Full wwPDB X-ray Structure Validation Report (i)

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 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

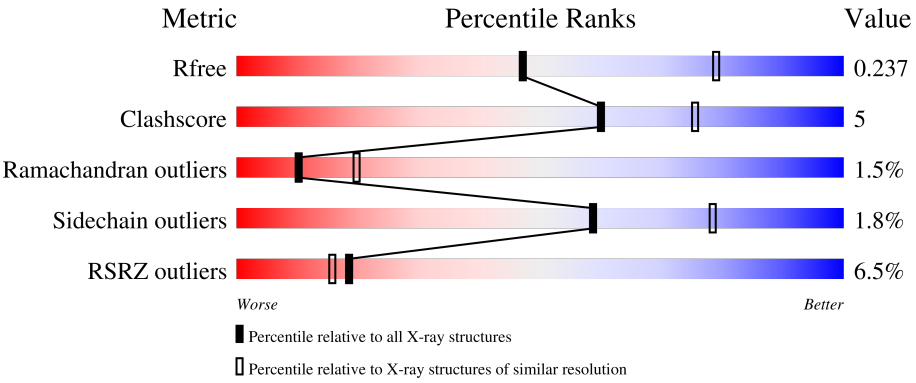
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

1 Overall quality at a glance (i)

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 <=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	10% 83% 15% ••
2	B	528	4% 85% 13% •
3	D	533	4% 81% 16% ••
4	C	528	7% 87% 11% ••
5	G	10	20% 90% 10%

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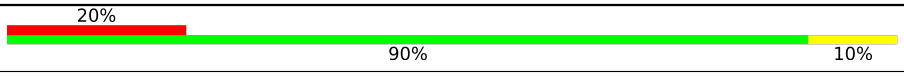
Mol	Chain	Length	Quality of chain
6	H	10	

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 (i)

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
3	D	521	Total	C	N	O	S	0	0	0
			4197	2716	725	733	23			

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
4	C	519	Total	C	N	O	S	0	0	0
			4164	2697	714	730	23			

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

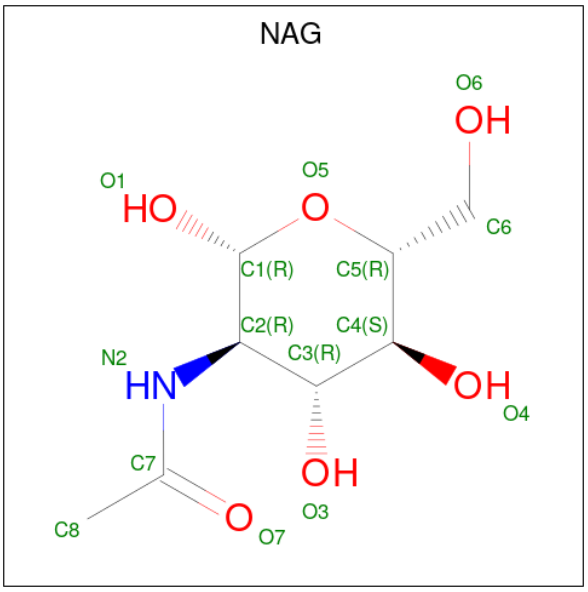
- Molecule 5 is a protein called ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

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

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

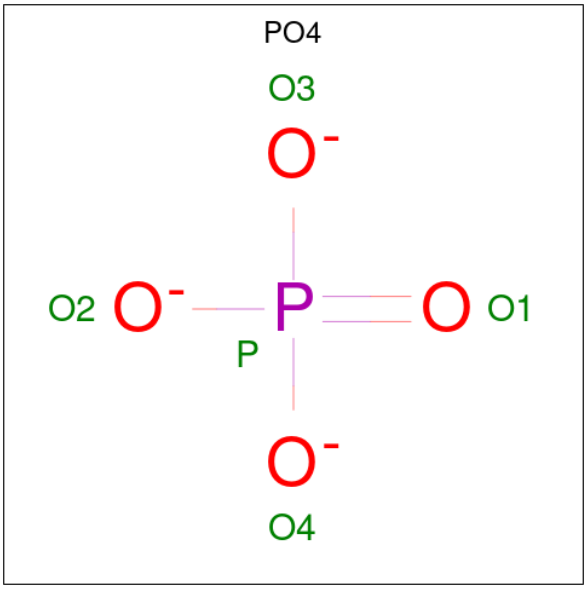
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	10	Total	C	N	O	0	0	0
			48	28	10	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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

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

- Molecule 9 is water.

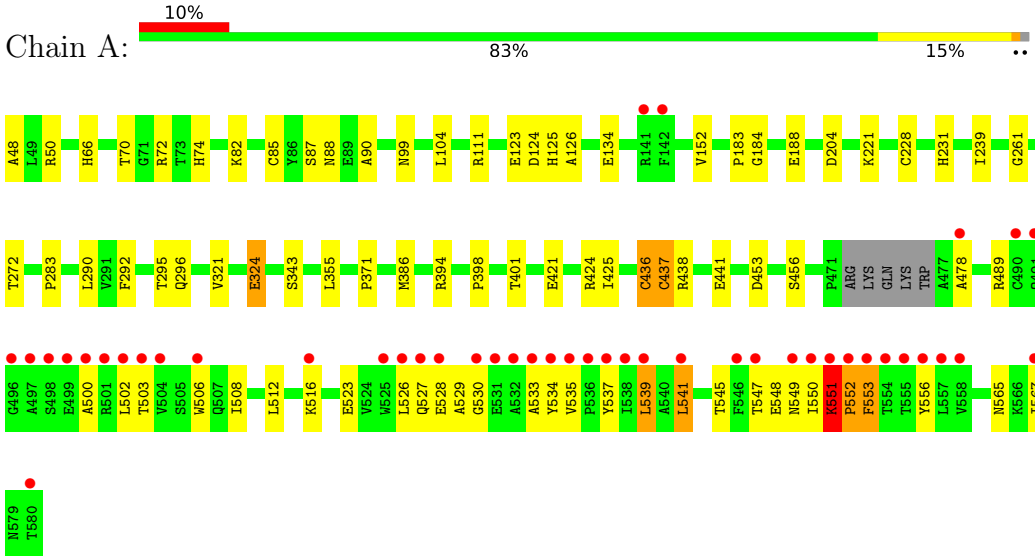
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	46	Total O 46 46	0	0
9	B	35	Total O 35 35	0	0
9	D	23	Total O 23 23	0	0
9	C	43	Total O 43 43	0	0
9	H	1	Total O 1 1	0	0

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.

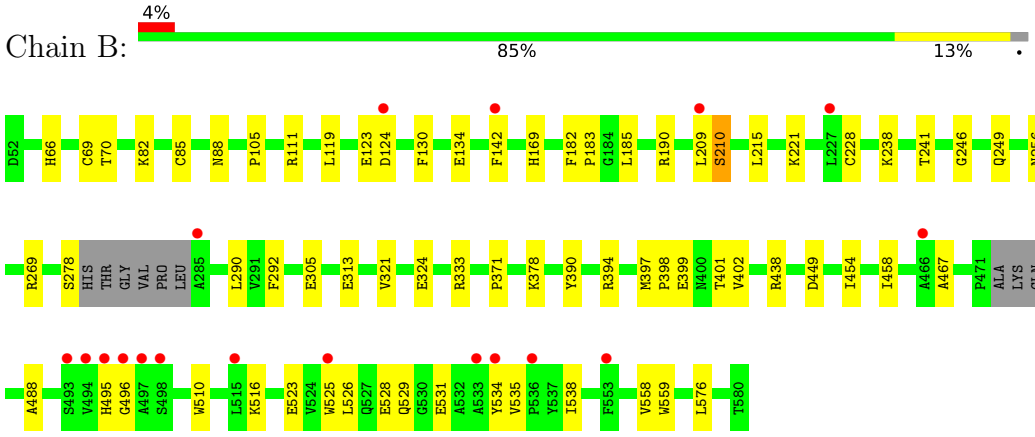
• Molecule 1: Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2

Chain A:



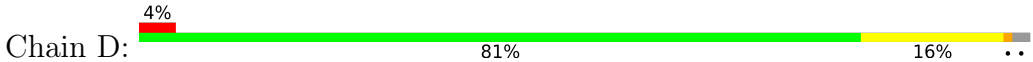
• Molecule 2: Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2

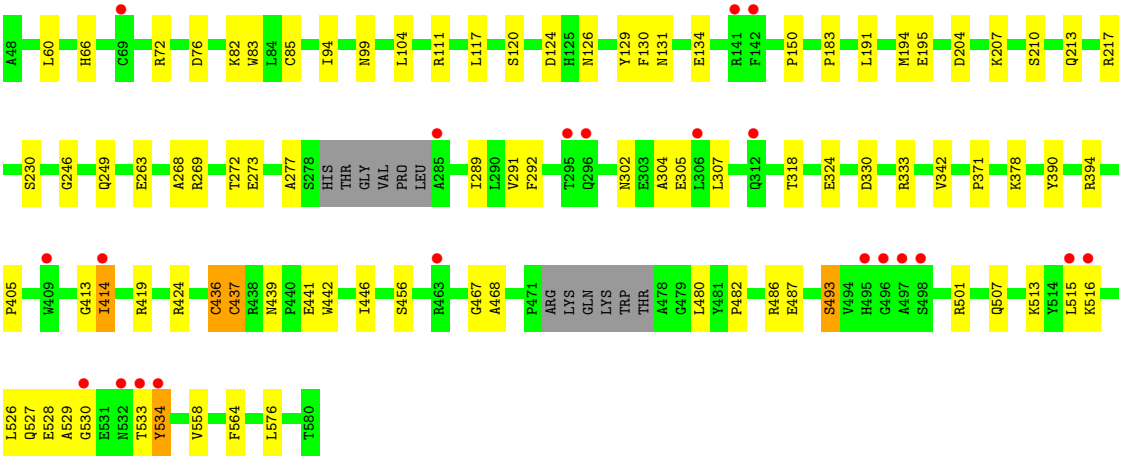
Chain B:



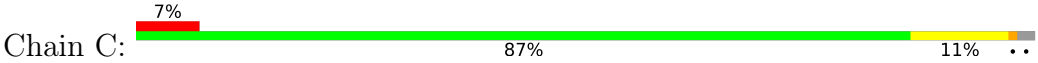
• Molecule 3: Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2

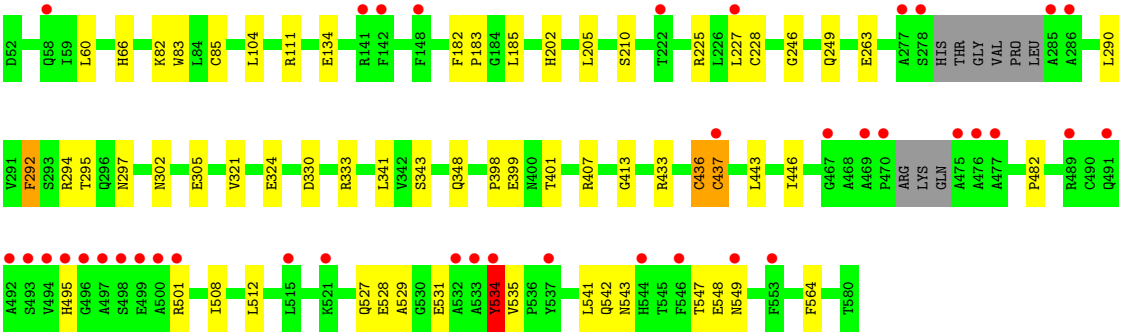
Chain D:



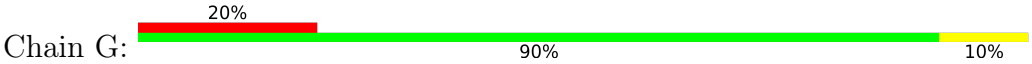


• Molecule 4: Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2

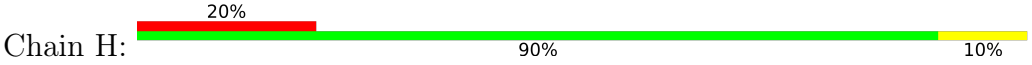


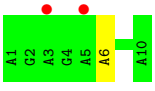


• Molecule 5: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA



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





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.16 (at 2.58Å)	Xtriage
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	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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 (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	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.

All (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
3:D:486:ARG:HH22	3:D:513:LYS:HE3	1.56	0.69
1:A:104:LEU:HD13	2:B:263:GLU:HG2	1.75	0.68
4:C:330:ASP:OD1	4:C:333:ARG:NH1	2.27	0.68
4:C:182:PHE:HB2	4:C:185:LEU:HD12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ARG:NH2	1:A:355:LEU:O	2.27	0.67
2:B:119:LEU:HG	2:B:130:PHE:HB2	1.77	0.67
1:A:527:GLN:HG3	1:A:533:ALA:HA	1.78	0.66
3:D:183:PRO:HD2	4:C:183:PRO:HD2	1.81	0.63
1:A:425:ILE:HG23	1:A:441:GLU:HG3	1.82	0.61
2:B:397:MET:HB3	2:B:399:GLU:OE1	2.01	0.59
4:C:66:HIS:HB3	4:C:82:LYS:HB2	1.84	0.59
3:D:99:ASN:ND2	9:D:1002:HOH:O	2.36	0.58
1:A:111:ARG:NH2	1:A:134:GLU:OE2	2.37	0.58
3:D:191:LEU:HG	3:D:210:SER:HB3	1.85	0.58
1:A:528:GLU:O	1:A:530:GLY:N	2.37	0.58
2:B:182:PHE:HB2	2:B:185:LEU:HD22	1.85	0.57
2:B:399:GLU:OE2	2:B:399:GLU:N	2.35	0.57
3:D:72:ARG:NH2	8:C:603:PO4:O2	2.36	0.57
4:C:527:GLN:HA	4:C:534:TYR:HB2	1.87	0.57
3:D:263:GLU:HG2	4:C:104:LEU:HG	1.87	0.56
2:B:190:ARG:HD3	2:B:215:LEU:HD13	1.87	0.56
4:C:111:ARG:NH2	4:C:134:GLU:OE2	2.39	0.56
2:B:66:HIS:HB3	2:B:82:LYS:HB2	1.87	0.56
2:B:526:LEU:HD12	2:B:558:VAL:HG22	1.88	0.55
2:B:111:ARG:NH2	2:B:134:GLU:OE2	2.39	0.55
3:D:111:ARG:NH2	3:D:134:GLU:OE2	2.39	0.54
1:A:183:PRO:HD2	2:B:183:PRO:HD2	1.89	0.54
2:B:398:PRO:O	2:B:401:THR:HG22	2.06	0.54
4:C:433:ARG:NH2	9:C:701:HOH:O	2.21	0.54
1:A:547:THR:O	1:A:550:ILE:HG12	2.07	0.54
3:D:424:ARG:NH2	3:D:441:GLU:OE1	2.31	0.54
3:D:439:ASN:HB3	3:D:442:TRP:HB3	1.90	0.53
1:A:88:ASN:HB3	1:A:221:LYS:HG3	1.90	0.53
3:D:526:LEU:O	3:D:534:TYR:HB3	2.08	0.53
2:B:324:GLU:N	2:B:324:GLU:OE1	2.41	0.53
1:A:292:PHE:HB2	1:A:343:SER:HB2	1.90	0.53
1:A:66:HIS:HB3	1:A:82:LYS:HB2	1.91	0.53
3:D:207:LYS:HE2	3:D:213:GLN:HE22	1.74	0.53
3:D:371:PRO:HD3	3:D:394:ARG:HD2	1.91	0.52
3:D:289:ILE:HB	3:D:318:THR:HG22	1.90	0.52
2:B:528:GLU:HB3	2:B:531:GLU:HG3	1.92	0.52
4:C:528:GLU:HB3	4:C:531:GLU:HG3	1.91	0.52
4:C:436:CYS:SG	4:C:437:CYS:N	2.82	0.52
3:D:413:GLY:O	3:D:414:ILE:HG12	2.10	0.52
1:A:526:LEU:C	1:A:534:TYR:HB2	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:GLU:HG3	2:B:238:LYS:HE2	1.92	0.51
4:C:246:GLY:HA2	4:C:249:GLN:O	2.11	0.51
1:A:268:ALA:O	1:A:272:THR:HG23	2.11	0.51
2:B:265:ARG:O	2:B:269:ARG:HG3	2.11	0.51
1:A:290:LEU:HD11	1:A:321:VAL:HB	1.93	0.51
1:A:204:ASP:OD1	1:A:204:ASP:N	2.45	0.50
2:B:313:GLU:HG2	2:B:458:ILE:HG23	1.93	0.50
1:A:549:ASN:O	1:A:556:TYR:OH	2.22	0.50
2:B:454:ILE:O	2:B:458:ILE:HG12	2.11	0.50
3:D:194:MET:HA	3:D:217:ARG:HB2	1.94	0.50
3:D:269:ARG:O	3:D:273:GLU:HG3	2.11	0.50
4:C:60:LEU:HD13	4:C:83:TRP:HB3	1.94	0.49
2:B:290:LEU:HD11	2:B:321:VAL:HB	1.94	0.49
3:D:85:CYS:O	3:D:94:ILE:N	2.40	0.49
3:D:324:GLU:OE1	3:D:324:GLU:N	2.45	0.49
1:A:70:THR:HB	2:B:70:THR:HG21	1.95	0.49
3:D:487:GLU:OE1	3:D:507:GLN:NE2	2.45	0.49
1:A:503:THR:HG23	1:A:545:THR:HG22	1.95	0.48
3:D:480:LEU:HD12	3:D:515:LEU:HD21	1.93	0.48
4:C:407:ARG:O	4:C:413:GLY:HA3	2.13	0.48
1:A:436:CYS:SG	1:A:437:CYS:N	2.86	0.48
2:B:402:VAL:HB	2:B:449:ASP:HB2	1.95	0.48
1:A:371:PRO:HD3	1:A:394:ARG:HD2	1.95	0.48
2:B:525:TRP:HB2	2:B:559:TRP:HB2	1.95	0.48
3:D:304:ALA:HA	3:D:307:LEU:HD12	1.94	0.48
3:D:493:SER:OG	3:D:501:ARG:HD3	2.14	0.47
1:A:261:GLY:O	1:A:265:ARG:HG3	2.15	0.47
1:A:551:LYS:HB3	1:A:552:PRO:CD	2.44	0.47
3:D:527:GLN:HA	3:D:534:TYR:HB3	1.96	0.47
4:C:290:LEU:HD11	4:C:321:VAL:HB	1.97	0.47
3:D:66:HIS:HB3	3:D:82:LYS:HB2	1.96	0.47
3:D:528:GLU:O	3:D:530:GLY:N	2.48	0.47
3:D:246:GLY:HA2	3:D:249:GLN:O	2.14	0.47
4:C:294:ARG:HD2	4:C:348:GLN:HE22	1.78	0.46
4:C:541:LEU:HG	4:C:542:GLN:H	1.80	0.46
2:B:371:PRO:HD3	2:B:394:ARG:HD2	1.97	0.46
2:B:523:GLU:HG3	2:B:538:ILE:HD13	1.96	0.46
1:A:74:HIS:NE2	1:A:124:ASP:OD1	2.40	0.46
3:D:204:ASP:OD1	3:D:204:ASP:N	2.45	0.46
1:A:239:ILE:HD11	2:B:105:PRO:HB3	1.97	0.46
1:A:539:LEU:HD13	1:A:541:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:405:PRO:HB3	3:D:414:ILE:HD11	1.98	0.46
2:B:69:CYS:HB2	2:B:105:PRO:HD3	1.98	0.46
3:D:436:CYS:SG	3:D:437:CYS:N	2.89	0.45
4:C:398:PRO:O	4:C:401:THR:HG22	2.17	0.45
1:A:265:ARG:NH1	1:A:386:MET:O	2.50	0.45
4:C:202:HIS:HB3	4:C:205:LEU:HD12	1.98	0.45
4:C:508:ILE:HB	4:C:512:LEU:HD23	1.99	0.45
3:D:117:LEU:HG	3:D:130:PHE:HB3	1.98	0.45
3:D:111:ARG:HD2	3:D:131:ASN:OD1	2.16	0.45
4:C:547:THR:OG1	4:C:548:GLU:N	2.50	0.45
4:C:495:HIS:CE1	4:C:501:ARG:HG3	2.52	0.45
3:D:150:PRO:HA	3:D:230:SER:HB2	1.99	0.44
4:C:443:LEU:HA	4:C:446:ILE:HG22	1.99	0.44
1:A:528:GLU:HB2	1:A:534:TYR:CE1	2.52	0.44
2:B:169:HIS:CE1	2:B:241:THR:HB	2.52	0.44
2:B:305:GLU:OE1	2:B:305:GLU:N	2.42	0.44
3:D:277:ALA:HA	3:D:333:ARG:NH2	2.32	0.44
1:A:506:TRP:HZ2	1:A:539:LEU:HD11	1.83	0.44
1:A:550:ILE:O	1:A:551:LYS:HB2	2.18	0.44
1:A:534:TYR:HB3	1:A:535:VAL:HG22	1.99	0.44
1:A:565:ASN:O	1:A:567:ILE:N	2.48	0.44
4:C:295:THR:OG1	4:C:324:GLU:OE2	2.37	0.43
1:A:152:VAL:HA	1:A:231:HIS:O	2.18	0.43
1:A:398:PRO:O	1:A:401:THR:HG22	2.19	0.43
1:A:421:GLU:HG3	1:A:424:ARG:HH21	1.84	0.43
3:D:60:LEU:HD13	3:D:83:TRP:HB3	2.00	0.43
3:D:126:ASN:HA	3:D:129:TYR:CE2	2.53	0.43
4:C:482:PRO:HB3	4:C:564:PHE:CZ	2.54	0.43
3:D:558:VAL:HB	3:D:576:LEU:HB2	2.00	0.43
2:B:88:ASN:HB3	2:B:221:LYS:HG2	2.01	0.43
3:D:268:ALA:O	3:D:272:THR:HG23	2.19	0.43
1:A:295:THR:OG1	1:A:324:GLU:OE1	2.37	0.43
1:A:508:ILE:HB	1:A:512:LEU:HD23	2.01	0.43
1:A:90:ALA:HB2	2:B:510:TRP:CE2	2.53	0.43
1:A:453:ASP:OD2	1:A:456:SER:HB2	2.19	0.43
3:D:446:ILE:HD12	3:D:446:ILE:HA	1.89	0.43
3:D:482:PRO:HG3	3:D:564:PHE:CG	2.54	0.43
1:A:500:ALA:O	1:A:550:ILE:HD13	2.19	0.42
4:C:534:TYR:HB3	4:C:535:VAL:H	1.46	0.42
2:B:558:VAL:HB	2:B:576:LEU:HB2	2.01	0.42
2:B:209:LEU:O	2:B:210:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:291:VAL:HG22	3:D:342:VAL:HB	2.01	0.42
2:B:378:LYS:HB2	2:B:390:TYR:CZ	2.54	0.42
1:A:551:LYS:HB3	1:A:552:PRO:HD2	2.00	0.41
1:A:184:GLY:O	1:A:188:GLU:HB2	2.20	0.41
4:C:85:CYS:HA	4:C:228:CYS:HA	2.02	0.41
1:A:502:LEU:HD23	1:A:502:LEU:HA	1.85	0.41
2:B:256:ASN:N	8:B:905:PO4:O4	2.40	0.41
1:A:85:CYS:HA	1:A:228:CYS:HA	2.03	0.41
1:A:506:TRP:CZ2	1:A:539:LEU:HD11	2.55	0.41
3:D:378:LYS:HB2	3:D:390:TYR:CZ	2.56	0.41
1:A:88:ASN:HB3	1:A:221:LYS:HE3	2.02	0.41
2:B:85:CYS:HA	2:B:228:CYS:HA	2.03	0.41
2:B:488:ALA:HB1	2:B:576:LEU:HD11	2.02	0.41
4:C:292:PHE:CD2	4:C:341:LEU:HD11	2.55	0.41
1:A:523:GLU:HA	1:A:537:TYR:O	2.20	0.40
4:C:302:ASN:HB2	4:C:305:GLU:HB3	2.04	0.40
3:D:302:ASN:HB2	3:D:305:GLU:HB3	2.03	0.40
1:A:99:ASN:ND2	9:A:1001:HOH:O	2.42	0.40
2:B:523:GLU:CD	2:B:525:TRP:HE1	2.25	0.40
4:C:495:HIS:ND1	4:C:501:ARG:HG3	2.36	0.40
4:C:399:GLU:H	4:C:399:GLU:CD	2.24	0.40
2:B:246:GLY:HA2	2:B:249:GLN:O	2.21	0.40
4:C:446:ILE:HD12	4:C:446:ILE:HA	1.93	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	524/533 (98%)	493 (94%)	20 (4%)	11 (2%)	7 12
2	B	512/528 (97%)	488 (95%)	17 (3%)	7 (1%)	11 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
2	B	124	ASP
2	B	529	GLN
2	B	534	TYR
3	D	124	ASP
3	D	414	ILE
4	C	437	CYS
4	C	529	ALA
1	A	126	ALA
1	A	283	PRO
1	A	553	PHE
2	B	496	GLY
3	D	437	CYS
3	D	529	ALA
4	C	534	TYR
4	C	549	ASN
1	A	125	HIS
1	A	478	ALA
2	B	535	VAL
2	B	467	ALA
6	H	6	ALA
1	A	552	PRO
3	D	468	ALA
5	G	2	ALA
3	D	533	THR
4	C	210	SER
2	B	210	SER
3	D	467	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	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
4	C	444/453 (98%)	438 (99%)	6 (1%)	67	84
All	All	1795/1830 (98%)	1762 (98%)	33 (2%)	59	78

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ARG
1	A	87	SER
1	A	324	GLU
1	A	438	ARG
1	A	489	ARG
1	A	516	LYS
1	A	539	LEU
1	A	541	LEU
1	A	548	GLU
1	A	553	PHE
2	B	142	PHE
2	B	278	SER
2	B	292	PHE
2	B	333	ARG
2	B	438	ARG
2	B	495	HIS
2	B	516	LYS
3	D	76	ASP
3	D	120	SER
3	D	195	GLU
3	D	292	PHE
3	D	330	ASP
3	D	419	ARG
3	D	456	SER

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Mol	Chain	Res	Type
3	D	493	SER
3	D	516	LYS
3	D	534	TYR
4	C	225	ARG
4	C	227	LEU
4	C	292	PHE
4	C	297	ASN
4	C	534	TYR
4	C	543	ASN

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

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, 95^{th} 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

All (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
1	A	500	ALA	8.1
1	A	498	SER	8.0
3	D	496	GLY	7.7
4	C	498	SER	7.6
3	D	497	ALA	7.2
3	D	534	TYR	7.2
4	C	494	VAL	6.6
4	C	286	ALA	6.6
1	A	546	PHE	6.5
1	A	550	ILE	6.4
2	B	496	GLY	6.4
1	A	577	VAL	6.1
1	A	537	TYR	6.0
1	A	549	ASN	5.8

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Mol	Chain	Res	Type	RSRZ
2	B	494	VAL	5.4
1	A	555	THR	5.4
1	A	552	PRO	5.3
2	B	495	HIS	5.2
4	C	534	TYR	5.2
2	B	498	SER	5.1
1	A	526	LEU	5.1
1	A	496	GLY	5.0
1	A	492	ALA	5.0
1	A	535	VAL	5.0
1	A	501	ARG	4.9
4	C	533	ALA	4.8
4	C	500	ALA	4.8
1	A	554	THR	4.7
3	D	285	ALA	4.7
1	A	530	GLY	4.5
1	A	478	ALA	4.5
3	D	498	SER	4.5
4	C	285	ALA	4.4
1	A	532	ALA	4.4
3	D	532	ASN	4.3
3	D	533	THR	4.3
2	B	534	TYR	4.2
1	A	556	TYR	4.1
2	B	525	TRP	4.1
2	B	477	ALA	4.1
4	C	475	ALA	4.1
4	C	496	GLY	4.1
2	B	533	ALA	4.1
1	A	499	GLU	4.0
4	C	499	GLU	4.0
2	B	124	ASP	4.0
4	C	553	PHE	4.0
1	A	533	ALA	3.8
1	A	536	PRO	3.7
1	A	491	GLN	3.7
1	A	557	LEU	3.7
2	B	536	PRO	3.6
4	C	495	HIS	3.6
1	A	494	VAL	3.5
4	C	501	ARG	3.5
4	C	546	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	578	CYS	3.5
1	A	547	THR	3.5
4	C	476	ALA	3.5
4	C	492	ALA	3.4
1	A	531	GLU	3.4
3	D	495	HIS	3.3
3	D	414	ILE	3.3
1	A	142	PHE	3.2
4	C	515	LEU	3.1
2	B	553	PHE	3.1
1	A	541	LEU	3.1
3	D	306	LEU	3.1
1	A	504	VAL	3.1
1	A	525	TRP	3.0
3	D	409	TRP	3.0
1	A	576	LEU	3.0
2	B	478	ALA	3.0
4	C	222	THR	3.0
1	A	551	LYS	2.9
1	A	493	SER	2.9
2	B	493	SER	2.9
1	A	527	GLN	2.9
3	D	530	GLY	2.9
1	A	528	GLU	2.9
1	A	506	TRP	2.8
1	A	539	LEU	2.8
4	C	493	SER	2.8
3	D	141	ARG	2.8
4	C	467	GLY	2.8
1	A	495	HIS	2.8
4	C	470	PRO	2.7
1	A	567	ILE	2.7
3	D	463	ARG	2.7
4	C	544	HIS	2.7
4	C	537	TYR	2.7
4	C	532	ALA	2.6
1	A	490	CYS	2.6
4	C	278	SER	2.6
1	A	580	THR	2.6
6	H	5	ALA	2.6
2	B	285	ALA	2.5
2	B	209	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
4	C	489	ARG	2.5
4	C	549	ASN	2.5
4	C	437	CYS	2.5
4	C	469	ALA	2.5
2	B	515	LEU	2.5
1	A	502	LEU	2.4
3	D	142	PHE	2.4
4	C	141	ARG	2.4
4	C	227	LEU	2.4
3	D	69	CYS	2.4
1	A	538	ILE	2.4
4	C	142	PHE	2.4
2	B	476	ALA	2.4
4	C	491	GLN	2.4
4	C	277	ALA	2.3
1	A	503	THR	2.3
1	A	516	LYS	2.3
3	D	295	THR	2.3
1	A	558	VAL	2.2
4	C	148	PHE	2.2
4	C	521	LYS	2.2
5	G	1	ALA	2.2
2	B	227	LEU	2.2
3	D	516	LYS	2.1
3	D	312	GLN	2.1
6	H	3	ALA	2.1
2	B	142	PHE	2.1
2	B	466	ALA	2.1
3	D	296	GLN	2.1
1	A	141	ARG	2.1
5	G	2	ALA	2.0
3	D	515	LEU	2.0
4	C	477	ALA	2.0
4	C	58	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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.