



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 12, 2021 – 12:26 PM EDT

PDB ID : 6XI2
Title : Apo form of POMGNT2
Authors : Halmo, S.M.; Yeh, J.; Wells, L.; Moremen, K.W.; Lanzilotta, W.N.
Deposited on : 2020-06-19
Resolution : 2.57 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 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 : 2.18
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) : 2.18

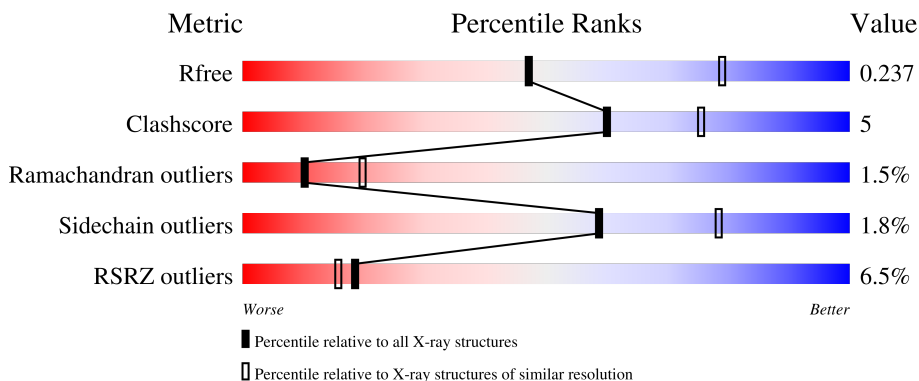
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

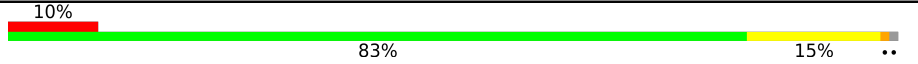
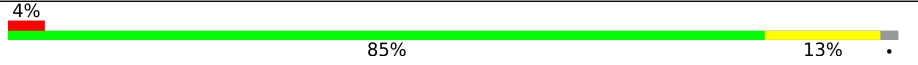



The reported resolution of this entry is 2.57 Å.

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.



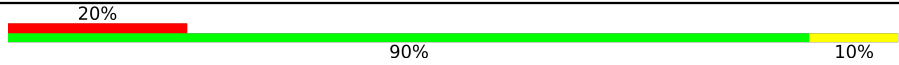
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	533	
2	B	528	
3	D	533	
4	C	528	
5	G	10	

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Mol	Chain	Length	Quality of chain
6	H	10	

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
8	PO4	D	907	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17188 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 Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	528	4246	2750	733	740	23	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	ALA	LYS	conflict	UNP Q8NAT1
A	126	ALA	ASN	conflict	UNP Q8NAT1
A	279	ALA	HIS	conflict	UNP Q8NAT1
A	427	ALA	GLN	conflict	UNP Q8NAT1
A	477	ALA	THR	conflict	UNP Q8NAT1
A	478	ALA	VAL	conflict	UNP Q8NAT1
A	518	ALA	ARG	conflict	UNP Q8NAT1
A	529	ALA	GLN	conflict	UNP Q8NAT1
A	532	ALA	ASN	conflict	UNP Q8NAT1
A	533	ALA	THR	conflict	UNP Q8NAT1

- Molecule 2 is a protein called Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	518	4168	2699	716	730	23	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	55	ALA	LYS	conflict	UNP Q8NAT1
B	126	ALA	ASN	conflict	UNP Q8NAT1
B	277	ALA	VAL	conflict	UNP Q8NAT1
B	285	ALA	GLY	conflict	UNP Q8NAT1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	421	GLN	GLU	conflict	UNP Q8NAT1
B	424	ALA	ARG	conflict	UNP Q8NAT1
B	466	ALA	LYS	conflict	UNP Q8NAT1
B	467	ALA	GLY	conflict	UNP Q8NAT1
B	?	-	ARG	deletion	UNP Q8NAT1
B	472	ALA	ARG	conflict	UNP Q8NAT1
B	476	ALA	TRP	conflict	UNP Q8NAT1
B	477	ALA	THR	conflict	UNP Q8NAT1
B	478	ALA	VAL	conflict	UNP Q8NAT1
B	518	ALA	ARG	conflict	UNP Q8NAT1
B	532	ALA	ASN	conflict	UNP Q8NAT1
B	533	ALA	THR	conflict	UNP Q8NAT1

- Molecule 3 is a protein called Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	521	4197	2716	725	733	23	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	55	ALA	LYS	conflict	UNP Q8NAT1
D	277	ALA	VAL	conflict	UNP Q8NAT1
D	285	ALA	GLY	conflict	UNP Q8NAT1
D	286	ALA	GLU	conflict	UNP Q8NAT1
D	293	ALA	SER	conflict	UNP Q8NAT1
D	308	ALA	LEU	conflict	UNP Q8NAT1
D	427	SER	GLN	conflict	UNP Q8NAT1
D	466	ALA	LYS	conflict	UNP Q8NAT1
D	468	ALA	ARG	conflict	UNP Q8NAT1
D	478	ALA	VAL	conflict	UNP Q8NAT1
D	518	ALA	ARG	conflict	UNP Q8NAT1
D	529	ALA	GLN	conflict	UNP Q8NAT1

- Molecule 4 is a protein called Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	519	4164	2697	714	730	23	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	55	ALA	LYS	conflict	UNP Q8NAT1
C	277	ALA	VAL	conflict	UNP Q8NAT1
C	285	ALA	GLY	conflict	UNP Q8NAT1
C	286	ALA	GLU	conflict	UNP Q8NAT1
C	419	ALA	ARG	conflict	UNP Q8NAT1
C	424	ALA	ARG	conflict	UNP Q8NAT1
C	?	-	ARG	deletion	UNP Q8NAT1
C	468	ALA	PRO	conflict	UNP Q8NAT1
C	469	ALA	GLY	conflict	UNP Q8NAT1
C	475	ALA	LYS	conflict	UNP Q8NAT1
C	476	ALA	TRP	conflict	UNP Q8NAT1
C	477	ALA	THR	conflict	UNP Q8NAT1
C	478	ALA	VAL	conflict	UNP Q8NAT1
C	518	ALA	ARG	conflict	UNP Q8NAT1
C	529	ALA	GLN	conflict	UNP Q8NAT1
C	532	ALA	ASN	conflict	UNP Q8NAT1
C	533	ALA	THR	conflict	UNP Q8NAT1

- Molecule 5 is a protein called ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
5	G	10	50	30	10	10	0	0	0

- Molecule 6 is a protein called ALA-GLY-ALA-GLY-ALA-ALA-ALA-ALA-ALA-ALA.

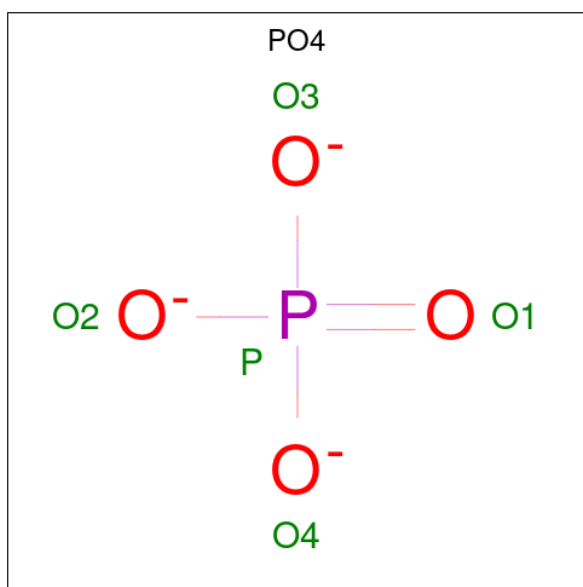
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
6	H	10	48	28	10	10	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	P	0	0
			5	4	1		
8	A	1	Total	O	P	0	0
			5	4	1		
8	A	1	Total	O	P	0	0
			5	4	1		
8	A	1	Total	O	P	0	0
			5	4	1		
8	A	1	Total	O	P	0	0
			5	4	1		
8	A	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		
8	D	1	Total	O	P	0	0
			5	4	1		
8	D	1	Total	O	P	0	0
			5	4	1		
8	D	1	Total	O	P	0	0
			5	4	1		
8	D	1	Total	O	P	0	0
			5	4	1		
8	D	1	Total	O	P	0	0
			5	4	1		
8	D	1	Total	O	P	0	0
			5	4	1		
8	C	1	Total	O	P	0	0
			5	4	1		
8	C	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	P	0	0
			5	4	1		
8	C	1	Total	O	P	0	0
			5	4	1		
8	C	1	Total	O	P	0	0
			5	4	1		

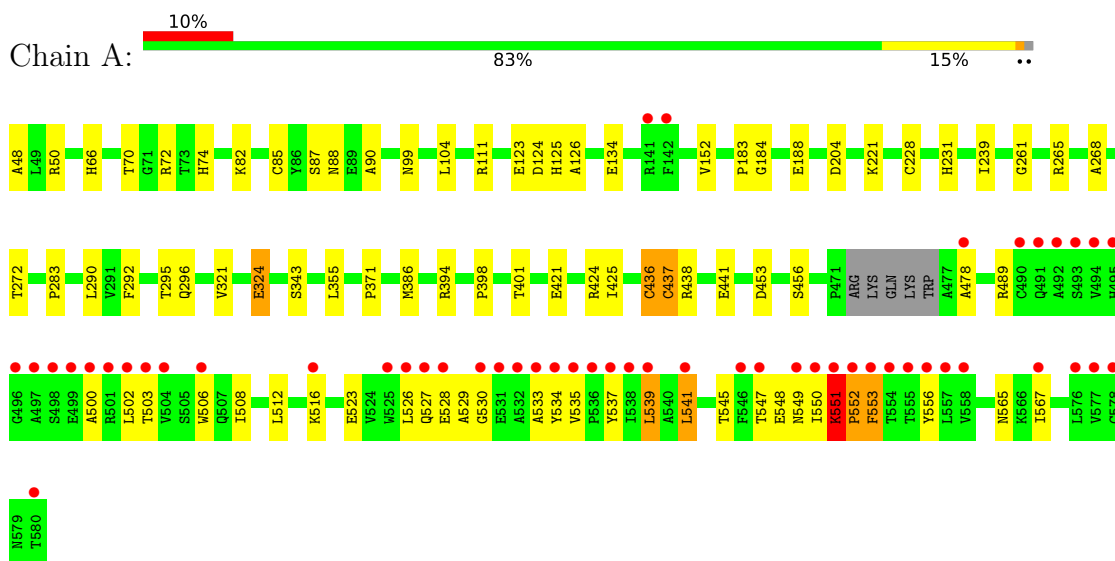
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	46	Total	O	0	0
			46	46		
9	B	35	Total	O	0	0
			35	35		
9	D	23	Total	O	0	0
			23	23		
9	C	43	Total	O	0	0
			43	43		
9	H	1	Total	O	0	0
			1	1		

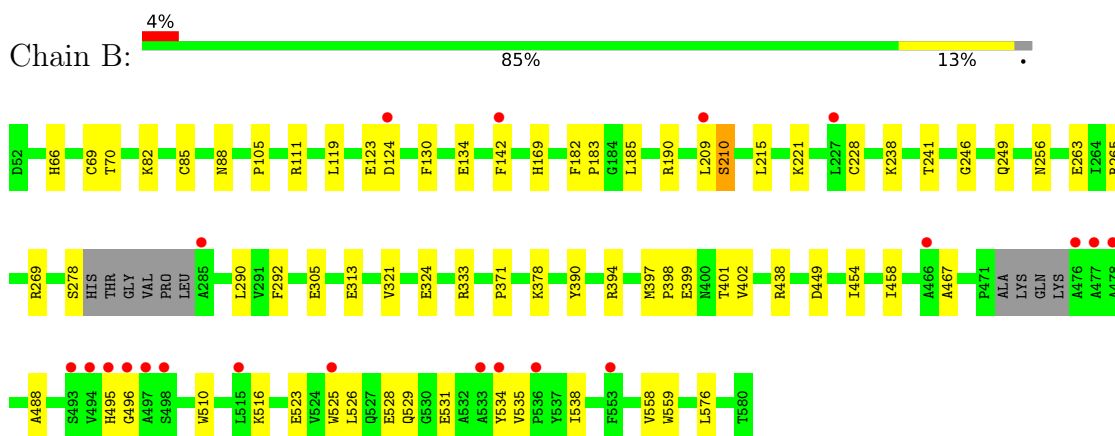
3 Residue-property plots

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.

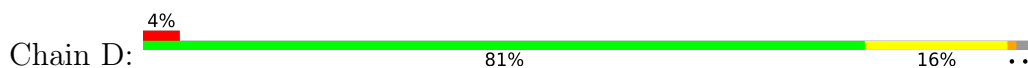
- Molecule 1: Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2

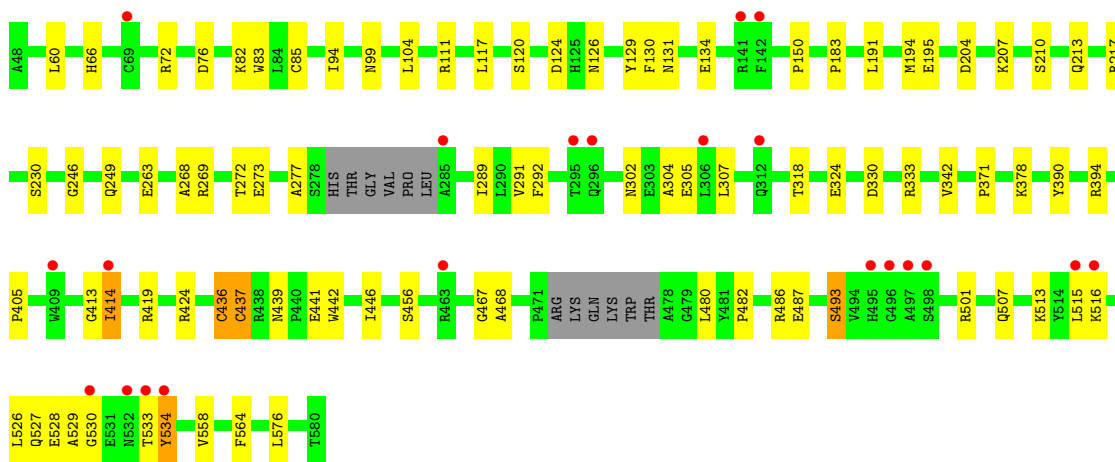


- Molecule 2: Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2

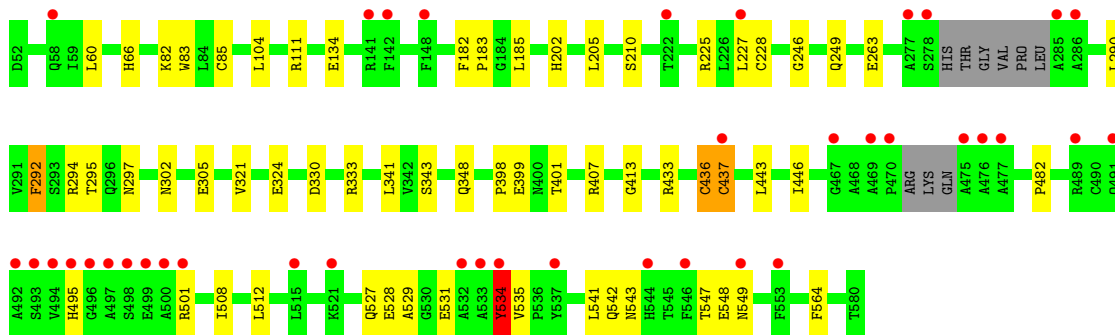
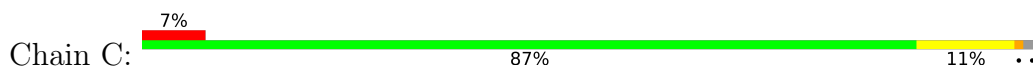


- Molecule 3: Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2

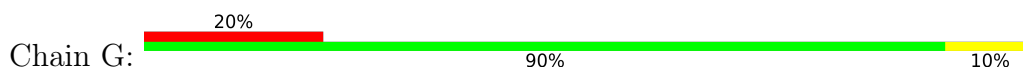




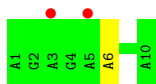
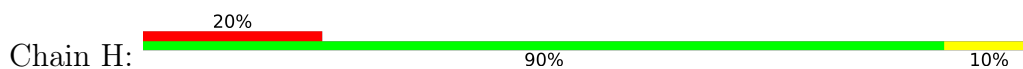
- Molecule 4: Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2



- Molecule 5: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA



- Molecule 6: ALA-GLY-ALA-GLY-ALA-ALA-ALA-ALA-ALA-ALA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	142.32Å 153.98Å 187.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.99 – 2.57 49.50 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.99-2.57) 95.7 (49.50-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.58Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.213 , 0.237 0.214 , 0.237	Depositor DCC
R_{free} test set	2020 reflections (1.55%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtrriage
Anisotropy	0.398	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17188	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: PO4, NAG

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	0.25	0/4364	0.45	0/5943
2	B	0.25	0/4284	0.45	0/5835
3	D	0.25	0/4313	0.44	0/5872
4	C	0.26	0/4279	0.44	0/5828
5	G	0.25	0/49	0.46	0/67
6	H	0.29	0/47	0.56	0/63
All	All	0.25	0/17336	0.45	0/23608

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
3	D	0	1
4	C	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	436	CYS	Peptide
1	A	551	LYS	Peptide
4	C	436	CYS	Peptide
3	D	436	CYS	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	4246	0	4225	48	0
2	B	4168	0	4128	39	0
3	D	4197	0	4167	43	0
4	C	4164	0	4125	33	0
5	G	50	0	52	0	0
6	H	48	0	48	0	0
7	A	14	0	13	0	0
7	B	14	0	13	0	0
7	D	14	0	13	0	0
8	A	40	0	0	0	0
8	B	30	0	0	1	0
8	C	25	0	0	1	0
8	D	30	0	0	0	0
9	A	46	0	0	1	0
9	B	35	0	0	1	0
9	C	43	0	0	1	0
9	D	23	0	0	1	0
9	H	1	0	0	0	0
All	All	17188	0	16784	155	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 5.

The worst 5 of 155 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:48:ALA:HB3	1:A:50:ARG:HH21	1.50	0.76
4:C:292:PHE:HB2	4:C:343:SER:HB2	1.70	0.74
2:B:399:GLU:H	2:B:399:GLU:CD	1.91	0.73
3:D:104:LEU:HD13	4:C:263:GLU:HG2	1.72	0.70
2:B:269:ARG:NH2	9:B:1001:HOH:O	2.25	0.69

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	524/533 (98%)	493 (94%)	20 (4%)	11 (2%)	7	12
2	B	512/528 (97%)	488 (95%)	17 (3%)	7 (1%)	11	21
3	D	515/533 (97%)	485 (94%)	23 (4%)	7 (1%)	11	21
4	C	513/528 (97%)	479 (93%)	29 (6%)	5 (1%)	15	31
5	G	8/10 (80%)	7 (88%)	0	1 (12%)	0	0
6	H	8/10 (80%)	4 (50%)	3 (38%)	1 (12%)	0	0
All	All	2080/2142 (97%)	1956 (94%)	92 (4%)	32 (2%)	10	20

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	A	296	GLN
1	A	437	CYS
1	A	529	ALA
1	A	551	LYS

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	455/461 (99%)	445 (98%)	10 (2%)	52	74
2	B	446/455 (98%)	439 (98%)	7 (2%)	62	81
3	D	450/461 (98%)	440 (98%)	10 (2%)	52	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	C	444/453 (98%)	438 (99%)	6 (1%)	67 84
All	All	1795/1830 (98%)	1762 (98%)	33 (2%)	59 78

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	227	LEU
4	C	292	PHE
4	C	543	ASN
2	B	292	PHE
2	B	278	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	579	ASN
3	D	491	GLN
4	C	126	ASN
4	C	579	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

28 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
8	PO4	A	903	-	4,4,4	0.93	0	6,6,6	0.44	0
8	PO4	A	904	-	4,4,4	0.92	0	6,6,6	0.41	0
8	PO4	A	902	-	4,4,4	0.92	0	6,6,6	0.46	0
8	PO4	D	904	-	4,4,4	0.91	0	6,6,6	0.45	0
8	PO4	C	604	-	4,4,4	0.91	0	6,6,6	0.42	0
8	PO4	B	906	-	4,4,4	0.91	0	6,6,6	0.45	0
8	PO4	A	908	-	4,4,4	0.91	0	6,6,6	0.41	0
8	PO4	D	903	-	4,4,4	0.92	0	6,6,6	0.44	0
8	PO4	D	907	-	4,4,4	0.92	0	6,6,6	0.45	0
8	PO4	D	905	-	4,4,4	0.92	0	6,6,6	0.48	0
8	PO4	B	905	-	4,4,4	0.93	0	6,6,6	0.42	0
8	PO4	B	902	-	4,4,4	0.91	0	6,6,6	0.43	0
8	PO4	C	603	-	4,4,4	0.93	0	6,6,6	0.44	0
8	PO4	C	601	-	4,4,4	0.93	0	6,6,6	0.44	0
8	PO4	A	906	-	4,4,4	0.90	0	6,6,6	0.43	0
8	PO4	D	902	-	4,4,4	0.92	0	6,6,6	0.43	0
7	NAG	A	901	1	14,14,15	0.92	1 (7%)	17,19,21	0.74	0
8	PO4	C	605	-	4,4,4	0.91	0	6,6,6	0.42	0
8	PO4	B	907	-	4,4,4	0.92	0	6,6,6	0.43	0
7	NAG	D	901	3	14,14,15	0.36	0	17,19,21	0.41	0
8	PO4	B	904	-	4,4,4	0.91	0	6,6,6	0.42	0
8	PO4	D	906	-	4,4,4	0.91	0	6,6,6	0.45	0
8	PO4	A	909	-	4,4,4	0.91	0	6,6,6	0.43	0
7	NAG	B	901	2	14,14,15	0.27	0	17,19,21	0.47	0
8	PO4	B	903	-	4,4,4	0.93	0	6,6,6	0.42	0
8	PO4	A	907	-	4,4,4	0.91	0	6,6,6	0.42	0
8	PO4	A	905	-	4,4,4	0.91	0	6,6,6	0.45	0
8	PO4	C	602	-	4,4,4	0.91	0	6,6,6	0.40	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
7	NAG	B	901	2	-	0/6/23/26	0/1/1/1
7	NAG	A	901	1	-	3/6/23/26	0/1/1/1
7	NAG	D	901	3	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	901	NAG	O5-C1	-3.37	1.38	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	901	NAG	O5-C5-C6-O6
7	A	901	NAG	C4-C5-C6-O6
7	D	901	NAG	O5-C5-C6-O6
7	A	901	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	905	PO4	1	0
8	C	603	PO4	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	528/533 (99%)	0.42	52 (9%) 7 6	26, 42, 104, 140	0
2	B	518/528 (98%)	0.16	21 (4%) 37 33	28, 42, 68, 113	0
3	D	521/533 (97%)	0.26	21 (4%) 38 34	32, 48, 75, 119	0
4	C	519/528 (98%)	0.39	39 (7%) 14 11	28, 43, 83, 137	0
5	G	10/10 (100%)	0.52	2 (20%) 1 0	40, 49, 61, 66	0
6	H	10/10 (100%)	1.13	2 (20%) 1 0	50, 52, 67, 72	0
All	All	2106/2142 (98%)	0.31	137 (6%) 18 16	26, 44, 82, 140	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	TYR	10.5
2	B	497	ALA	9.3
1	A	553	PHE	9.1
4	C	497	ALA	9.1
1	A	497	ALA	8.1

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 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(Å ²)	Q<0.9
8	PO4	D	906	5/5	0.71	0.30	65,65,75,85	0
8	PO4	D	907	5/5	0.72	0.41	75,81,100,105	0
8	PO4	A	906	5/5	0.79	0.24	62,70,81,98	0
7	NAG	A	901	14/15	0.80	0.29	58,68,74,76	0
7	NAG	D	901	14/15	0.82	0.29	61,72,75,81	0
8	PO4	A	909	5/5	0.82	0.27	78,80,89,103	0
8	PO4	C	605	5/5	0.85	0.33	81,82,91,97	0
8	PO4	A	908	5/5	0.87	0.14	75,81,96,99	0
8	PO4	B	905	5/5	0.91	0.14	57,62,77,78	0
7	NAG	B	901	14/15	0.92	0.18	56,61,67,68	0
8	PO4	C	602	5/5	0.93	0.28	78,82,97,98	0
8	PO4	C	603	5/5	0.93	0.13	57,62,69,70	0
8	PO4	B	903	5/5	0.93	0.15	70,73,91,103	0
8	PO4	A	904	5/5	0.94	0.23	58,64,82,84	0
8	PO4	A	902	5/5	0.95	0.16	41,44,45,63	0
8	PO4	B	904	5/5	0.95	0.14	60,60,71,81	0
8	PO4	A	907	5/5	0.95	0.15	59,71,77,84	0
8	PO4	D	903	5/5	0.95	0.11	60,63,69,69	0
8	PO4	C	604	5/5	0.95	0.14	41,43,49,49	0
8	PO4	D	904	5/5	0.95	0.15	69,71,74,81	0
8	PO4	C	601	5/5	0.96	0.21	44,54,58,66	0
8	PO4	B	906	5/5	0.96	0.15	40,43,52,55	0
8	PO4	D	905	5/5	0.96	0.19	44,48,59,65	0
8	PO4	D	902	5/5	0.96	0.17	46,50,55,64	0
8	PO4	A	905	5/5	0.96	0.16	37,45,53,59	0
8	PO4	B	907	5/5	0.97	0.23	60,63,65,70	0
8	PO4	A	903	5/5	0.98	0.15	49,52,63,67	0
8	PO4	B	902	5/5	0.98	0.12	43,52,56,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.