



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 03:09 PM GMT

PDB ID : 2O26
Title : Structure of a class III RTK signaling assembly
Authors : Liu, H.; Chen, X.; Focia, P.J.; He, X.
Deposited on : 2006-11-29
Resolution : 2.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

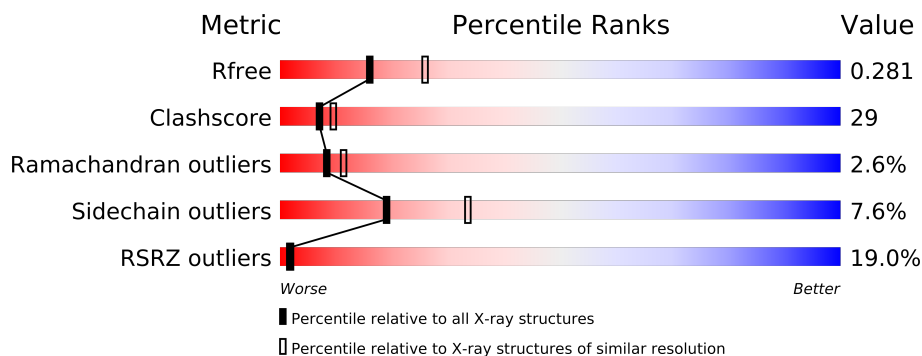
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	145	
1	B	145	
1	E	145	
1	F	145	
2	U	290	
2	W	290	
2	X	290	
2	Y	290	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15104 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Kit ligand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1140	722	189	220	9			
1	B	139	Total	C	N	O	S	0	0	0
			1090	692	174	215	9			
1	E	139	Total	C	N	O	S	0	0	0
			1090	692	174	215	9			
1	F	139	Total	C	N	O	S	0	0	0
			1090	692	174	215	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	HIS	-	EXPRESSION TAG	UNP P20826
A	143	HIS	-	EXPRESSION TAG	UNP P20826
A	144	HIS	-	EXPRESSION TAG	UNP P20826
A	145	HIS	-	EXPRESSION TAG	UNP P20826
A	146	HIS	-	EXPRESSION TAG	UNP P20826
A	147	HIS	-	EXPRESSION TAG	UNP P20826
B	142	HIS	-	EXPRESSION TAG	UNP P20826
B	143	HIS	-	EXPRESSION TAG	UNP P20826
B	144	HIS	-	EXPRESSION TAG	UNP P20826
B	145	HIS	-	EXPRESSION TAG	UNP P20826
B	146	HIS	-	EXPRESSION TAG	UNP P20826
B	147	HIS	-	EXPRESSION TAG	UNP P20826
E	142	HIS	-	EXPRESSION TAG	UNP P20826
E	143	HIS	-	EXPRESSION TAG	UNP P20826
E	144	HIS	-	EXPRESSION TAG	UNP P20826
E	145	HIS	-	EXPRESSION TAG	UNP P20826
E	146	HIS	-	EXPRESSION TAG	UNP P20826
E	147	HIS	-	EXPRESSION TAG	UNP P20826
F	142	HIS	-	EXPRESSION TAG	UNP P20826
F	143	HIS	-	EXPRESSION TAG	UNP P20826
F	144	HIS	-	EXPRESSION TAG	UNP P20826

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Chain	Residue	Modelled	Actual	Comment	Reference
F	145	HIS	-	EXPRESSION TAG	UNP P20826
F	146	HIS	-	EXPRESSION TAG	UNP P20826
F	147	HIS	-	EXPRESSION TAG	UNP P20826

- Molecule 2 is a protein called Mast/stem cell growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	275	Total	C	N	O	S	0	0	0
			2164	1369	372	411	12			
2	Y	275	Total	C	N	O	S	0	0	0
			2164	1369	372	411	12			
2	U	275	Total	C	N	O	S	0	0	0
			2164	1369	372	411	12			
2	W	275	Total	C	N	O	S	0	0	0
			2164	1369	372	411	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	146	GLN	ASN	ENGINEERED	UNP P05532
Y	146	GLN	ASN	ENGINEERED	UNP P05532
U	146	GLN	ASN	ENGINEERED	UNP P05532
W	146	GLN	ASN	ENGINEERED	UNP P05532

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	X	3	Total	C	N	O	0	0
			38	22	2	14		
3	Y	3	Total	C	N	O	0	0
			38	22	2	14		
3	U	3	Total	C	N	O	0	0
			38	22	2	14		
3	W	3	Total	C	N	O	0	0
			38	22	2	14		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	146	GLN	ASN	ENGINEERED	UNP P05532
Y	146	GLN	ASN	ENGINEERED	UNP P05532
U	146	GLN	ASN	ENGINEERED	UNP P05532

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Chain	Residue	Modelled	Actual	Comment	Reference
W	146	GLN	ASN	ENGINEERED	UNP P05532

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	X	3	Total	C	N	O	0	0
			39	22	2	15		
4	Y	3	Total	C	N	O	0	0
			39	22	2	15		
4	U	3	Total	C	N	O	0	0
			39	22	2	15		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	146	GLN	ASN	ENGINEERED	UNP P05532
Y	146	GLN	ASN	ENGINEERED	UNP P05532
U	146	GLN	ASN	ENGINEERED	UNP P05532

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	W	3	Total	C	N	O	0	0
			39	22	2	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	146	GLN	ASN	ENGINEERED	UNP P05532

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	171	Total	O	0	0
			171	171		
6	B	144	Total	O	0	0
			144	144		
6	E	152	Total	O	0	0
			152	152		
6	F	143	Total	O	0	0
			143	143		

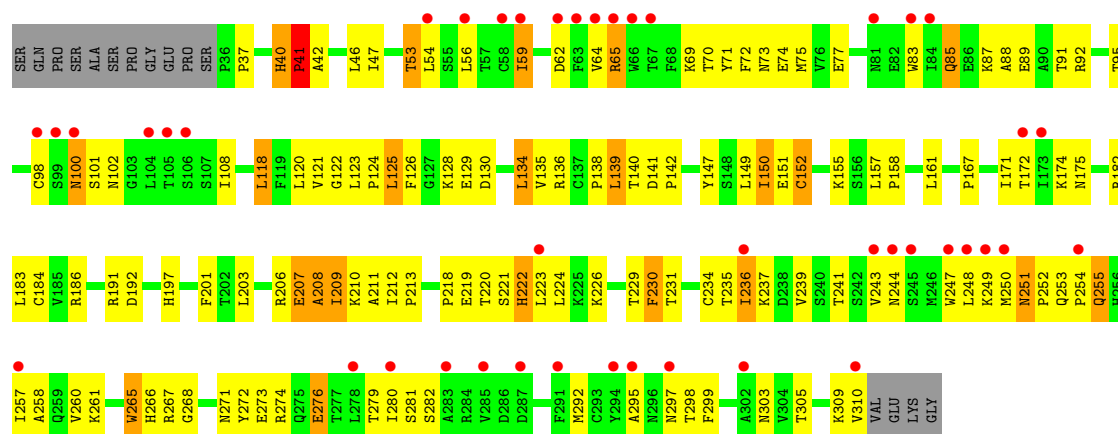
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	U	270	Total 270	O 270	0	0
6	W	267	Total 267	O 267	0	0
6	X	273	Total 273	O 273	0	0
6	Y	310	Total 310	O 310	0	0

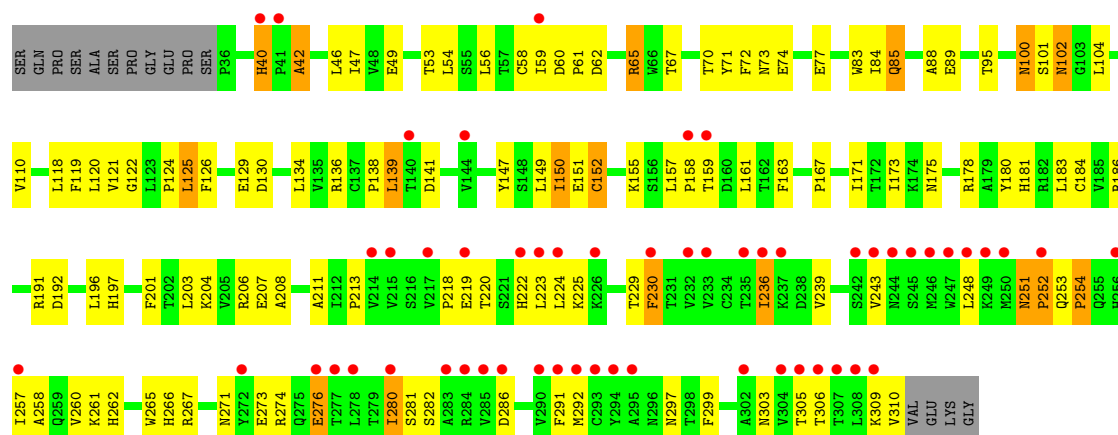
• Molecule 2: Mast/stem cell growth factor receptor

Chain X:



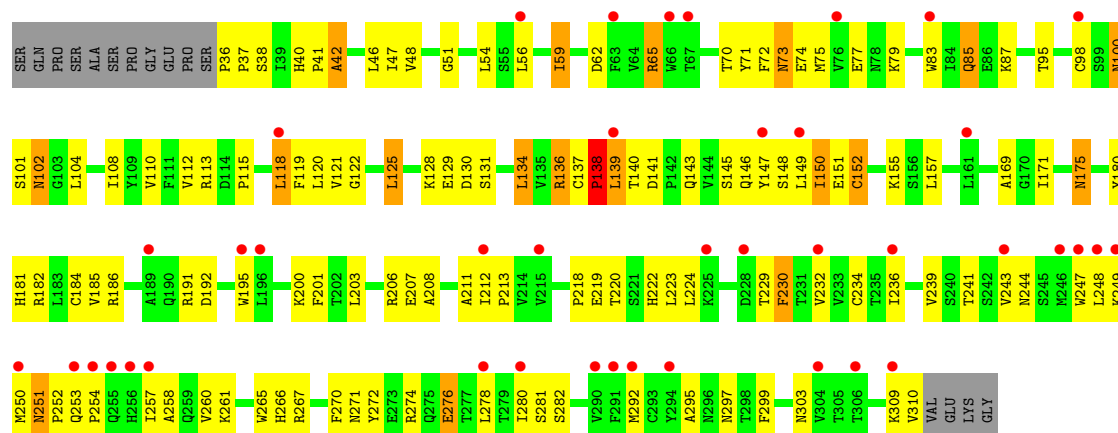
• Molecule 2: Mast/stem cell growth factor receptor

Chain Y:



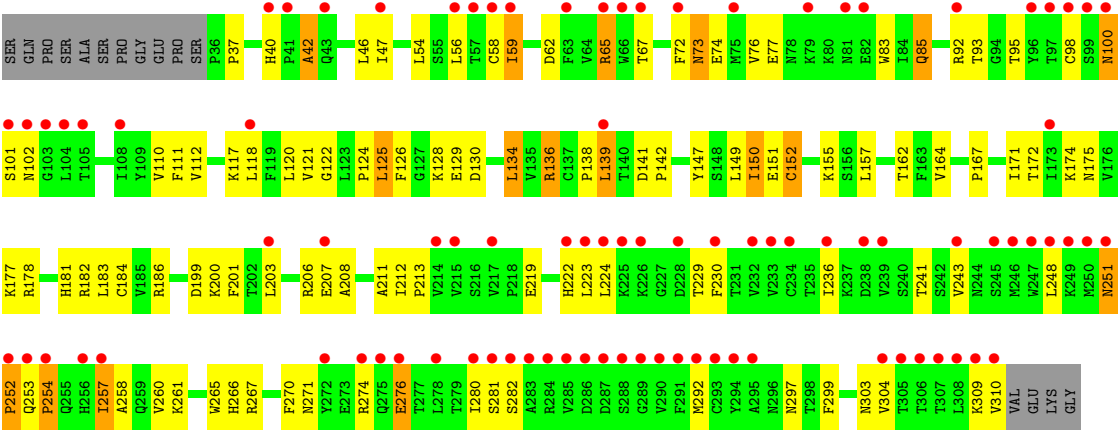
• Molecule 2: Mast/stem cell growth factor receptor

Chain U:



• Molecule 2: Mast/stem cell growth factor receptor

Chain W: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.85Å 200.15Å 82.02Å 90.00° 91.42° 90.00°	Depositor
Resolution (Å)	19.93 – 2.50 48.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.93-2.50) 96.8 (48.46-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.270 0.251 , 0.281	Depositor DCC
R_{free} test set	4160 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 75.7	EDS
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 82592 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15104	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUL, NAG, NDG, 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	A	0.40	0/1164	0.70	1/1579 (0.1%)
1	B	0.48	1/1109 (0.1%)	0.67	0/1504
1	E	0.40	0/1109	0.64	1/1504 (0.1%)
1	F	0.41	0/1109	0.65	1/1504 (0.1%)
2	U	0.38	0/2214	0.72	1/3011 (0.0%)
2	W	0.35	0/2214	0.64	0/3011
2	X	0.37	0/2214	0.69	2/3011 (0.1%)
2	Y	0.36	0/2214	0.65	0/3011
All	All	0.39	1/13347 (0.0%)	0.67	6/18135 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	SER	CA-CB	7.77	1.64	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	138	PRO	CA-N-CD	-14.78	90.81	111.50
2	X	41	PRO	CA-N-CD	-12.45	94.08	111.50
1	A	102	PRO	CA-N-CD	-8.86	99.09	111.50
1	F	134	ASP	C-N-CA	-5.22	108.64	121.70
2	X	208	ALA	N-CA-C	-5.22	96.92	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1140	0	1121	62	0
1	B	1090	0	1086	68	0
1	E	1090	0	1086	65	0
1	F	1090	0	1086	54	0
2	U	2164	0	2140	139	0
2	W	2164	0	2140	117	0
2	X	2164	0	2140	145	0
2	Y	2164	0	2140	125	0
3	U	38	0	34	3	0
3	W	38	0	34	0	0
3	X	38	0	34	1	0
3	Y	38	0	34	2	0
4	U	39	0	34	0	0
4	X	39	0	34	1	0
4	Y	39	0	34	1	0
5	W	39	0	34	2	0
6	A	171	0	0	24	0
6	B	144	0	0	32	0
6	E	152	0	0	24	0
6	F	143	0	0	23	0
6	U	270	0	0	37	0
6	W	267	0	0	35	0
6	X	273	0	0	50	0
6	Y	310	0	0	46	0
All	All	15104	0	13211	761	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 29.

The worst 5 of 761 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:W:184:CYS:HB2	6:W:321:HOH:O	1.50	1.08
2:U:251:ASN:HB2	2:U:252:PRO:HD3	1.36	1.06
2:Y:251:ASN:HB2	2:Y:252:PRO:HD3	1.34	1.06

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:W:251:ASN:HB2	2:W:252:PRO:HD3	1.37	1.06
2:X:251:ASN:HB2	2:X:252:PRO:HD3	1.35	1.03

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	142/145 (98%)	124 (87%)	13 (9%)	5 (4%)	6	7
1	B	137/145 (94%)	122 (89%)	10 (7%)	5 (4%)	5	6
1	E	137/145 (94%)	124 (90%)	9 (7%)	4 (3%)	7	9
1	F	137/145 (94%)	121 (88%)	12 (9%)	4 (3%)	7	9
2	U	273/290 (94%)	252 (92%)	15 (6%)	6 (2%)	10	15
2	W	273/290 (94%)	255 (93%)	12 (4%)	6 (2%)	10	15
2	X	273/290 (94%)	253 (93%)	15 (6%)	5 (2%)	13	20
2	Y	273/290 (94%)	249 (91%)	16 (6%)	8 (3%)	7	9
All	All	1645/1740 (94%)	1500 (91%)	102 (6%)	43 (3%)	8	11

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	102	PRO
1	E	102	PRO
1	F	102	PRO
2	X	73	ASN
2	Y	73	ASN

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	135/136 (99%)	124 (92%)	11 (8%)	17	30
1	B	130/136 (96%)	119 (92%)	11 (8%)	15	28
1	E	130/136 (96%)	120 (92%)	10 (8%)	18	33
1	F	130/136 (96%)	120 (92%)	10 (8%)	18	33
2	U	247/259 (95%)	231 (94%)	16 (6%)	24	42
2	W	247/259 (95%)	230 (93%)	17 (7%)	22	39
2	X	247/259 (95%)	224 (91%)	23 (9%)	13	23
2	Y	247/259 (95%)	230 (93%)	17 (7%)	22	39
All	All	1513/1580 (96%)	1398 (92%)	115 (8%)	19	33

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	X	125	LEU
2	X	276	GLU
2	W	134	LEU
2	X	134	LEU
2	X	209	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	X	255	GLN
2	Y	100	ASN
2	W	251	ASN
2	X	297	ASN
2	Y	102	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

24 carbohydrates 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	$\# Z > 2$
3	FUL	U	1	3	9,10,11	0.44	0	10,14,16	0.39	0
3	NAG	U	2	3,2	12,14,15	0.71	0	15,19,21	1.07	1 (6%)
3	NAG	U	3	3	12,14,15	0.48	0	15,19,21	0.79	0
4	NAG	U	4	2,4	12,14,15	0.79	0	15,19,21	1.13	2 (13%)
4	NAG	U	5	4	12,14,15	0.71	0	15,19,21	0.68	0
4	MAN	U	6	4	10,11,12	0.46	0	11,15,17	0.52	0
3	FUL	W	1	3	9,10,11	0.41	0	10,14,16	0.38	0
3	NAG	W	2	3,2	12,14,15	0.60	0	15,19,21	0.84	0
3	NAG	W	3	3	12,14,15	0.45	0	15,19,21	0.53	0
5	NDG	W	4	2,5	12,14,15	0.65	0	15,19,21	0.50	0
5	NAG	W	5	5	12,14,15	0.63	0	15,19,21	0.77	0
5	MAN	W	6	5	10,11,12	0.50	0	11,15,17	0.51	0
3	FUL	X	1	3	9,10,11	0.40	0	10,14,16	0.34	0
3	NAG	X	2	3,2	12,14,15	0.60	0	15,19,21	0.97	1 (6%)
3	NAG	X	3	3	12,14,15	0.48	0	15,19,21	0.63	0
4	NAG	X	4	2,4	12,14,15	0.72	0	15,19,21	1.22	1 (6%)
4	NAG	X	5	4	12,14,15	0.71	0	15,19,21	0.67	0
4	MAN	X	6	4	10,11,12	0.46	0	11,15,17	0.48	0
3	FUL	Y	1	3	9,10,11	0.39	0	10,14,16	0.36	0
3	NAG	Y	2	3,2	12,14,15	0.68	0	15,19,21	1.12	0
3	NAG	Y	3	3	12,14,15	0.46	0	15,19,21	0.68	0
4	NAG	Y	4	2,4	12,14,15	0.83	0	15,19,21	1.36	2 (13%)
4	NAG	Y	5	4	12,14,15	0.62	0	15,19,21	0.89	0
4	MAN	Y	6	4	10,11,12	0.37	0	11,15,17	0.31	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
3	FUL	U	1	3	-	0/0/17/20	0/1/1/1
3	NAG	U	2	3,2	-	0/6/23/26	0/1/1/1
3	NAG	U	3	3	-	0/6/23/26	0/1/1/1
4	NAG	U	4	2,4	-	1/6/23/26	0/1/1/1
4	NAG	U	5	4	-	0/6/23/26	0/1/1/1
4	MAN	U	6	4	-	0/2/19/22	0/1/1/1
3	FUL	W	1	3	-	0/0/17/20	0/1/1/1
3	NAG	W	2	3,2	-	0/6/23/26	0/1/1/1
3	NAG	W	3	3	-	0/6/23/26	0/1/1/1
5	NDG	W	4	2,5	-	0/6/23/26	0/1/1/1
5	NAG	W	5	5	-	0/6/23/26	0/1/1/1
5	MAN	W	6	5	-	0/2/19/22	0/1/1/1
3	FUL	X	1	3	-	0/0/17/20	0/1/1/1
3	NAG	X	2	3,2	-	0/6/23/26	0/1/1/1
3	NAG	X	3	3	-	0/6/23/26	0/1/1/1
4	NAG	X	4	2,4	-	0/6/23/26	0/1/1/1
4	NAG	X	5	4	-	0/6/23/26	0/1/1/1
4	MAN	X	6	4	-	0/2/19/22	0/1/1/1
3	FUL	Y	1	3	-	0/0/17/20	0/1/1/1
3	NAG	Y	2	3,2	-	0/6/23/26	0/1/1/1
3	NAG	Y	3	3	-	0/6/23/26	0/1/1/1
4	NAG	Y	4	2,4	-	1/6/23/26	0/1/1/1
4	NAG	Y	5	4	-	0/6/23/26	0/1/1/1
4	MAN	Y	6	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	4	NAG	C3-C4-C5	3.12	115.77	110.20
4	U	4	NAG	C3-C4-C5	2.97	115.50	110.20
4	Y	4	NAG	C4-C3-C2	2.84	118.27	111.32
4	X	4	NAG	C3-C4-C5	2.80	115.20	110.20
3	U	2	NAG	C2-N2-C7	-2.23	119.34	123.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Y	4	NAG	O7-C7-N2-C2
4	U	4	NAG	O7-C7-N2-C2

There are no ring outliers.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	144/145 (99%)	0.67	11 (7%) 14 13	42, 68, 170, 188	0
1	B	139/145 (95%)	1.24	25 (17%) 2 2	39, 76, 187, 194	0
1	E	139/145 (95%)	1.40	20 (14%) 3 3	39, 69, 184, 200	0
1	F	139/145 (95%)	1.49	34 (24%) 1 1	45, 86, 185, 197	0
2	U	275/290 (94%)	0.82	41 (14%) 3 3	44, 85, 168, 187	0
2	W	275/290 (94%)	1.67	91 (33%) 1 1	59, 104, 183, 193	0
2	X	275/290 (94%)	0.95	43 (15%) 3 2	49, 90, 162, 189	0
2	Y	275/290 (94%)	1.24	55 (20%) 2 1	46, 81, 180, 191	0
All	All	1661/1740 (95%)	1.18	320 (19%) 2 1	39, 87, 177, 200	0

The worst 5 of 320 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	34	ALA	12.2
2	W	96	TYR	11.3
2	W	246	MET	10.9
1	F	36	MET	10.7
2	W	224	LEU	10.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	FUL	U	1	10/11	0.40	1.16	124,131,139,141	0
4	NAG	X	4	14/15	0.20	-0.49	112,143,156,171	0
3	NAG	Y	2	14/15	0.23	-0.50	156,169,179,192	0
3	FUL	W	1	10/11	0.27	-0.83	160,171,172,173	0
3	NAG	W	2	14/15	0.12	-0.96	145,156,169,178	0
5	NDG	W	4	14/15	0.23	-1.37	164,180,187,190	0
3	NAG	U	2	14/15	0.16	-1.61	97,118,131,148	0
3	NAG	X	2	14/15	0.15	-1.64	111,124,133,143	0
4	NAG	U	4	14/15	0.15	-1.94	151,162,169,171	0
3	FUL	X	1	10/11	0.18	-2.14	112,119,127,129	0
4	NAG	Y	4	14/15	0.19	-4.53	137,150,160,170	0
3	FUL	Y	1	10/11	0.39	-146.00	154,171,175,177	0
4	NAG	X	5	14/15	0.22	-	183,193,195,196	0
3	NAG	W	3	14/15	0.18	-	185,191,194,196	0
3	NAG	U	3	14/15	0.23	-	170,189,193,194	0
4	NAG	Y	5	14/15	0.18	-	180,190,198,198	0
4	NAG	U	5	14/15	0.21	-	179,186,194,197	0
3	NAG	Y	3	14/15	0.19	-	185,191,194,196	0
3	NAG	X	3	14/15	0.17	-	156,163,170,171	0
4	MAN	X	6	11/12	0.12	-	193,197,198,198	0
4	MAN	U	6	11/12	0.10	-	191,196,198,198	0
5	MAN	W	6	11/12	0.23	-	190,196,198,198	0
5	NAG	W	5	14/15	0.26	-	187,195,198,198	0
4	MAN	Y	6	11/12	0.11	-	161,171,175,177	0

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.