



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2020 – 12:19 PM JST

PDB ID : 6L4Y
Title : Turning an asparaginyl endopeptidase into a peptide ligase
Authors : El Sahili, A.; Lescar, J.
Deposited on : 2019-10-21
Resolution : 1.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

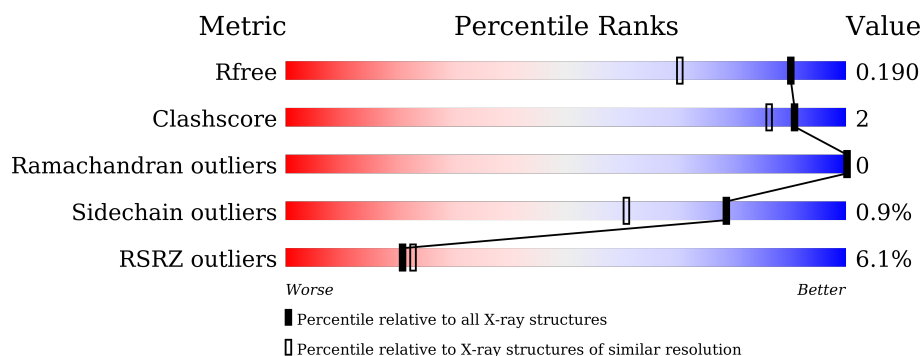
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 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	502	<div> <div>5%</div> <div>77%</div> <div>5%</div> <div>18%</div> </div>
1	B	502	<div> <div>5%</div> <div>79%</div> <div>•</div> <div>18%</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
1	SNN	A	179	-	X	-	-
1	SNN	B	179	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7513 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 Asparaginyl endopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	9	0
			3295	2074	565	631	25			
1	B	413	Total	C	N	O	S	0	6	0
			3284	2068	564	627	25			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A0A0P0QM28
A	-12	VAL	-	expression tag	UNP A0A0P0QM28
A	-11	SER	-	expression tag	UNP A0A0P0QM28
A	-10	ALA	-	expression tag	UNP A0A0P0QM28
A	-9	ILE	-	expression tag	UNP A0A0P0QM28
A	-8	VAL	-	expression tag	UNP A0A0P0QM28
A	-7	LEU	-	expression tag	UNP A0A0P0QM28
A	-6	TYR	-	expression tag	UNP A0A0P0QM28
A	-5	VAL	-	expression tag	UNP A0A0P0QM28
A	-4	LEU	-	expression tag	UNP A0A0P0QM28
A	-3	LEU	-	expression tag	UNP A0A0P0QM28
A	-2	ALA	-	expression tag	UNP A0A0P0QM28
A	-1	ALA	-	expression tag	UNP A0A0P0QM28
A	0	ALA	-	expression tag	UNP A0A0P0QM28
A	1	ALA	-	expression tag	UNP A0A0P0QM28
A	2	HIS	-	expression tag	UNP A0A0P0QM28
A	3	SER	-	expression tag	UNP A0A0P0QM28
A	4	ALA	-	expression tag	UNP A0A0P0QM28
A	5	PHE	-	expression tag	UNP A0A0P0QM28
A	6	ALA	-	expression tag	UNP A0A0P0QM28
A	7	ALA	-	expression tag	UNP A0A0P0QM28
A	8	ALA	-	expression tag	UNP A0A0P0QM28
A	9	MET	-	expression tag	UNP A0A0P0QM28
A	10	GLY	-	expression tag	UNP A0A0P0QM28
A	11	HIS	-	expression tag	UNP A0A0P0QM28

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Chain	Residue	Modelled	Actual	Comment	Reference
A	12	HIS	-	expression tag	UNP A0A0P0QM28
A	13	HIS	-	expression tag	UNP A0A0P0QM28
A	14	HIS	-	expression tag	UNP A0A0P0QM28
A	15	HIS	-	expression tag	UNP A0A0P0QM28
A	16	HIS	-	expression tag	UNP A0A0P0QM28
A	17	SER	-	expression tag	UNP A0A0P0QM28
A	18	SER	-	expression tag	UNP A0A0P0QM28
A	19	GLY	-	expression tag	UNP A0A0P0QM28
A	20	VAL	-	expression tag	UNP A0A0P0QM28
A	21	ASP	-	expression tag	UNP A0A0P0QM28
A	22	LEU	-	expression tag	UNP A0A0P0QM28
A	23	GLY	-	expression tag	UNP A0A0P0QM28
A	24	THR	-	expression tag	UNP A0A0P0QM28
A	25	GLU	-	expression tag	UNP A0A0P0QM28
A	26	ASN	-	expression tag	UNP A0A0P0QM28
A	27	LEU	-	expression tag	UNP A0A0P0QM28
A	28	TYR	-	expression tag	UNP A0A0P0QM28
A	29	PHE	-	expression tag	UNP A0A0P0QM28
A	30	GLN	-	expression tag	UNP A0A0P0QM28
A	31	SER	-	expression tag	UNP A0A0P0QM28
A	32	MET	-	expression tag	UNP A0A0P0QM28
A	74	VAL	GLU	engineered mutation	UNP A0A0P0QM28
A	252	VAL	GLY	engineered mutation	UNP A0A0P0QM28
B	-13	MET	-	expression tag	UNP A0A0P0QM28
B	-12	VAL	-	expression tag	UNP A0A0P0QM28
B	-11	SER	-	expression tag	UNP A0A0P0QM28
B	-10	ALA	-	expression tag	UNP A0A0P0QM28
B	-9	ILE	-	expression tag	UNP A0A0P0QM28
B	-8	VAL	-	expression tag	UNP A0A0P0QM28
B	-7	LEU	-	expression tag	UNP A0A0P0QM28
B	-6	TYR	-	expression tag	UNP A0A0P0QM28
B	-5	VAL	-	expression tag	UNP A0A0P0QM28
B	-4	LEU	-	expression tag	UNP A0A0P0QM28
B	-3	LEU	-	expression tag	UNP A0A0P0QM28
B	-2	ALA	-	expression tag	UNP A0A0P0QM28
B	-1	ALA	-	expression tag	UNP A0A0P0QM28
B	0	ALA	-	expression tag	UNP A0A0P0QM28
B	1	ALA	-	expression tag	UNP A0A0P0QM28
B	2	HIS	-	expression tag	UNP A0A0P0QM28
B	3	SER	-	expression tag	UNP A0A0P0QM28
B	4	ALA	-	expression tag	UNP A0A0P0QM28
B	5	PHE	-	expression tag	UNP A0A0P0QM28

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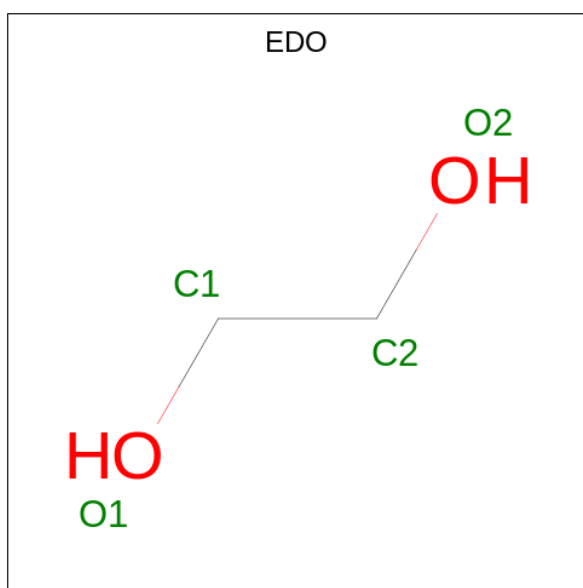
Chain	Residue	Modelled	Actual	Comment	Reference
B	6	ALA	-	expression tag	UNP A0A0P0QM28
B	7	ALA	-	expression tag	UNP A0A0P0QM28
B	8	ALA	-	expression tag	UNP A0A0P0QM28
B	9	MET	-	expression tag	UNP A0A0P0QM28
B	10	GLY	-	expression tag	UNP A0A0P0QM28
B	11	HIS	-	expression tag	UNP A0A0P0QM28
B	12	HIS	-	expression tag	UNP A0A0P0QM28
B	13	HIS	-	expression tag	UNP A0A0P0QM28
B	14	HIS	-	expression tag	UNP A0A0P0QM28
B	15	HIS	-	expression tag	UNP A0A0P0QM28
B	16	HIS	-	expression tag	UNP A0A0P0QM28
B	17	SER	-	expression tag	UNP A0A0P0QM28
B	18	SER	-	expression tag	UNP A0A0P0QM28
B	19	GLY	-	expression tag	UNP A0A0P0QM28
B	20	VAL	-	expression tag	UNP A0A0P0QM28
B	21	ASP	-	expression tag	UNP A0A0P0QM28
B	22	LEU	-	expression tag	UNP A0A0P0QM28
B	23	GLY	-	expression tag	UNP A0A0P0QM28
B	24	THR	-	expression tag	UNP A0A0P0QM28
B	25	GLU	-	expression tag	UNP A0A0P0QM28
B	26	ASN	-	expression tag	UNP A0A0P0QM28
B	27	LEU	-	expression tag	UNP A0A0P0QM28
B	28	TYR	-	expression tag	UNP A0A0P0QM28
B	29	PHE	-	expression tag	UNP A0A0P0QM28
B	30	GLN	-	expression tag	UNP A0A0P0QM28
B	31	SER	-	expression tag	UNP A0A0P0QM28
B	32	MET	-	expression tag	UNP A0A0P0QM28
B	74	VAL	GLU	engineered mutation	UNP A0A0P0QM28
B	252	VAL	GLY	engineered mutation	UNP A0A0P0QM28

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

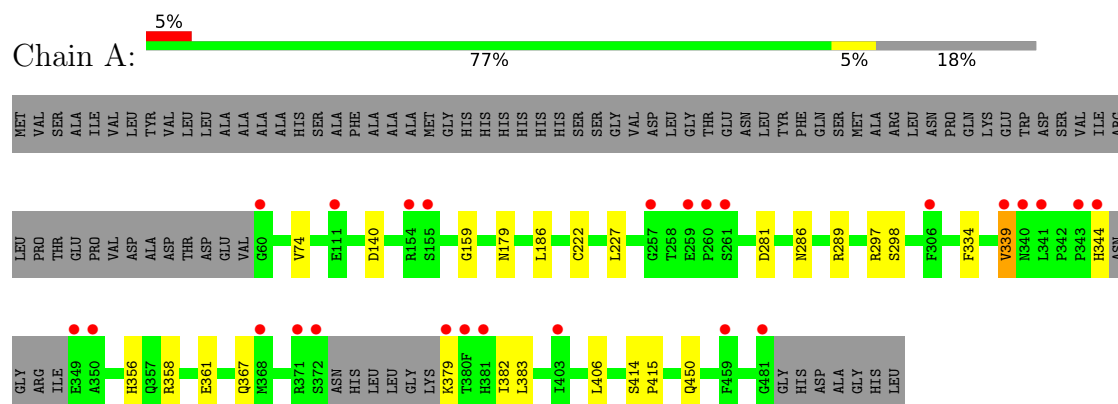
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	452	Total	O	0	0
			452	452		
5	B	443	Total	O	0	0
			443	443		

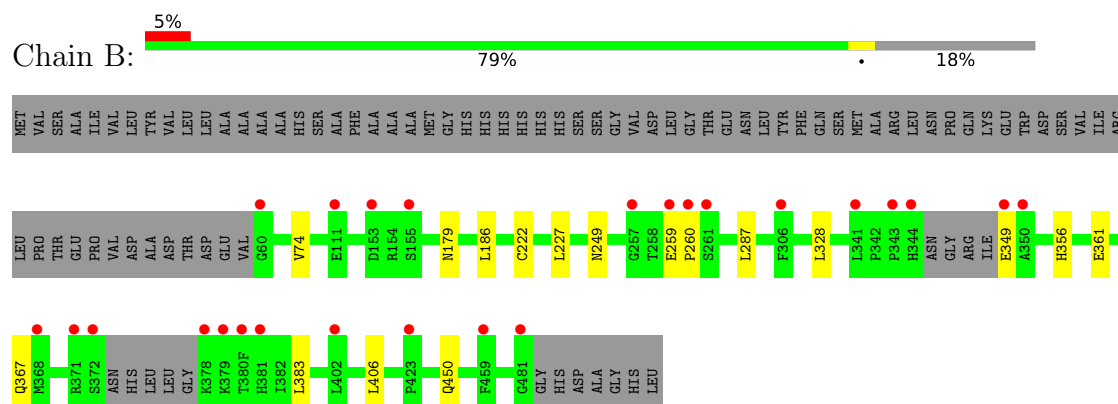
3 Residue-property plots [i](#)

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: Asparaginyl endopeptidase



• Molecule 1: Asparaginyl endopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.61Å 79.60Å 136.47Å 90.00° 93.95° 90.00°	Depositor
Resolution (Å)	21.84 – 1.50 21.84 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (21.84-1.50) 99.9 (21.84-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.50Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.172 , 0.190 0.174 , 0.190	Depositor DCC
R_{free} test set	7598 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7513	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SNN, OCS, PEG, NAG, EDO

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	0.43	0/3354	0.58	0/4537
1	B	0.43	0/3342	0.59	0/4520
All	All	0.43	0/6696	0.58	0/9057

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3295	0	3164	17	0
1	B	3284	0	3163	7	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	4	0	6	3	0
4	A	7	0	10	3	0
5	A	452	0	0	0	0
5	B	443	0	0	0	0
All	All	7513	0	6369	22	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 2.

All (22) 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:297:ARG:HE	4:A:503:PEG:H22	1.42	0.83
1:A:281:ASP:OD1	1:A:344:HIS:HE1	1.79	0.65
1:A:297:ARG:NE	4:A:503:PEG:H22	2.13	0.61
1:A:334:PHE:HZ	1:A:339:VAL:HG13	1.67	0.59
1:A:140:ASP:OD1	3:A:502:EDO:H12	2.04	0.57
1:A:356:HIS:HD2	1:A:358:ARG:H	1.54	0.55
1:B:287:LEU:HD22	1:B:328:LEU:HD23	1.87	0.55
1:A:297:ARG:HE	4:A:503:PEG:C2	2.16	0.54
1:A:286:ASN:HD22	1:A:289:ARG:NH1	2.08	0.51
1:B:249[A]:ASN:ND2	1:B:356:HIS:CD2	2.79	0.50
1:B:74:VAL:HG21	1:B:361:GLU:HA	1.95	0.49
1:A:298:SER:OG	1:A:344:HIS:NE2	2.31	0.48
1:A:74:VAL:HG21	1:A:361:GLU:HA	1.96	0.48
1:A:186:LEU:HD21	1:A:227:LEU:HD11	1.97	0.47
1:B:259:GLU:HA	1:B:260:PRO:C	2.35	0.47
1:A:406:LEU:HD22	1:B:383:LEU:HG	1.97	0.46
1:B:186:LEU:HD21	1:B:227:LEU:HD11	1.98	0.45
1:A:140:ASP:OD1	3:A:502:EDO:C1	2.65	0.44
1:A:159:GLY:HA3	3:A:502:EDO:H12	2.00	0.43
1:A:414:SER:OG	1:A:415:PRO:HD3	2.18	0.43
1:A:379:LYS:HB3	1:A:382:ILE:HD12	2.00	0.42
1:A:383:LEU:HG	1:B:406:LEU:HD22	2.02	0.42

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	411/502 (82%)	404 (98%)	7 (2%)	0	100	100
1	B	409/502 (82%)	403 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	820/1004 (82%)	807 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	357/420 (85%)	354 (99%)	3 (1%)	81	66
1	B	356/420 (85%)	353 (99%)	3 (1%)	81	66
All	All	713/840 (85%)	707 (99%)	6 (1%)	78	66

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	339	VAL
1	A	367	GLN
1	A	450	GLN
1	B	349	GLU
1	B	367	GLN
1	B	450	GLN

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	121	ASN
1	A	356	HIS
1	A	385	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	OCS	A	222	1	7,8,9	1.50	2 (28%)	6,11,13	2.37	4 (66%)
1	SNN	A	179	1	5,6,8	3.92	4 (80%)	3,6,11	2.43	2 (66%)
1	OCS	B	222	1	7,8,9	1.39	1 (14%)	6,11,13	2.95	3 (50%)
1	SNN	B	179	1	5,6,8	3.69	4 (80%)	3,6,11	2.50	2 (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	OCS	A	222	1	-	0/4/7/9	-
1	SNN	A	179	1	-	3/3/5/12	-
1	OCS	B	222	1	-	0/4/7/9	-
1	SNN	B	179	1	-	3/3/5/12	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	SNN	C4-C3	-6.54	1.39	1.54
1	B	179	SNN	C4-C3	-5.56	1.41	1.54
1	B	179	SNN	O2-C2	4.01	1.35	1.19
1	A	179	SNN	O2-C2	3.87	1.35	1.19
1	B	179	SNN	C4-C5	-3.16	1.41	1.49
1	A	179	SNN	O5-C5	3.04	1.37	1.19
1	B	179	SNN	O5-C5	3.04	1.37	1.19
1	A	179	SNN	C4-C5	-2.89	1.42	1.49
1	B	222	OCS	OD1-SG	-2.66	1.37	1.45
1	A	222	OCS	CB-CA	2.33	1.56	1.53
1	A	222	OCS	OD1-SG	-2.22	1.38	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	OCS	OD2-SG-OD1	5.12	123.79	111.27
1	B	222	OCS	OD2-SG-OD3	-3.38	103.02	111.27
1	B	222	OCS	OD3-SG-CB	3.19	110.73	106.94
1	B	179	SNN	C4-C3-C2	-3.12	105.61	111.44
1	A	222	OCS	OD2-SG-CB	3.08	110.64	105.74
1	A	179	SNN	C4-C3-C2	-3.03	105.78	111.44
1	B	179	SNN	C3-C4-C5	-3.00	103.09	114.44
1	A	222	OCS	OD3-SG-CB	-2.95	103.43	106.94
1	A	179	SNN	C3-C4-C5	-2.91	103.42	114.44
1	A	222	OCS	OD2-SG-OD3	-2.62	104.87	111.27
1	A	222	OCS	OD3-SG-OD1	2.33	122.00	113.95

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	179	SNN	O2-C2-C3-C4
1	A	179	SNN	C3-C4-C5-O5
1	B	179	SNN	O2-C2-C3-C4
1	B	179	SNN	C3-C4-C5-O5
1	A	179	SNN	N3-C3-C4-C5
1	B	179	SNN	N3-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
2	NAG	B	501	1	14,14,15	0.32	0	17,19,21	0.85	1 (5%)
2	NAG	A	501	1	14,14,15	0.29	0	17,19,21	0.40	0
3	EDO	A	502	-	3,3,3	0.61	0	2,2,2	0.30	0
4	PEG	A	503	-	6,6,6	0.07	0	5,5,5	0.03	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	NAG	B	501	1	-	3/6/23/26	0/1/1/1
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	EDO	A	502	-	-	0/1/1/1	-
4	PEG	A	503	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAG	C1-C2-N2	-2.56	106.11	110.49

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	NAG	C1-C2-N2-C7
2	B	501	NAG	C8-C7-N2-C2
4	A	503	PEG	C1-C2-O2-C3
4	A	503	PEG	C4-C3-O2-C2
2	B	501	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	EDO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	PEG	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 [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	410/502 (81%)	0.14	25 (6%)	21 23	18, 27, 47, 67	0
1	B	411/502 (81%)	0.18	25 (6%)	21 23	18, 26, 46, 72	0
All	All	821/1004 (81%)	0.16	50 (6%)	21 23	18, 26, 46, 72	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	PRO	6.1
1	B	349	GLU	6.0
1	B	378	LYS	5.4
1	B	306	PHE	5.4
1	B	380(F)	THR	5.4
1	B	344	HIS	5.2
1	B	343	PRO	5.0
1	A	306	PHE	5.0
1	A	380(F)	THR	5.0
1	A	339	VAL	4.5
1	B	481	GLY	4.2
1	B	372	SER	4.2
1	A	259	GLU	4.0
1	A	340	ASN	3.9
1	B	368	MET	3.6
1	A	350	ALA	3.6
1	B	350	ALA	3.6
1	A	349	GLU	3.4
1	A	368	MET	3.4
1	A	381	HIS	3.4
1	B	379	LYS	3.4
1	A	379	LYS	3.3
1	A	261	SER	3.3
1	B	260	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	423	PRO	3.2
1	A	344	HIS	3.1
1	B	261	SER	3.1
1	A	372	SER	3.0
1	B	259	GLU	3.0
1	A	481	GLY	2.9
1	A	341	LEU	2.9
1	B	60	GLY	2.7
1	A	154	ARG	2.6
1	A	403	ILE	2.6
1	A	343	PRO	2.6
1	A	60	GLY	2.5
1	B	381	HIS	2.4
1	B	257	GLY	2.4
1	B	155	SER	2.4
1	A	371	ARG	2.4
1	B	111	GLU	2.3
1	B	153[A]	ASP	2.3
1	A	257	GLY	2.3
1	B	341	LEU	2.2
1	B	402	LEU	2.2
1	A	459	PHE	2.1
1	A	155	SER	2.1
1	B	371	ARG	2.1
1	B	459	PHE	2.1
1	A	111	GLU	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	SNN	A	179	7/8	0.94	0.08	19,19,21,23	0
1	SNN	B	179	7/8	0.94	0.07	18,19,20,22	0
1	OCS	A	222	9/10	0.96	0.08	23,24,29,30	0
1	OCS	B	222	9/10	0.97	0.07	22,24,29,31	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
2	NAG	A	501	14/15	0.49	0.37	49,51,52,52	0
2	NAG	B	501	14/15	0.66	0.39	49,51,54,56	0
4	PEG	A	503	7/7	0.71	0.28	60,61,61,61	0
3	EDO	A	502	4/4	0.78	0.26	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.