



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:46 am GMT

PDB ID : 4MQW  
Title : Structure of follicle-stimulating hormone in complex with the entire ectodomain of its receptor (P31)  
Authors : Jiang, X.; Liu, H.; Chen, X.; He, X.  
Deposited on : 2013-09-16  
Resolution : 2.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

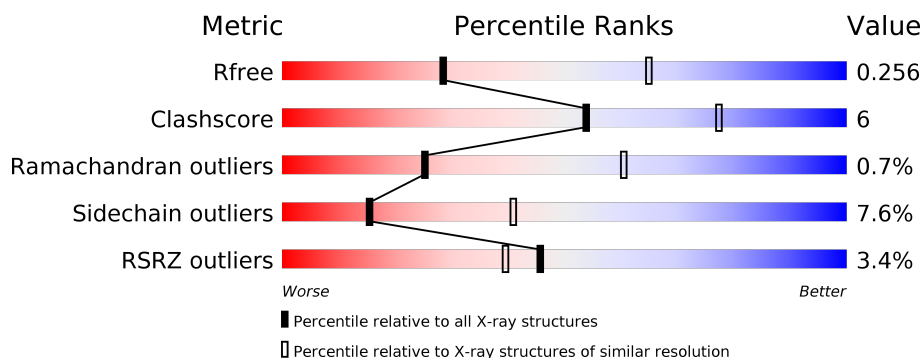
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	102	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>20%</div> <div>•</div> <div>14%</div> </div> </div>
1	D	102	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>13%</div> </div> </div>
1	G	102	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div></div> <div>14%</div> </div> </div>
2	B	111	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>• •</div> </div> </div>
2	E	111	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• •</div> </div> </div>
2	H	111	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	X	361	
3	Y	361	
3	Z	361	

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
5	EDO	X	401	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11798 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			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	ALA	-	EXPRESSION TAG	UNP Q96QJ4
A	94	ALA	-	EXPRESSION TAG	UNP Q96QJ4
A	95	ALA	-	EXPRESSION TAG	UNP Q96QJ4
A	96	HIS	-	EXPRESSION TAG	UNP Q96QJ4
A	97	HIS	-	EXPRESSION TAG	UNP Q96QJ4
A	98	HIS	-	EXPRESSION TAG	UNP Q96QJ4
A	99	HIS	-	EXPRESSION TAG	UNP Q96QJ4
A	100	HIS	-	EXPRESSION TAG	UNP Q96QJ4
A	101	HIS	-	EXPRESSION TAG	UNP Q96QJ4
A	102	HIS	-	EXPRESSION TAG	UNP Q96QJ4
D	93	ALA	-	EXPRESSION TAG	UNP Q96QJ4
D	94	ALA	-	EXPRESSION TAG	UNP Q96QJ4
D	95	ALA	-	EXPRESSION TAG	UNP Q96QJ4
D	96	HIS	-	EXPRESSION TAG	UNP Q96QJ4
D	97	HIS	-	EXPRESSION TAG	UNP Q96QJ4
D	98	HIS	-	EXPRESSION TAG	UNP Q96QJ4
D	99	HIS	-	EXPRESSION TAG	UNP Q96QJ4
D	100	HIS	-	EXPRESSION TAG	UNP Q96QJ4
D	101	HIS	-	EXPRESSION TAG	UNP Q96QJ4
D	102	HIS	-	EXPRESSION TAG	UNP Q96QJ4
G	93	ALA	-	EXPRESSION TAG	UNP Q96QJ4
G	94	ALA	-	EXPRESSION TAG	UNP Q96QJ4
G	95	ALA	-	EXPRESSION TAG	UNP Q96QJ4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	96	HIS	-	EXPRESSION TAG	UNP Q96QJ4
G	97	HIS	-	EXPRESSION TAG	UNP Q96QJ4
G	98	HIS	-	EXPRESSION TAG	UNP Q96QJ4
G	99	HIS	-	EXPRESSION TAG	UNP Q96QJ4
G	100	HIS	-	EXPRESSION TAG	UNP Q96QJ4
G	101	HIS	-	EXPRESSION TAG	UNP Q96QJ4
G	102	HIS	-	EXPRESSION TAG	UNP Q96QJ4

- Molecule 2 is a protein called Follitropin subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	109	Total	C	N	O	S	0	0	0
			848	527	142	166	13			
2	E	108	Total	C	N	O	S	0	0	0
			840	522	141	165	12			
2	H	108	Total	C	N	O	S	0	0	0
			840	522	141	165	12			

- Molecule 3 is a protein called Follicle-stimulating hormone receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	289	Total	C	N	O	S	0	0	0
			2275	1439	397	427	12			
3	Y	284	Total	C	N	O	S	0	0	0
			2258	1428	392	428	10			
3	Z	290	Total	C	N	O	S	0	0	0
			2312	1463	406	431	12			

There are 33 discrepancies between the modelled and reference sequences:

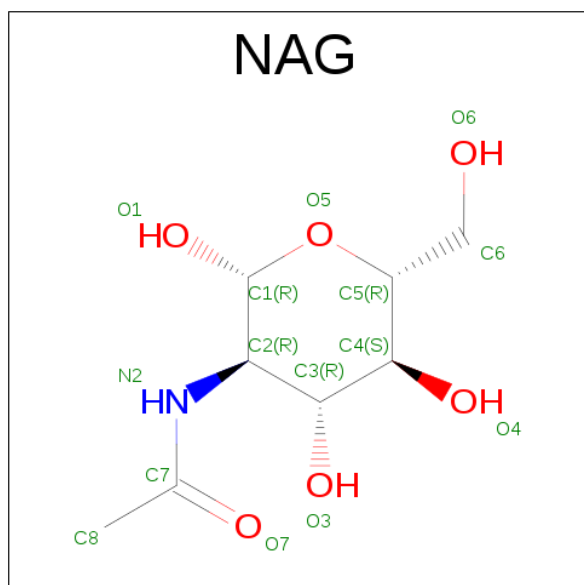
Chain	Residue	Modelled	Actual	Comment	Reference
X	188	SER	CYS	ENGINEERED MUTATION	UNP P23945
X	367	ALA	-	EXPRESSION TAG	UNP P23945
X	368	ALA	-	EXPRESSION TAG	UNP P23945
X	369	ALA	-	EXPRESSION TAG	UNP P23945
X	370	HIS	-	EXPRESSION TAG	UNP P23945
X	371	HIS	-	EXPRESSION TAG	UNP P23945
X	372	HIS	-	EXPRESSION TAG	UNP P23945
X	373	HIS	-	EXPRESSION TAG	UNP P23945
X	374	HIS	-	EXPRESSION TAG	UNP P23945
X	375	HIS	-	EXPRESSION TAG	UNP P23945
X	376	HIS	-	EXPRESSION TAG	UNP P23945

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	188	SER	CYS	ENGINEERED MUTATION	UNP P23945
Y	367	ALA	-	EXPRESSION TAG	UNP P23945
Y	368	ALA	-	EXPRESSION TAG	UNP P23945
Y	369	ALA	-	EXPRESSION TAG	UNP P23945
Y	370	HIS	-	EXPRESSION TAG	UNP P23945
Y	371	HIS	-	EXPRESSION TAG	UNP P23945
Y	372	HIS	-	EXPRESSION TAG	UNP P23945
Y	373	HIS	-	EXPRESSION TAG	UNP P23945
Y	374	HIS	-	EXPRESSION TAG	UNP P23945
Y	375	HIS	-	EXPRESSION TAG	UNP P23945
Y	376	HIS	-	EXPRESSION TAG	UNP P23945
Z	188	SER	CYS	ENGINEERED MUTATION	UNP P23945
Z	367	ALA	-	EXPRESSION TAG	UNP P23945
Z	368	ALA	-	EXPRESSION TAG	UNP P23945
Z	369	ALA	-	EXPRESSION TAG	UNP P23945
Z	370	HIS	-	EXPRESSION TAG	UNP P23945
Z	371	HIS	-	EXPRESSION TAG	UNP P23945
Z	372	HIS	-	EXPRESSION TAG	UNP P23945
Z	373	HIS	-	EXPRESSION TAG	UNP P23945
Z	374	HIS	-	EXPRESSION TAG	UNP P23945
Z	375	HIS	-	EXPRESSION TAG	UNP P23945
Z	376	HIS	-	EXPRESSION TAG	UNP P23945

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (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		
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		

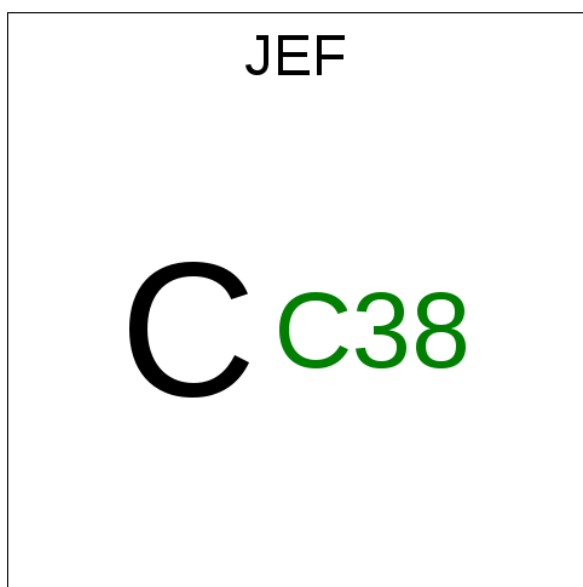
- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	X	1	Total	C	O	0	0
			4	2	2		
5	X	1	Total	C	O	0	0
			4	2	2		
5	Y	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is O-(O-(2-AMINOPROPYL)-O'-(2-METHOXYETHYL)POLYPROPYLENE GLYCOL 500) (three-letter code: JEF) (formula: C<sub>30</sub>H<sub>63</sub>NO<sub>10</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	Z	1	Total	C	O	0	0
			8	5	3		

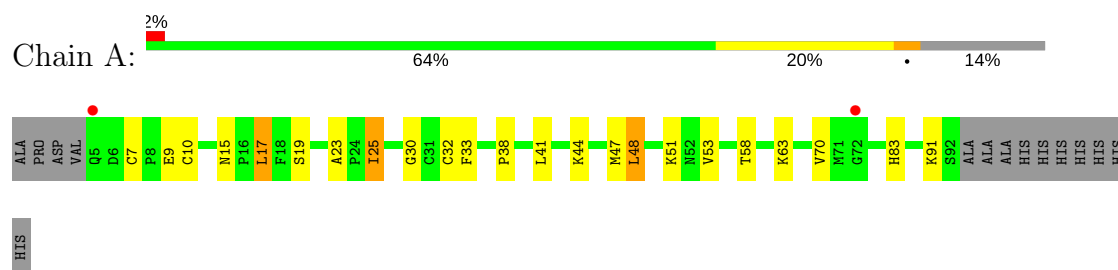
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	13	Total	O	0	0
			13	13		
7	B	16	Total	O	0	0
			16	16		
7	X	22	Total	O	0	0
			22	22		
7	D	10	Total	O	0	0
			10	10		
7	E	13	Total	O	0	0
			13	13		
7	Y	28	Total	O	0	0
			28	28		
7	G	15	Total	O	0	0
			15	15		
7	H	20	Total	O	0	0
			20	20		
7	Z	18	Total	O	0	0
			18	18		

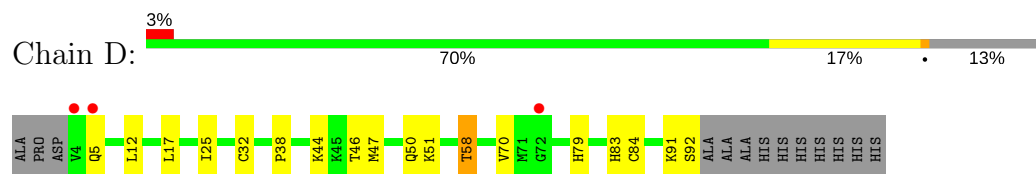
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

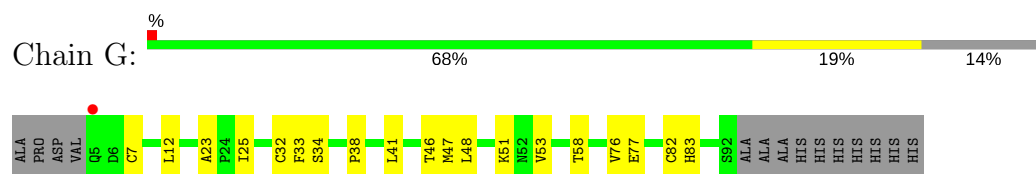
- Molecule 1: Glycoprotein hormones, alpha polypeptide



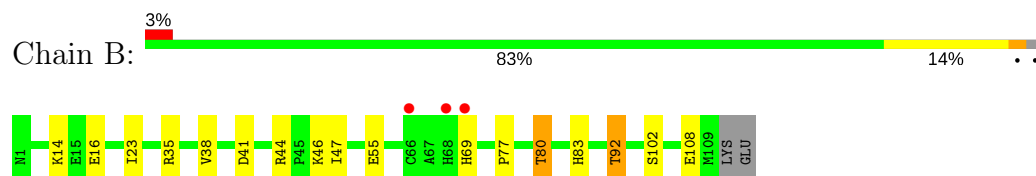
- Molecule 1: Glycoprotein hormones, alpha polypeptide



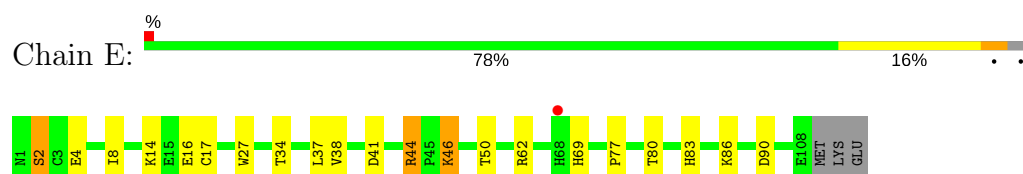
- Molecule 1: Glycoprotein hormones, alpha polypeptide



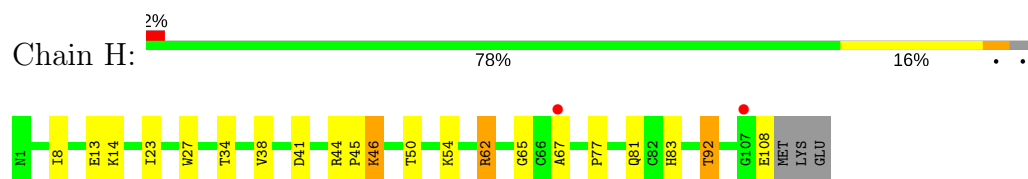
- Molecule 2: Follitropin subunit beta



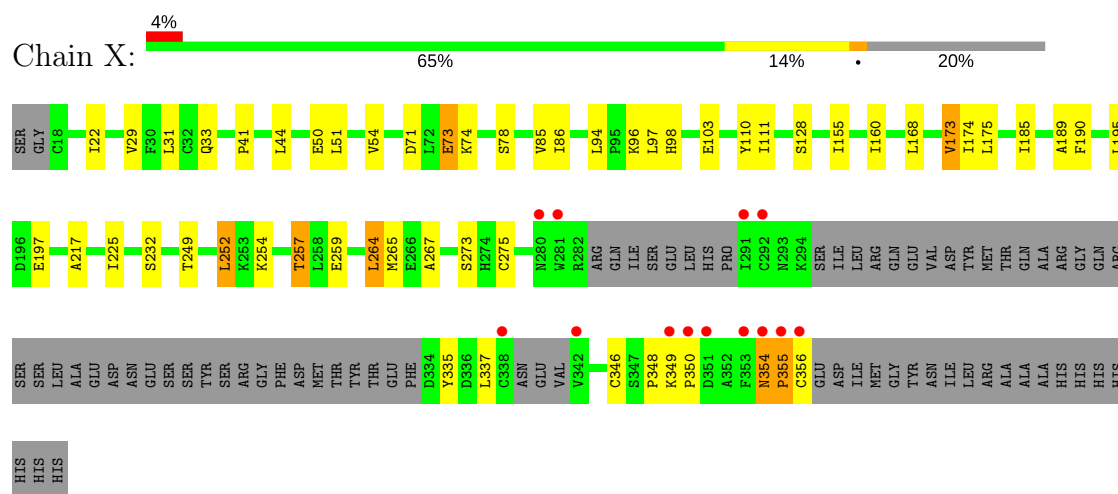
- Molecule 2: Follitropin subunit beta



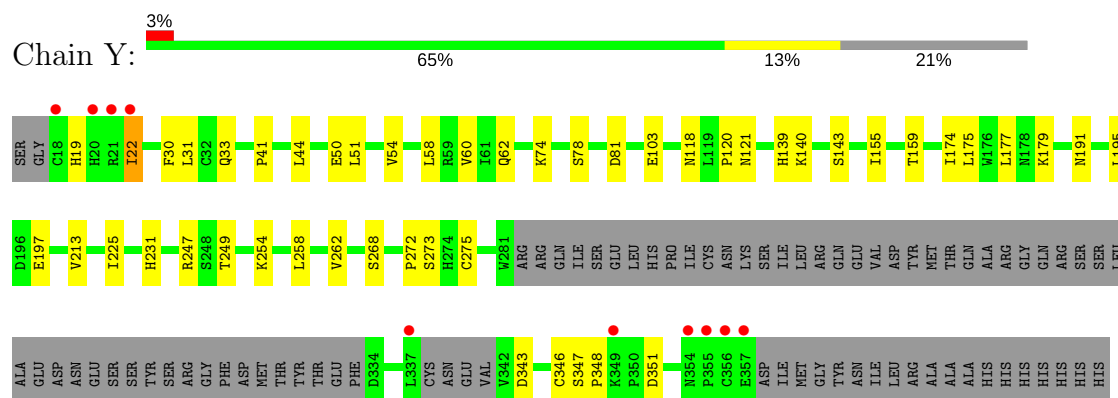
- Molecule 2: Follitropin subunit beta



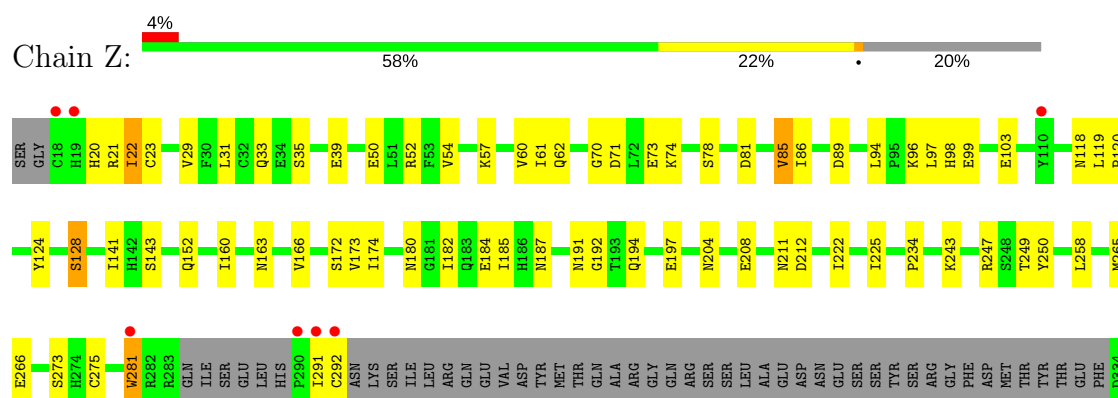
- Molecule 3: Follicle-stimulating hormone receptor

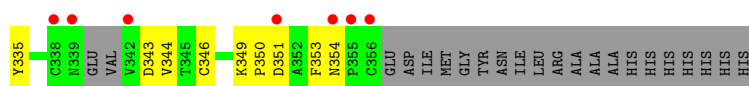


- Molecule 3: Follicle-stimulating hormone receptor



- Molecule 3: Follicle-stimulating hormone receptor





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.90Å 95.90Å 204.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.93 – 2.90 24.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.6 (24.93-2.90) 95.5 (24.93-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.89Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, $R_{free}$	0.174 , 0.237 0.192 , 0.256	Depositor DCC
$R_{free}$ test set	2226 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.3	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 58.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11798	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.94 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4222e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, JEF, 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	0.46	0/690	0.65	0/933
1	D	0.44	0/697	0.67	0/943
1	G	0.44	0/690	0.67	0/933
2	B	0.44	0/867	0.74	0/1177
2	E	0.44	0/859	0.72	0/1167
2	H	0.46	0/859	0.72	0/1167
3	X	0.44	0/2299	0.73	0/3115
3	Y	0.46	0/2283	0.73	0/3094
3	Z	0.45	0/2339	0.73	0/3168
All	All	0.45	0/11583	0.72	0/15697

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	675	0	647	14	0
1	D	682	0	656	12	0
1	G	675	0	647	14	0
2	B	848	0	798	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	840	0	789	12	0
2	H	840	0	789	14	0
3	X	2275	0	2240	33	0
3	Y	2258	0	2235	19	0
3	Z	2312	0	2293	36	0
4	A	28	0	26	1	0
4	B	28	0	26	0	0
4	D	28	0	26	0	0
4	E	28	0	26	0	0
4	G	28	0	26	1	0
4	H	28	0	26	0	0
4	X	14	0	13	0	0
4	Y	14	0	13	0	0
4	Z	14	0	13	0	0
5	B	8	0	12	0	0
5	X	8	0	12	0	0
5	Y	4	0	6	0	0
6	Z	8	0	8	0	0
7	A	13	0	0	0	0
7	B	16	0	0	0	0
7	D	10	0	0	0	0
7	E	13	0	0	0	0
7	G	15	0	0	0	0
7	H	20	0	0	0	0
7	X	22	0	0	0	0
7	Y	28	0	0	0	0
7	Z	18	0	0	1	0
All	All	11798	0	11327	138	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 6.

All (138) 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:275:CYS:HG	3:Y:346:CYS:HG	1.05	0.84
1:G:32:CYS:HB3	1:G:58:THR:HG23	1.62	0.81
3:Z:275:CYS:HG	3:Z:346:CYS:HG	0.86	0.81
1:G:47:MET:HE3	1:G:51:LYS:H	1.48	0.78
2:E:41:ASP:O	2:E:44:ARG:HD2	1.85	0.76
1:A:32:CYS:HB3	1:A:58:THR:HG23	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:MET:HE3	1:D:51:LYS:H	1.59	0.68
3:X:29:VAL:HG13	3:X:50:GLU:HB3	1.76	0.68
1:D:92:SER:HB3	2:E:86:LYS:HD2	1.75	0.67
1:G:25:ILE:HD13	2:H:38:VAL:HG11	1.77	0.66
1:G:33:PHE:O	1:G:58:THR:HG22	1.95	0.65
3:Z:33:GLN:HG3	3:Z:54:VAL:HB	1.81	0.63
1:G:25:ILE:CD1	2:H:38:VAL:HG11	2.30	0.62
3:X:354:ASN:HB3	3:X:356:CYS:H	1.64	0.62
3:X:50:GLU:HG3	3:X:74:LYS:HB2	1.82	0.62
3:Y:50:GLU:HG3	3:Y:74:LYS:HB2	1.81	0.62
2:E:41:ASP:HB3	2:E:44:ARG:HB3	1.82	0.61
1:D:25:ILE:HD11	1:D:70:VAL:HG11	1.83	0.60
3:Z:258:LEU:HD12	3:Z:281:TRP:HB3	1.84	0.59
1:A:47:MET:HE3	1:A:51:LYS:H	1.68	0.58
3:Z:160:ILE:HD12	3:Z:185:ILE:HG12	1.85	0.58
3:Y:33:GLN:HA	3:Y:54:VAL:O	2.03	0.58
3:Z:335:TYS:N	3:Z:335:TYS:HD2	2.19	0.58
1:A:44:LYS:HA	1:A:47:MET:HE2	1.86	0.58
1:A:25:ILE:HD11	1:A:70:VAL:HG11	1.85	0.57
2:H:14:LYS:HE2	2:H:65:GLY:HA2	1.86	0.57
3:Z:50:GLU:HG3	3:Z:74:LYS:HB2	1.87	0.57
1:D:12:LEU:HD21	1:D:79:HIS:HB2	1.87	0.56
3:X:354:ASN:CB	3:X:355:PRO:HA	2.36	0.56
1:D:32:CYS:HB3	1:D:58:THR:HG23	1.87	0.55
3:Y:174:ILE:HG23	3:Y:197:GLU:HB3	1.88	0.55
3:Z:21:ARG:HH21	3:Z:22:ILE:HD11	1.72	0.55
3:Z:166:VAL:HG23	3:Z:192:GLY:HA3	1.89	0.54
3:Z:60:VAL:HG13	3:Z:85:VAL:HG23	1.89	0.54
1:A:17:LEU:HD13	3:X:335:TYS:HD2	1.90	0.54
1:G:38:PRO:HB3	2:H:77:PRO:HD2	1.91	0.52
2:B:55:GLU:HB2	2:B:80:THR:HG22	1.91	0.52
3:X:85:VAL:HG12	3:X:110:TYR:HB3	1.92	0.52
1:G:76:VAL:HB	2:H:38:VAL:HG12	1.92	0.52
3:Z:243:LYS:HG2	3:Z:266:GLU:HB3	1.91	0.52
3:X:160:ILE:HD12	3:X:185:ILE:HG12	1.92	0.51
3:X:73:GLU:HA	3:X:97:LEU:HA	1.92	0.51
2:E:46:LYS:HE2	3:Y:197:GLU:OE1	2.11	0.51
3:Y:175:LEU:HD12	3:Y:195:LEU:HD21	1.92	0.51
3:Z:33:GLN:HA	3:Z:54:VAL:O	2.11	0.51
3:Z:78:SER:HA	3:Z:103:GLU:O	2.11	0.51
3:Z:275:CYS:HG	3:Z:346:CYS:CB	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:PHE:O	1:A:58:THR:HG22	2.11	0.50
2:E:37:LEU:HD12	2:E:44:ARG:CG	2.42	0.50
1:A:23:ALA:HB1	4:A:202:NAG:H83	1.93	0.50
1:G:23:ALA:HB1	4:G:202:NAG:H83	1.93	0.50
3:X:257:THR:HB	3:X:259:GLU:HG2	1.94	0.50
1:D:47:MET:CE	1:D:51:LYS:H	2.25	0.50
3:X:94:LEU:HD13	3:X:97:LEU:HD22	1.93	0.49
1:D:44:LYS:HA	1:D:47:MET:HE2	1.93	0.49
1:D:5:GLN:HB2	2:E:2:SER:HB3	1.95	0.49
3:X:174:ILE:HG23	3:X:197:GLU:HB3	1.95	0.49
3:Z:180:ASN:HB2	3:Z:182:ILE:HD12	1.94	0.49
1:G:76:VAL:HB	2:H:38:VAL:CG1	2.42	0.49
1:A:47:MET:CE	1:A:51:LYS:H	2.26	0.48
1:G:46:THR:HG22	3:Z:81:ASP:HB3	1.94	0.48
3:Z:349:LYS:HD3	3:Z:350:PRO:HD2	1.94	0.48
1:A:15:ASN:O	1:A:19:SER:HB2	2.13	0.48
2:E:37:LEU:HD12	2:E:44:ARG:HG3	1.95	0.48
3:Z:61:ILE:HD12	3:Z:86:ILE:HG12	1.96	0.48
2:H:41:ASP:N	2:H:44:ARG:HD3	2.28	0.48
3:X:354:ASN:HB3	3:X:356:CYS:N	2.28	0.48
1:A:38:PRO:HB3	2:B:77:PRO:HD2	1.94	0.48
3:X:71:ASP:HA	3:X:96:LYS:HD2	1.96	0.48
3:Z:197:GLU:HB2	3:Z:222:ILE:HB	1.95	0.48
1:A:53:VAL:HG12	2:B:92:THR:HG23	1.96	0.48
3:X:190:PHE:O	3:X:217:ALA:HB2	2.14	0.47
3:Z:119:LEU:HB2	3:Z:141:ILE:HG23	1.96	0.47
2:E:14:LYS:HD3	2:E:17:CYS:HB2	1.97	0.47
3:X:225:ILE:HD12	3:X:249:THR:HG21	1.96	0.47
3:X:168:LEU:HD23	3:X:173:VAL:HG21	1.97	0.47
1:D:58:THR:HG23	1:D:84:CYS:HB3	1.96	0.46
3:X:175:LEU:HD12	3:X:195:LEU:HD21	1.97	0.46
3:Y:272:PRO:HG3	3:Y:348:PRO:HG2	1.97	0.46
3:X:78:SER:HA	3:X:103:GLU:O	2.15	0.46
3:Y:41:PRO:HB2	3:Y:44:LEU:HG	1.97	0.46
3:Z:211:ASN:HA	3:Z:234:PRO:HB3	1.98	0.46
3:Y:30:PHE:HB2	3:Y:51:LEU:HD23	1.98	0.45
2:E:16:GLU:HB2	2:E:69:HIS:CD2	2.52	0.45
3:Z:73:GLU:HB3	3:Z:98:HIS:CE1	2.52	0.45
3:Z:120:PRO:HA	3:Z:143:SER:HA	1.98	0.45
1:G:41:LEU:HD12	2:H:13:GLU:H	1.82	0.45
3:X:335:TYS:HD1	3:X:335:TYS:HA	1.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:349:LYS:N	3:X:350:PRO:HD3	2.32	0.45
3:Y:120:PRO:HA	3:Y:143:SER:HA	1.98	0.45
3:X:41:PRO:HD2	3:X:44:LEU:HD11	2.00	0.44
3:Y:268:SER:HA	3:Y:347:SER:HB3	1.99	0.44
3:Y:33:GLN:HG3	3:Y:54:VAL:HB	1.99	0.44
1:A:48:LEU:HD22	3:X:155:ILE:HD11	2.00	0.44
3:X:22:ILE:HD11	3:X:41:PRO:HG3	2.00	0.44
3:X:33:GLN:HA	3:X:54:VAL:O	2.18	0.44
3:X:275:CYS:HG	3:X:346:CYS:CB	2.29	0.43
2:E:41:ASP:O	2:E:44:ARG:CD	2.63	0.43
3:Y:139:HIS:CD2	3:Y:140:LYS:HG3	2.54	0.43
3:Y:22:ILE:HD12	3:Y:41:PRO:HG3	1.99	0.43
2:B:16:GLU:HB2	2:B:69:HIS:CD2	2.54	0.43
2:H:46:LYS:H	2:H:46:LYS:HD3	1.83	0.43
1:D:46:THR:HG22	3:Y:81:ASP:HB3	2.00	0.43
3:X:354:ASN:HB2	3:X:355:PRO:HA	2.01	0.43
3:Z:174:ILE:HG12	3:Z:197:GLU:HG2	2.00	0.43
2:H:54:LYS:HB3	2:H:81:GLN:HB3	2.00	0.43
3:Z:35:SER:HA	3:Z:57:LYS:HG2	2.00	0.43
3:Z:94:LEU:HD13	3:Z:97:LEU:HD22	2.01	0.43
3:Z:29:VAL:HG13	3:Z:50:GLU:HB3	2.00	0.42
3:X:354:ASN:HB3	3:X:355:PRO:HA	2.00	0.42
3:X:264:LEU:HD21	3:X:267:ALA:HB2	2.01	0.42
3:Y:231:HIS:CE1	3:Z:250:TYR:HB3	2.54	0.42
3:Z:20:HIS:HB3	3:Z:23:CYS:O	2.20	0.42
3:Z:71:ASP:HA	3:Z:96:LYS:HD2	2.01	0.42
1:G:53:VAL:HG12	2:H:92:THR:HG23	2.01	0.42
3:Z:31:LEU:HA	3:Z:52:ARG:HB2	2.01	0.42
3:Y:225:ILE:O	3:Y:249:THR:HG21	2.20	0.42
3:Y:60:VAL:HG21	2:H:62:ARG:NH2	2.35	0.42
3:Z:187:ASN:OD1	3:Z:212:ASP:HB2	2.20	0.42
3:X:73:GLU:HB2	3:X:98:HIS:CE1	2.55	0.42
3:Z:184:GLU:HA	7:Z:504:HOH:O	2.19	0.42
3:X:348:PRO:C	3:X:350:PRO:HD3	2.40	0.42
3:Y:78:SER:HA	3:Y:103:GLU:O	2.20	0.42
1:A:41:LEU:HD23	1:A:44:LYS:HD2	2.02	0.42
1:A:10:CYS:HA	1:A:30:GLY:HA3	2.01	0.41
1:G:12:LEU:HG	1:G:82:CYS:SG	2.59	0.41
3:X:252:LEU:HD12	3:X:252:LEU:HA	1.93	0.41
3:X:86:ILE:HB	3:X:111:ILE:HG12	2.03	0.41
3:Z:225:ILE:O	3:Z:249:THR:HG21	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:PRO:HB3	2:E:77:PRO:HD2	2.02	0.41
2:E:8:ILE:HG12	2:E:27:TRP:HB2	2.03	0.41
1:D:47:MET:HE3	1:D:50:GLN:HA	2.02	0.41
1:G:77:GLU:O	2:H:38:VAL:HG13	2.21	0.40
3:X:160:ILE:HG22	3:X:189:ALA:HB1	2.03	0.40
3:Z:172:SER:HA	3:Z:194:GLN:HB2	2.03	0.40
3:Z:99:GLU:HG3	3:Z:124:TYR:HD2	1.85	0.40
2:H:8:ILE:HG12	2:H:27:TRP:HB2	2.03	0.40
3:Z:128:SER:HA	3:Z:152:GLN:O	2.22	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	86/102 (84%)	80 (93%)	6 (7%)	0	100	100
1	D	87/102 (85%)	80 (92%)	7 (8%)	0	100	100
1	G	86/102 (84%)	79 (92%)	7 (8%)	0	100	100
2	B	107/111 (96%)	103 (96%)	4 (4%)	0	100	100
2	E	106/111 (96%)	103 (97%)	2 (2%)	1 (1%)	20	54
2	H	106/111 (96%)	101 (95%)	3 (3%)	2 (2%)	9	33
3	X	280/361 (78%)	244 (87%)	32 (11%)	4 (1%)	13	41
3	Y	277/361 (77%)	246 (89%)	30 (11%)	1 (0%)	38	72
3	Z	281/361 (78%)	241 (86%)	38 (14%)	2 (1%)	25	60
All	All	1416/1722 (82%)	1277 (90%)	129 (9%)	10 (1%)	25	60

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	X	354	ASN
2	H	67	ALA
3	Z	70	GLY
3	X	252	LEU
3	X	337	LEU
3	Z	353	PHE
2	E	2	SER
3	Y	155	ILE
2	H	45	PRO
3	X	355	PRO

### 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	80/90 (89%)	72 (90%)	8 (10%)	9	27
1	D	81/90 (90%)	77 (95%)	4 (5%)	29	63
1	G	80/90 (89%)	76 (95%)	4 (5%)	28	62
2	B	97/99 (98%)	84 (87%)	13 (13%)	4	13
2	E	96/99 (97%)	86 (90%)	10 (10%)	8	25
2	H	96/99 (97%)	88 (92%)	8 (8%)	13	36
3	X	256/328 (78%)	245 (96%)	11 (4%)	33	68
3	Y	257/328 (78%)	238 (93%)	19 (7%)	16	42
3	Z	263/328 (80%)	241 (92%)	22 (8%)	13	36
All	All	1306/1551 (84%)	1207 (92%)	99 (8%)	15	41

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	CYS
1	A	9	GLU
1	A	17	LEU
1	A	25	ILE
1	A	48	LEU

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Mol	Chain	Res	Type
1	A	63	LYS
1	A	83	HIS
1	A	91	LYS
2	B	14	LYS
2	B	23	ILE
2	B	35	ARG
2	B	38	VAL
2	B	41	ASP
2	B	44	ARG
2	B	46	LYS
2	B	47	ILE
2	B	80	THR
2	B	83	HIS
2	B	92	THR
2	B	102	SER
2	B	108	GLU
3	X	31	LEU
3	X	51	LEU
3	X	73	GLU
3	X	128	SER
3	X	173	VAL
3	X	232	SER
3	X	254	LYS
3	X	257	THR
3	X	264	LEU
3	X	265	MET
3	X	273	SER
1	D	17	LEU
1	D	58	THR
1	D	83	HIS
1	D	91	LYS
2	E	4	GLU
2	E	34	THR
2	E	38	VAL
2	E	44	ARG
2	E	46	LYS
2	E	50	THR
2	E	62	ARG
2	E	80	THR
2	E	83	HIS
2	E	90	ASP
3	Y	19	HIS

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Mol	Chain	Res	Type
3	Y	22	ILE
3	Y	31	LEU
3	Y	58	LEU
3	Y	62	GLN
3	Y	118	ASN
3	Y	121	ASN
3	Y	159	THR
3	Y	177	LEU
3	Y	179	LYS
3	Y	191	ASN
3	Y	213	VAL
3	Y	247	ARG
3	Y	254	LYS
3	Y	258	LEU
3	Y	262	VAL
3	Y	273	SER
3	Y	343	ASP
3	Y	351	ASP
1	G	7	CYS
1	G	34	SER
1	G	48	LEU
1	G	83	HIS
2	H	23	ILE
2	H	34	THR
2	H	46	LYS
2	H	50	THR
2	H	62	ARG
2	H	83	HIS
2	H	92	THR
2	H	108	GLU
3	Z	22	ILE
3	Z	39	GLU
3	Z	62	GLN
3	Z	85	VAL
3	Z	89	ASP
3	Z	118	ASN
3	Z	128	SER
3	Z	163	ASN
3	Z	173	VAL
3	Z	191	ASN
3	Z	204	ASN
3	Z	208	GLU

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Mol	Chain	Res	Type
3	Z	247	ARG
3	Z	265	MET
3	Z	273	SER
3	Z	281	TRP
3	Z	291	ILE
3	Z	292	CYS
3	Z	343	ASP
3	Z	344	VAL
3	Z	351	ASP
3	Z	354	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	69	HIS
3	X	251	ASN
3	Y	118	ASN
3	Y	240	ASN
3	Y	251	ASN
3	Y	354	ASN
2	H	69	HIS
3	Z	93	ASN
3	Z	118	ASN
3	Z	163	ASN
3	Z	251	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	16,16,17	3.20	7 (43%)	19,22,24	2.08	10 (52%)
3	TYS	Y	335	3	16,16,17	3.64	9 (56%)	19,22,24	2.11	6 (31%)
3	TYS	Z	335	3	16,16,17	3.40	10 (62%)	19,22,24	1.47	2 (10%)

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	-	0/9/11/13	0/1/1/1
3	TYS	Y	335	3	-	0/9/11/13	0/1/1/1
3	TYS	Z	335	3	-	0/9/11/13	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	335	TYS	OH-S	-10.47	1.44	1.63
3	X	335	TYS	OH-S	-10.00	1.45	1.63
3	Z	335	TYS	OH-S	-9.90	1.45	1.63
3	X	335	TYS	OH-CZ	-3.20	1.37	1.42
3	Y	335	TYS	OH-CZ	-2.82	1.38	1.42
3	Z	335	TYS	OH-CZ	-2.20	1.39	1.42
3	X	335	TYS	CD2-CG	2.01	1.43	1.38
3	Z	335	TYS	CE2-CZ	2.12	1.43	1.38
3	X	335	TYS	CE1-CZ	2.31	1.43	1.38
3	X	335	TYS	CA-C	2.42	1.53	1.50
3	Y	335	TYS	CB-CA	2.49	1.59	1.53
3	Z	335	TYS	CB-CG	2.64	1.57	1.51
3	Y	335	TYS	CB-CG	2.85	1.58	1.51
3	Z	335	TYS	CD2-CG	2.87	1.44	1.38
3	Z	335	TYS	CE1-CD1	3.13	1.44	1.38
3	Z	335	TYS	CD1-CG	3.21	1.45	1.38
3	Y	335	TYS	CA-C	3.22	1.54	1.50
3	Y	335	TYS	CE1-CD1	3.50	1.45	1.38
3	Y	335	TYS	CD1-CG	3.50	1.46	1.38
3	Z	335	TYS	CB-CA	3.54	1.61	1.53
3	Z	335	TYS	CA-C	3.62	1.55	1.50
3	X	335	TYS	CE2-CZ	3.74	1.46	1.38
3	Z	335	TYS	CE1-CZ	3.74	1.46	1.38
3	X	335	TYS	CD1-CG	3.86	1.46	1.38
3	Y	335	TYS	CD2-CG	3.94	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	335	TYS	CE1-CZ	4.94	1.48	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	335	TYS	OH-CZ-CE2	-4.16	111.03	118.73
3	X	335	TYS	CB-CG-CD2	-2.81	115.24	120.91
3	X	335	TYS	O3-S-O1	-2.70	99.21	108.79
3	X	335	TYS	OH-CZ-CE1	-2.42	114.26	118.73
3	X	335	TYS	O3-S-O2	-2.32	100.56	108.79
3	X	335	TYS	OH-S-O1	-2.31	101.10	107.59
3	Y	335	TYS	O3-S-O1	-2.09	101.40	108.79
3	X	335	TYS	CB-CA-C	-2.02	107.52	111.41
3	X	335	TYS	CB-CG-CD1	2.04	125.03	120.91
3	Y	335	TYS	O2-S-O1	2.44	122.78	112.25
3	X	335	TYS	OH-S-O2	2.44	114.44	107.59
3	Y	335	TYS	CE2-CD2-CG	2.63	124.65	121.02
3	Z	335	TYS	CG-CB-CA	2.88	120.11	114.29
3	Y	335	TYS	CG-CB-CA	3.11	120.57	114.29
3	X	335	TYS	OH-CZ-CE2	3.51	125.23	118.73
3	Z	335	TYS	O2-S-O1	3.60	127.81	112.25
3	X	335	TYS	O2-S-O1	4.16	130.23	112.25
3	Y	335	TYS	OH-CZ-CE1	5.25	128.45	118.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	335	TYS	2	0
3	Z	335	TYS	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

21 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	A	201	1	14,14,15	0.26	0	15,19,21	2.50	4 (26%)
4	NAG	A	202	1	14,14,15	0.29	0	15,19,21	0.78	0
4	NAG	B	201	2	14,14,15	0.32	0	15,19,21	1.24	3 (20%)
4	NAG	B	202	2	14,14,15	0.36	0	15,19,21	0.74	0
5	EDO	B	203	-	3,3,3	0.77	0	2,2,2	0.07	0
5	EDO	B	204	-	3,3,3	0.66	0	2,2,2	0.18	0
4	NAG	D	201	1	14,14,15	0.26	0	15,19,21	1.86	3 (20%)
4	NAG	D	202	1	14,14,15	0.29	0	15,19,21	0.75	1 (6%)
4	NAG	E	201	2	14,14,15	0.31	0	15,19,21	0.72	1 (6%)
4	NAG	E	202	2	14,14,15	0.30	0	15,19,21	0.88	2 (13%)
4	NAG	G	201	1	14,14,15	0.30	0	15,19,21	2.07	3 (20%)
4	NAG	G	202	1	14,14,15	0.27	0	15,19,21	0.50	0
4	NAG	H	201	2	14,14,15	0.30	0	15,19,21	0.71	1 (6%)
4	NAG	H	202	2	14,14,15	0.28	0	15,19,21	0.50	0
5	EDO	X	401	-	3,3,3	0.76	0	2,2,2	0.10	0
5	EDO	X	402	-	3,3,3	0.65	0	2,2,2	0.26	0
4	NAG	X	403	3	14,14,15	0.27	0	15,19,21	0.65	0
5	EDO	Y	401	-	3,3,3	0.67	0	2,2,2	0.31	0
4	NAG	Y	402	3	14,14,15	0.29	0	15,19,21	0.73	0
6	JEF	Z	401	-	7,7,40	1.85	2 (28%)	5,7,48	1.76	1 (20%)
4	NAG	Z	402	3	14,14,15	0.27	0	15,19,21	0.50	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
4	NAG	A	201	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	202	1	-	0/6/23/26	0/1/1/1
4	NAG	B	201	2	-	0/6/23/26	0/1/1/1
4	NAG	B	202	2	-	0/6/23/26	0/1/1/1
5	EDO	B	203	-	-	0/1/1/1	0/0/0/0
5	EDO	B	204	-	-	0/1/1/1	0/0/0/0
4	NAG	D	201	1	-	0/6/23/26	0/1/1/1
4	NAG	D	202	1	-	0/6/23/26	0/1/1/1
4	NAG	E	201	2	-	0/6/23/26	0/1/1/1
4	NAG	E	202	2	-	0/6/23/26	0/1/1/1
4	NAG	G	201	1	-	0/6/23/26	0/1/1/1
4	NAG	G	202	1	-	0/6/23/26	0/1/1/1
4	NAG	H	201	2	-	0/6/23/26	0/1/1/1
4	NAG	H	202	2	-	0/6/23/26	0/1/1/1
5	EDO	X	401	-	-	0/1/1/1	0/0/0/0
5	EDO	X	402	-	-	0/1/1/1	0/0/0/0
4	NAG	X	403	3	-	0/6/23/26	0/1/1/1
5	EDO	Y	401	-	-	0/1/1/1	0/0/0/0
4	NAG	Y	402	3	-	0/6/23/26	0/1/1/1
6	JEF	Z	401	-	-	0/6/6/46	0/0/0/0
4	NAG	Z	402	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	401	JEF	C10-C11	2.76	1.55	1.51
6	Z	401	JEF	O4-C11	3.58	1.47	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	201	NAG	O5-C1-C2	-7.21	101.44	111.47
4	D	201	NAG	O5-C1-C2	-5.33	104.06	111.47
4	G	201	NAG	O5-C1-C2	-5.11	104.37	111.47
4	B	201	NAG	O5-C1-C2	-2.05	108.62	111.47
4	D	202	NAG	C1-C2-N2	-2.00	107.07	110.49
4	E	202	NAG	C1-O5-C5	2.00	114.92	112.17
4	D	201	NAG	C2-N2-C7	2.04	125.92	122.94
4	B	201	NAG	C2-N2-C7	2.25	126.22	122.94
4	E	202	NAG	O5-C1-C2	2.25	114.60	111.47
4	H	201	NAG	C1-O5-C5	2.28	115.31	112.17
4	A	201	NAG	C2-N2-C7	2.33	126.34	122.94
4	E	201	NAG	C1-O5-C5	2.38	115.45	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	201	NAG	C2-N2-C7	2.42	126.47	122.94
4	A	201	NAG	C1-O5-C5	2.62	115.78	112.17
4	B	201	NAG	C1-C2-N2	3.01	115.63	110.49
6	Z	401	JEF	C8-O4-C11	3.86	124.22	115.34
4	D	201	NAG	C1-C2-N2	4.18	117.62	110.49
4	A	201	NAG	C1-C2-N2	5.06	119.14	110.49
4	G	201	NAG	C1-C2-N2	5.47	119.84	110.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	202	NAG	1	0
4	G	202	NAG	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	88/102 (86%)	-0.48	2 (2%) 61 57	40, 67, 114, 147	0
1	D	89/102 (87%)	-0.43	3 (3%) 46 39	41, 67, 121, 159	0
1	G	88/102 (86%)	-0.47	1 (1%) 80 79	48, 71, 114, 145	0
2	B	109/111 (98%)	-0.40	3 (2%) 53 48	43, 72, 126, 162	0
2	E	108/111 (97%)	-0.44	1 (0%) 84 83	48, 75, 116, 158	0
2	H	108/111 (97%)	-0.32	2 (1%) 67 64	49, 76, 126, 152	0
3	X	288/361 (79%)	-0.18	13 (4%) 34 29	41, 86, 140, 210	0
3	Y	283/361 (78%)	-0.23	10 (3%) 44 38	44, 86, 144, 187	0
3	Z	289/361 (80%)	-0.10	14 (4%) 31 27	42, 92, 143, 195	0
All	All	1450/1722 (84%)	-0.27	49 (3%) 46 39	40, 82, 139, 210	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Z	356	CYS	8.1
3	X	351	ASP	5.9
1	D	4	VAL	5.5
3	Z	342	VAL	5.0
3	Z	290	PRO	5.0
3	Z	291	ILE	4.5
3	Y	357	GLU	4.4
3	Z	351	ASP	4.2
3	Z	338	CYS	3.9
3	Z	339	ASN	3.9
3	X	350	PRO	3.6
3	Z	355	PRO	3.6
3	X	354	ASN	3.4
3	Y	349	LYS	3.4
1	D	72	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	68	HIS	3.3
1	G	5	GLN	3.2
3	Y	356	CYS	3.2
3	X	355	PRO	3.2
3	Y	354	ASN	3.1
3	Z	354	ASN	3.1
3	Z	292	CYS	3.1
3	X	280	ASN	3.0
3	X	281	TRP	3.0
3	X	353	PHE	2.9
3	Y	21	ARG	2.9
1	D	5	GLN	2.9
3	Z	281	TRP	2.8
2	E	68	HIS	2.8
3	Z	19	HIS	2.8
2	H	67	ALA	2.8
3	X	291	ILE	2.7
3	Z	18	CYS	2.7
1	A	5	GLN	2.5
3	Y	22	ILE	2.5
3	Y	355	PRO	2.4
3	X	338	CYS	2.4
2	B	66	CYS	2.3
2	H	107	GLY	2.3
3	Y	20	HIS	2.2
3	Z	110	TYR	2.2
1	A	72	GLY	2.2
3	Y	337	LEU	2.2
3	X	342	VAL	2.2
3	X	356	CYS	2.2
3	Y	18	CYS	2.1
3	X	292	CYS	2.1
2	B	69	HIS	2.0
3	X	349	LYS	2.0

## 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. 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, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TYS	Z	335	16/17	0.84	0.29	-	105,114,138,139	0
3	TYS	X	335	16/17	0.90	0.26	-	107,121,139,141	0
3	TYS	Y	335	16/17	0.89	0.24	-	114,125,145,147	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	X	401	4/4	0.82	0.30	11.34	66,67,68,68	0
4	NAG	Y	402	14/15	0.93	0.27	1.63	106,118,125,127	0
4	NAG	Z	402	14/15	0.92	0.21	0.99	103,118,123,124	0
4	NAG	X	403	14/15	0.85	0.24	0.87	109,117,127,127	0
5	EDO	Y	401	4/4	0.87	0.17	-0.16	74,76,77,77	0
4	NAG	D	202	14/15	0.94	0.14	-0.31	75,78,86,87	0
4	NAG	D	201	14/15	0.92	0.14	-0.31	71,76,80,83	0
4	NAG	A	201	14/15	0.95	0.13	-0.59	70,77,86,89	0
4	NAG	A	202	14/15	0.98	0.12	-0.63	72,78,86,92	0
5	EDO	X	402	4/4	0.90	0.14	-0.73	97,98,99,99	0
4	NAG	G	201	14/15	0.93	0.13	-0.80	69,79,88,92	0
4	NAG	G	202	14/15	0.96	0.13	-0.91	85,88,95,98	0
4	NAG	H	202	14/15	0.72	0.38	-	135,143,151,154	0
5	EDO	B	204	4/4	0.79	0.35	-	109,109,110,110	0
5	EDO	B	203	4/4	0.80	0.22	-	76,77,78,79	0
4	NAG	E	201	14/15	0.78	0.31	-	145,152,158,163	0
4	NAG	B	201	14/15	0.82	0.41	-	126,136,146,146	0
4	NAG	B	202	14/15	0.81	0.39	-	162,171,176,179	0
6	JEF	Z	401	8/41	0.71	0.26	-	108,114,116,117	0
4	NAG	H	201	14/15	0.69	0.41	-	140,145,153,154	0
4	NAG	E	202	14/15	0.70	0.47	-	144,150,159,164	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.