



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 06:55 AM BST

PDB ID : 4AY9
Title : Structure of follicle-stimulating hormone in complex with the entire ectodomain of its receptor
Authors : Jiang, X.; Liu, H.; Chen, X.; He, X.
Deposited on : 2012-06-19
Resolution : 2.50 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

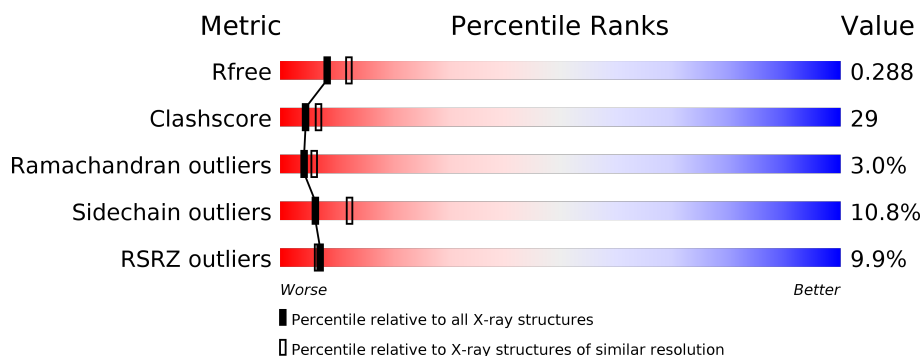
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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	92	
1	D	92	
1	G	92	
2	B	111	
2	E	111	
2	H	111	

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Mol	Chain	Length	Quality of chain
3	X	350	
3	Y	350	
3	Z	350	

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
3	TYS	Y	335	-	-	X	-
3	TYS	Z	335	-	-	X	-
4	NAG	E	1007	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12344 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 GLYCOPROTEIN HORMONES, ALPHA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	88	Total	C	N	O	S	0	0	0
			675	417	118	127	13			
1	D	89	Total	C	N	O	S	0	0	0
			682	422	119	128	13			
1	G	88	Total	C	N	O	S	0	0	0
			675	417	118	127	13			

- Molecule 2 is a protein called FOLLITROPIN SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	107	Total	C	N	O	S	0	0	0
			831	517	140	162	12			
2	E	107	Total	C	N	O	S	0	0	0
			831	517	140	162	12			
2	H	107	Total	C	N	O	S	0	0	0
			831	517	140	162	12			

- Molecule 3 is a protein called FOLLICLE-STIMULATING HORMONE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	307	Total	C	N	O	S	0	0	0
			2462	1555	429	466	12			
3	Y	307	Total	C	N	O	S	0	0	0
			2462	1555	429	466	12			
3	Z	307	Total	C	N	O	S	0	0	0
			2462	1555	429	466	12			

There are 3 discrepancies between the modelled and reference sequences:

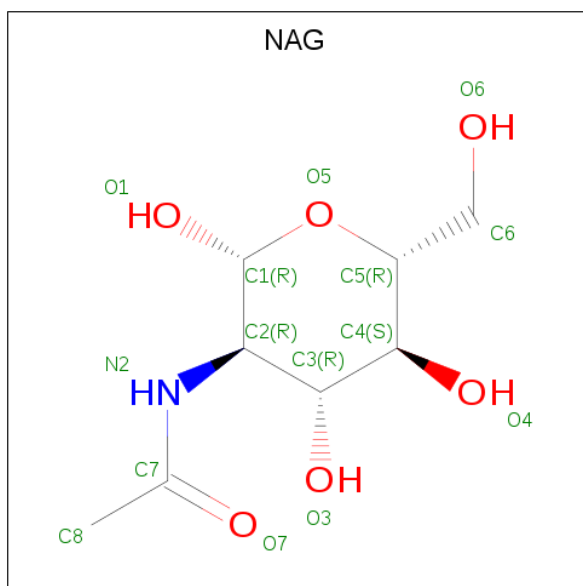
Chain	Residue	Modelled	Actual	Comment	Reference
X	188	SER	CYS	conflict	UNP P23945
Y	188	SER	CYS	conflict	UNP P23945

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	188	SER	CYS	conflict	UNP P23945

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		
4	Z	1	Total	C	N	O	0	0
			14	8	1	5		

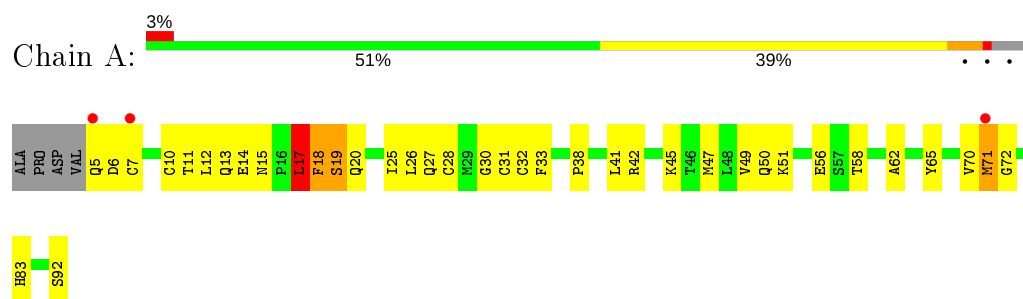
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	O	0	0
			19	19		
5	B	15	Total	O	0	0
			15	15		
5	D	18	Total	O	0	0
			18	18		
5	E	21	Total	O	0	0
			21	21		
5	G	18	Total	O	0	0
			18	18		
5	H	14	Total	O	0	0
			14	14		
5	X	28	Total	O	0	0
			28	28		
5	Y	45	Total	O	0	0
			45	45		
5	Z	45	Total	O	0	0
			45	45		

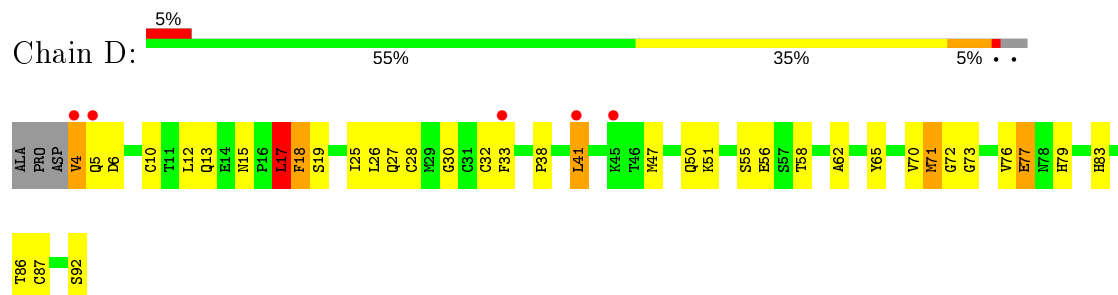
3 Residue-property plots [i](#)

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.

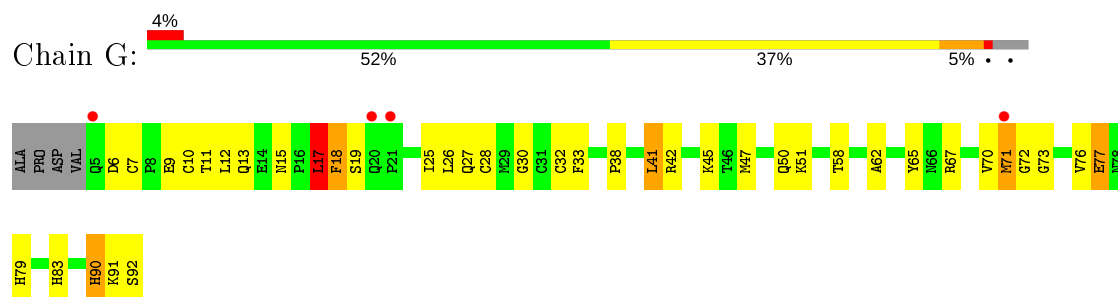
- Molecule 1: GLYCOPROTEIN HORMONES, ALPHA POLYPEPTIDE



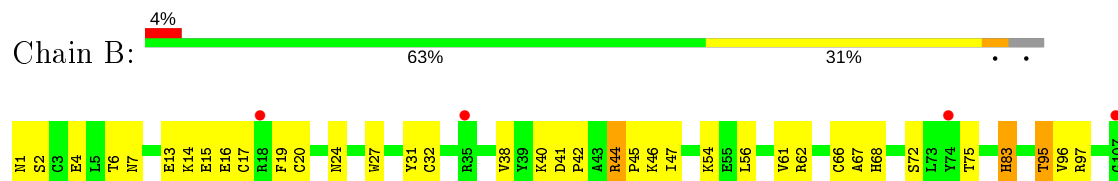
- Molecule 1: GLYCOPROTEIN HORMONES, ALPHA POLYPEPTIDE



- Molecule 1: GLYCOPROTEIN HORMONES, ALPHA POLYPEPTIDE



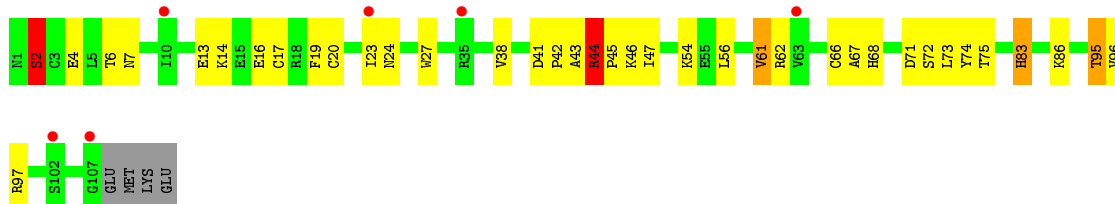
- Molecule 2: FOLLITROPIN SUBUNIT BETA



GLU
MET
LYS
GLU

• Molecule 2: FOLLITROPIN SUBUNIT BETA

Chain E: 



• Molecule 2: FOLLITROPIN SUBUNIT BETA

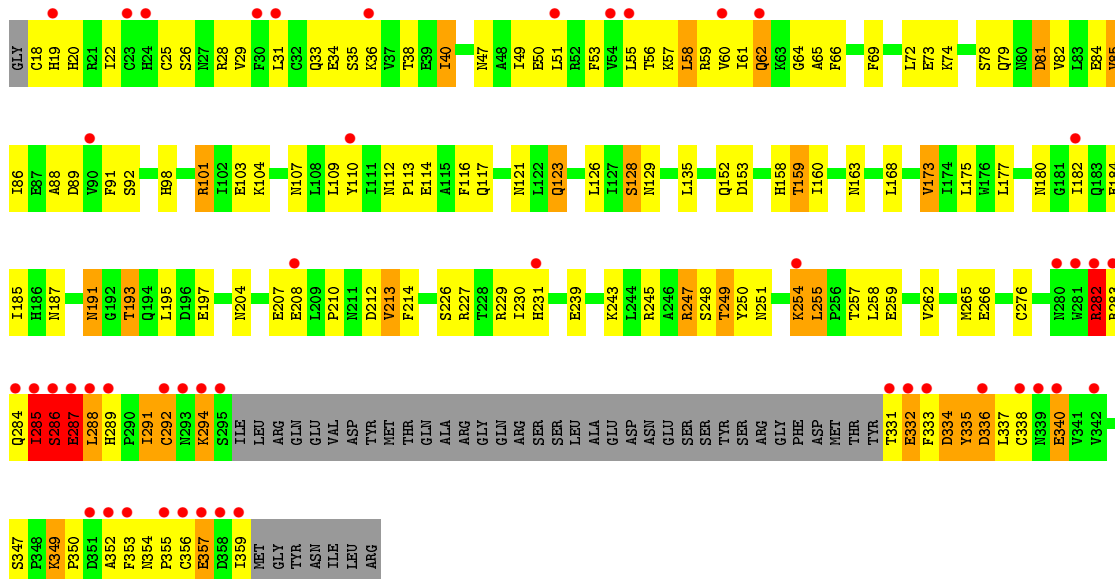
Chain H: 



GLU
MET
LYS
GLU

• Molecule 3: FOLLICLE-STIMULATING HORMONE RECEPTOR

Chain X: 



• Molecule 3: FOLLICLE-STIMULATING HORMONE RECEPTOR

Chain Y: 

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.72Å 95.48Å 95.67Å 60.30° 80.02° 75.35°	Depositor
Resolution (Å)	47.90 – 2.50 47.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.90-2.50) 97.5 (47.90-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.235 , 0.269 0.260 , 0.288	Depositor DCC
R_{free} test set	3599 reflections (2.54%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12344	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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, TYS

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	0.38	0/690	0.56	0/933
1	D	0.37	0/697	0.53	0/943
1	G	0.38	0/690	0.57	0/933
2	B	0.34	0/850	0.55	0/1155
2	E	0.39	0/850	0.60	0/1155
2	H	0.35	0/850	0.57	0/1155
3	X	0.33	0/2493	0.60	0/3380
3	Y	0.34	0/2493	0.61	0/3380
3	Z	0.34	0/2493	0.60	0/3380
All	All	0.35	0/12106	0.59	0/16414

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
3	Y	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	Y	340	GLU	Peptide
3	Y	341	VAL	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	675	0	647	40	0
1	D	682	0	656	49	0
1	G	675	0	647	43	0
2	B	831	0	782	43	0
2	E	831	0	782	51	0
2	H	831	0	782	36	0
3	X	2462	0	2439	153	0
3	Y	2462	0	2440	162	0
3	Z	2462	0	2438	137	0
4	A	28	0	26	3	0
4	B	28	0	26	9	0
4	D	28	0	26	1	0
4	E	28	0	26	12	0
4	G	28	0	26	4	0
4	H	28	0	26	5	0
4	X	14	0	13	5	0
4	Y	14	0	13	5	0
4	Z	14	0	13	1	0
5	A	19	0	0	6	0
5	B	15	0	0	7	0
5	D	18	0	0	4	0
5	E	21	0	0	4	0
5	G	18	0	0	3	0
5	H	14	0	0	0	0
5	X	28	0	0	20	0
5	Y	45	0	0	21	0
5	Z	45	0	0	21	0
All	All	12344	0	11808	681	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 29.

The worst 5 of 681 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)
3:Y:191:ASN:HD21	4:Y:1191:NAG:C1	1.07	1.58
3:Y:276:CYS:SG	3:Y:350:PRO:HG3	1.58	1.41
4:E:1007:NAG:O6	5:E:2021:HOH:O	1.54	1.25
3:Y:335:TYS:HE2	3:Y:335:TYS:O3	1.38	1.18
3:Z:335:TYS:HD2	3:Z:335:TYS:N	1.53	1.17

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	86/92 (94%)	82 (95%)	1 (1%)	3 (4%)	3	4
1	D	87/92 (95%)	80 (92%)	4 (5%)	3 (3%)	3	5
1	G	86/92 (94%)	81 (94%)	0	5 (6%)	1	1
2	B	105/111 (95%)	103 (98%)	1 (1%)	1 (1%)	15	28
2	E	105/111 (95%)	102 (97%)	1 (1%)	2 (2%)	8	13
2	H	105/111 (95%)	101 (96%)	3 (3%)	1 (1%)	15	28
3	X	302/350 (86%)	269 (89%)	26 (9%)	7 (2%)	6	10
3	Y	302/350 (86%)	266 (88%)	23 (8%)	13 (4%)	2	3
3	Z	302/350 (86%)	274 (91%)	18 (6%)	10 (3%)	4	5
All	All	1480/1659 (89%)	1358 (92%)	77 (5%)	45 (3%)	4	6

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	18	PHE
2	B	44	ARG
1	D	18	PHE
2	E	44	ARG

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	80/83 (96%)	71 (89%)	9 (11%)	6	11
1	D	81/83 (98%)	75 (93%)	6 (7%)	13	27
1	G	80/83 (96%)	73 (91%)	7 (9%)	10	19
2	B	95/99 (96%)	88 (93%)	7 (7%)	13	27
2	E	95/99 (96%)	86 (90%)	9 (10%)	8	17
2	H	95/99 (96%)	88 (93%)	7 (7%)	13	27
3	X	283/320 (88%)	245 (87%)	38 (13%)	4	7
3	Y	283/320 (88%)	253 (89%)	30 (11%)	6	13
3	Z	283/320 (88%)	248 (88%)	35 (12%)	4	9
All	All	1375/1506 (91%)	1227 (89%)	148 (11%)	6	12

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	X	262	VAL
3	X	359	ILE
3	Z	282	ARG
3	X	282	ARG
3	X	331	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	X	284	GLN
3	Y	62	GLN
3	Y	163	ASN
3	Y	191	ASN
3	Y	339	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	TYS	X	335	3	15,16,17	1.12	1 (6%)	18,22,24	0.61	0
3	TYS	Y	335	3	15,16,17	2.11	3 (20%)	18,22,24	1.33	2 (11%)
3	TYS	Z	335	3	15,16,17	1.13	1 (6%)	18,22,24	0.56	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	TYS	X	335	3	-	5/10/11/13	0/1/1/1
3	TYS	Y	335	3	-	6/10/11/13	0/1/1/1
3	TYS	Z	335	3	-	5/10/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	335	TYS	OH-CZ	-4.59	1.35	1.42
3	Y	335	TYS	CE2-CD2	-4.30	1.30	1.38
3	Y	335	TYS	OH-S	-3.81	1.52	1.58
3	Z	335	TYS	OH-CZ	-3.17	1.37	1.42
3	X	335	TYS	OH-CZ	-3.09	1.37	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	335	TYS	OH-CZ-CE1	2.87	124.28	118.64
3	Y	335	TYS	OH-CZ-CE2	-2.49	113.75	118.64

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	335	TYS	C-CA-CB-CG
3	X	335	TYS	CE1-CZ-OH-S
3	X	335	TYS	CE2-CZ-OH-S
3	Y	335	TYS	C-CA-CB-CG
3	Z	335	TYS	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	335	TYS	1	0
3	Y	335	TYS	12	0
3	Z	335	TYS	8	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 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	$\# Z > 2$
4	NAG	Y	1191	3	14,14,15	0.58	0	17,19,21	1.27	2 (11%)
4	NAG	B	1007	2	14,14,15	0.74	0	17,19,21	2.32	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1078	1	14,14,15	0.69	0	17,19,21	1.94	5 (29%)
4	NAG	H	1007	2	14,14,15	0.67	0	17,19,21	1.95	4 (23%)
4	NAG	G	1052	1	14,14,15	0.73	0	17,19,21	3.34	5 (29%)
4	NAG	D	1052	1	14,14,15	0.72	0	17,19,21	3.01	4 (23%)
4	NAG	A	1052	1	14,14,15	0.98	0	17,19,21	3.68	5 (29%)
4	NAG	E	1024	-	14,14,15	0.85	0	17,19,21	2.40	4 (23%)
4	NAG	G	1078	1	14,14,15	0.66	0	17,19,21	1.71	4 (23%)
4	NAG	D	1078	1	14,14,15	0.73	0	17,19,21	1.73	3 (17%)
4	NAG	E	1007	2	14,14,15	0.48	0	17,19,21	1.52	2 (11%)
4	NAG	H	1024	2	14,14,15	0.78	0	17,19,21	2.06	6 (35%)
4	NAG	B	1024	2	14,14,15	0.48	0	17,19,21	1.90	5 (29%)
4	NAG	X	1191	3	14,14,15	0.57	0	17,19,21	1.36	2 (11%)
4	NAG	Z	1191	3	14,14,15	0.56	0	17,19,21	1.26	2 (11%)

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
4	NAG	Y	1191	3	-	0/6/23/26	0/1/1/1
4	NAG	B	1007	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1078	1	-	0/6/23/26	0/1/1/1
4	NAG	H	1007	2	-	3/6/23/26	0/1/1/1
4	NAG	G	1052	1	-	1/6/23/26	0/1/1/1
4	NAG	D	1052	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1052	1	-	3/6/23/26	0/1/1/1
4	NAG	E	1024	-	-	2/6/23/26	0/1/1/1
4	NAG	G	1078	1	-	2/6/23/26	0/1/1/1
4	NAG	D	1078	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1007	2	-	2/6/23/26	0/1/1/1
4	NAG	H	1024	2	-	4/6/23/26	0/1/1/1
4	NAG	B	1024	2	-	3/6/23/26	0/1/1/1
4	NAG	X	1191	3	-	0/6/23/26	0/1/1/1
4	NAG	Z	1191	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1052	NAG	O5-C1-C2	-11.71	92.80	111.29
4	G	1052	NAG	O5-C1-C2	-9.85	95.73	111.29
4	D	1052	NAG	O5-C1-C2	-9.10	96.92	111.29
4	G	1052	NAG	C4-C3-C2	-7.62	99.85	111.02
4	A	1052	NAG	C4-C3-C2	-7.31	100.31	111.02

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1007	NAG	C3-C2-N2-C7
4	G	1052	NAG	C3-C2-N2-C7
4	D	1052	NAG	C3-C2-N2-C7
4	A	1052	NAG	C3-C2-N2-C7
4	E	1024	NAG	C3-C2-N2-C7

There are no ring outliers.

12 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	1191	NAG	5	0
4	B	1007	NAG	5	0
4	H	1007	NAG	3	0
4	G	1052	NAG	4	0
4	D	1052	NAG	1	0
4	A	1052	NAG	3	0
4	E	1024	NAG	4	0
4	E	1007	NAG	8	0
4	H	1024	NAG	2	0
4	B	1024	NAG	4	0
4	X	1191	NAG	5	0
4	Z	1191	NAG	1	0

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	88/92 (95%)	0.42	3 (3%) 45 48	38, 50, 81, 100	0
1	D	89/92 (96%)	0.62	5 (5%) 24 25	36, 48, 82, 112	0
1	G	88/92 (95%)	0.51	4 (4%) 33 36	38, 48, 82, 100	0
2	B	107/111 (96%)	0.58	4 (3%) 41 45	40, 56, 89, 101	0
2	E	107/111 (96%)	0.47	6 (5%) 24 25	40, 56, 88, 100	0
2	H	107/111 (96%)	0.54	6 (5%) 24 25	39, 56, 88, 103	0
3	X	306/350 (87%)	0.96	47 (15%) 2 1	27, 64, 155, 165	0
3	Y	306/350 (87%)	1.10	42 (13%) 3 2	24, 63, 154, 187	0
3	Z	306/350 (87%)	0.77	32 (10%) 6 6	27, 62, 149, 179	0
All	All	1504/1659 (90%)	0.78	149 (9%) 7 7	24, 58, 139, 187	0

The worst 5 of 149 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	285	ILE	21.5
3	X	331	THR	13.0
3	X	285	ILE	12.7
3	Y	333	PHE	12.5
3	Y	281	TRP	12.5

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	TYS	Y	335	16/17	0.63	0.37	104,127,145,145	0
3	TYS	Z	335	16/17	0.71	0.38	101,124,144,144	0
3	TYS	X	335	16/17	0.78	0.31	103,127,146,146	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	E	1024	14/15	0.84	0.35	23,24,26,27	0
4	NAG	B	1024	14/15	0.86	0.34	27,32,34,34	0
4	NAG	E	1007	14/15	0.87	0.39	24,26,29,29	0
4	NAG	H	1007	14/15	0.88	0.33	26,29,30,33	0
4	NAG	X	1191	14/15	0.88	0.23	14,15,16,17	0
4	NAG	H	1024	14/15	0.90	0.39	32,32,35,36	0
4	NAG	B	1007	14/15	0.91	0.30	28,30,32,33	0
4	NAG	D	1078	14/15	0.91	0.11	23,25,27,27	0
4	NAG	Y	1191	14/15	0.91	0.31	10,11,12,12	0
4	NAG	G	1078	14/15	0.92	0.14	22,23,24,26	0
4	NAG	Z	1191	14/15	0.92	0.21	9,10,11,12	0
4	NAG	D	1052	14/15	0.93	0.13	17,21,24,26	0
4	NAG	G	1052	14/15	0.94	0.10	20,22,26,29	0
4	NAG	A	1052	14/15	0.94	0.12	19,20,24,26	0
4	NAG	A	1078	14/15	0.95	0.13	22,24,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.