



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:44 AM UTC

PDB ID : 3HFH / pdb_00003hfh
Title : Crystal structure of tandem FF domains
Authors : Lu, M.; Yang, J.; Ren, Z.; Subir, S.; Bedford, M.T.; Jacobson, R.H.; McMurray, J.S.; Chen, X.
Deposited on : 2009-05-11
Resolution : 2.70 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

<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

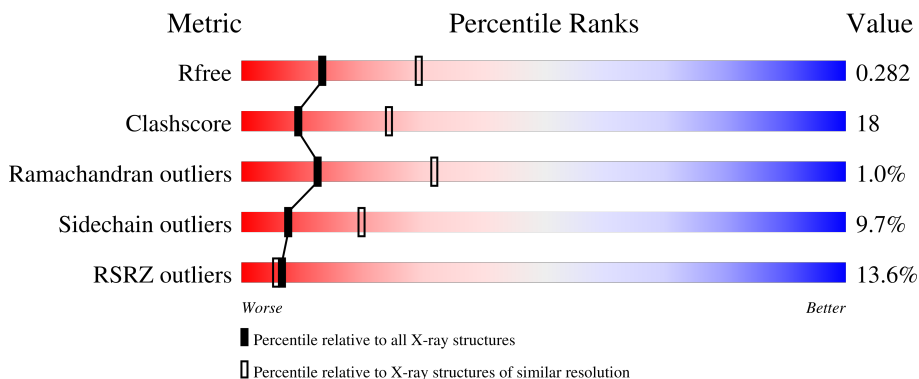
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	190	15% 46% 33% 10% 12%
1	B	190	6% 56% 33% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3178 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 Transcription elongation regulator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	Se	0	0	0
			1475	951	255	262	7			
1	B	190	Total	C	N	O	Se	0	0	0
			1648	1061	285	295	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	656	GLY	-	expression tag	UNP O14776
A	657	PRO	-	expression tag	UNP O14776
A	658	LEU	-	expression tag	UNP O14776
A	659	GLY	-	expression tag	UNP O14776
A	660	SER	-	expression tag	UNP O14776
B	656	GLY	-	expression tag	UNP O14776
B	657	PRO	-	expression tag	UNP O14776
B	658	LEU	-	expression tag	UNP O14776
B	659	GLY	-	expression tag	UNP O14776
B	660	SER	-	expression tag	UNP O14776

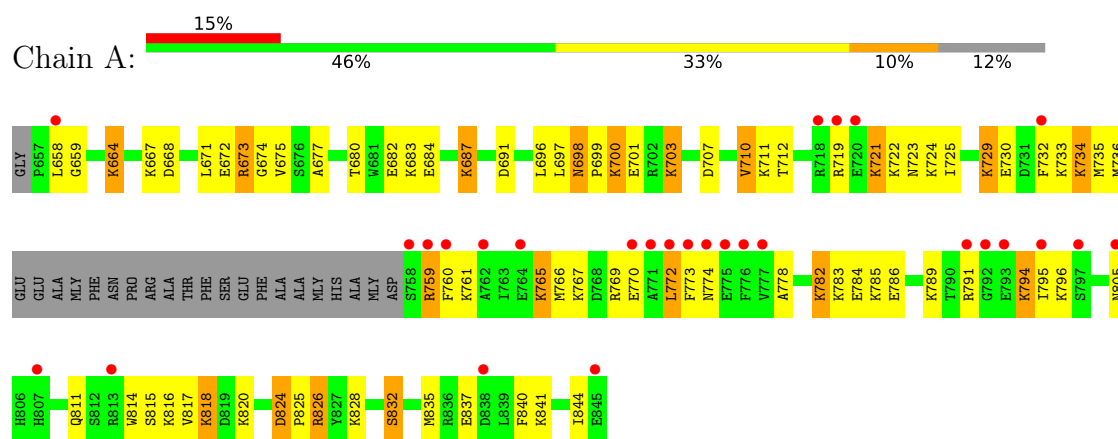
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	O	0	0
			15	15		
2	B	40	Total	O	0	0
			40	40		

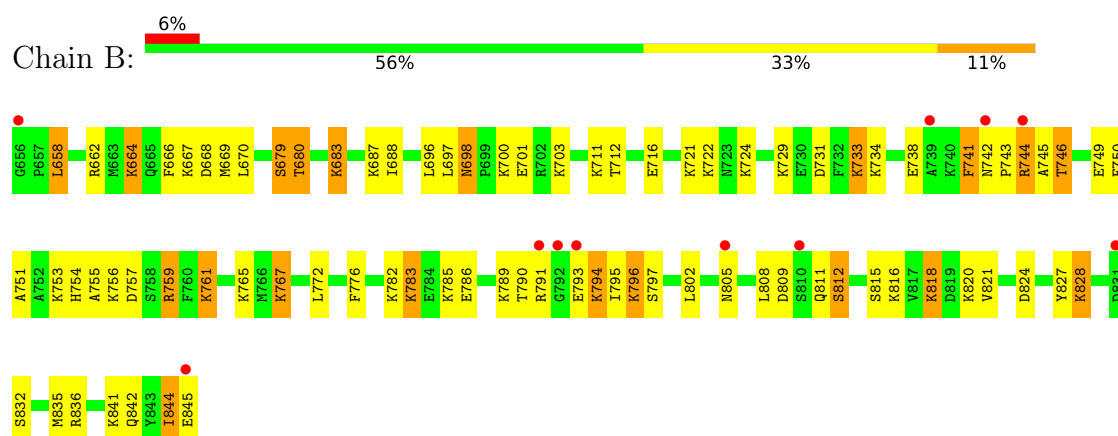
3 Residue-property plots [i](#)

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: Transcription elongation regulator 1



• Molecule 1: Transcription elongation regulator 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α , β , γ	141.30Å 141.30Å 155.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.02 – 2.70 20.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.02-2.70) 92.7 (20.02-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.71Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.230 , 0.283 0.234 , 0.282	Depositor DCC
R_{free} test set	4631 reflections (9.77%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtrriage
Anisotropy	0.354	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3178	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0327e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MLY

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	0.42	0/1195	0.81	3/1595 (0.2%)
1	B	0.50	0/1347	0.81	5/1804 (0.3%)
All	All	0.47	0/2542	0.81	8/3399 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	679	SER	CB-CA-C	-7.72	95.94	112.78
1	A	824	ASP	CA-C-N	7.14	127.14	119.28
1	A	824	ASP	C-N-CA	7.14	127.14	119.28
1	B	679	SER	N-CA-C	-7.01	98.98	108.24
1	B	745	ALA	N-CA-C	6.91	119.23	110.24
1	B	679	SER	CA-C-N	5.27	131.08	122.81
1	B	679	SER	C-N-CA	5.27	131.08	122.81
1	A	805	ASN	N-CA-C	-5.20	106.89	113.18

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	1475	0	1519	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1648	0	1676	53	0
2	A	15	0	0	0	0
2	B	40	0	0	2	0
All	All	3178	0	3195	114	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 18.

All (114) 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:A:826:ARG:HG3	1:A:826:ARG:HH11	1.13	1.12
1:B:679:SER:O	2:B:9:HOH:O	1.77	1.02
1:A:765:MLY:HG2	1:A:766:MSE:H	1.38	0.87
1:A:826:ARG:HH11	1:A:826:ARG:CG	1.88	0.86
1:A:826:ARG:HG3	1:A:826:ARG:NH1	1.92	0.84
1:A:698:ASN:HD21	1:A:701:GLU:HG3	1.43	0.83
1:B:746:THR:HG22	1:B:749:GLU:H	1.45	0.82
1:B:698:ASN:C	1:B:698:ASN:HD22	1.89	0.80
1:A:680:THR:HG22	1:A:682:GLU:H	1.55	0.72
1:A:736:MSE:HE1	1:A:773:PHE:CE1	2.25	0.71
1:B:680:THR:HG22	1:B:683:MLY:H	1.56	0.71
1:B:664:MLY:HH22	1:B:668:ASP:OD2	1.90	0.70
1:B:698:ASN:ND2	1:B:701:GLU:H	1.90	0.69
1:B:786:GLU:O	1:B:790:THR:HG23	1.94	0.68
1:A:832:SER:OG	1:A:835:MSE:HB3	1.94	0.67
1:A:784:GLU:C	1:A:786:GLU:H	2.02	0.67
1:A:703:MLY:HE3	1:A:707:ASP:OD1	1.96	0.66
1:A:674:GLY:O	1:A:687:MLY:HH23	1.97	0.65
1:A:698:ASN:ND2	1:A:701:GLU:H	1.96	0.64
1:B:733:MLY:HB3	1:B:776:PHE:CZ	2.35	0.62
1:A:698:ASN:C	1:A:698:ASN:HD22	2.08	0.61
1:B:751:ALA:O	1:B:755:ALA:HB2	2.01	0.61
1:A:698:ASN:ND2	1:A:701:GLU:HG3	2.13	0.61
1:A:734:MLY:C	1:A:736:MSE:H	2.13	0.61
1:A:658:LEU:H	1:A:658:LEU:HD23	1.65	0.61
1:B:741:PHE:CE1	1:B:743:PRO:HG3	2.36	0.60
1:A:765:MLY:HG2	1:A:766:MSE:N	2.12	0.60
1:B:757:ASP:OD1	1:B:759:ARG:HD3	2.02	0.59
1:A:736:MSE:HE1	1:A:773:PHE:CD1	2.39	0.58
1:B:743:PRO:HD2	1:B:744:ARG:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:802:LEU:HD21	1:B:821:VAL:HB	1.87	0.56
1:A:730:GLU:O	1:A:734:MLY:HB3	2.07	0.55
1:A:784:GLU:C	1:A:786:GLU:N	2.64	0.55
1:B:698:ASN:HD21	1:B:701:GLU:HG3	1.70	0.55
1:B:742:ASN:OD1	1:B:744:ARG:HB2	2.07	0.54
1:B:696:LEU:O	1:B:697:LEU:HD23	2.08	0.54
1:A:826:ARG:CG	1:A:826:ARG:NH1	2.61	0.53
1:B:658:LEU:CD2	1:B:658:LEU:H	2.22	0.52
1:A:673:ARG:NH1	1:A:691:ASP:OD1	2.43	0.52
1:A:760:PHE:CE2	1:A:769:ARG:HD3	2.46	0.51
1:A:668:ASP:O	1:A:672:GLU:HG3	2.11	0.50
1:B:793:GLU:O	1:B:797:SER:HB2	2.10	0.50
1:A:794:MLY:CG	1:A:794:MLY:HH22	2.43	0.49
1:B:750:PHE:CE1	1:B:754:HIS:CD2	3.01	0.49
1:B:698:ASN:C	1:B:698:ASN:ND2	2.62	0.49
1:B:791:ARG:O	1:B:795:ILE:HG12	2.12	0.48
1:B:790:THR:O	1:B:794:MLY:HB3	2.14	0.48
1:B:698:ASN:HD21	1:B:701:GLU:H	1.60	0.48
1:B:832:SER:O	1:B:836:ARG:HG3	2.13	0.48
1:B:662:ARG:HD2	1:B:696:LEU:O	2.14	0.48
1:A:719:ARG:NH1	1:A:723:ASN:HD21	2.12	0.48
1:A:734:MLY:C	1:A:736:MSE:N	2.77	0.48
1:A:732:PHE:HE2	1:A:772:LEU:HB3	1.78	0.47
1:B:697:LEU:HB3	1:B:701:GLU:HB2	1.96	0.47
1:B:742:ASN:OD1	1:B:744:ARG:HD3	2.15	0.47
1:A:680:THR:HG22	1:A:682:GLU:N	2.27	0.46
1:B:809:ASP:O	1:B:844:ILE:HG13	2.14	0.46
1:A:700:MLY:HH22	1:A:700:MLY:HD2	1.70	0.46
1:A:696:LEU:C	1:A:697:LEU:HD23	2.40	0.46
1:A:721:MLY:O	1:A:725:ILE:HD13	2.16	0.46
1:B:844:ILE:O	1:B:845:GLU:CB	2.63	0.46
1:B:731:ASP:HB3	1:B:759:ARG:HG2	1.98	0.45
1:B:805:ASN:ND2	2:B:49:HOH:O	2.48	0.45
1:A:658:LEU:H	1:A:658:LEU:CD2	2.29	0.45
1:A:735:MSE:HG3	1:A:759:ARG:HH12	1.82	0.45
1:B:796:MLY:HD2	1:B:796:MLY:HH22	1.68	0.45
1:A:824:ASP:OD2	1:A:826:ARG:NH1	2.50	0.45
1:B:761:MLY:HH22	1:B:761:MLY:HD2	1.72	0.45
1:A:824:ASP:CG	1:A:826:ARG:HH12	2.24	0.45
1:A:840:PHE:O	1:A:844:ILE:HG12	2.16	0.45
1:B:712:THR:O	1:B:716:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:767:MLY:HH22	1:B:767:MLY:HD2	1.86	0.45
1:B:783:MLY:O	1:B:783:MLY:HG2	2.12	0.44
1:B:818:MLY:HH22	1:B:818:MLY:HD2	1.69	0.44
1:B:827:TYR:C	1:B:827:TYR:CD1	2.95	0.44
1:B:696:LEU:C	1:B:697:LEU:HD23	2.41	0.44
1:A:735:MSE:O	1:A:735:MSE:HG2	2.18	0.44
1:A:765:MLY:CG	1:A:766:MSE:H	2.18	0.43
1:B:783:MLY:HH23	1:B:783:MLY:HD3	1.78	0.43
1:A:729:MLY:HH23	1:A:729:MLY:HD2	1.83	0.43
1:A:698:ASN:HD22	1:A:701:GLU:H	1.65	0.43
1:A:814:TRP:CD1	1:A:837:GLU:HG3	2.53	0.43
1:B:742:ASN:O	1:B:743:PRO:C	2.61	0.43
1:A:677:ALA:HA	1:A:710:VAL:HG22	2.01	0.43
1:A:844:ILE:O	1:A:844:ILE:HG22	2.18	0.43
1:B:828:MLY:HH23	1:B:828:MLY:HD3	1.90	0.43
1:A:824:ASP:HA	1:A:825:PRO:HD3	1.77	0.43
1:B:808:LEU:HB3	1:B:844:ILE:HD11	2.00	0.42
1:A:817:VAL:O	1:A:818:MLY:C	2.67	0.42
1:A:774:ASN:O	1:A:778:ALA:HB3	2.19	0.42
1:B:669:MSE:HG3	1:B:670:LEU:N	2.34	0.42
1:A:697:LEU:HB3	1:A:701:GLU:HB2	2.02	0.42
1:A:732:PHE:CE2	1:A:772:LEU:HB3	2.54	0.42
1:A:766:MSE:SE	1:A:769:ARG:HH11	2.52	0.42
1:B:738:GLU:CD	1:B:759:ARG:HH22	2.27	0.42
1:B:683:MLY:HH22	1:B:683:MLY:HD2	1.84	0.42
1:A:765:MLY:CG	1:A:766:MSE:N	2.82	0.41
1:B:698:ASN:ND2	1:B:701:GLU:HG3	2.35	0.41
1:A:675:VAL:HG13	1:A:684:GLU:HB3	2.02	0.41
1:A:818:MLY:HH23	1:A:818:MLY:HD3	1.75	0.41
1:B:845:GLU:O	1:B:845:GLU:HG2	2.20	0.41
1:A:698:ASN:HB2	1:A:699:PRO:HD2	2.02	0.41
1:A:735:MSE:HG3	1:A:759:ARG:NH1	2.35	0.41
1:A:765:MLY:HE2	1:A:765:MLY:HB3	1.61	0.41
1:A:791:ARG:O	1:A:794:MLY:HB2	2.21	0.41
1:B:796:MLY:HH13	1:B:842:GLN:OE1	2.21	0.41
1:A:658:LEU:HD21	1:A:664:MLY:HG3	2.03	0.41
1:B:741:PHE:C	1:B:741:PHE:CD2	2.99	0.41
1:A:782:MLY:O	1:A:782:MLY:HG2	2.21	0.41
1:B:666:PHE:CE1	1:B:669:MSE:HE2	2.56	0.41
1:B:688:ILE:HD13	1:B:688:ILE:HG21	1.88	0.41
1:B:746:THR:HG22	1:B:749:GLU:N	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:ILE:HD12	1:A:844:ILE:HG23	1.89	0.41
1:A:698:ASN:ND2	1:A:698:ASN:C	2.78	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	137/190 (72%)	127 (93%)	9 (7%)	1 (1%)	18	41
1	B	158/190 (83%)	147 (93%)	9 (6%)	2 (1%)	9	25
All	All	295/380 (78%)	274 (93%)	18 (6%)	3 (1%)	12	32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	741	PHE
1	B	812	SER
1	A	659	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	128/134 (96%)	115 (90%)	13 (10%)	7	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	141/134 (105%)	128 (91%)	13 (9%)	8	22
All	All	269/268 (100%)	243 (90%)	26 (10%)	8	20

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	671	LEU
1	A	673	ARG
1	A	698	ASN
1	A	710	VAL
1	A	712	THR
1	A	759	ARG
1	A	770	GLU
1	A	772	LEU
1	A	795	ILE
1	A	811	GLN
1	A	815	SER
1	A	826	ARG
1	A	832	SER
1	B	658	LEU
1	B	680	THR
1	B	698	ASN
1	B	744	ARG
1	B	746	THR
1	B	759	ARG
1	B	772	LEU
1	B	811	GLN
1	B	812	SER
1	B	815	SER
1	B	824	ASP
1	B	835	MSE
1	B	844	ILE

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

Mol	Chain	Res	Type
1	A	698	ASN
1	A	708	GLN
1	A	723	ASN
1	A	727	GLN
1	A	805	ASN

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Mol	Chain	Res	Type
1	B	686	HIS
1	B	698	ASN
1	B	704	GLN
1	B	708	GLN
1	B	754	HIS
1	B	805	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

57 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	MLY	B	733	1	9,10,11	0.43	0	6,11,13	2.48	4 (66%)
1	MLY	B	783	1	9,10,11	0.39	0	6,11,13	2.37	4 (66%)
1	MLY	B	761	1	9,10,11	0.35	0	6,11,13	2.40	4 (66%)
1	MLY	A	729	1	9,10,11	0.37	0	6,11,13	2.26	4 (66%)
1	MLY	B	703	1	9,10,11	0.44	0	6,11,13	2.39	4 (66%)
1	MLY	A	733	1	9,10,11	0.38	0	6,11,13	2.26	4 (66%)
1	MLY	B	756	1	9,10,11	0.54	0	6,11,13	2.15	3 (50%)
1	MLY	B	789	1	9,10,11	0.38	0	6,11,13	2.33	4 (66%)
1	MLY	A	761	1	9,10,11	0.43	0	6,11,13	2.46	4 (66%)
1	MLY	B	683	1	9,10,11	0.40	0	6,11,13	2.87	3 (50%)
1	MLY	B	740	1	3,4,11	0.83	0	2,4,13	1.07	0
1	MLY	A	711	1	9,10,11	0.41	0	6,11,13	2.52	4 (66%)
1	MLY	B	841	1	9,10,11	0.34	0	6,11,13	2.29	3 (50%)
1	MLY	A	794	1	9,10,11	0.47	0	6,11,13	2.14	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	B	828	1	9,10,11	0.37	0	6,11,13	2.46	4 (66%)
1	MLY	B	711	1	9,10,11	0.48	0	6,11,13	2.45	4 (66%)
1	MLY	A	785	1	9,10,11	0.45	0	6,11,13	2.24	4 (66%)
1	MLY	B	724	1	9,10,11	0.42	0	6,11,13	2.56	4 (66%)
1	MLY	B	722	1	9,10,11	0.45	0	6,11,13	2.37	4 (66%)
1	MLY	B	767	1	9,10,11	0.41	0	6,11,13	2.49	4 (66%)
1	MLY	A	721	1	9,10,11	0.44	0	6,11,13	2.51	4 (66%)
1	MLY	B	667	1	9,10,11	0.63	0	6,11,13	2.77	5 (83%)
1	MLY	B	729	1	9,10,11	0.39	0	6,11,13	2.25	4 (66%)
1	MLY	B	753	1	9,10,11	0.42	0	6,11,13	2.33	4 (66%)
1	MLY	B	818	1	9,10,11	0.44	0	6,11,13	2.46	4 (66%)
1	MLY	A	687	1	9,10,11	0.48	0	6,11,13	2.58	4 (66%)
1	MLY	A	841	1	9,10,11	0.34	0	6,11,13	2.43	4 (66%)
1	MLY	B	664	1	9,10,11	0.56	0	6,11,13	2.48	3 (50%)
1	MLY	A	722	1	9,10,11	0.46	0	6,11,13	2.36	4 (66%)
1	MLY	A	765	1	9,10,11	0.42	0	6,11,13	2.55	4 (66%)
1	MLY	A	683	1	9,10,11	0.46	0	6,11,13	2.69	3 (50%)
1	MLY	A	816	1	9,10,11	0.58	0	6,11,13	2.25	4 (66%)
1	MLY	A	820	1	9,10,11	0.40	0	6,11,13	2.60	3 (50%)
1	MLY	A	782	1	9,10,11	0.47	0	6,11,13	2.42	4 (66%)
1	MLY	B	765	1	9,10,11	0.59	0	6,11,13	2.25	4 (66%)
1	MLY	B	785	1	9,10,11	0.42	0	6,11,13	2.40	4 (66%)
1	MLY	B	796	1	9,10,11	0.41	0	6,11,13	2.37	4 (66%)
1	MLY	B	700	1	9,10,11	0.45	0	6,11,13	2.43	4 (66%)
1	MLY	A	828	1	9,10,11	0.42	0	6,11,13	2.36	4 (66%)
1	MLY	A	703	1	9,10,11	0.40	0	6,11,13	2.32	4 (66%)
1	MLY	A	724	1	9,10,11	0.41	0	6,11,13	2.47	4 (66%)
1	MLY	A	789	1	9,10,11	0.45	0	6,11,13	2.34	4 (66%)
1	MLY	A	796	1	9,10,11	0.46	0	6,11,13	2.19	3 (50%)
1	MLY	B	721	1	9,10,11	0.50	0	6,11,13	2.45	4 (66%)
1	MLY	A	700	1	9,10,11	0.47	0	6,11,13	2.36	4 (66%)
1	MLY	B	782	1	9,10,11	0.45	0	6,11,13	2.45	4 (66%)
1	MLY	B	687	1	9,10,11	0.55	0	6,11,13	2.60	4 (66%)
1	MLY	B	816	1	9,10,11	0.39	0	6,11,13	2.53	4 (66%)
1	MLY	A	767	1	9,10,11	0.41	0	6,11,13	2.46	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	B	794	1	9,10,11	0.45	0	6,11,13	2.60	3 (50%)
1	MLY	A	664	1	9,10,11	0.39	0	6,11,13	2.46	4 (66%)
1	MLY	B	734	1	9,10,11	0.41	0	6,11,13	2.51	4 (66%)
1	MLY	A	734	1	9,10,11	0.46	0	6,11,13	2.35	4 (66%)
1	MLY	A	667	1	9,10,11	0.52	0	6,11,13	2.43	4 (66%)
1	MLY	A	818	1	9,10,11	0.39	0	6,11,13	2.49	4 (66%)
1	MLY	A	783	1	9,10,11	0.41	0	6,11,13	2.57	4 (66%)
1	MLY	B	820	1	9,10,11	0.37	0	6,11,13	2.41	4 (66%)

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
1	MLY	B	733	1	-	4/8/9/11	-
1	MLY	B	783	1	-	5/8/9/11	-
1	MLY	B	761	1	-	4/8/9/11	-
1	MLY	A	729	1	-	3/8/9/11	-
1	MLY	B	703	1	-	4/8/9/11	-
1	MLY	A	733	1	-	5/8/9/11	-
1	MLY	B	756	1	-	1/8/9/11	-
1	MLY	B	789	1	-	3/8/9/11	-
1	MLY	A	761	1	-	2/8/9/11	-
1	MLY	B	683	1	-	4/8/9/11	-
1	MLY	B	740	1	-	0/1/2/11	-
1	MLY	A	711	1	-	5/8/9/11	-
1	MLY	B	841	1	-	2/8/9/11	-
1	MLY	A	794	1	-	2/8/9/11	-
1	MLY	B	828	1	-	1/8/9/11	-
1	MLY	B	711	1	-	1/8/9/11	-
1	MLY	A	785	1	-	3/8/9/11	-
1	MLY	B	724	1	-	1/8/9/11	-
1	MLY	B	722	1	-	1/8/9/11	-
1	MLY	B	767	1	-	3/8/9/11	-
1	MLY	A	721	1	-	5/8/9/11	-
1	MLY	B	667	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	729	1	-	4/8/9/11	-
1	MLY	B	753	1	-	2/8/9/11	-
1	MLY	B	818	1	-	3/8/9/11	-
1	MLY	A	687	1	-	1/8/9/11	-
1	MLY	A	841	1	-	3/8/9/11	-
1	MLY	B	664	1	-	4/8/9/11	-
1	MLY	A	722	1	-	3/8/9/11	-
1	MLY	A	765	1	-	4/8/9/11	-
1	MLY	A	683	1	-	2/8/9/11	-
1	MLY	A	816	1	-	4/8/9/11	-
1	MLY	A	820	1	-	4/8/9/11	-
1	MLY	A	782	1	-	2/8/9/11	-
1	MLY	B	765	1	-	3/8/9/11	-
1	MLY	B	785	1	-	3/8/9/11	-
1	MLY	B	796	1	-	3/8/9/11	-
1	MLY	B	700	1	-	4/8/9/11	-
1	MLY	A	828	1	-	1/8/9/11	-
1	MLY	A	703	1	-	3/8/9/11	-
1	MLY	A	724	1	-	2/8/9/11	-
1	MLY	A	789	1	-	1/8/9/11	-
1	MLY	A	796	1	-	3/8/9/11	-
1	MLY	B	721	1	-	1/8/9/11	-
1	MLY	A	700	1	-	3/8/9/11	-
1	MLY	B	782	1	-	2/8/9/11	-
1	MLY	B	687	1	-	2/8/9/11	-
1	MLY	B	816	1	-	5/8/9/11	-
1	MLY	A	767	1	-	2/8/9/11	-
1	MLY	B	794	1	-	5/8/9/11	-
1	MLY	A	664	1	-	5/8/9/11	-
1	MLY	B	734	1	-	5/8/9/11	-
1	MLY	A	734	1	-	5/8/9/11	-
1	MLY	A	667	1	-	1/8/9/11	-
1	MLY	A	818	1	-	2/8/9/11	-
1	MLY	A	783	1	-	3/8/9/11	-
1	MLY	B	820	1	-	2/8/9/11	-

There are no bond length outliers.

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	683	MLY	CH2-NZ-CH1	4.82	122.08	109.72
1	B	683	MLY	CD-CE-NZ	-4.62	101.76	113.71
1	B	794	MLY	CH2-NZ-CH1	4.29	120.70	109.72
1	B	687	MLY	CH2-NZ-CH1	4.28	120.68	109.72
1	A	820	MLY	CH2-NZ-CH1	4.23	120.56	109.72
1	B	664	MLY	CH2-NZ-CH1	4.22	120.54	109.72
1	B	667	MLY	CH2-NZ-CH1	4.22	120.53	109.72
1	A	687	MLY	CH2-NZ-CH1	4.20	120.49	109.72
1	A	711	MLY	CH2-NZ-CH1	4.19	120.46	109.72
1	A	783	MLY	CH2-NZ-CH1	4.17	120.40	109.72
1	A	818	MLY	CH2-NZ-CH1	4.11	120.24	109.72
1	B	703	MLY	CH2-NZ-CH1	4.11	120.24	109.72
1	A	664	MLY	CH2-NZ-CH1	4.10	120.23	109.72
1	A	761	MLY	CH2-NZ-CH1	4.10	120.23	109.72
1	A	841	MLY	CH2-NZ-CH1	4.09	120.19	109.72
1	B	734	MLY	CH2-NZ-CH1	4.08	120.18	109.72
1	B	828	MLY	CH2-NZ-CH1	4.07	120.16	109.72
1	A	721	MLY	CH2-NZ-CH1	4.07	120.15	109.72
1	B	700	MLY	CH2-NZ-CH1	4.07	120.14	109.72
1	B	818	MLY	CH2-NZ-CH1	4.04	120.08	109.72
1	B	761	MLY	CH2-NZ-CH1	4.03	120.06	109.72
1	A	724	MLY	CH2-NZ-CH1	4.03	120.05	109.72
1	A	765	MLY	CH2-NZ-CH1	4.01	120.01	109.72
1	B	683	MLY	CH2-NZ-CH1	4.01	119.98	109.72
1	B	724	MLY	CH2-NZ-CH1	3.98	119.92	109.72
1	A	703	MLY	CH2-NZ-CH1	3.96	119.87	109.72
1	A	767	MLY	CH2-NZ-CH1	3.96	119.86	109.72
1	B	782	MLY	CH2-NZ-CH1	3.95	119.84	109.72
1	A	789	MLY	CH2-NZ-CH1	3.94	119.83	109.72
1	A	828	MLY	CH2-NZ-CH1	3.92	119.78	109.72
1	B	820	MLY	CH2-NZ-CH1	3.92	119.78	109.72
1	B	733	MLY	CH2-NZ-CH1	3.92	119.77	109.72
1	B	841	MLY	CH2-NZ-CH1	3.92	119.77	109.72
1	A	700	MLY	CH2-NZ-CH1	3.88	119.65	109.72
1	A	816	MLY	CH2-NZ-CH1	3.86	119.62	109.72
1	B	789	MLY	CH2-NZ-CH1	3.84	119.56	109.72
1	A	722	MLY	CH2-NZ-CH1	3.83	119.53	109.72
1	A	782	MLY	CH2-NZ-CH1	3.82	119.51	109.72
1	B	816	MLY	CH2-NZ-CH1	3.82	119.50	109.72
1	B	753	MLY	CH2-NZ-CH1	3.82	119.50	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	722	MLY	CH2-NZ-CH1	3.79	119.43	109.72
1	B	729	MLY	CH2-NZ-CH1	3.79	119.42	109.72
1	B	711	MLY	CH2-NZ-CH1	3.78	119.42	109.72
1	A	733	MLY	CH2-NZ-CH1	3.77	119.39	109.72
1	B	767	MLY	CH2-NZ-CH1	3.77	119.39	109.72
1	A	734	MLY	CH2-NZ-CH1	3.77	119.39	109.72
1	B	721	MLY	CH2-NZ-CH1	3.77	119.37	109.72
1	B	783	MLY	CH2-NZ-CH1	3.76	119.36	109.72
1	B	785	MLY	CH2-NZ-CH1	3.75	119.34	109.72
1	A	667	MLY	CH2-NZ-CH1	3.74	119.31	109.72
1	B	796	MLY	CH2-NZ-CH1	3.72	119.25	109.72
1	B	667	MLY	CD-CE-NZ	-3.70	104.16	113.71
1	A	794	MLY	CH2-NZ-CH1	3.65	119.08	109.72
1	A	729	MLY	CH2-NZ-CH1	3.63	119.01	109.72
1	A	785	MLY	CH2-NZ-CH1	3.61	118.97	109.72
1	B	756	MLY	CH2-NZ-CH1	3.57	118.87	109.72
1	A	796	MLY	CH2-NZ-CH1	3.55	118.82	109.72
1	B	765	MLY	CH2-NZ-CH1	3.54	118.78	109.72
1	A	820	MLY	CD-CE-NZ	-3.46	104.76	113.71
1	B	816	MLY	CD-CE-NZ	-3.38	104.97	113.71
1	A	765	MLY	CD-CE-NZ	-3.38	104.98	113.71
1	B	724	MLY	CD-CE-NZ	-3.36	105.04	113.71
1	A	687	MLY	CD-CE-NZ	-3.32	105.12	113.71
1	A	783	MLY	CD-CE-NZ	-3.30	105.18	113.71
1	B	794	MLY	CD-CE-NZ	-3.29	105.22	113.71
1	B	687	MLY	CD-CE-NZ	-3.25	105.32	113.71
1	B	767	MLY	CD-CE-NZ	-3.21	105.41	113.71
1	B	721	MLY	CD-CE-NZ	-3.16	105.53	113.71
1	B	733	MLY	CD-CE-NZ	-3.16	105.55	113.71
1	A	711	MLY	CD-CE-NZ	-3.12	105.66	113.71
1	B	734	MLY	CD-CE-NZ	-3.09	105.71	113.71
1	B	711	MLY	CD-CE-NZ	-3.05	105.82	113.71
1	A	724	MLY	CD-CE-NZ	-3.03	105.88	113.71
1	A	667	MLY	CD-CE-NZ	-3.03	105.89	113.71
1	A	721	MLY	CD-CE-NZ	-3.01	105.92	113.71
1	B	818	MLY	CD-CE-NZ	-3.01	105.94	113.71
1	A	767	MLY	CD-CE-NZ	-2.97	106.03	113.71
1	A	782	MLY	CD-CE-NZ	-2.96	106.07	113.71
1	B	828	MLY	CD-CE-NZ	-2.93	106.13	113.71
1	B	782	MLY	CD-CE-NZ	-2.93	106.13	113.71
1	A	683	MLY	CD-CE-NZ	-2.93	106.15	113.71
1	A	818	MLY	CD-CE-NZ	-2.91	106.18	113.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	820	MLY	CD-CE-NZ	-2.87	106.29	113.71
1	B	785	MLY	CD-CE-NZ	-2.86	106.31	113.71
1	B	683	MLY	CH1-NZ-CE	2.85	122.03	110.75
1	A	761	MLY	CD-CE-NZ	-2.84	106.36	113.71
1	B	796	MLY	CD-CE-NZ	-2.83	106.39	113.71
1	B	700	MLY	CD-CE-NZ	-2.83	106.41	113.71
1	A	664	MLY	CD-CE-NZ	-2.82	106.43	113.71
1	B	841	MLY	CH2-NZ-CE	2.73	121.57	110.75
1	A	841	MLY	CD-CE-NZ	-2.72	106.67	113.71
1	B	783	MLY	CD-CE-NZ	-2.72	106.68	113.71
1	A	794	MLY	CH2-NZ-CE	2.71	121.50	110.75
1	A	796	MLY	CH2-NZ-CE	2.70	121.47	110.75
1	A	734	MLY	CD-CE-NZ	-2.68	106.79	113.71
1	A	700	MLY	CD-CE-NZ	-2.67	106.81	113.71
1	B	729	MLY	CH2-NZ-CE	2.67	121.34	110.75
1	B	753	MLY	CH2-NZ-CE	2.67	121.34	110.75
1	A	683	MLY	CH2-NZ-CE	2.66	121.29	110.75
1	B	722	MLY	CD-CE-NZ	-2.66	106.85	113.71
1	A	729	MLY	CH2-NZ-CE	2.65	121.24	110.75
1	B	721	MLY	CH2-NZ-CE	2.64	121.22	110.75
1	A	733	MLY	CH2-NZ-CE	2.63	121.17	110.75
1	B	756	MLY	CH2-NZ-CE	2.61	121.09	110.75
1	A	785	MLY	CH2-NZ-CE	2.59	121.03	110.75
1	A	667	MLY	CH2-NZ-CE	2.59	121.00	110.75
1	A	828	MLY	CH2-NZ-CE	2.59	121.00	110.75
1	B	761	MLY	CD-CE-NZ	-2.58	107.03	113.71
1	B	765	MLY	CH2-NZ-CE	2.58	121.00	110.75
1	B	785	MLY	CH2-NZ-CE	2.58	120.97	110.75
1	A	722	MLY	CH2-NZ-CE	2.58	120.96	110.75
1	B	722	MLY	CH2-NZ-CE	2.57	120.94	110.75
1	A	703	MLY	CH2-NZ-CE	2.57	120.94	110.75
1	B	664	MLY	CD-CE-NZ	-2.56	107.09	113.71
1	B	796	MLY	CH2-NZ-CE	2.56	120.89	110.75
1	B	703	MLY	CD-CE-NZ	-2.55	107.11	113.71
1	A	820	MLY	CH1-NZ-CE	2.55	120.86	110.75
1	A	724	MLY	CH2-NZ-CE	2.55	120.85	110.75
1	B	664	MLY	CH2-NZ-CE	2.54	120.84	110.75
1	B	711	MLY	CH2-NZ-CE	2.54	120.83	110.75
1	A	722	MLY	CD-CE-NZ	-2.54	107.15	113.71
1	A	721	MLY	CH2-NZ-CE	2.53	120.77	110.75
1	A	664	MLY	CH2-NZ-CE	2.52	120.76	110.75
1	A	700	MLY	CH2-NZ-CE	2.51	120.72	110.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	783	MLY	CH2-NZ-CE	2.51	120.72	110.75
1	B	794	MLY	CH2-NZ-CE	2.51	120.71	110.75
1	A	789	MLY	CH2-NZ-CE	2.50	120.67	110.75
1	B	733	MLY	CH2-NZ-CE	2.49	120.64	110.75
1	B	753	MLY	CD-CE-NZ	-2.49	107.28	113.71
1	B	782	MLY	CH2-NZ-CE	2.48	120.60	110.75
1	A	828	MLY	CD-CE-NZ	-2.47	107.32	113.71
1	A	734	MLY	CH2-NZ-CE	2.47	120.56	110.75
1	B	667	MLY	CH2-NZ-CE	2.47	120.56	110.75
1	B	828	MLY	CH2-NZ-CE	2.47	120.54	110.75
1	B	789	MLY	CD-CE-NZ	-2.46	107.34	113.71
1	B	789	MLY	CH2-NZ-CE	2.46	120.50	110.75
1	B	703	MLY	CH2-NZ-CE	2.45	120.46	110.75
1	B	816	MLY	CH1-NZ-CE	2.44	120.44	110.75
1	A	782	MLY	CH2-NZ-CE	2.44	120.44	110.75
1	A	767	MLY	CH2-NZ-CE	2.44	120.43	110.75
1	B	767	MLY	CH1-NZ-CE	2.44	120.42	110.75
1	B	700	MLY	CH2-NZ-CE	2.42	120.36	110.75
1	A	789	MLY	CD-CE-NZ	-2.42	107.45	113.71
1	B	724	MLY	CH2-NZ-CE	2.42	120.35	110.75
1	B	687	MLY	CH1-NZ-CE	2.40	120.28	110.75
1	A	816	MLY	CH1-NZ-CE	2.39	120.25	110.75
1	A	818	MLY	CH2-NZ-CE	2.39	120.22	110.75
1	B	765	MLY	CH1-NZ-CE	2.39	120.21	110.75
1	B	767	MLY	CH2-NZ-CE	2.38	120.19	110.75
1	B	820	MLY	CH2-NZ-CE	2.38	120.19	110.75
1	A	816	MLY	CH2-NZ-CE	2.37	120.13	110.75
1	A	783	MLY	CH2-NZ-CE	2.36	120.12	110.75
1	B	818	MLY	CH2-NZ-CE	2.36	120.11	110.75
1	B	761	MLY	CH2-NZ-CE	2.35	120.08	110.75
1	B	734	MLY	CH2-NZ-CE	2.35	120.06	110.75
1	A	782	MLY	CH1-NZ-CE	2.35	120.06	110.75
1	B	816	MLY	CH2-NZ-CE	2.35	120.05	110.75
1	A	734	MLY	CH1-NZ-CE	2.35	120.05	110.75
1	A	765	MLY	CH2-NZ-CE	2.34	120.05	110.75
1	B	756	MLY	CH1-NZ-CE	2.34	120.04	110.75
1	B	820	MLY	CH1-NZ-CE	2.34	120.03	110.75
1	A	841	MLY	CH2-NZ-CE	2.34	120.03	110.75
1	A	687	MLY	CH1-NZ-CE	2.34	120.02	110.75
1	A	761	MLY	CH1-NZ-CE	2.34	120.01	110.75
1	A	785	MLY	CH1-NZ-CE	2.33	119.99	110.75
1	A	765	MLY	CH1-NZ-CE	2.32	119.95	110.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	789	MLY	CH1-NZ-CE	2.32	119.94	110.75
1	B	783	MLY	CH1-NZ-CE	2.31	119.92	110.75
1	A	711	MLY	CH1-NZ-CE	2.31	119.89	110.75
1	B	796	MLY	CH1-NZ-CE	2.30	119.86	110.75
1	B	761	MLY	CH1-NZ-CE	2.30	119.85	110.75
1	B	818	MLY	CH1-NZ-CE	2.29	119.81	110.75
1	A	841	MLY	CH1-NZ-CE	2.27	119.77	110.75
1	A	761	MLY	CH2-NZ-CE	2.27	119.76	110.75
1	B	734	MLY	CH1-NZ-CE	2.27	119.76	110.75
1	B	711	MLY	CH1-NZ-CE	2.27	119.75	110.75
1	A	729	MLY	CH1-NZ-CE	2.27	119.75	110.75
1	B	724	MLY	CH1-NZ-CE	2.26	119.73	110.75
1	A	767	MLY	CH1-NZ-CE	2.26	119.71	110.75
1	A	796	MLY	CH1-NZ-CE	2.26	119.70	110.75
1	A	667	MLY	CH1-NZ-CE	2.25	119.69	110.75
1	B	785	MLY	CH1-NZ-CE	2.25	119.69	110.75
1	A	711	MLY	CH2-NZ-CE	2.24	119.65	110.75
1	B	722	MLY	CH1-NZ-CE	2.24	119.63	110.75
1	A	700	MLY	CH1-NZ-CE	2.24	119.62	110.75
1	B	733	MLY	CH1-NZ-CE	2.23	119.59	110.75
1	A	785	MLY	CD-CE-NZ	-2.22	107.97	113.71
1	B	782	MLY	CH1-NZ-CE	2.22	119.56	110.75
1	B	765	MLY	CD-CE-NZ	-2.22	107.98	113.71
1	A	818	MLY	CH1-NZ-CE	2.22	119.54	110.75
1	A	722	MLY	CH1-NZ-CE	2.21	119.51	110.75
1	A	789	MLY	CH1-NZ-CE	2.21	119.50	110.75
1	B	700	MLY	CH1-NZ-CE	2.21	119.50	110.75
1	A	687	MLY	CH2-NZ-CE	2.20	119.48	110.75
1	A	783	MLY	CH1-NZ-CE	2.20	119.48	110.75
1	A	733	MLY	CH1-NZ-CE	2.19	119.44	110.75
1	A	703	MLY	CD-CE-NZ	-2.19	108.06	113.71
1	B	721	MLY	CH1-NZ-CE	2.18	119.41	110.75
1	A	794	MLY	CH1-NZ-CE	2.18	119.39	110.75
1	B	828	MLY	CH1-NZ-CE	2.16	119.30	110.75
1	B	703	MLY	CH1-NZ-CE	2.16	119.30	110.75
1	B	729	MLY	CH1-NZ-CE	2.14	119.23	110.75
1	A	828	MLY	CH1-NZ-CE	2.14	119.22	110.75
1	A	729	MLY	CD-CE-NZ	-2.13	108.20	113.71
1	A	703	MLY	CH1-NZ-CE	2.13	119.19	110.75
1	A	733	MLY	CD-CE-NZ	-2.13	108.22	113.71
1	B	753	MLY	CH1-NZ-CE	2.12	119.15	110.75
1	A	724	MLY	CH1-NZ-CE	2.11	119.10	110.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	721	MLY	CH1-NZ-CE	2.10	119.08	110.75
1	B	687	MLY	CH2-NZ-CE	2.09	119.03	110.75
1	A	664	MLY	CH1-NZ-CE	2.08	119.00	110.75
1	B	667	MLY	CD-CG-CB	-2.07	105.80	113.62
1	B	667	MLY	CH1-NZ-CE	2.06	118.91	110.75
1	B	841	MLY	CD-CE-NZ	-2.05	108.41	113.71
1	B	729	MLY	CD-CE-NZ	-2.01	108.51	113.71
1	A	816	MLY	CD-CE-NZ	-2.01	108.51	113.71

There are no chirality outliers.

All (165) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	711	MLY	N-CA-CB-CG
1	A	711	MLY	C-CA-CB-CG
1	A	721	MLY	N-CA-CB-CG
1	A	721	MLY	C-CA-CB-CG
1	A	722	MLY	N-CA-CB-CG
1	A	722	MLY	C-CA-CB-CG
1	A	734	MLY	O-C-CA-CB
1	A	765	MLY	O-C-CA-CB
1	A	783	MLY	O-C-CA-CB
1	A	785	MLY	C-CA-CB-CG
1	A	785	MLY	O-C-CA-CB
1	A	796	MLY	C-CA-CB-CG
1	A	820	MLY	C-CA-CB-CG
1	B	664	MLY	N-CA-CB-CG
1	B	664	MLY	C-CA-CB-CG
1	B	667	MLY	N-CA-CB-CG
1	B	667	MLY	C-CA-CB-CG
1	B	683	MLY	N-CA-CB-CG
1	B	683	MLY	C-CA-CB-CG
1	B	700	MLY	N-CA-CB-CG
1	B	700	MLY	C-CA-CB-CG
1	B	703	MLY	N-CA-CB-CG
1	B	703	MLY	C-CA-CB-CG
1	B	729	MLY	N-CA-CB-CG
1	B	729	MLY	C-CA-CB-CG
1	B	733	MLY	C-CA-CB-CG
1	B	734	MLY	N-CA-CB-CG
1	B	734	MLY	C-CA-CB-CG
1	B	761	MLY	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	B	783	MLY	N-CA-CB-CG
1	B	783	MLY	C-CA-CB-CG
1	B	785	MLY	C-CA-CB-CG
1	B	789	MLY	C-CA-CB-CG
1	B	789	MLY	O-C-CA-CB
1	B	794	MLY	N-CA-CB-CG
1	B	794	MLY	C-CA-CB-CG
1	B	816	MLY	C-CA-CB-CG
1	A	765	MLY	CE-CD-CG-CB
1	A	687	MLY	CD-CE-NZ-CH2
1	A	703	MLY	CD-CE-NZ-CH1
1	A	721	MLY	CD-CE-NZ-CH2
1	A	722	MLY	CD-CE-NZ-CH2
1	A	729	MLY	CD-CE-NZ-CH2
1	A	733	MLY	CD-CE-NZ-CH2
1	A	767	MLY	CD-CE-NZ-CH2
1	A	782	MLY	CD-CE-NZ-CH2
1	A	783	MLY	CD-CE-NZ-CH2
1	A	789	MLY	CD-CE-NZ-CH2
1	A	796	MLY	CD-CE-NZ-CH2
1	A	816	MLY	CD-CE-NZ-CH1
1	A	841	MLY	CD-CE-NZ-CH1
1	B	722	MLY	CD-CE-NZ-CH2
1	B	724	MLY	CD-CE-NZ-CH2
1	B	729	MLY	CD-CE-NZ-CH1
1	B	733	MLY	CD-CE-NZ-CH2
1	B	782	MLY	CD-CE-NZ-CH2
1	B	783	MLY	CD-CE-NZ-CH2
1	B	785	MLY	CD-CE-NZ-CH2
1	A	664	MLY	CD-CE-NZ-CH2
1	A	700	MLY	CD-CE-NZ-CH2
1	A	711	MLY	CD-CE-NZ-CH1
1	A	724	MLY	CD-CE-NZ-CH2
1	A	734	MLY	CD-CE-NZ-CH2
1	A	765	MLY	CD-CE-NZ-CH1
1	A	794	MLY	CD-CE-NZ-CH1
1	A	820	MLY	CD-CE-NZ-CH1
1	A	828	MLY	CD-CE-NZ-CH2
1	B	664	MLY	CD-CE-NZ-CH2
1	B	667	MLY	CD-CE-NZ-CH2
1	B	700	MLY	CD-CE-NZ-CH2
1	B	703	MLY	CD-CE-NZ-CH2

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Mol	Chain	Res	Type	Atoms
1	B	711	MLY	CD-CE-NZ-CH2
1	B	721	MLY	CD-CE-NZ-CH2
1	B	734	MLY	CD-CE-NZ-CH1
1	B	761	MLY	CD-CE-NZ-CH2
1	B	765	MLY	CD-CE-NZ-CH1
1	B	767	MLY	CD-CE-NZ-CH2
1	B	816	MLY	CD-CE-NZ-CH2
1	B	820	MLY	CD-CE-NZ-CH2
1	B	828	MLY	CD-CE-NZ-CH2
1	B	841	MLY	CD-CE-NZ-CH2
1	A	700	MLY	CG-CD-CE-NZ
1	A	733	MLY	CG-CD-CE-NZ
1	B	687	MLY	CG-CD-CE-NZ
1	A	729	MLY	CG-CD-CE-NZ
1	A	667	MLY	CD-CE-NZ-CH2
1	A	683	MLY	CD-CE-NZ-CH2
1	A	818	MLY	CD-CE-NZ-CH2
1	B	683	MLY	CD-CE-NZ-CH2
1	B	753	MLY	CD-CE-NZ-CH2
1	B	756	MLY	CD-CE-NZ-CH2
1	B	789	MLY	CD-CE-NZ-CH2
1	B	796	MLY	CD-CE-NZ-CH2
1	B	818	MLY	CD-CE-NZ-CH2
1	B	796	MLY	CG-CD-CE-NZ
1	B	761	MLY	CG-CD-CE-NZ
1	A	761	MLY	CD-CE-NZ-CH2
1	A	785	MLY	CD-CE-NZ-CH2
1	B	794	MLY	CD-CE-NZ-CH2
1	B	783	MLY	CG-CD-CE-NZ
1	A	711	MLY	CD-CE-NZ-CH2
1	A	820	MLY	CD-CE-NZ-CH2
1	B	687	MLY	CD-CE-NZ-CH1
1	A	765	MLY	CA-CB-CG-CD
1	B	703	MLY	CA-CB-CG-CD
1	A	729	MLY	CE-CD-CG-CB
1	A	721	MLY	CE-CD-CG-CB
1	A	820	MLY	CE-CD-CG-CB
1	B	782	MLY	CA-CB-CG-CD
1	B	767	MLY	CE-CD-CG-CB
1	B	734	MLY	CE-CD-CG-CB
1	B	796	MLY	CE-CD-CG-CB
1	A	703	MLY	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	B	733	MLY	CG-CD-CE-NZ
1	A	700	MLY	CE-CD-CG-CB
1	B	818	MLY	CE-CD-CG-CB
1	A	733	MLY	CE-CD-CG-CB
1	A	734	MLY	CG-CD-CE-NZ
1	A	664	MLY	CG-CD-CE-NZ
1	B	818	MLY	CG-CD-CE-NZ
1	B	765	MLY	CA-CB-CG-CD
1	B	767	MLY	CA-CB-CG-CD
1	B	683	MLY	CA-CB-CG-CD
1	B	667	MLY	CG-CD-CE-NZ
1	A	796	MLY	CG-CD-CE-NZ
1	A	794	MLY	CE-CD-CG-CB
1	A	664	MLY	CA-CB-CG-CD
1	B	816	MLY	CD-CE-NZ-CH1
1	B	733	MLY	CE-CD-CG-CB
1	A	664	MLY	C-CA-CB-CG
1	A	733	MLY	C-CA-CB-CG
1	A	816	MLY	C-CA-CB-CG
1	B	820	MLY	C-CA-CB-CG
1	B	765	MLY	CG-CD-CE-NZ
1	B	794	MLY	CA-CB-CG-CD
1	A	724	MLY	CD-CE-NZ-CH1
1	A	841	MLY	CE-CD-CG-CB
1	A	664	MLY	N-CA-CB-CG
1	A	733	MLY	N-CA-CB-CG
1	A	734	MLY	N-CA-CB-CG
1	A	767	MLY	N-CA-CB-CG
1	A	816	MLY	N-CA-CB-CG
1	B	816	MLY	N-CA-CB-CG
1	A	782	MLY	CG-CD-CE-NZ
1	A	816	MLY	CE-CD-CG-CB
1	B	794	MLY	CG-CD-CE-NZ
1	A	761	MLY	CE-CD-CG-CB
1	B	783	MLY	CA-CB-CG-CD
1	B	753	MLY	CG-CD-CE-NZ
1	A	711	MLY	CE-CD-CG-CB
1	B	664	MLY	CA-CB-CG-CD
1	B	734	MLY	CA-CB-CG-CD
1	A	683	MLY	CD-CE-NZ-CH1
1	B	816	MLY	CA-CB-CG-CD
1	A	721	MLY	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	A	734	MLY	CA-CB-CG-CD
1	B	729	MLY	CD-CE-NZ-CH2
1	B	761	MLY	CE-CD-CG-CB
1	A	783	MLY	CA-CB-CG-CD
1	A	841	MLY	C-CA-CB-CG
1	A	703	MLY	CA-CB-CG-CD
1	B	700	MLY	CE-CD-CG-CB
1	B	785	MLY	N-CA-CB-CG
1	A	818	MLY	CG-CD-CE-NZ
1	B	841	MLY	CE-CD-CG-CB

There are no ring outliers.

21 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	733	MLY	1	0
1	B	783	MLY	2	0
1	B	761	MLY	1	0
1	A	729	MLY	1	0
1	B	683	MLY	2	0
1	A	794	MLY	2	0
1	B	828	MLY	1	0
1	B	767	MLY	1	0
1	A	721	MLY	1	0
1	B	818	MLY	1	0
1	A	687	MLY	1	0
1	B	664	MLY	1	0
1	A	765	MLY	5	0
1	A	782	MLY	1	0
1	B	796	MLY	2	0
1	A	703	MLY	1	0
1	A	700	MLY	1	0
1	B	794	MLY	1	0
1	A	664	MLY	1	0
1	A	734	MLY	3	0
1	A	818	MLY	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	134/190 (70%)	0.88	28 (20%) 2 2	51, 94, 161, 172	0
1	B	153/190 (80%)	0.28	11 (7%) 21 18	44, 71, 123, 144	0
All	All	287/380 (75%)	0.56	39 (13%) 7 6	44, 79, 145, 172	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	773	PHE	5.8
1	B	744	ARG	4.9
1	A	758	SER	4.7
1	B	805	ASN	4.1
1	A	845	GLU	3.8
1	A	732	PHE	3.7
1	A	774	ASN	3.2
1	A	658	LEU	3.1
1	A	772	LEU	3.1
1	B	739	ALA	3.1
1	B	656	GLY	2.9
1	A	771	ALA	2.9
1	A	775	GLU	2.9
1	B	791	ARG	2.9
1	A	838	ASP	2.8
1	A	762	ALA	2.7
1	A	807	HIS	2.7
1	A	720	GLU	2.7
1	A	777	VAL	2.7
1	B	845	GLU	2.6
1	A	760	PHE	2.6
1	A	791	ARG	2.6
1	A	793	GLU	2.6
1	A	795	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	770	GLU	2.4
1	B	831	ASP	2.4
1	A	776	PHE	2.4
1	B	810	SER	2.4
1	B	793	GLU	2.4
1	A	805	ASN	2.3
1	B	792	GLY	2.3
1	A	813	ARG	2.2
1	A	719	ARG	2.2
1	A	718	ARG	2.1
1	A	764	GLU	2.1
1	B	742	ASN	2.0
1	A	792	GLY	2.0
1	A	759	ARG	2.0
1	A	797	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	MLY	A	785	11/12	0.41	0.30	153,163,167,167	0
1	MLY	A	820	11/12	0.45	0.23	113,120,127,129	0
1	MLY	B	816	11/12	0.49	0.30	103,117,148,149	0
1	MLY	A	789	11/12	0.55	0.26	147,154,170,171	0
1	MLY	A	765	11/12	0.56	0.29	123,133,139,139	0
1	MLY	B	756	11/12	0.60	0.26	70,86,102,107	0
1	MLY	A	816	11/12	0.60	0.27	100,113,131,132	0
1	MLY	B	789	11/12	0.61	0.28	113,134,169,169	0
1	MLY	A	782	11/12	0.67	0.24	164,175,190,191	0
1	MLY	B	740	5/12	0.68	0.18	120,134,137,138	0
1	MLY	A	767	11/12	0.70	0.25	114,125,148,148	0
1	MLY	A	734	11/12	0.70	0.30	144,157,170,170	0
1	MLY	A	783	11/12	0.73	0.19	158,166,170,170	0
1	MLY	B	785	11/12	0.73	0.20	103,109,132,133	0
1	MLY	A	711	11/12	0.79	0.20	67,83,120,120	0
1	MLY	A	733	11/12	0.79	0.23	146,157,169,171	0
1	MLY	B	782	11/12	0.80	0.18	93,113,142,143	0
1	MLY	A	683	11/12	0.81	0.17	65,73,85,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MLY	A	722	11/12	0.81	0.18	113,149,155,157	0
1	MLY	A	729	11/12	0.83	0.17	119,126,148,150	0
1	MLY	A	794	11/12	0.83	0.16	105,111,116,116	0
1	MLY	B	783	11/12	0.84	0.16	103,106,131,134	0
1	MLY	B	721	11/12	0.84	0.17	74,86,124,128	0
1	MLY	B	828	11/12	0.84	0.18	91,102,126,128	0
1	MLY	A	761	11/12	0.85	0.18	133,143,155,158	0
1	MLY	A	703	11/12	0.85	0.15	54,75,122,122	0
1	MLY	B	794	11/12	0.85	0.16	86,96,115,115	0
1	MLY	A	796	11/12	0.85	0.18	100,105,120,121	0
1	MLY	B	722	11/12	0.85	0.18	63,82,122,126	0
1	MLY	B	765	11/12	0.86	0.17	64,74,107,107	0
1	MLY	B	729	11/12	0.86	0.14	70,86,125,128	0
1	MLY	B	820	11/12	0.87	0.16	95,106,121,123	0
1	MLY	B	753	11/12	0.87	0.17	69,72,108,109	0
1	MLY	A	818	11/12	0.88	0.27	98,115,159,162	0
1	MLY	A	828	11/12	0.88	0.19	103,119,136,141	0
1	MLY	A	841	11/12	0.88	0.16	69,82,120,121	0
1	MLY	B	711	11/12	0.89	0.13	55,71,115,116	0
1	MLY	A	721	11/12	0.89	0.15	109,116,121,122	0
1	MLY	B	734	11/12	0.89	0.20	84,96,136,138	0
1	MLY	B	767	11/12	0.90	0.16	60,75,102,109	0
1	MLY	B	818	11/12	0.90	0.22	91,98,133,133	0
1	MLY	A	700	11/12	0.90	0.19	56,68,111,111	0
1	MLY	A	724	11/12	0.90	0.16	110,118,122,122	0
1	MLY	B	841	11/12	0.90	0.13	64,84,111,111	0
1	MLY	B	703	11/12	0.91	0.14	55,61,100,103	0
1	MLY	B	724	11/12	0.91	0.17	60,79,105,107	0
1	MLY	B	667	11/12	0.91	0.13	52,64,84,89	0
1	MLY	B	733	11/12	0.91	0.14	72,86,114,117	0
1	MLY	B	700	11/12	0.91	0.14	53,66,98,101	0
1	MLY	B	796	11/12	0.92	0.14	77,82,110,111	0
1	MLY	B	761	11/12	0.92	0.15	64,69,95,100	0
1	MLY	A	667	11/12	0.92	0.14	53,63,100,100	0
1	MLY	B	683	11/12	0.93	0.11	51,54,65,68	0
1	MLY	B	664	11/12	0.95	0.10	52,60,74,75	0
1	MLY	A	664	11/12	0.96	0.09	54,58,78,81	0
1	MLY	A	687	11/12	0.96	0.10	51,58,80,84	0
1	MLY	B	687	11/12	0.97	0.07	47,52,71,73	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.