



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 06:07 AM BST

PDB ID : 3QUM
Title : Crystal structure of human prostate specific antigen (PSA) in Fab sandwich with a high affinity and a PCa selective antibody
Authors : Stura, E.A.; Muller, B.H.; Michel, S.; Ducancel, F.
Deposited on : 2011-02-24
Resolution : 3.20 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 : 2.13.1
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) : 2.13.1

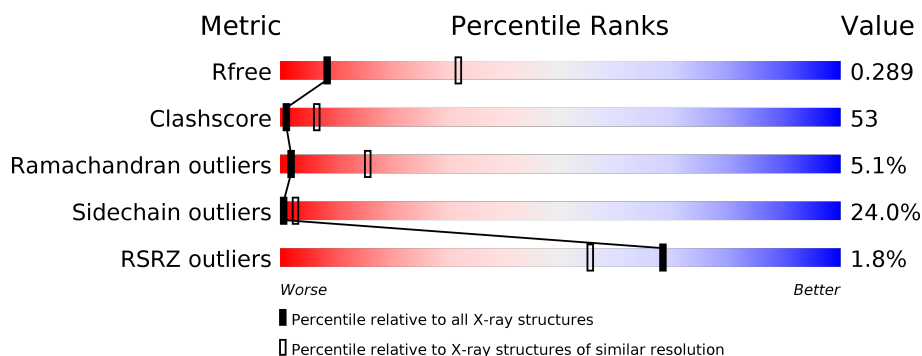
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	P	237	
1	Q	237	
2	L	219	
2	M	219	
3	H	219	
3	K	219	

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Mol	Chain	Length	Quality of chain
4	A	218	
4	C	218	
5	B	219	
5	D	219	
6	E	15	
7	F	2	
8	G	15	

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
6	GAL	E	10	-	-	-	X
6	SIA	E	11	-	-	-	X
6	NAG	E	12	-	-	-	X
6	SIA	E	14	-	-	-	X
6	SIA	E	7	-	-	-	X
6	NAG	E	9	-	-	-	X
8	GAL	G	10	-	-	-	X
8	GAL	G	13	-	-	-	X
8	SIA	G	14	-	-	-	X
8	NAG	G	2	-	-	-	X
8	MAN	G	4	-	-	-	X
8	GAL	G	6	-	-	-	X
8	SIA	G	7	-	-	-	X
8	NAG	G	9	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17606 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 Prostate-specific antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	237	Total	C	N	O	S	4	0	0
			1832	1162	323	333	14			
1	Q	237	Total	C	N	O	S	0	0	0
			1832	1162	323	333	14			

- Molecule 2 is a protein called Fab 5D3D11 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	219	Total	C	N	O	S	0	0	0
			1704	1063	289	343	9			
2	M	219	Total	C	N	O	S	0	0	0
			1704	1063	289	343	9			

- Molecule 3 is a protein called Fab 5D3D11 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	217	Total	C	N	O	S	0	0	0
			1637	1040	267	323	7			
3	K	219	Total	C	N	O	S	0	0	0
			1657	1050	272	328	7			

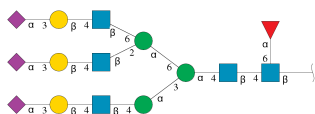
- Molecule 4 is a protein called Fab 5D5A5 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	218	Total	C	N	O	S	0	0	0
			1701	1062	287	345	7			
4	C	218	Total	C	N	O	S	0	0	0
			1701	1062	287	345	7			

- Molecule 5 is a protein called Fab 5D5A5 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	219	Total	C	N	O	S	0	0	0
			1655	1043	273	330	9			
5	D	219	Total	C	N	O	S	0	0	0
			1655	1043	273	330	9			

- Molecule 6 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



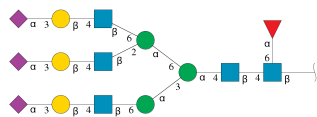
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	E	15	Total	C	N	O	0	0	0
			206	115	8	83			

- Molecule 7 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	F	2	Total	C	N	O	0	0	0
			25	14	1	10			

- Molecule 8 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

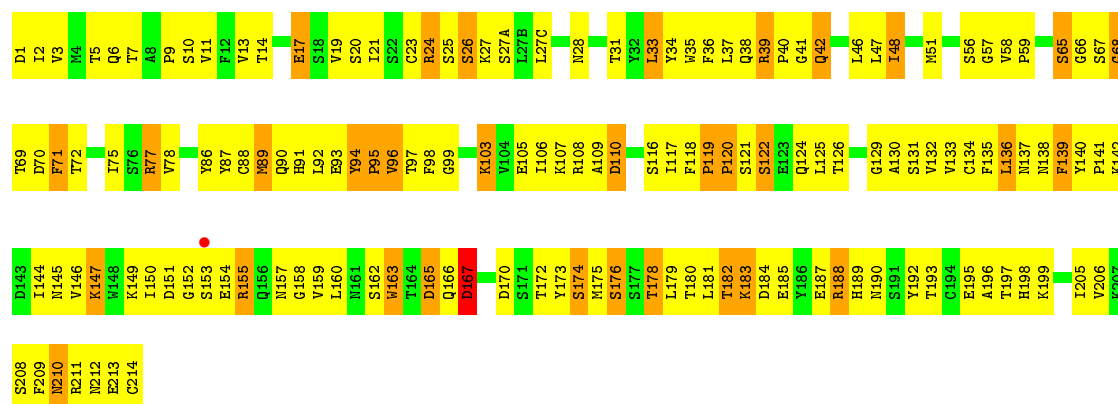


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	G	15	Total	C	N	O	0	0	0
			206	115	8	83			

- Molecule 9 is water.

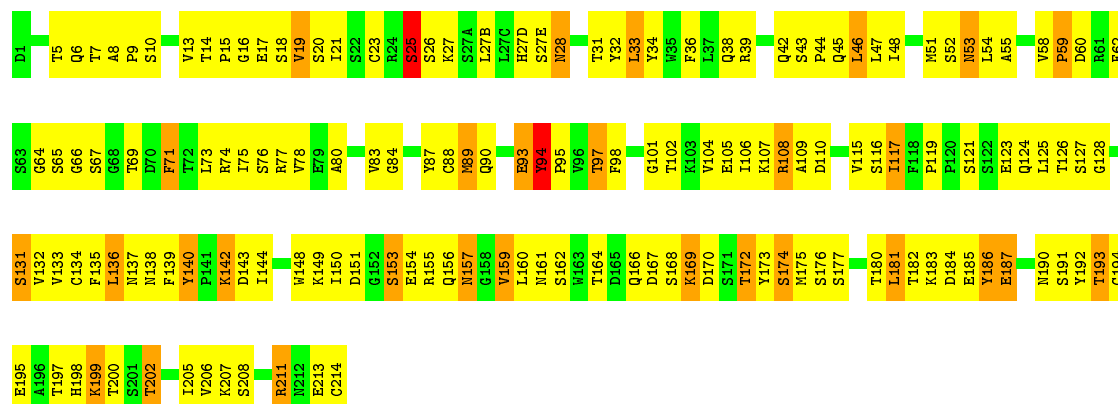
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	P	26	Total	O	0	0
			26	26		
9	L	4	Total	O	0	0
			4	4		
9	H	10	Total	O	0	0
			10	10		
9	A	4	Total	O	0	0
			4	4		
9	B	4	Total	O	0	0
			4	4		
9	Q	5	Total	O	0	0
			5	5		
9	M	6	Total	O	0	0
			6	6		
9	K	14	Total	O	0	0
			14	14		
9	C	11	Total	O	0	0
			11	11		
9	D	7	Total	O	0	0
			7	7		

Chain L:  31% 54% 15%

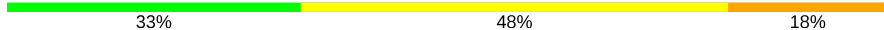


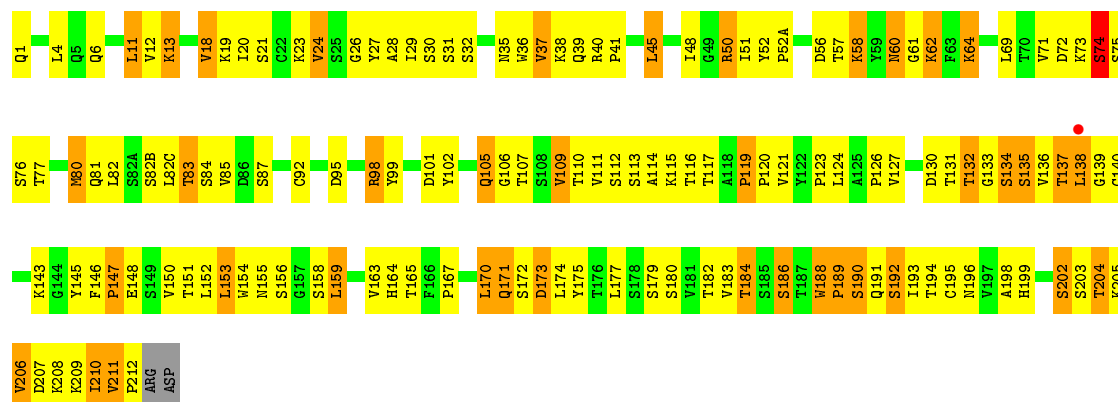
• Molecule 2: Fab 5D3D11 Light Chain

Chain M:  30% 56% 13%

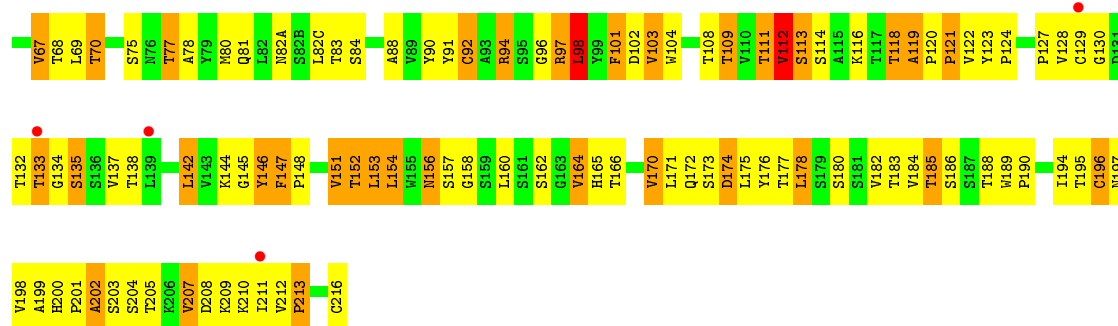


• Molecule 3: Fab 5D3D11 Heavy Chain

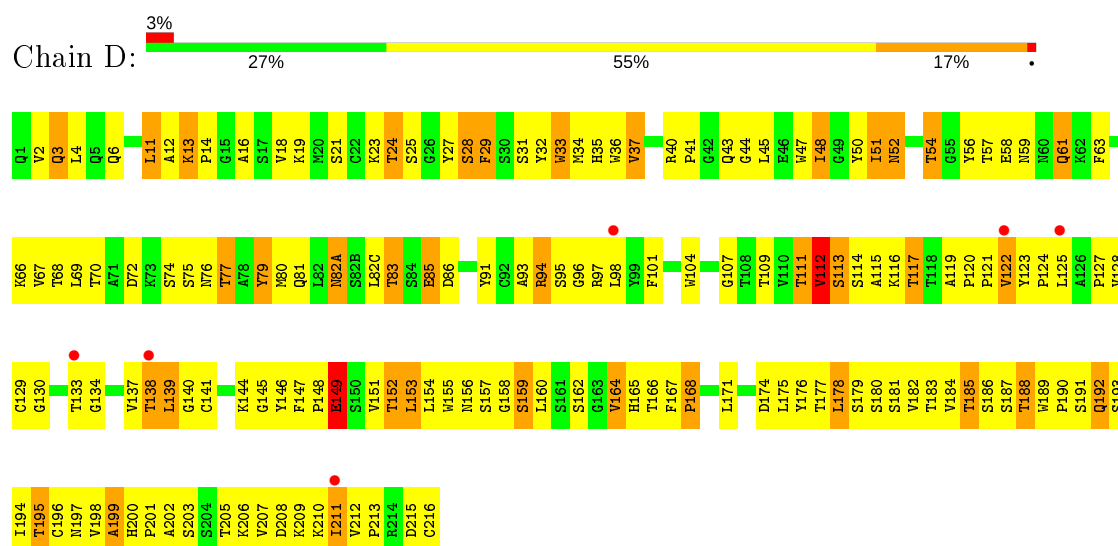
Chain H:  33% 48% 18%



• Molecule 3: Fab 5D3D11 Heavy Chain



• Molecule 5: Fab 5D5A5 Heavy Chain



• Molecule 6: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 7: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose



• Molecule 8: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid

-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.31Å 226.88Å 118.69Å 90.00° 96.51° 90.00°	Depositor
Resolution (Å)	58.97 – 3.20 81.76 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (58.97-3.20) 98.3 (81.76-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.198 , 0.294 0.194 , 0.289	Depositor DCC
R_{free} test set	2370 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	78.1	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 75.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17606	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: NAG, SIA, GAL, FUC, A2G, MAN

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	P	0.73	2/1883 (0.1%)	0.87	1/2564 (0.0%)
1	Q	0.45	0/1883	0.67	0/2564
2	L	0.58	0/1743	0.76	2/2366 (0.1%)
2	M	0.63	0/1743	0.76	0/2366
3	H	0.64	0/1680	0.80	1/2294 (0.0%)
3	K	0.71	0/1700	0.76	0/2319
4	A	0.53	0/1742	0.71	0/2368
4	C	0.58	0/1742	0.72	0/2368
5	B	0.57	0/1697	0.72	2/2316 (0.1%)
5	D	0.51	0/1697	0.72	0/2316
All	All	0.60	2/17510 (0.0%)	0.75	6/23841 (0.0%)

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	P	0	2
2	M	0	1
3	H	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	168	CYS	CB-SG	-6.03	1.72	1.82
1	P	220	CYS	CA-C	-5.33	1.39	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	113	SER	N-CA-C	6.26	127.91	111.00
2	L	33	LEU	CA-CB-CG	5.68	128.37	115.30
5	B	98	LEU	CA-CB-CG	-5.64	102.33	115.30
2	L	27(C)	LEU	CA-CB-CG	5.44	127.82	115.30
3	H	45	LEU	CA-CB-CG	5.24	127.34	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	98	ARG	Sidechain
2	M	93	GLU	Peptide
1	P	153	LYS	Peptide
1	P	95(J)	ARG	Sidechain

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	P	1832	0	1802	208	0
1	Q	1832	0	1803	255	0
2	L	1704	0	1636	176	0
2	M	1704	0	1636	161	0
3	H	1637	0	1607	149	0
3	K	1657	0	1624	144	0
4	A	1701	0	1624	189	0
4	C	1701	0	1624	184	0
5	B	1655	0	1612	217	0
5	D	1655	0	1612	211	0
6	E	206	0	172	10	0
7	F	25	0	21	1	0
8	G	206	0	172	13	0
9	A	4	0	0	0	0
9	B	4	0	0	3	0
9	C	11	0	0	0	0
9	D	7	0	0	2	0
9	H	10	0	0	1	0
9	K	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	4	0	0	3	0
9	M	6	0	0	2	0
9	P	26	0	0	5	0
9	Q	5	0	0	2	0
All	All	17606	0	16945	1821	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 53.

The worst 5 of 1821 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)
5:D:120:PRO:HG2	5:D:146:TYR:CD1	1.76	1.20
1:P:161:HIS:CE1	1:P:185:ARG:HH21	1.64	1.15
1:Q:73:PHE:HE2	1:Q:153:LYS:HA	1.09	1.14
5:B:111:THR:O	5:B:112:VAL:HG12	1.48	1.14
1:P:237:TRP:O	1:P:241:THR:HG22	1.46	1.12

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	P	235/237 (99%)	195 (83%)	31 (13%)	9 (4%)	3	22
1	Q	235/237 (99%)	186 (79%)	39 (17%)	10 (4%)	2	20
2	L	217/219 (99%)	166 (76%)	39 (18%)	12 (6%)	2	14
2	M	217/219 (99%)	177 (82%)	31 (14%)	9 (4%)	3	21
3	H	215/219 (98%)	186 (86%)	18 (8%)	11 (5%)	2	15
3	K	217/219 (99%)	181 (83%)	32 (15%)	4 (2%)	8	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	216/218 (99%)	177 (82%)	22 (10%)	17 (8%)	1	6
4	C	216/218 (99%)	173 (80%)	30 (14%)	13 (6%)	1	12
5	B	217/219 (99%)	166 (76%)	35 (16%)	16 (7%)	1	7
5	D	217/219 (99%)	163 (75%)	42 (19%)	12 (6%)	2	14
All	All	2202/2224 (99%)	1770 (80%)	319 (14%)	113 (5%)	2	15

5 of 113 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	95	PRO
2	L	167	ASP
2	L	174	SER
3	H	173	ASP
4	A	17	GLN

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	P	205/205 (100%)	161 (78%)	44 (22%)	1	5
1	Q	205/205 (100%)	150 (73%)	55 (27%)	0	2
2	L	196/196 (100%)	160 (82%)	36 (18%)	1	8
2	M	196/196 (100%)	146 (74%)	50 (26%)	0	2
3	H	187/189 (99%)	135 (72%)	52 (28%)	0	1
3	K	189/189 (100%)	148 (78%)	41 (22%)	1	5
4	A	193/193 (100%)	152 (79%)	41 (21%)	1	5
4	C	193/193 (100%)	143 (74%)	50 (26%)	0	2
5	B	189/189 (100%)	135 (71%)	54 (29%)	0	1
5	D	189/189 (100%)	145 (77%)	44 (23%)	1	3
All	All	1942/1944 (100%)	1475 (76%)	467 (24%)	0	3

5 of 467 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	152	THR
1	Q	155	LEU
5	D	37	VAL
5	B	164	VAL
1	Q	67	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	30	GLN
2	M	38	GLN
5	D	52	ASN
1	Q	70	HIS
1	Q	174	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

32 monosaccharides 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$
6	NAG	E	1	1,6	14,14,15	1.14	1 (7%)	17,19,21	1.83	4 (23%)
6	GAL	E	10	6	11,11,12	1.26	2 (18%)	15,15,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SIA	E	11	6	17,20,21	2.19	5 (29%)	21,28,31	1.68	3 (14%)
6	NAG	E	12	6	14,14,15	0.54	0	17,19,21	0.99	1 (5%)
6	GAL	E	13	6	11,11,12	0.55	0	15,15,17	1.91	5 (33%)
6	SIA	E	14	6	17,20,21	0.62	0	21,28,31	2.26	6 (28%)
6	FUC	E	15	6	10,10,11	0.67	0	14,14,16	0.73	0
6	NAG	E	2	6	14,14,15	0.60	0	17,19,21	1.15	2 (11%)
6	MAN	E	3	6	11,11,12	1.14	1 (9%)	15,15,17	2.11	5 (33%)
6	MAN	E	4	6	11,11,12	0.73	0	15,15,17	1.62	3 (20%)
6	NAG	E	5	6	14,14,15	0.80	1 (7%)	17,19,21	1.91	3 (17%)
6	GAL	E	6	6	11,11,12	0.66	0	15,15,17	1.38	2 (13%)
6	SIA	E	7	6	17,20,21	0.81	0	21,28,31	1.29	2 (9%)
6	MAN	E	8	6	11,11,12	0.68	0	15,15,17	2.57	5 (33%)
6	NAG	E	9	6	14,14,15	0.69	0	17,19,21	1.58	2 (11%)
7	A2G	F	1	1,7	14,14,15	0.70	0	17,19,21	1.13	2 (11%)
7	GAL	F	2	7	11,11,12	0.74	0	15,15,17	1.37	3 (20%)
8	NAG	G	1	1,8	14,14,15	0.58	0	17,19,21	2.07	5 (29%)
8	GAL	G	10	8	11,11,12	0.82	0	15,15,17	1.98	5 (33%)
8	SIA	G	11	8	17,20,21	0.52	0	21,28,31	1.24	1 (4%)
8	NAG	G	12	8	14,14,15	0.57	0	17,19,21	2.64	6 (35%)
8	GAL	G	13	8	11,11,12	0.93	1 (9%)	15,15,17	1.30	2 (13%)
8	SIA	G	14	8	17,20,21	0.69	0	21,28,31	1.68	3 (14%)
8	FUC	G	15	8	10,10,11	0.64	0	14,14,16	1.83	4 (28%)
8	NAG	G	2	8	14,14,15	0.57	0	17,19,21	1.70	4 (23%)
8	MAN	G	3	8	11,11,12	0.73	0	15,15,17	2.56	7 (46%)
8	MAN	G	4	8	11,11,12	0.68	0	15,15,17	1.69	3 (20%)
8	NAG	G	5	8	14,14,15	0.63	0	17,19,21	1.69	5 (29%)
8	GAL	G	6	8	11,11,12	0.74	0	15,15,17	1.18	1 (6%)
8	SIA	G	7	8	17,20,21	0.71	0	21,28,31	1.56	1 (4%)
8	MAN	G	8	8	11,11,12	0.74	0	15,15,17	2.32	4 (26%)
8	NAG	G	9	8	14,14,15	1.36	1 (7%)	17,19,21	1.63	5 (29%)

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
6	NAG	E	1	1,6	-	0/6/23/26	0/1/1/1
6	GAL	E	10	6	-	2/2/19/22	0/1/1/1
6	SIA	E	11	6	-	12/14/34/38	0/1/1/1
6	NAG	E	12	6	-	0/6/23/26	0/1/1/1
6	GAL	E	13	6	-	1/2/19/22	0/1/1/1
6	SIA	E	14	6	-	8/14/34/38	0/1/1/1
6	FUC	E	15	6	-	-	0/1/1/1
6	NAG	E	2	6	-	1/6/23/26	0/1/1/1
6	MAN	E	3	6	-	1/2/19/22	0/1/1/1
6	MAN	E	4	6	-	1/2/19/22	1/1/1/1
6	NAG	E	5	6	-	2/6/23/26	0/1/1/1
6	GAL	E	6	6	-	2/2/19/22	0/1/1/1
6	SIA	E	7	6	-	10/14/34/38	0/1/1/1
6	MAN	E	8	6	-	2/2/19/22	0/1/1/1
6	NAG	E	9	6	-	2/6/23/26	0/1/1/1
7	A2G	F	1	1,7	-	2/6/23/26	0/1/1/1
7	GAL	F	2	7	-	1/2/19/22	0/1/1/1
8	NAG	G	1	1,8	-	2/6/23/26	0/1/1/1
8	GAL	G	10	8	-	1/2/19/22	0/1/1/1
8	SIA	G	11	8	-	8/14/34/38	0/1/1/1
8	NAG	G	12	8	-	3/6/23/26	0/1/1/1
8	GAL	G	13	8	-	1/2/19/22	0/1/1/1
8	SIA	G	14	8	-	3/14/34/38	0/1/1/1
8	FUC	G	15	8	-	-	0/1/1/1
8	NAG	G	2	8	-	2/6/23/26	0/1/1/1
8	MAN	G	3	8	-	0/2/19/22	0/1/1/1
8	MAN	G	4	8	-	1/2/19/22	0/1/1/1
8	NAG	G	5	8	-	2/6/23/26	0/1/1/1
8	GAL	G	6	8	-	2/2/19/22	0/1/1/1
8	SIA	G	7	8	-	2/14/34/38	0/1/1/1
8	MAN	G	8	8	-	2/2/19/22	0/1/1/1
8	NAG	G	9	8	-	0/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	11	SIA	C11-C10	-4.91	1.40	1.50
6	E	11	SIA	O10-C10	-4.61	1.12	1.23
8	G	9	NAG	O5-C1	-4.53	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	11	SIA	C10-N5	3.77	1.47	1.34
6	E	10	GAL	O3-C3	2.95	1.49	1.43

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	8	MAN	C1-O5-C5	7.58	122.47	112.19
8	G	3	MAN	C1-O5-C5	6.08	120.43	112.19
8	G	7	SIA	C6-O6-C2	5.99	124.16	111.34
8	G	8	MAN	O2-C2-C1	5.79	121.00	109.15
8	G	12	NAG	C1-O5-C5	5.77	120.01	112.19

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	7	SIA	C5-C6-C7-C8
6	E	7	SIA	C5-C6-C7-O7
6	E	7	SIA	O6-C6-C7-C8
6	E	7	SIA	O6-C6-C7-O7
6	E	7	SIA	O7-C7-C8-C9

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	4	MAN	C1-C2-C3-C4-C5-O5

18 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	7	SIA	2	0
6	E	3	MAN	3	0
8	G	1	NAG	2	0
8	G	5	NAG	1	0
8	G	11	SIA	3	0
6	E	4	MAN	2	0
8	G	8	MAN	2	0
6	E	13	GAL	1	0
8	G	3	MAN	1	0
8	G	4	MAN	1	0
6	E	14	SIA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	12	NAG	4	0
8	G	9	NAG	2	0
7	F	1	A2G	1	0
6	E	2	NAG	2	0
6	E	5	NAG	1	0
6	E	6	GAL	1	0
8	G	6	GAL	1	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	P	237/237 (100%)	0.01	11 (4%) 32 20	28, 49, 123, 155	4 (1%)
1	Q	237/237 (100%)	0.22	12 (5%) 28 16	58, 94, 155, 193	0
2	L	219/219 (100%)	-0.03	1 (0%) 91 86	36, 76, 123, 155	0
2	M	219/219 (100%)	-0.21	0 100 100	46, 71, 104, 154	0
3	H	217/219 (99%)	-0.16	1 (0%) 91 86	27, 52, 139, 172	0
3	K	219/219 (100%)	-0.28	0 100 100	33, 56, 83, 142	0
4	A	218/218 (100%)	-0.03	1 (0%) 91 86	51, 79, 104, 141	0
4	C	218/218 (100%)	0.03	5 (2%) 60 47	50, 76, 109, 150	0
5	B	219/219 (100%)	0.04	4 (1%) 68 55	48, 84, 118, 157	0
5	D	219/219 (100%)	0.01	6 (2%) 54 39	53, 85, 113, 140	0
All	All	2222/2224 (99%)	-0.04	41 (1%) 68 55	27, 74, 124, 193	4 (0%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	152	PRO	9.4
1	P	192	SER	7.3
1	Q	192	SER	5.4
1	P	150	LEU	4.9
1	P	146	PRO	4.6

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

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

6.3 Carbohydrates ⓘ

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	SIA	G	7	20/21	0.36	0.54	116,118,118,118	20
8	NAG	G	12	14/15	0.39	0.36	134,136,137,139	14
8	MAN	G	4	11/12	0.39	0.52	119,121,122,122	11
8	NAG	G	9	14/15	0.40	0.49	130,131,132,132	14
6	MAN	E	3	11/12	0.41	0.23	112,114,118,118	0
8	NAG	G	5	14/15	0.41	0.40	115,117,117,118	14
8	GAL	G	6	11/12	0.42	0.45	116,117,118,118	11
6	MAN	E	4	11/12	0.45	0.37	120,121,122,122	0
8	GAL	G	13	11/12	0.45	0.79	141,142,143,143	0
6	NAG	E	9	14/15	0.48	0.45	119,121,121,121	14
6	SIA	E	11	20/21	0.49	0.47	115,119,119,119	20
6	GAL	E	10	11/12	0.49	0.48	118,119,119,119	11
8	SIA	G	14	20/21	0.50	0.52	144,145,146,146	0
6	SIA	E	14	20/21	0.51	0.43	106,108,110,110	20
8	MAN	G	3	11/12	0.54	0.32	123,124,127,129	0
8	MAN	G	8	11/12	0.55	0.39	130,132,133,134	11
6	SIA	E	7	20/21	0.60	0.41	117,119,120,120	20
6	NAG	E	12	14/15	0.62	0.47	114,116,117,117	14
6	GAL	E	6	11/12	0.62	0.37	122,122,123,123	11
8	GAL	G	10	11/12	0.64	0.53	131,132,132,132	11
8	SIA	G	11	20/21	0.68	0.35	131,132,133,133	20
8	NAG	G	2	14/15	0.70	0.41	112,114,116,120	14
6	NAG	E	5	14/15	0.75	0.34	123,123,124,124	0
7	A2G	F	1	14/15	0.77	0.36	60,63,65,65	14
6	MAN	E	8	11/12	0.78	0.25	117,119,120,120	11
7	GAL	F	2	11/12	0.80	0.43	65,66,66,66	11
6	GAL	E	13	11/12	0.80	0.29	111,112,112,112	11
8	NAG	G	1	14/15	0.82	0.19	96,99,101,104	0
6	NAG	E	2	14/15	0.83	0.19	97,99,102,107	0
8	FUC	G	15	10/11	0.86	0.33	100,101,101,101	0
6	NAG	E	1	14/15	0.90	0.15	73,77,83,89	0
6	FUC	E	15	10/11	0.95	0.11	88,88,89,89	0

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.