



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:13 PM UTC

PDB ID : 3LK6 / pdb_00003lk6
Title : Beta-N-hexosaminidase N318D mutant (YBBD_N318D) from bacillus subtilis
Authors : Krug, M.
Deposited on : 2010-01-27
Resolution : 2.88 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

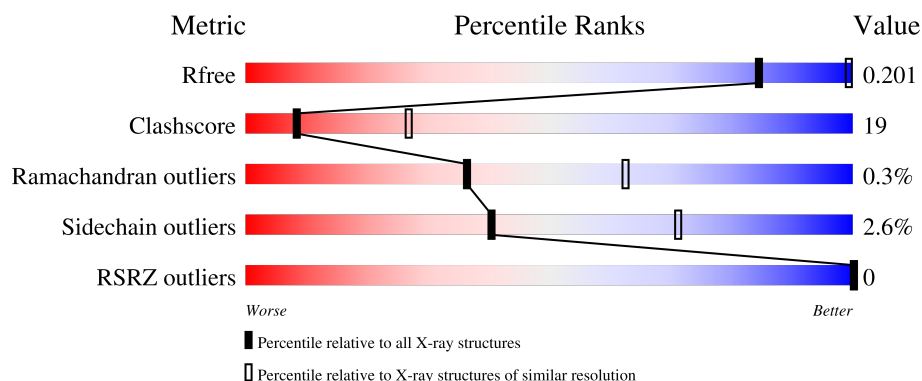
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	616	 65% 33% .
1	B	616	 64% 34% ..
1	C	616	 65% 33% .
1	D	616	 64% 34% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19416 atoms, of which 188 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 Lipoprotein ybbD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	615	Total	C	N	O	S	0	2	0
			4767	3019	829	900	19			
1	B	612	Total	C	N	O	S	0	1	0
			4738	3002	824	893	19			
1	C	616	Total	C	N	O	S	0	0	0
			4758	3013	829	897	19			
1	D	614	Total	C	N	O	S	0	1	0
			4753	3011	827	896	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	318	ASN	ASP	engineered mutation	UNP P40406
B	318	ASN	ASP	engineered mutation	UNP P40406
C	318	ASN	ASP	engineered mutation	UNP P40406
D	318	ASN	ASP	engineered mutation	UNP P40406

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			15	4	8	3		
2	A	1	Total	C	H	O	0	0
			17	4	10	3		
2	A	1	Total	C	H	O	0	0
			17	4	10	3		
2	A	1	Total	C	H	O	0	0
			17	4	10	3		
2	B	1	Total	C	H	O	0	0
			17	4	10	3		
2	B	1	Total	C	H	O	0	0
			17	4	10	3		
2	B	1	Total	C	H	O	0	0
			17	4	10	3		
2	B	1	Total	C	H	O	0	0
			17	4	10	3		
2	B	1	Total	C	H	O	0	0
			17	4	10	3		
2	C	1	Total	C	H	O	0	0
			17	4	10	3		
2	C	1	Total	C	H	O	0	0
			17	4	10	3		
2	C	1	Total	C	H	O	0	0
			17	4	10	3		
2	C	1	Total	C	H	O	0	0
			17	4	10	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	0	0
			17	4	10	3		
2	D	1	Total	C	H	O	0	0
			17	4	10	3		
2	D	1	Total	C	H	O	0	0
			17	4	10	3		
2	D	1	Total	C	H	O	0	0
			17	4	10	3		
2	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

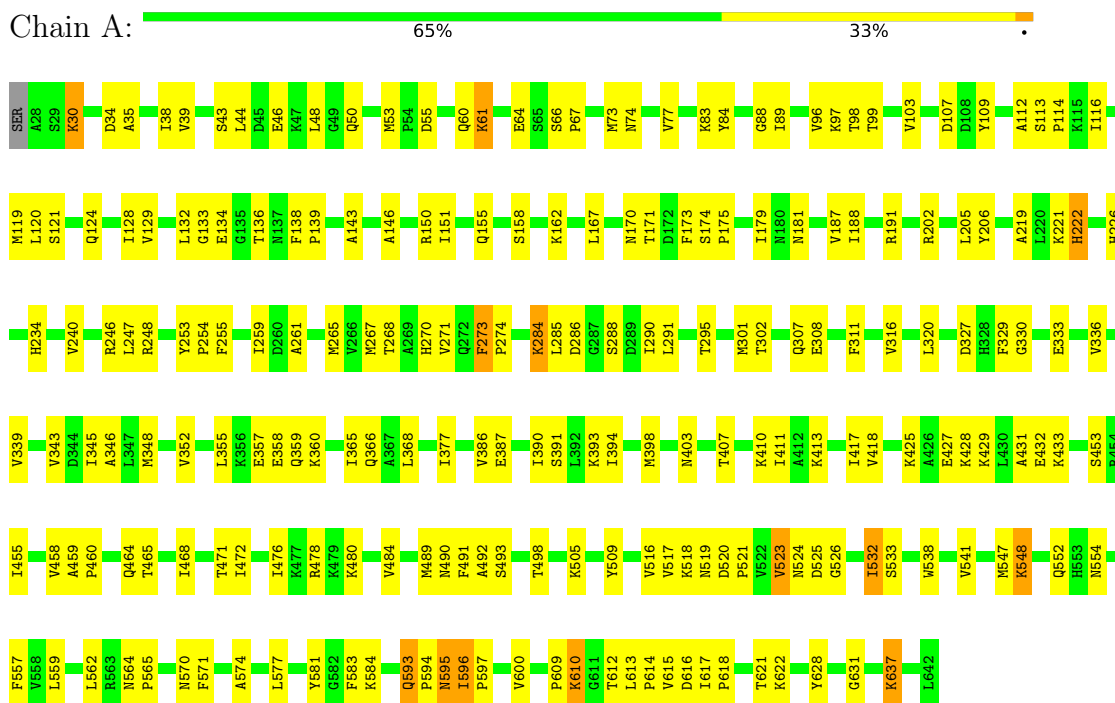
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	23	Total	O	0	0
			23	23		
4	C	19	Total	O	0	0
			19	19		
4	D	15	Total	O	0	0
			15	15		

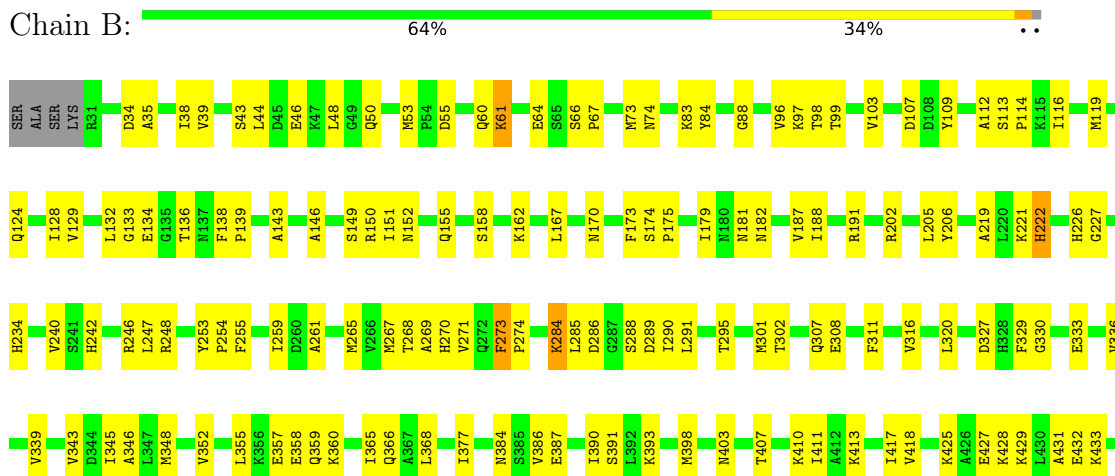
3 Residue-property plots

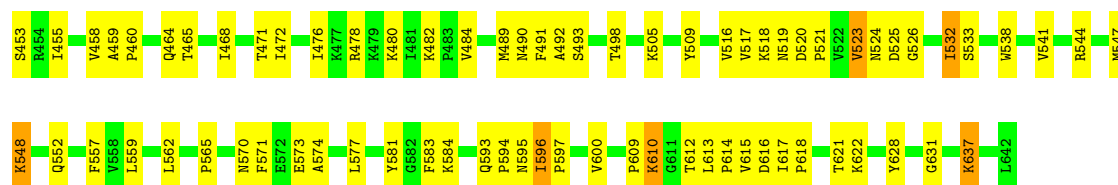
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Lipoprotein ybbD



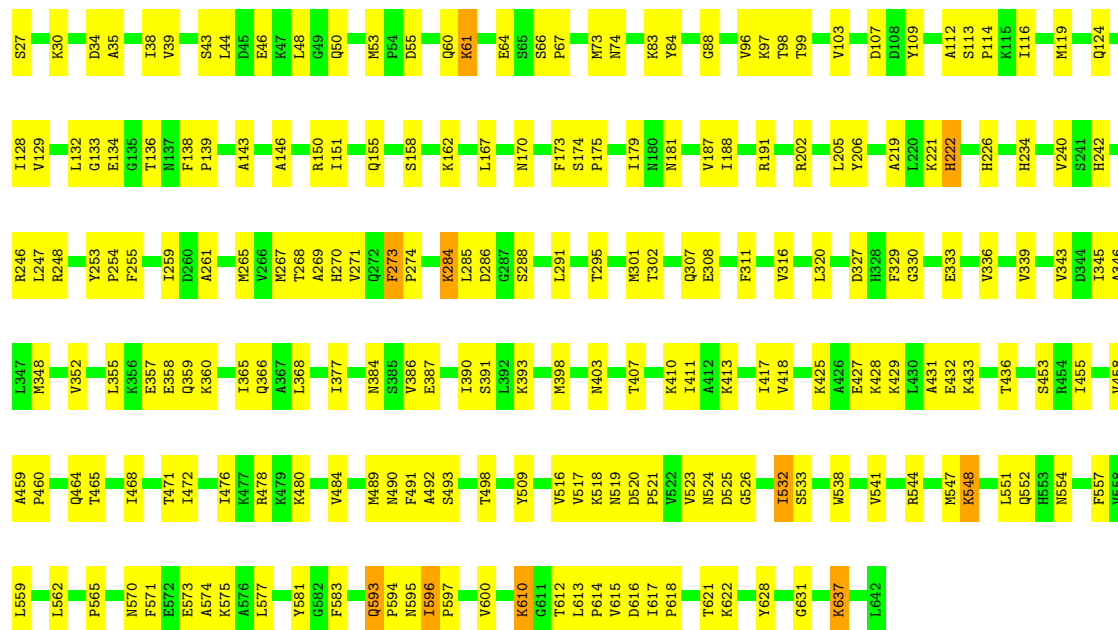
• Molecule 1: Lipoprotein ybbD





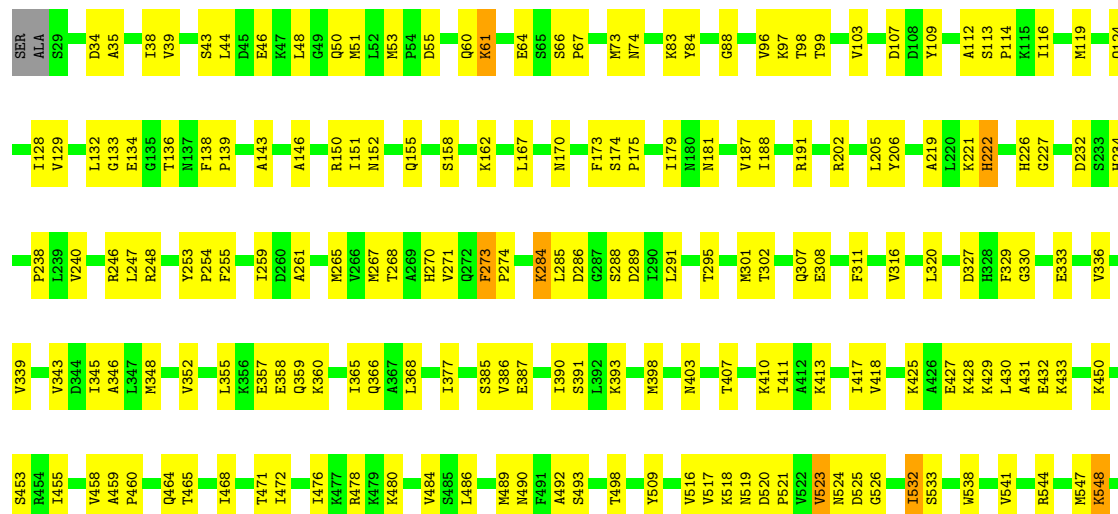
• Molecule 1: Lipoprotein ybbD

Chain C: 65% 33% .



• Molecule 1: Lipoprotein ybbD

Chain D: 64% 34% .



L551	Q552		F557	V558	L559		L562	R563	N564	P565		N570	F571	E572	E573	A574		L577		Y581	G582	F583	K584		Q593	P594	N595	I596	P597		V600		P609	K610	G611	T612	L613	P614	V615	D616	I617	P618		T621		Y628		G631		K637	T638	G639	R640	P641	L642
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.31Å 99.15Å 139.86Å 90.11° 90.05° 89.94°	Depositor
Resolution (Å)	48.99 – 2.88 48.99 – 2.88	Depositor EDS
% Data completeness (in resolution range)	93.9 (48.99-2.88) 93.8 (48.99-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.171 , 0.201 0.171 , 0.201	Depositor DCC
R_{free} test set	3270 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.958	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.418 for h,-k,-l 0.420 for -h,k,-l 0.418 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19416	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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: PEG, NA

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	0.40	0/4854	0.85	9/6553 (0.1%)
1	B	0.41	0/4825	0.85	7/6515 (0.1%)
1	C	0.40	0/4842	0.85	8/6537 (0.1%)
1	D	0.40	0/4840	0.85	5/6534 (0.1%)
All	All	0.40	0/19361	0.85	29/26139 (0.1%)

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	SER	CA-C-N	9.55	131.78	119.84
1	C	113	SER	C-N-CA	9.55	131.78	119.84
1	A	113	SER	CA-C-N	9.51	131.73	119.84
1	A	113	SER	C-N-CA	9.51	131.73	119.84
1	B	113	SER	CA-C-N	9.21	131.35	119.84

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	4767	0	4886	186	0
1	B	4738	0	4858	192	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4758	0	4880	184	0
1	D	4753	0	4876	189	0
2	A	28	38	40	3	0
2	B	42	60	60	10	0
2	C	35	50	50	3	0
2	D	28	40	40	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	18	0	0	1	0
4	B	23	0	0	1	0
4	C	19	0	0	1	0
4	D	15	0	0	2	0
All	All	19228	188	19690	740	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 19.

The worst 5 of 740 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:53:MET:HE1	1:B:119:MET:HE3	1.33	1.11
1:A:53:MET:HE1	1:A:119:MET:HE3	1.33	1.10
1:B:53:MET:CE	1:B:119:MET:HE3	1.83	1.08
1:A:53:MET:CE	1:A:119:MET:HE3	1.84	1.07
1:D:53:MET:HE1	1:D:119:MET:HE3	1.31	1.07

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	615/616 (100%)	575 (94%)	38 (6%)	2 (0%)	36	62
1	B	611/616 (99%)	573 (94%)	36 (6%)	2 (0%)	36	62
1	C	614/616 (100%)	575 (94%)	37 (6%)	2 (0%)	36	62
1	D	613/616 (100%)	573 (94%)	38 (6%)	2 (0%)	36	62
All	All	2453/2464 (100%)	2296 (94%)	149 (6%)	8 (0%)	36	62

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	222	HIS
1	C	61	LYS
1	C	222	HIS
1	D	222	HIS
1	A	61	LYS

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	520/519 (100%)	506 (97%)	14 (3%)	39	70
1	B	517/519 (100%)	504 (98%)	13 (2%)	42	72
1	C	519/519 (100%)	506 (98%)	13 (2%)	42	72
1	D	519/519 (100%)	505 (97%)	14 (3%)	39	70
All	All	2075/2076 (100%)	2021 (97%)	54 (3%)	40	71

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	343	VAL
1	C	548	LYS
1	D	548	LYS
1	C	365	ILE
1	C	516	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	101	GLN
1	C	606	GLN
1	C	374	ASN
1	D	50	GLN
1	B	60	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PEG	D	643	-	6,6,6	0.59	0	5,5,5	0.68	0
2	PEG	B	650	-	6,6,6	0.56	0	5,5,5	0.62	0
2	PEG	A	644	-	6,6,6	0.52	0	5,5,5	0.72	0
2	PEG	D	644	-	6,6,6	0.57	0	5,5,5	0.69	0
2	PEG	A	646	-	6,6,6	0.70	0	5,5,5	0.74	0
2	PEG	D	646	-	6,6,6	0.63	0	5,5,5	0.62	0
2	PEG	A	645	-	6,6,6	0.59	0	5,5,5	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEG	C	646	-	6,6,6	0.60	0	5,5,5	0.56	0
2	PEG	C	645	-	6,6,6	0.53	0	5,5,5	0.71	0
2	PEG	C	643	-	6,6,6	0.64	0	5,5,5	0.85	0
2	PEG	B	649	-	6,6,6	0.63	0	5,5,5	0.77	0
2	PEG	C	647	-	6,6,6	0.62	0	5,5,5	0.81	0
2	PEG	A	643	-	6,6,6	0.66	0	5,5,5	0.79	0
2	PEG	C	644	-	6,6,6	0.66	0	5,5,5	0.68	0
2	PEG	B	648	-	6,6,6	0.62	0	5,5,5	0.61	0
2	PEG	B	643	-	6,6,6	0.61	0	5,5,5	1.05	1 (20%)
2	PEG	B	645	-	6,6,6	0.60	0	5,5,5	0.54	0
2	PEG	B	644	-	6,6,6	0.67	0	5,5,5	0.70	0
2	PEG	D	645	-	6,6,6	0.68	0	5,5,5	0.71	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
2	PEG	D	643	-	-	0/4/4/4	-
2	PEG	B	650	-	-	0/4/4/4	-
2	PEG	A	644	-	-	0/4/4/4	-
2	PEG	D	644	-	-	1/4/4/4	-
2	PEG	A	646	-	-	0/4/4/4	-
2	PEG	D	646	-	-	0/4/4/4	-
2	PEG	A	645	-	-	0/4/4/4	-
2	PEG	C	646	-	-	1/4/4/4	-
2	PEG	C	645	-	-	1/4/4/4	-
2	PEG	C	643	-	-	0/4/4/4	-
2	PEG	B	649	-	-	0/4/4/4	-
2	PEG	C	647	-	-	0/4/4/4	-
2	PEG	A	643	-	-	1/4/4/4	-
2	PEG	C	644	-	-	1/4/4/4	-
2	PEG	B	648	-	-	0/4/4/4	-
2	PEG	B	643	-	-	2/4/4/4	-
2	PEG	B	645	-	-	2/4/4/4	-
2	PEG	B	644	-	-	2/4/4/4	-
2	PEG	D	645	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	643	PEG	C3-O2-C2	2.28	123.23	113.26

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	645	PEG	O1-C1-C2-O2
2	B	643	PEG	O2-C3-C4-O4
2	B	645	PEG	O1-C1-C2-O2
2	A	643	PEG	O2-C3-C4-O4
2	B	643	PEG	C1-C2-O2-C3

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	650	PEG	2	0
2	A	644	PEG	1	0
2	D	644	PEG	3	0
2	A	646	PEG	2	0
2	C	645	PEG	2	0
2	B	649	PEG	1	0
2	C	644	PEG	1	0
2	B	643	PEG	3	0
2	B	645	PEG	2	0
2	B	644	PEG	2	0
2	D	645	PEG	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 [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	615/616 (99%)	-1.65	0 100 100	18, 43, 80, 138	2 (0%)
1	B	612/616 (99%)	-1.66	0 100 100	17, 43, 79, 123	1 (0%)
1	C	616/616 (100%)	-1.64	0 100 100	18, 43, 82, 126	0
1	D	614/616 (99%)	-1.64	0 100 100	18, 43, 80, 123	1 (0%)
All	All	2457/2464 (99%)	-1.65	0 100 100	17, 43, 80, 138	4 (0%)

There are no RSRZ outliers to report.

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
2	PEG	C	647	7/7	0.97	0.07	65,93,112,112	0
3	NA	C	648	1/1	0.98	0.06	69,69,69,69	0
2	PEG	A	645	7/7	0.99	0.05	50,74,98,98	0
2	PEG	A	646	7/7	0.99	0.05	74,100,127,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PEG	B	643	7/7	0.99	0.03	62,74,88,88	0
2	PEG	B	644	7/7	0.99	0.04	61,73,86,86	0
2	PEG	B	645	7/7	0.99	0.07	55,93,115,117	0
2	PEG	B	648	7/7	0.99	0.04	47,72,87,87	0
2	PEG	B	649	7/7	0.99	0.04	76,96,125,125	0
2	PEG	B	650	7/7	0.99	0.03	53,82,99,99	0
2	PEG	A	643	7/7	0.99	0.05	66,78,93,93	0
2	PEG	C	643	7/7	0.99	0.04	72,86,92,94	0
2	PEG	C	644	7/7	0.99	0.04	70,89,107,107	0
2	PEG	C	646	7/7	0.99	0.04	32,67,81,81	0
2	PEG	D	644	7/7	0.99	0.05	53,83,100,100	0
2	PEG	D	645	7/7	0.99	0.05	71,88,97,98	0
3	NA	A	647	1/1	0.99	0.05	63,63,63,63	0
2	PEG	A	644	7/7	0.99	0.04	55,80,96,96	0
3	NA	D	647	1/1	0.99	0.04	71,71,71,71	0
2	PEG	C	645	7/7	1.00	0.03	39,69,89,89	0
3	NA	B	651	1/1	1.00	0.03	51,51,51,51	0
2	PEG	D	643	7/7	1.00	0.03	50,61,73,73	0
2	PEG	D	646	7/7	1.00	0.03	51,62,72,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.