



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:43 PM UTC

PDB ID : 4N8S / pdb_00004n8s
Title : Crystal Structure of the ternary complex of lipase from *Thermomyces lanuginosa* with Ethylacetoacetate and P-nitrobenzaldehyde at 2.3 Å resolution
Authors : Kumar, M.; Mukherjee, J.; Gupta, M.N.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2013-10-18
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

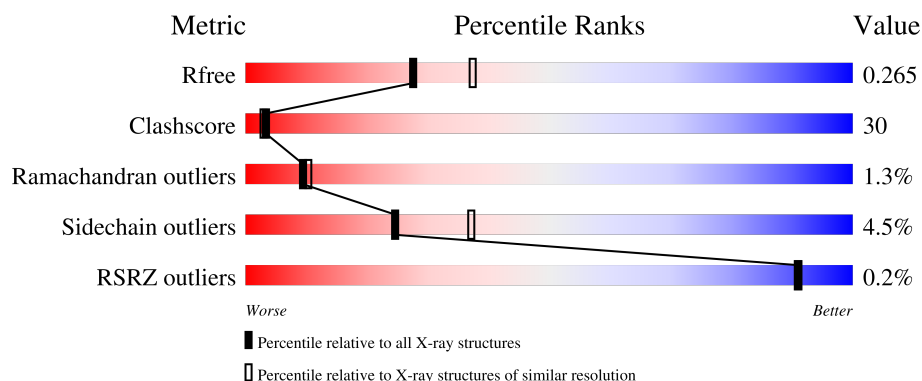
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	269	 60% 34% 6%
1	B	269	 52% 38% 9%

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
3	XXH	A	302	-	X	X	-
4	EAC	A	303	-	-	X	-

2 Entry composition [i](#)

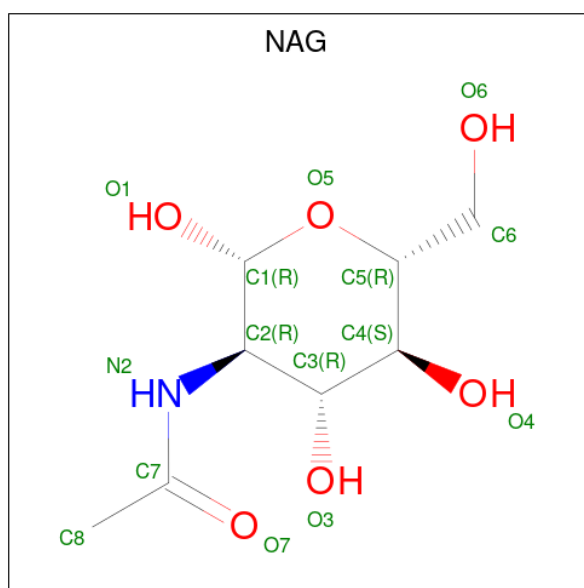
There are 6 unique types of molecules in this entry. The entry contains 4379 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lipase.

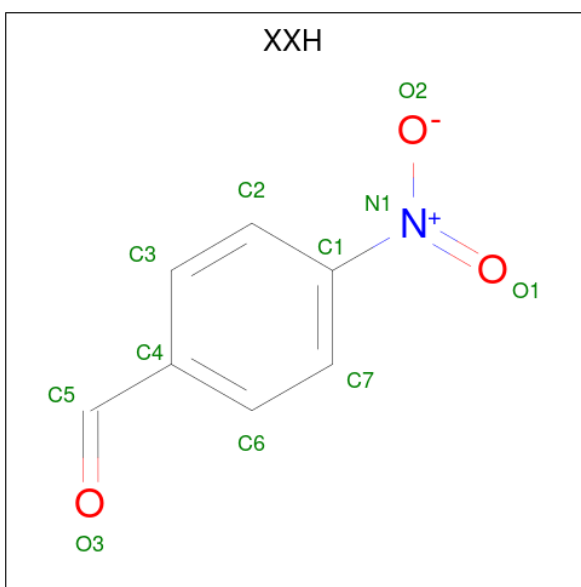
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	B	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



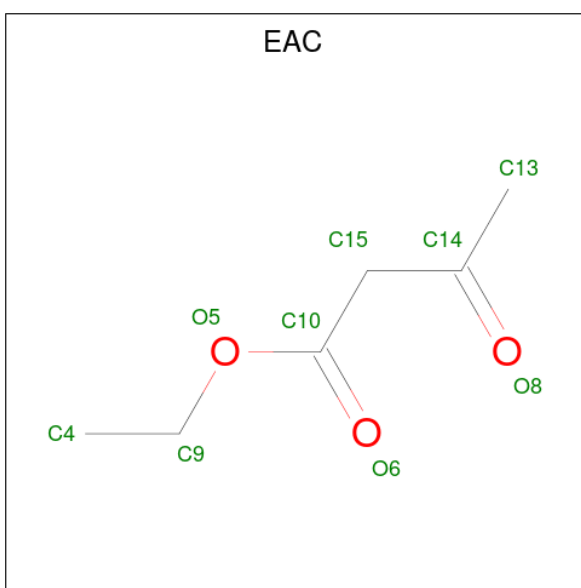
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 4-nitrobenzaldehyde (CCD ID: XXH) (formula: $C_7H_5NO_3$).



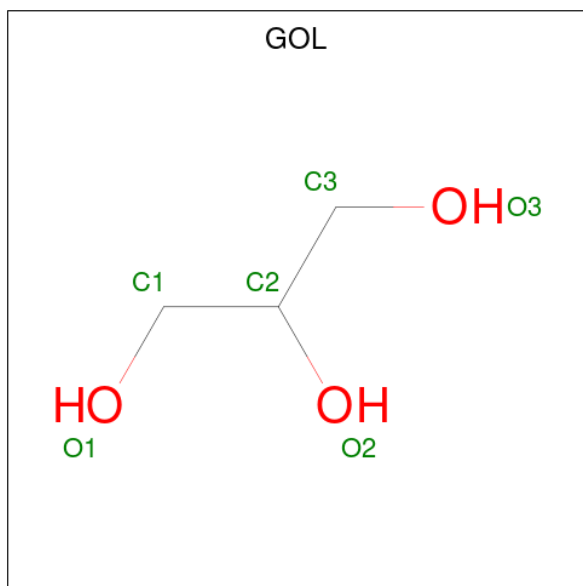
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	7	1	3		
3	B	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 4 is ethyl 3-oxobutanoate (CCD ID: EAC) (formula: $C_6H_{10}O_3$).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

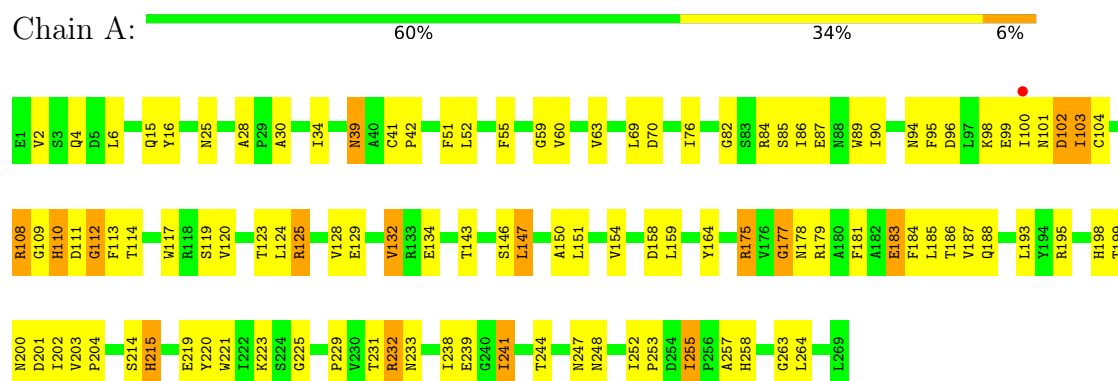
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	67	Total	O	0	0
			67	67		
6	B	96	Total	O	0	0
			96	96		

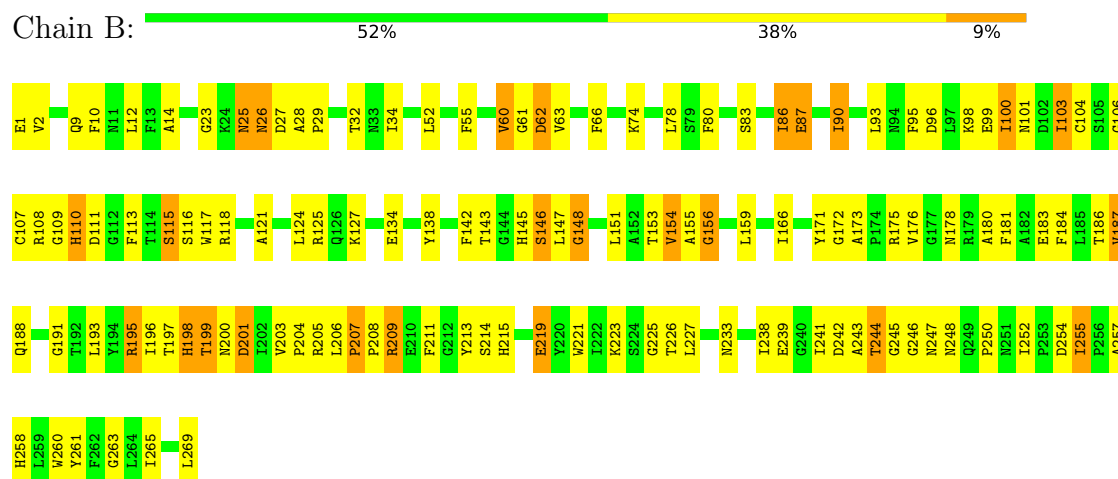
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Lipase



• Molecule 1: Lipase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	140.46Å 140.46Å 80.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.30) 99.5 (50.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.221 , 0.266 0.228 , 0.265	Depositor DCC
R_{free} test set	2011 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.138 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.829 for H, K, L 0.171 for K, H, -L	Depositor
Outliers	0 of 40186 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4379	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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, NAG, EAC, XXH

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	1.33	11/2121 (0.5%)	1.28	13/2887 (0.5%)
1	B	1.32	9/2121 (0.4%)	1.34	24/2887 (0.8%)
All	All	1.32	20/4242 (0.5%)	1.31	37/5774 (0.6%)

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	A	0	2
1	B	0	1
All	All	0	3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	GLU	N-CA	8.31	1.56	1.46
1	B	146	SER	CA-C	6.55	1.59	1.52
1	A	221	TRP	NE1-CE2	-6.31	1.30	1.37
1	B	255	ILE	CA-C	6.12	1.58	1.52
1	A	143	THR	CA-C	-6.03	1.45	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ILE	N-CA-C	8.32	119.12	110.72
1	A	111	ASP	N-CA-C	7.30	118.88	111.07
1	B	10	PHE	N-CA-C	7.04	118.60	111.07
1	B	86	ILE	N-CA-C	6.63	116.76	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	ALA	N-CA-C	-6.60	104.09	111.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	ARG	Sidechain
1	A	232	ARG	Sidechain
1	B	244	THR	Peptide

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	2071	0	1964	92	0
1	B	2071	0	1964	156	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	11	0	5	11	0
3	B	11	0	5	1	0
4	A	9	0	10	4	0
4	B	9	0	10	2	0
5	B	6	0	8	2	0
6	A	67	0	0	2	0
6	B	96	0	0	5	0
All	All	4379	0	3992	249	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 30.

The worst 5 of 249 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:B:86:ILE:HG22	1:B:90:ILE:CD1	1.77	1.14
1:B:86:ILE:HG22	1:B:90:ILE:HD11	1.14	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:303:EAC:H6	4:A:303:EAC:O6	1.51	1.08
1:A:264:LEU:N	3:A:302:XXH:H2	1.67	1.07
1:B:86:ILE:CG2	1:B:90:ILE:HD11	1.84	1.06

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	267/269 (99%)	249 (93%)	18 (7%)	0	100	100
1	B	267/269 (99%)	238 (89%)	22 (8%)	7 (3%)	4	3
All	All	534/538 (99%)	487 (91%)	40 (8%)	7 (1%)	9	10

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	201	ASP
1	B	62	ASP
1	B	209	ARG
1	B	110	HIS
1	B	156	GLY

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	220/220 (100%)	206 (94%)	14 (6%)	16	23
1	B	220/220 (100%)	214 (97%)	6 (3%)	39	58
All	All	440/440 (100%)	420 (96%)	20 (4%)	24	37

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	25	ASN
1	B	134	GLU
1	B	195	ARG
1	B	181	PHE
1	A	134	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	215	HIS
1	B	248	ASN
1	A	248	ASN
1	B	25	ASN
1	B	26	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	$\# Z > 2$
5	GOL	B	304	-	5,5,5	0.89	0	5,5,5	1.17	0
3	XXH	B	302	-	11,11,11	1.02	0	12,14,14	1.23	2 (16%)
3	XXH	A	302	-	11,11,11	1.48	3 (27%)	12,14,14	2.68	8 (66%)
4	EAC	B	303	-	8,8,8	1.60	1 (12%)	9,9,9	1.38	1 (11%)
2	NAG	A	301	1	14,14,15	0.76	0	17,19,21	1.53	4 (23%)
4	EAC	A	303	-	8,8,8	1.50	1 (12%)	9,9,9	1.46	2 (22%)
2	NAG	B	301	1	14,14,15	0.76	0	17,19,21	1.53	4 (23%)

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
5	GOL	B	304	-	-	2/4/4/4	-
3	XXH	B	302	-	-	0/4/6/6	0/1/1/1
3	XXH	A	302	-	-	4/4/6/6	0/1/1/1
4	EAC	B	303	-	-	5/7/7/7	-
2	NAG	A	301	1	-	2/6/23/26	0/1/1/1
4	EAC	A	303	-	-	5/7/7/7	-
2	NAG	B	301	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	303	EAC	O5-C10	4.27	1.45	1.33
4	A	303	EAC	O5-C10	3.96	1.44	1.33
3	A	302	XXH	C1-N1	-3.30	1.37	1.45
3	A	302	XXH	C3-C4	-2.16	1.35	1.39
3	A	302	XXH	O2-N1	-2.10	1.21	1.35

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	XXH	C2-C1-N1	-5.13	114.86	119.34
3	A	302	XXH	C7-C1-N1	4.62	123.37	119.34
2	A	301	NAG	C2-N2-C7	-3.35	118.41	122.90
2	B	301	NAG	C2-N2-C7	-3.35	118.41	122.90
3	A	302	XXH	C3-C4-C5	-3.19	112.05	120.33

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	XXH	C7-C1-N1-O1
3	A	302	XXH	C2-C1-N1-O1
4	A	303	EAC	C13-C14-C15-C10
4	A	303	EAC	O8-C14-C15-C10
4	B	303	EAC	C13-C14-C15-C10

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	304	GOL	2	0
3	B	302	XXH	1	0
3	A	302	XXH	11	0
4	B	303	EAC	2	0
4	A	303	EAC	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	269/269 (100%)	-0.79	1 (0%) 88 89	24, 48, 93, 126	1 (0%)
1	B	269/269 (100%)	-0.67	0 100 100	25, 54, 92, 124	1 (0%)
All	All	538/538 (100%)	-0.73	1 (0%) 91 91	24, 51, 93, 126	2 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	ILE	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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
4	EAC	B	303	9/9	0.94	0.08	44,47,52,53	9
4	EAC	A	303	9/9	0.96	0.07	46,53,57,59	9
2	NAG	A	301	14/15	0.97	0.06	43,49,57,57	14
2	NAG	B	301	14/15	0.98	0.05	43,49,53,55	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	XXH	B	302	11/11	0.98	0.08	40,43,58,62	11
3	XXH	A	302	11/11	0.99	0.06	42,48,51,51	11
5	GOL	B	304	6/6	0.99	0.09	34,34,36,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.