



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:30 PM GMT

PDB ID : 4LRS
Title : Crystal and solution structures of the bifunctional enzyme (Aldolase/Aldehyde dehydrogenase) from *Thermomonospora curvata*, reveal a cofactor-binding domain motion during NAD⁺ and CoA accommodation within the shared cofactor-binding site
Authors : Fischer, B.; Branlant, G.; Talfournier, F.; Gruez, A.
Deposited on : 2013-07-20
Resolution : 1.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

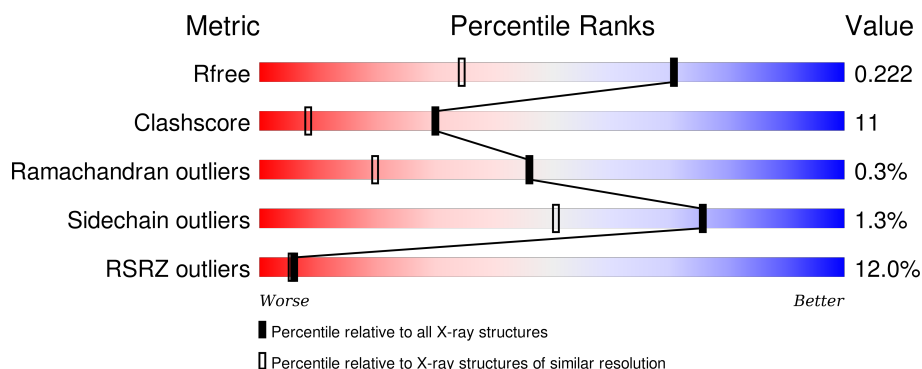
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

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	355	<div> <div>9%</div> <div>85%</div> <div>10%</div> <div>5%</div> </div>
2	B	323	<div> <div>12%</div> <div>80%</div> <div>10%</div> <div>9%</div> </div>
3	N	3	<div> <div>100%</div> <div>100%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAD	B	401	-	-	-	X
11	FOR	B	410	-	-	X	X
6	CL	A	403	-	-	-	X
7	MG	A	404	-	-	-	X
8	GOL	A	405	-	-	-	X
8	GOL	B	403	-	-	-	X
8	GOL	B	405	-	-	X	X
8	GOL	B	406	-	-	-	X
8	GOL	B	407	-	-	-	X
9	PEG	A	406	-	-	X	X
9	PEG	A	408[A]	-	-	X	X
9	PEG	A	408[B]	-	-	X	X
9	PEG	A	410	-	-	X	X
9	PEG	B	408	-	-	-	X
9	PEG	B	409	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 5807 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 4-hydroxy-2-oxovalerate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	9	26	0
			2715	1687	505	514	9			

- Molecule 2 is a protein called Acetaldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	294	Total	C	N	O	S	9	22	0
			2360	1489	411	448	12			

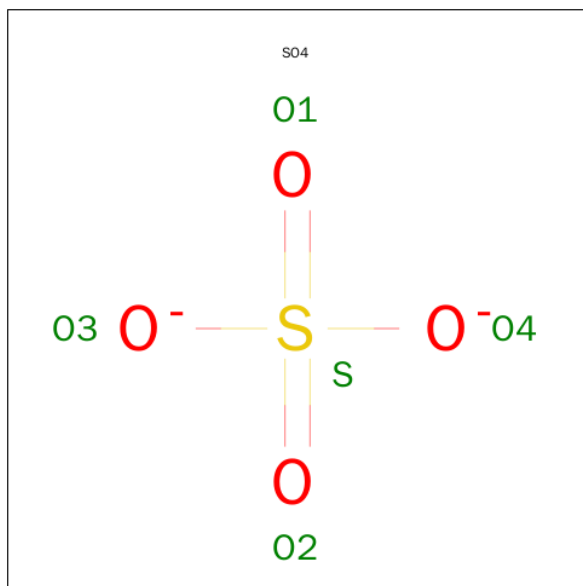
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	INITIATING METHIONINE	UNP D1A3K7
B	2	GLY	-	EXPRESSION TAG	UNP D1A3K7
B	3	SER	-	EXPRESSION TAG	UNP D1A3K7
B	4	SER	-	EXPRESSION TAG	UNP D1A3K7
B	5	HIS	-	EXPRESSION TAG	UNP D1A3K7
B	6	HIS	-	EXPRESSION TAG	UNP D1A3K7
B	7	HIS	-	EXPRESSION TAG	UNP D1A3K7
B	8	HIS	-	EXPRESSION TAG	UNP D1A3K7
B	9	HIS	-	EXPRESSION TAG	UNP D1A3K7
B	10	HIS	-	EXPRESSION TAG	UNP D1A3K7
B	11	SER	-	EXPRESSION TAG	UNP D1A3K7
B	12	SER	-	EXPRESSION TAG	UNP D1A3K7
B	13	GLY	-	EXPRESSION TAG	UNP D1A3K7
B	14	LEU	-	EXPRESSION TAG	UNP D1A3K7
B	15	VAL	-	EXPRESSION TAG	UNP D1A3K7
B	16	PRO	-	EXPRESSION TAG	UNP D1A3K7
B	17	ARG	-	EXPRESSION TAG	UNP D1A3K7
B	18	GLY	-	EXPRESSION TAG	UNP D1A3K7
B	19	SER	-	EXPRESSION TAG	UNP D1A3K7
B	20	HIS	-	EXPRESSION TAG	UNP D1A3K7

- Molecule 3 is a protein called Symmetric aldolase, C-terminal disordered residues.

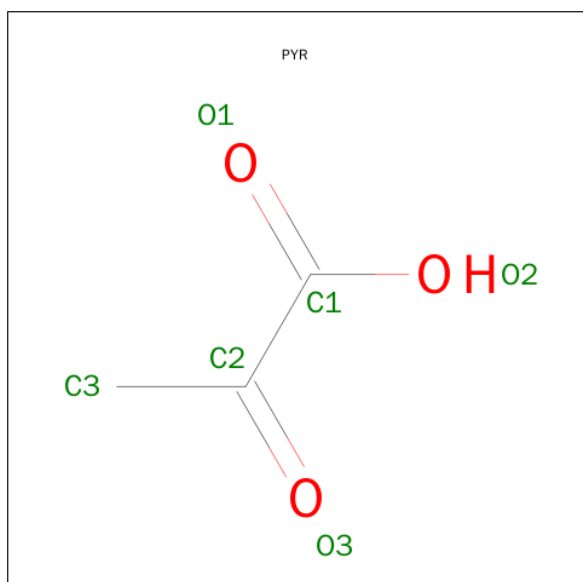
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	N	3	Total	C	N	O	0	0	0
			15	9	3	3			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is PYRUVIC ACID (three-letter code: PYR) (formula: C₃H₄O₃).



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

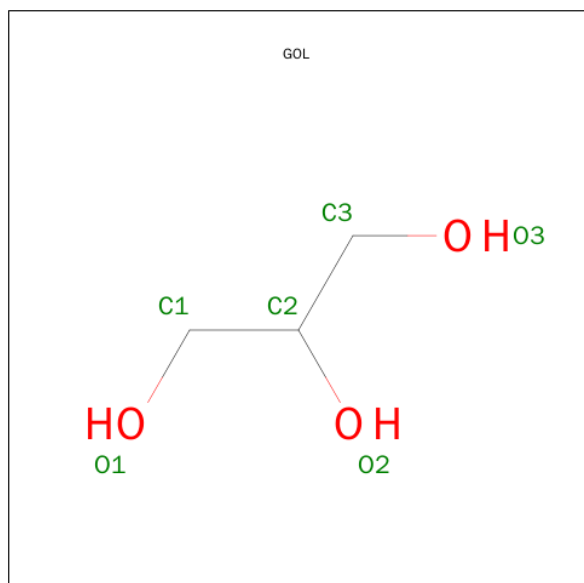
- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Cl		0	0
			1	1			
6	A	1	Total	Cl		0	0
			1	1			

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Mg		0	0
			1	1			

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



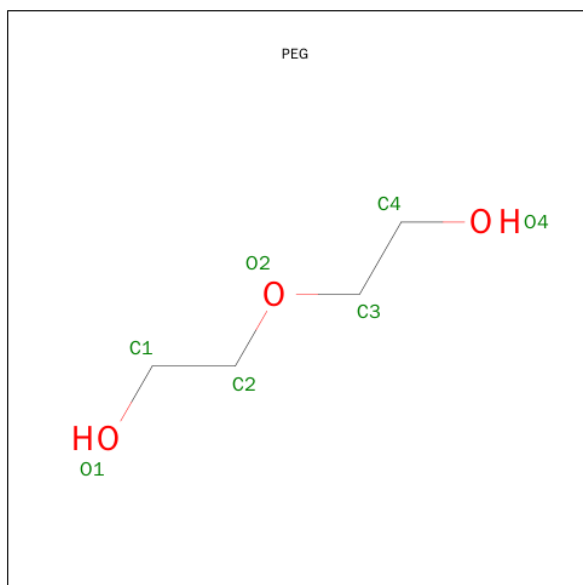
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

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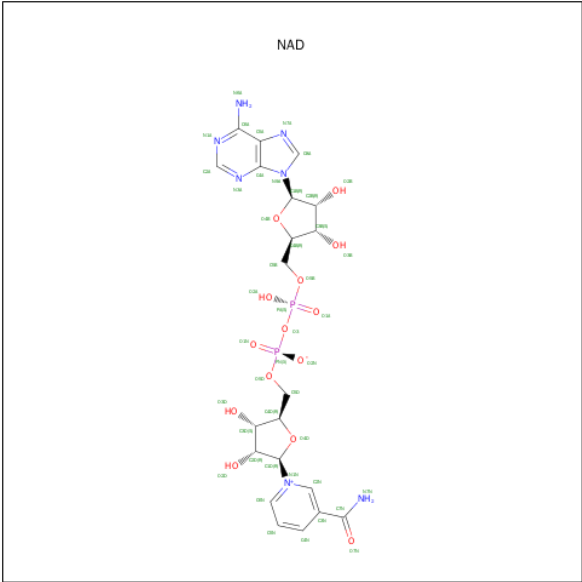
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



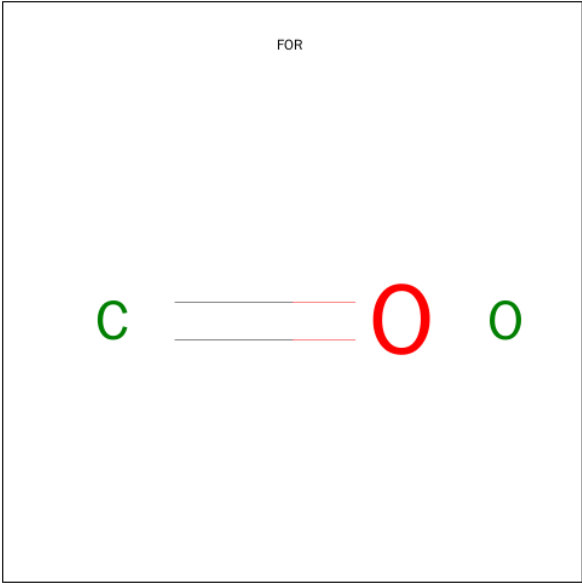
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	1
			14	8	6		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 11 is FORMYL GROUP (three-letter code: FOR) (formula: CH₂O).



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

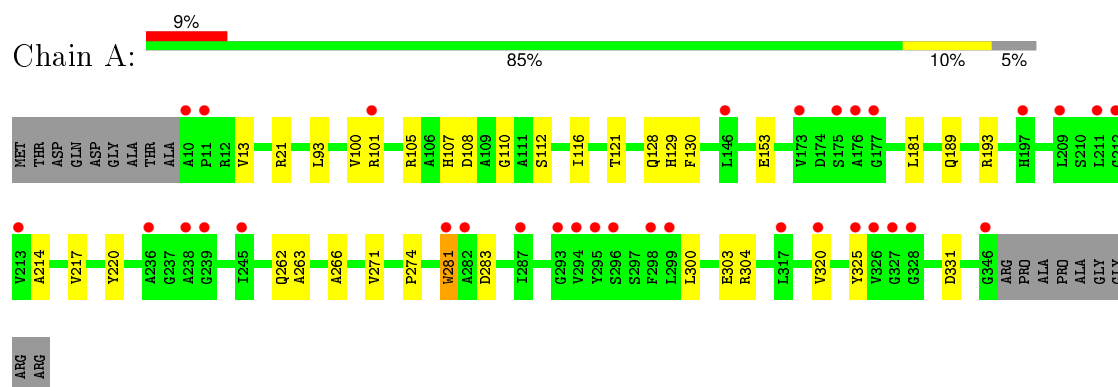
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	296	Total 296	O 296	0	0
12	B	265	Total 265	O 265	0	0
12	N	4	Total 4	O 4	0	0

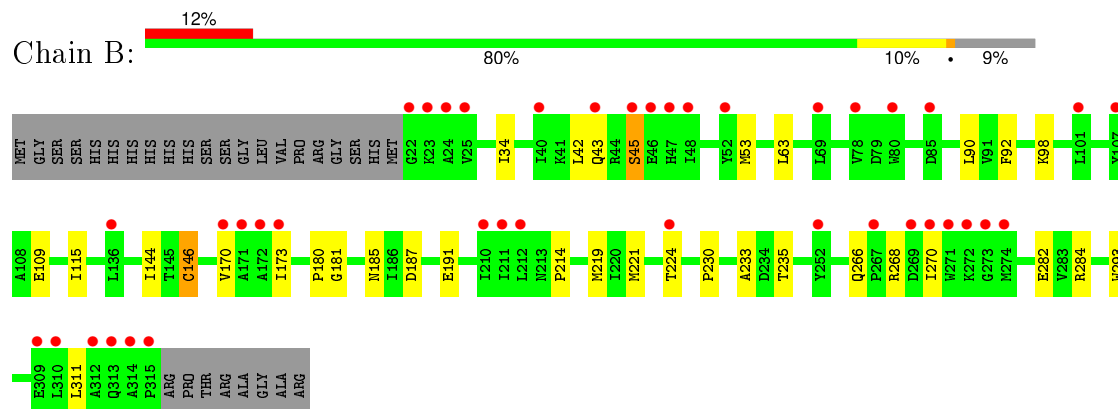
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

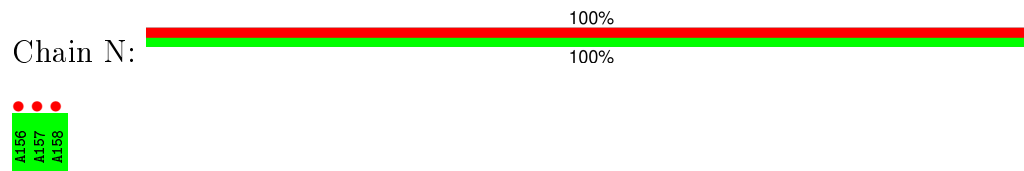
- Molecule 1: 4-hydroxy-2-oxovalerate aldolase



- Molecule 2: Acetaldehyde dehydrogenase



- Molecule 3: Symmetric aldolase, C-terminal disordered residues



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.88Å 92.21Å 56.48Å 90.00° 100.59° 90.00°	Depositor
Resolution (Å)	25.00 – 1.55 43.35 – 1.55	Depositor EDS
% Data completeness (in resolution range)	97.7 (25.00-1.55) 97.7 (43.35-1.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.164 , 0.200 0.194 , 0.222	Depositor DCC
R_{free} test set	5337 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 106731 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5807	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: GOL, MG, FOR, NAD, CL, PYR, SO4, 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	0.63	2/2776 (0.1%)	0.71	0/3768
2	B	0.54	1/2418 (0.0%)	0.66	0/3303
3	N	0.58	0/14	0.49	0/18
All	All	0.59	3/5208 (0.1%)	0.69	0/7089

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281[A]	TRP	CD2-CE2	5.27	1.47	1.41
1	A	281[B]	TRP	CD2-CE2	5.27	1.47	1.41
2	B	293	TRP	CD2-CE2	5.08	1.47	1.41

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	2715	0	2665	50	0
2	B	2360	0	2390	36	0
3	N	15	0	14	0	0
4	A	5	0	0	0	0
5	A	6	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
8	A	6	0	8	0	0
8	B	30	0	40	7	0
9	A	42	0	60	39	0
9	B	14	0	20	11	0
10	B	44	0	26	11	0
11	B	2	0	0	3	0
12	A	296	0	0	5	0
12	B	265	0	0	4	0
12	N	4	0	0	0	0
All	All	5807	0	5226	117	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 11.

All (117) 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)
9:A:408[B]:PEG:H12	9:A:410:PEG:C4	1.62	1.28
9:A:408[A]:PEG:C2	9:A:410:PEG:H42	1.64	1.25
9:A:408[B]:PEG:C1	9:A:410:PEG:H31	1.67	1.22
9:A:408[A]:PEG:C1	9:A:410:PEG:H42	1.68	1.22
9:A:408[B]:PEG:H12	9:A:410:PEG:C3	1.73	1.19
9:A:408[A]:PEG:H21	9:A:410:PEG:H42	1.21	1.15
2:B:146[A]:CYS:SG	10:B:401:NAD:C4N	2.35	1.15
9:A:408[B]:PEG:C1	9:A:410:PEG:C3	2.26	1.11
9:A:408[B]:PEG:C1	9:A:410:PEG:C4	2.31	1.08
9:A:408[A]:PEG:H11	9:A:410:PEG:C4	1.81	1.08
9:A:408[A]:PEG:H11	9:A:410:PEG:H42	1.29	1.08
1:A:101[B]:ARG:HH11	1:A:101[B]:ARG:HG3	1.15	1.08
9:A:408[B]:PEG:C1	9:A:410:PEG:H42	1.86	1.04
2:B:180:PRO:HB2	9:B:409:PEG:H42	1.43	1.00
10:B:401:NAD:H2B	9:B:409:PEG:H32	1.48	0.96
9:A:408[A]:PEG:H21	9:A:410:PEG:C4	1.96	0.95
9:A:408[B]:PEG:H12	9:A:410:PEG:H31	1.35	0.94
9:A:408[B]:PEG:H11	9:A:410:PEG:H31	1.51	0.91
1:A:101[B]:ARG:HH11	1:A:101[B]:ARG:CG	1.83	0.91
1:A:101[A]:ARG:NH2	2:B:191[A]:GLU:OE1	2.03	0.91
9:A:408[B]:PEG:H11	9:A:410:PEG:C3	2.00	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:PRO:HG2	9:B:408:PEG:H32	1.53	0.89
9:A:408[B]:PEG:C2	9:A:410:PEG:H42	1.98	0.89
2:B:235:THR:OG1	8:B:403:GOL:H2	1.75	0.86
9:A:408[B]:PEG:H22	9:A:410:PEG:H42	1.56	0.85
2:B:146[A]:CYS:SG	10:B:401:NAD:H4N	2.17	0.82
9:A:408[A]:PEG:H11	9:A:410:PEG:C3	2.10	0.81
10:B:401:NAD:H2B	9:B:409:PEG:C3	2.10	0.81
1:A:281[A]:TRP:CD1	1:A:283[A]:ASP:HB3	2.15	0.81
1:A:101[B]:ARG:HD3	1:A:105[B]:ARG:HH12	1.46	0.81
1:A:101[B]:ARG:HD2	1:A:105[B]:ARG:HH22	1.44	0.80
9:A:408[A]:PEG:C2	9:A:410:PEG:C4	2.55	0.79
1:A:101[B]:ARG:CD	1:A:105[B]:ARG:HH12	1.96	0.77
2:B:266:GLN:HA	8:B:405:GOL:H31	1.67	0.76
10:B:401:NAD:H8A	9:B:409:PEG:H32	1.67	0.76
2:B:173[B]:ILE:HG22	2:B:221:MET:HG3	1.69	0.75
2:B:233:ALA:HA	9:B:408:PEG:H11	1.69	0.74
1:A:262[B]:GLN:HG2	9:A:408[B]:PEG:C4	2.17	0.74
9:A:408[B]:PEG:H12	9:A:410:PEG:H41	1.67	0.74
1:A:101[B]:ARG:NH1	1:A:101[B]:ARG:HG3	1.98	0.73
1:A:262[B]:GLN:HG2	9:A:408[B]:PEG:H42	1.71	0.72
2:B:170:VAL:HB	2:B:224[B]:THR:HG22	1.72	0.71
1:A:112:SER:HA	9:A:406:PEG:H42	1.72	0.71
1:A:271:VAL:HG23	9:A:410:PEG:H21	1.71	0.71
2:B:90[B]:LEU:HD13	2:B:92:PHE:CE1	2.27	0.69
1:A:107:HIS:CD2	9:A:406:PEG:H41	2.28	0.68
9:A:408[B]:PEG:H32	12:A:730:HOH:O	1.92	0.68
1:A:101[B]:ARG:NH1	1:A:101[B]:ARG:CG	2.51	0.67
2:B:146[B]:CYS:HB3	10:B:401:NAD:H4N	1.76	0.66
2:B:90[B]:LEU:HD12	2:B:90[B]:LEU:O	1.96	0.66
2:B:53:MET:HG3	2:B:63:LEU:HD23	1.80	0.63
2:B:268[A]:ARG:HE	8:B:404:GOL:H31	1.63	0.63
2:B:146[A]:CYS:SG	10:B:401:NAD:C5N	2.88	0.62
1:A:281[A]:TRP:HD1	1:A:283[A]:ASP:HB3	1.63	0.60
1:A:101[B]:ARG:HG2	1:A:105[B]:ARG:NH1	2.19	0.58
1:A:93[B]:LEU:HD21	1:A:129[B]:HIS:CE1	2.38	0.58
1:A:266:ALA:HB3	9:A:410:PEG:H41	1.84	0.58
2:B:115[B]:ILE:HD11	2:B:311:LEU:HD12	1.85	0.57
2:B:235:THR:HG21	8:B:405:GOL:H12	1.87	0.57
2:B:92:PHE:CE2	2:B:115[B]:ILE:HD12	2.39	0.56
1:A:274:PRO:HB2	9:A:407:PEG:H41	1.87	0.56
1:A:271:VAL:CG2	9:A:410:PEG:H21	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98[C]:LYS:HD2	12:B:671:HOH:O	2.06	0.56
2:B:266:GLN:HA	8:B:405:GOL:C3	2.36	0.56
1:A:101[B]:ARG:NH1	1:A:101[B]:ARG:HB2	2.20	0.55
1:A:262[B]:GLN:HG2	9:A:408[B]:PEG:C3	2.36	0.55
2:B:180:PRO:HB2	9:B:409:PEG:C4	2.29	0.54
9:A:408[A]:PEG:H11	9:A:410:PEG:H32	1.89	0.53
10:B:401:NAD:O1A	9:B:409:PEG:H41	2.09	0.53
1:A:107:HIS:NE2	9:A:406:PEG:H41	2.23	0.53
1:A:110:GLY:HA2	9:A:406:PEG:H11	1.89	0.53
1:A:129[C]:HIS:N	1:A:129[C]:HIS:ND1	2.52	0.53
2:B:146[B]:CYS:HB3	10:B:401:NAD:C4N	2.38	0.53
10:B:401:NAD:H8A	9:B:409:PEG:C3	2.36	0.53
1:A:153:GLU:OE2	1:A:193[B]:ARG:NH2	2.41	0.52
2:B:42:LEU:O	2:B:45:SER:HB3	2.09	0.52
9:A:408[B]:PEG:O1	9:A:410:PEG:H11	2.09	0.52
1:A:112:SER:HB3	9:A:406:PEG:H31	1.91	0.51
1:A:100:VAL:HG23	2:B:187[B]:ASP:OD2	2.10	0.51
2:B:90[B]:LEU:HD12	2:B:90[B]:LEU:C	2.31	0.51
2:B:181:GLY:HA2	9:B:409:PEG:H11	1.92	0.50
9:B:409:PEG:H21	12:B:673:HOH:O	2.12	0.50
8:B:403:GOL:O3	8:B:405:GOL:H11	2.12	0.50
8:B:403:GOL:O3	8:B:405:GOL:C1	2.61	0.48
1:A:13[B]:VAL:HG22	1:A:220:TYR:CD1	2.49	0.48
1:A:101[B]:ARG:NH1	1:A:101[B]:ARG:CB	2.77	0.47
1:A:303[A]:GLU:OE2	12:A:769:HOH:O	2.20	0.47
1:A:21:ARG:HD2	1:A:21:ARG:C	2.33	0.47
1:A:116[B]:ILE:HD12	1:A:130:PHE:CD1	2.49	0.47
1:A:129[B]:HIS:NE2	2:B:187[B]:ASP:OD1	2.46	0.47
1:A:189[B]:GLN:NE2	12:A:728:HOH:O	2.48	0.46
1:A:128:GLN:HB2	1:A:129[C]:HIS:CE1	2.51	0.46
1:A:304[B]:ARG:HG3	12:A:616:HOH:O	2.14	0.46
2:B:34:ILE:HD11	10:B:401:NAD:C4N	2.46	0.45
2:B:90[B]:LEU:CD1	2:B:92:PHE:CE1	2.99	0.45
1:A:263:ALA:HA	9:A:408[B]:PEG:H31	1.98	0.45
11:B:410:FOR:C	12:B:510:HOH:O	2.54	0.45
9:A:408[B]:PEG:C1	9:A:410:PEG:H11	2.48	0.44
1:A:214:ALA:O	1:A:217[B]:VAL:HG22	2.19	0.43
1:A:300[B]:LEU:O	1:A:304[B]:ARG:HG3	2.19	0.43
1:A:101[B]:ARG:CD	1:A:105[B]:ARG:NH1	2.73	0.43
1:A:108[B]:ASP:O	1:A:108[B]:ASP:OD1	2.36	0.43
1:A:262[A]:GLN:HB3	9:A:408[A]:PEG:H42	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43[B]:GLN:HB2	12:B:584:HOH:O	2.18	0.43
2:B:170:VAL:HB	2:B:224[B]:THR:CG2	2.46	0.41
1:A:331:ASP:CB	2:B:224[B]:THR:HG21	2.51	0.41
1:A:320:VAL:HG13	1:A:325:TYR:HD2	1.85	0.41
9:A:409:PEG:H42	12:A:763:HOH:O	2.21	0.41
1:A:101[B]:ARG:CG	1:A:105[B]:ARG:HH12	2.33	0.41
1:A:121:THR:OG1	2:B:214:PRO:HG3	2.20	0.41
2:B:224[B]:THR:O	2:B:224[B]:THR:HG23	2.20	0.40
2:B:282:GLU:OE1	2:B:284[A]:ARG:NH1	2.55	0.40
1:A:300[B]:LEU:HD23	1:A:300[B]:LEU:HA	1.83	0.40
1:A:101[B]:ARG:HH11	1:A:101[B]:ARG:CB	2.33	0.40
1:A:13[B]:VAL:CG2	1:A:220:TYR:CD1	3.05	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	362/355 (102%)	357 (99%)	4 (1%)	1 (0%)	46	20
2	B	316/323 (98%)	308 (98%)	7 (2%)	1 (0%)	46	20
3	N	1/3 (33%)	0	1 (100%)	0	100	100
All	All	679/681 (100%)	665 (98%)	12 (2%)	2 (0%)	46	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	LEU
2	B	144	ILE

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	272/257 (106%)	272 (100%)	0	100	100
2	B	246/245 (100%)	238 (97%)	8 (3%)	45	13
All	All	518/502 (103%)	510 (98%)	8 (2%)	76	44

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	45	SER
2	B	109	GLU
2	B	146[A]	CYS
2	B	146[B]	CYS
2	B	185	ASN
2	B	219[A]	MET
2	B	219[B]	MET
2	B	270	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	318	GLN
2	B	84	GLN
2	B	263	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 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	$\# Z > 2$
4	SO4	A	401	-	4,4,4	0.45	0	6,6,6	0.67	0
5	PYR	A	402	7	2,5,5	0.97	0	2,6,6	1.94	1 (50%)
8	GOL	A	405	-	5,5,5	0.28	0	5,5,5	0.17	0
9	PEG	A	406	-	6,6,6	0.59	0	5,5,5	0.50	0
9	PEG	A	407	-	6,6,6	0.42	0	5,5,5	0.40	0
9	PEG	A	408[A]	-	6,6,6	0.59	0	5,5,5	0.61	0
9	PEG	A	408[B]	-	6,6,6	0.49	0	5,5,5	0.12	0
9	PEG	A	409	-	6,6,6	0.48	0	5,5,5	0.14	0
9	PEG	A	410	-	6,6,6	0.38	0	5,5,5	0.70	0
10	NAD	B	401	-	38,48,48	0.97	3 (7%)	47,73,73	1.50	5 (10%)
8	GOL	B	403	-	5,5,5	0.20	0	5,5,5	0.27	0
8	GOL	B	404	-	5,5,5	0.30	0	5,5,5	0.40	0
8	GOL	B	405	-	5,5,5	0.58	0	5,5,5	1.06	0
8	GOL	B	406	-	5,5,5	0.37	0	5,5,5	0.37	0
8	GOL	B	407	-	5,5,5	0.18	0	5,5,5	0.36	0
9	PEG	B	408	-	6,6,6	0.45	0	5,5,5	0.57	0
9	PEG	B	409	-	6,6,6	0.38	0	5,5,5	0.35	0
11	FOR	B	410	-	0,1,1	0.00	-	0,0,0	0.00	-

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
4	SO4	A	401	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PYR	A	402	7	-	0/0/4/4	0/0/0/0
8	GOL	A	405	-	-	0/4/4/4	0/0/0/0
9	PEG	A	406	-	-	0/4/4/4	0/0/0/0
9	PEG	A	407	-	-	0/4/4/4	0/0/0/0
9	PEG	A	408[A]	-	-	0/4/4/4	0/0/0/0
9	PEG	A	408[B]	-	-	0/4/4/4	0/0/0/0
9	PEG	A	409	-	-	0/4/4/4	0/0/0/0
9	PEG	A	410	-	-	0/4/4/4	0/0/0/0
10	NAD	B	401	-	-	0/22/62/62	0/5/5/5
8	GOL	B	403	-	-	0/4/4/4	0/0/0/0
8	GOL	B	404	-	-	0/4/4/4	0/0/0/0
8	GOL	B	405	-	-	0/4/4/4	0/0/0/0
8	GOL	B	406	-	-	0/4/4/4	0/0/0/0
8	GOL	B	407	-	-	0/4/4/4	0/0/0/0
9	PEG	B	408	-	-	0/4/4/4	0/0/0/0
9	PEG	B	409	-	-	0/4/4/4	0/0/0/0
11	FOR	B	410	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	401	NAD	C5A-C4A	2.56	1.46	1.40
10	B	401	NAD	O4D-C1D	2.68	1.44	1.41
10	B	401	NAD	O4B-C1B	2.97	1.45	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	401	NAD	N3A-C2A-N1A	-7.46	123.18	128.89
10	B	401	NAD	C1B-N9A-C4A	-3.30	121.97	126.94
10	B	401	NAD	O4B-C1B-N9A	-2.19	103.52	108.10
10	B	401	NAD	C4B-O4B-C1B	-2.16	107.34	109.72
5	A	402	PYR	O3-C2-C3	2.19	125.38	120.13
10	B	401	NAD	C2A-N1A-C6A	2.58	123.38	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	406	PEG	5	0
9	A	407	PEG	1	0
9	A	408[A]	PEG	10	0
9	A	408[B]	PEG	19	0
9	A	409	PEG	1	0
9	A	410	PEG	26	0
10	B	401	NAD	11	0
8	B	403	GOL	3	0
8	B	404	GOL	1	0
8	B	405	GOL	5	0
9	B	408	PEG	2	0
9	B	409	PEG	9	0
11	B	410	FOR	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	337/355 (94%)	0.51	33 (9%)	10 10	5, 8, 14, 29	9 (2%)
2	B	294/323 (91%)	0.58	40 (13%)	4 4	6, 9, 16, 28	11 (3%)
3	N	3/3 (100%)	8.49	3 (100%)	0 0	32, 32, 32, 32	3 (100%)
All	All	634/681 (93%)	0.58	76 (11%)	6 5	5, 9, 16, 32	23 (3%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	158	ALA	10.0
2	B	315	PRO	9.3
3	N	156	ALA	9.1
2	B	22	GLY	8.7
3	N	157	ALA	6.4
2	B	314	ALA	5.4
1	A	10	ALA	5.3
1	A	326	VAL	4.7
2	B	313	GLN	4.6
2	B	273	GLY	4.4
2	B	211[A]	ILE	4.3
2	B	271	TRP	4.2
2	B	312	ALA	4.1
1	A	211	LEU	4.0
1	A	295	TYR	3.9
1	A	346	GLY	3.9
1	A	213[A]	VAL	3.8
2	B	269	ASP	3.7
1	A	176	ALA	3.7
2	B	46	GLU	3.7
2	B	270	ILE	3.6
2	B	43[A]	GLN	3.5
1	A	146	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	24	ALA	3.3
2	B	272[A]	LYS	3.3
2	B	310	LEU	3.3
2	B	69	LEU	3.1
1	A	209	LEU	3.1
2	B	210	ILE	3.0
2	B	85	ASP	3.0
1	A	287	ILE	3.0
1	A	173	VAL	2.9
2	B	212	LEU	2.9
1	A	245	ILE	2.9
2	B	52	TYR	2.9
1	A	197	HIS	2.9
1	A	212	GLY	2.8
1	A	294	VAL	2.8
2	B	107	TYR	2.7
1	A	11	PRO	2.6
2	B	136	LEU	2.6
2	B	171	ALA	2.6
2	B	48	ILE	2.6
2	B	274	MET	2.5
1	A	296[A]	SER	2.5
2	B	47	HIS	2.5
1	A	236	ALA	2.5
2	B	252	TYR	2.5
1	A	282	ALA	2.4
1	A	239	GLY	2.4
1	A	328	GLY	2.4
2	B	78	VAL	2.4
2	B	267	PRO	2.4
2	B	25	VAL	2.4
1	A	317	LEU	2.4
1	A	101[A]	ARG	2.4
2	B	80	TRP	2.4
2	B	172	ALA	2.3
2	B	173[A]	ILE	2.3
2	B	40[A]	ILE	2.3
2	B	23	LYS	2.3
1	A	299	LEU	2.2
2	B	45	SER	2.2
1	A	177	GLY	2.2
2	B	101[A]	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	175	SER	2.1
1	A	281[A]	TRP	2.1
1	A	327	GLY	2.1
1	A	325	TYR	2.1
1	A	238	ALA	2.1
1	A	298	PHE	2.1
2	B	309	GLU	2.1
1	A	293	GLY	2.1
1	A	320	VAL	2.0
2	B	170	VAL	2.0
2	B	224[A]	THR	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
9	PEG	A	410	7/7	0.77	0.35	22.47	14,16,23,24	7
9	PEG	A	408[B]	7/7	0.70	0.41	14.25	28,29,39,45	7
9	PEG	A	408[A]	7/7	0.70	0.41	12.03	21,26,33,36	7
8	GOL	B	403	6/6	0.84	0.24	9.59	18,24,31,38	6
9	PEG	B	408	7/7	0.72	0.26	8.18	23,24,37,39	7
7	MG	A	404	1/1	1.00	0.38	7.55	9,9,9,9	0
8	GOL	B	407	6/6	0.87	0.24	6.46	27,36,36,37	6
8	GOL	B	406	6/6	0.67	0.30	5.63	37,51,55,59	0
8	GOL	B	405	6/6	0.64	0.34	5.60	22,24,26,28	6
8	GOL	A	405	6/6	0.60	0.25	4.93	37,46,48,51	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	CL	A	403	1/1	0.99	0.15	3.74	24,24,24,24	0
11	FOR	B	410	2/2	0.89	0.29	3.07	20,20,20,23	0
9	PEG	A	406	7/7	0.80	0.27	2.69	19,24,28,36	7
10	NAD	B	401	44/44	0.95	0.14	2.02	16,19,20,24	0
8	GOL	B	404	6/6	0.55	0.27	1.48	33,44,45,46	6
5	PYR	A	402	6/6	0.90	0.18	0.81	16,18,24,26	0
9	PEG	B	409	7/7	0.77	0.22	0.57	21,26,35,36	7
6	CL	B	402	1/1	0.99	0.06	-1.39	29,29,29,29	0
4	SO4	A	401	5/5	0.93	0.14	-	22,24,28,31	5
9	PEG	A	409	7/7	0.78	0.28	-	23,28,32,33	7
9	PEG	A	407	7/7	0.54	0.27	-	23,29,31,33	7

6.5 Other polymers ⓘ

There are no such residues in this entry.