122.58
4	A	400	NAD	C4D-O4D-C1D	-2.23	107.40	109.77
4	A	400	NAD	O7N-C7N-N7N	-2.16	119.51	122.58
2	A	398	PPI	C3-C2-C1	2.71	116.33	112.59
4	D	400	NAD	O2N-PN-O1N	3.22	128.95	112.28
4	C	400	NAD	O2N-PN-O1N	3.27	129.20	112.28
2	B	398	PPI	C3-C2-C1	3.80	117.84	112.59
4	C	400	NAD	C3N-C7N-N7N	4.46	122.87	117.77
4	B	400	NAD	C3N-C7N-N7N	5.25	123.77	117.77
4	A	400	NAD	C3N-C7N-N7N	5.74	124.33	117.77
4	D	400	NAD	C3N-C7N-N7N	6.46	125.14	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	399	LAC	1	0
4	A	400	NAD	1	0
2	A	453	PPI	1	0
5	A	701	PEG	6	0
5	A	772	PEG	1	0
2	B	398	PPI	1	0
3	B	399	LAC	1	0
4	B	400	NAD	2	0
6	B	404	1PE	2	0
6	B	407	1PE	6	0
6	B	804	1PE	2	0
2	C	398	PPI	1	0
3	C	399	LAC	1	0
4	C	400	NAD	1	0
6	C	404	1PE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	399	LAC	1	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	327/334 (97%)	-0.38	4 (1%) 79 82	13, 23, 46, 54	16 (4%)
1	B	326/334 (97%)	-0.45	2 (0%) 89 91	13, 23, 36, 43	17 (5%)
1	C	327/334 (97%)	-0.16	12 (3%) 42 49	17, 28, 53, 60	11 (3%)
1	D	327/334 (97%)	-0.25	1 (0%) 93 94	17, 27, 50, 55	16 (4%)
All	All	1307/1336 (97%)	-0.31	19 (1%) 74 77	13, 25, 48, 60	60 (4%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	334	SER	6.2
1	C	23	LEU	3.1
1	C	318	VAL	3.0
1	C	20	LEU	2.7
1	C	332	GLY	2.6
1	C	22	ASP	2.5
1	C	19	ALA	2.5
1	B	321	ASP	2.4
1	A	63	PRO	2.4
1	A	334	SER	2.3
1	B	319	LYS	2.3
1	C	319	LYS	2.2
1	C	316	ALA	2.2
1	A	318	VAL	2.1
1	C	333	PRO	2.1
1	C	323	GLU	2.1
1	A	22	ASP	2.1
1	D	22	ASP	2.1
1	C	17	GLN	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(Å ²)	Q<0.9
2	PPI	A	453	5/5	0.90	0.25	11.97	47,49,50,52	0
5	PEG	A	701	7/7	0.87	0.27	9.76	34,42,45,47	0
7	GOL	A	800	6/6	0.59	0.34	9.41	61,64,65,66	0
7	GOL	C	401	6/6	0.49	0.37	8.16	71,72,73,73	0
5	PEG	A	555	7/7	0.63	0.29	7.94	39,47,56,56	0
7	GOL	B	777	6/6	0.66	0.23	7.32	60,61,61,61	0
2	PPI	D	398	5/5	0.90	0.20	6.97	43,44,46,46	0
6	1PE	C	404	10/16	0.87	0.24	6.34	53,55,55,56	0
6	1PE	B	804	10/16	0.67	0.40	6.32	47,59,62,63	0
7	GOL	B	711	6/6	0.81	0.20	5.67	56,61,61,62	0
7	GOL	B	770	6/6	0.64	0.24	5.61	59,61,62,62	0
5	PEG	A	803	6/7	0.71	0.20	5.52	55,58,60,60	0
6	1PE	A	335	10/16	0.74	0.21	5.34	69,69,70,70	0
5	PEG	A	772	7/7	0.74	0.22	4.77	75,76,76,76	0
7	GOL	B	800	6/6	0.74	0.24	4.58	70,71,71,71	0
6	1PE	A	404	13/16	0.88	0.18	4.07	42,49,61,62	0
2	PPI	A	398	5/5	0.92	0.17	4.06	38,39,42,42	0
6	1PE	A	444	13/16	0.78	0.20	3.79	64,66,69,69	0
5	PEG	C	771	7/7	0.65	0.24	3.28	63,65,65,65	0
7	GOL	B	801	6/6	0.79	0.17	3.21	59,60,60,61	0
6	1PE	B	407	13/16	0.81	0.20	3.20	53,54,57,57	13
2	PPI	B	398	5/5	0.91	0.18	3.18	36,39,42,42	0
6	1PE	B	404	15/16	0.78	0.20	2.72	50,52,55,55	15
5	PEG	A	403	7/7	0.83	0.16	2.67	58,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PPI	C	398	5/5	0.93	0.12	2.12	47,48,49,49	0
6	1PE	A	700	8/16	0.81	0.17	1.99	45,46,48,48	8
5	PEG	A	454	7/7	0.84	0.31	1.98	63,63,65,66	0
5	PEG	C	702	7/7	0.92	0.12	1.69	28,33,40,44	0
7	GOL	C	650	6/6	0.82	0.15	1.65	68,69,69,70	0
7	GOL	D	777	6/6	0.88	0.15	0.88	66,67,67,68	0
3	LAC	B	399	6/6	0.97	0.12	0.87	14,17,20,26	0
3	LAC	D	399	6/6	0.95	0.12	0.24	20,21,23,24	1
5	PEG	D	405	7/7	0.86	0.12	0.12	48,50,52,53	0
3	LAC	C	399	6/6	0.97	0.09	0.09	22,25,26,31	0
4	NAD	A	400	44/44	0.97	0.09	-0.44	9,16,19,22	0
4	NAD	D	400	44/44	0.97	0.09	-0.75	14,23,25,27	0
3	LAC	A	399	6/6	0.95	0.10	-0.77	13,15,20,23	0
4	NAD	B	400	44/44	0.97	0.08	-0.78	9,18,21,23	0
4	NAD	C	400	44/44	0.98	0.08	-1.17	15,23,25,26	0
7	GOL	D	401	6/6	0.83	0.23	-	62,63,63,63	0
5	PEG	A	802	7/7	0.82	0.24	-	55,55,59,59	0
7	GOL	A	710	6/6	0.86	0.28	-	70,71,71,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.