wwPDB X-ray Structure Validation Summary Report (i)

Jan 2, 2024 – 04:09 PM EST

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 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

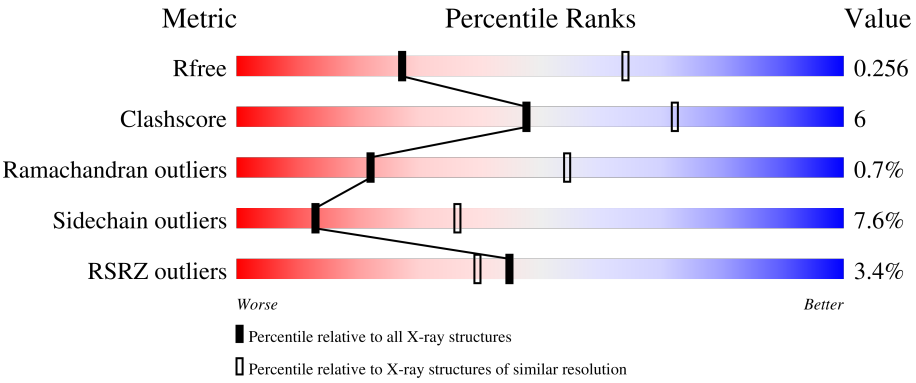
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	102	2% 64% 20% 14%
1	D	102	3% 70% 17% 13%
1	G	102	% 68% 19% 14%
2	B	111	3% 83% 14%
2	E	111	% 78% 16%

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Mol	Chain	Length	Quality of chain
2	H	111	2% 78% 16%
3	X	361	3% 65% 13% 20%
3	Y	361	3% 65% 14% 21%
3	Z	361	4% 58% 21% 20%

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	X	335	-	X	-	-
4	NAG	E	202	-	-	-	X
4	NAG	H	201	-	-	-	X

2 Entry composition (i)

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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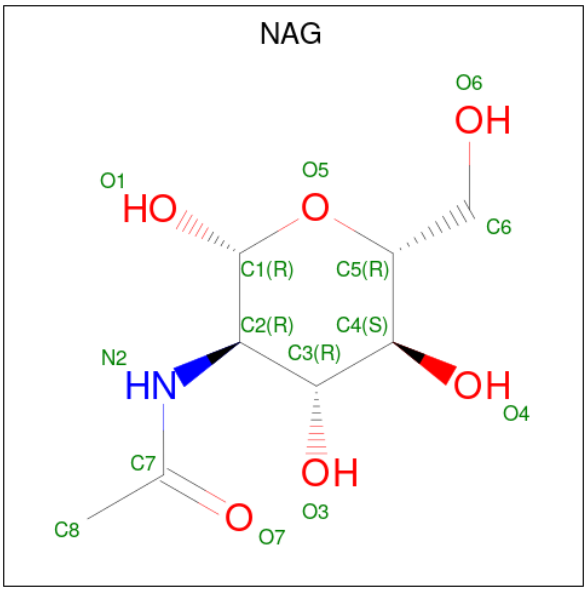
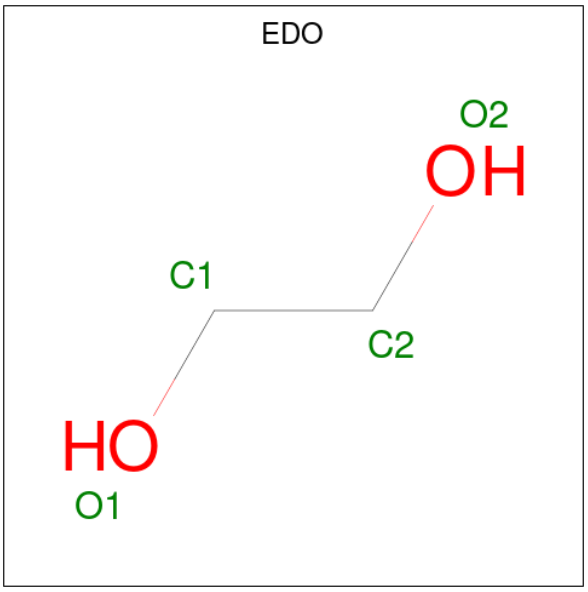
Chain	Residue	Modelled	Actual	Comment	Reference
Y	188	SER	CYS	engineered mutation	UNP P23945
Y	367	ALA	-	expression tag	UNP P23945
Y	368	ALA	-	expression tag	UNP P23945
Y	369	ALA	-	expression tag	UNP P23945
Y	370	HIS	-	expression tag	UNP P23945
Y	371	HIS	-	expression tag	UNP P23945
Y	372	HIS	-	expression 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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



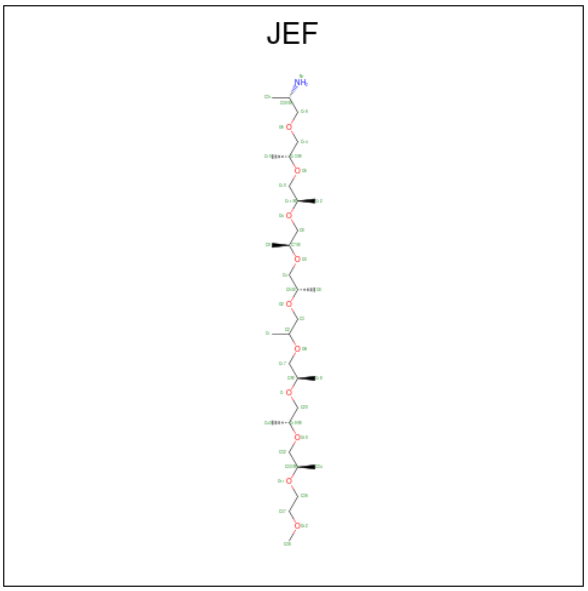
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is O-(O-(2-AMINOPROPYL)-O'-(2-METHOXYETHYL)POLYPROPYLENE GLYCOL 500) (three-letter code: JEF) (formula: $C_{30}H_{63}NO_{10}$).



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

- Molecule 7 is water.

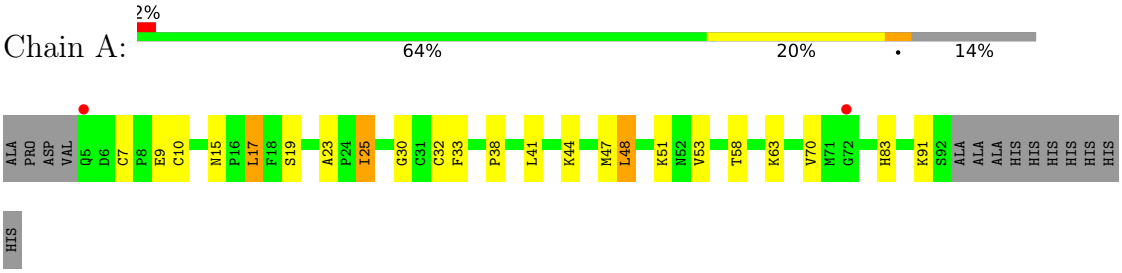
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	13	Total O 13 13	0	0
7	B	16	Total O 16 16	0	0
7	X	22	Total O 22 22	0	0
7	D	10	Total O 10 10	0	0
7	E	13	Total O 13 13	0	0
7	Y	28	Total O 28 28	0	0
7	G	15	Total O 15 15	0	0
7	H	20	Total O 20 20	0	0
7	Z	18	Total O 18 18	0	0

3 Residue-property plots

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.

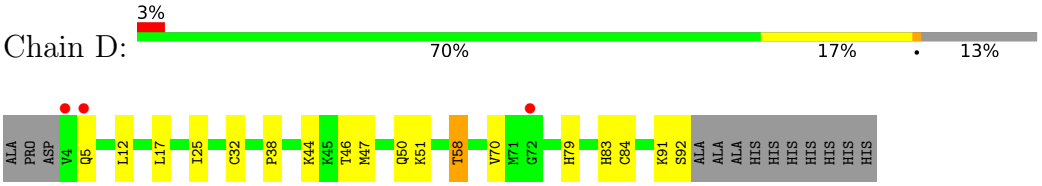
• Molecule 1: Glycoprotein hormones, alpha polypeptide

Chain A:



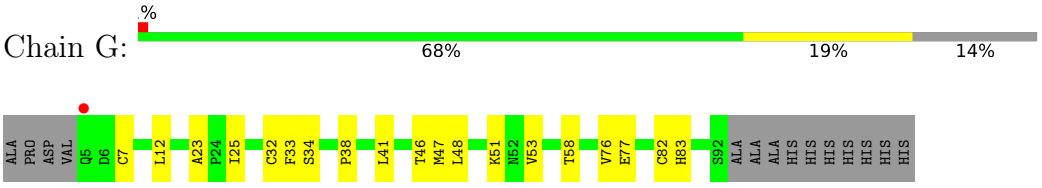
• Molecule 1: Glycoprotein hormones, alpha polypeptide

Chain D:



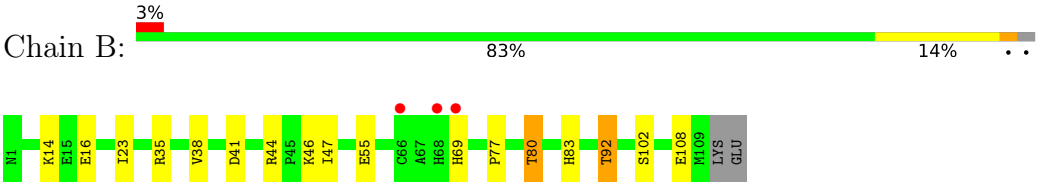
• Molecule 1: Glycoprotein hormones, alpha polypeptide

Chain G:



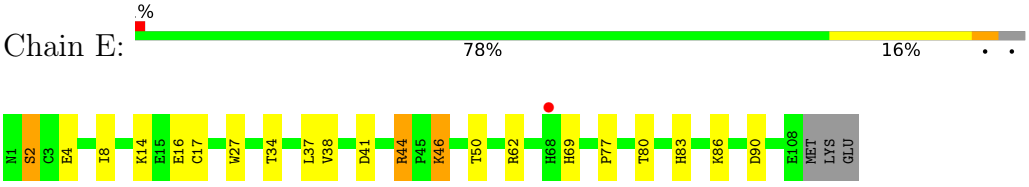
• Molecule 2: Follitropin subunit beta

Chain B:



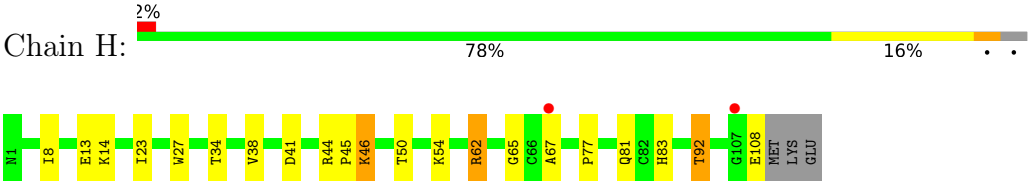
• Molecule 2: Follitropin subunit beta

Chain E:



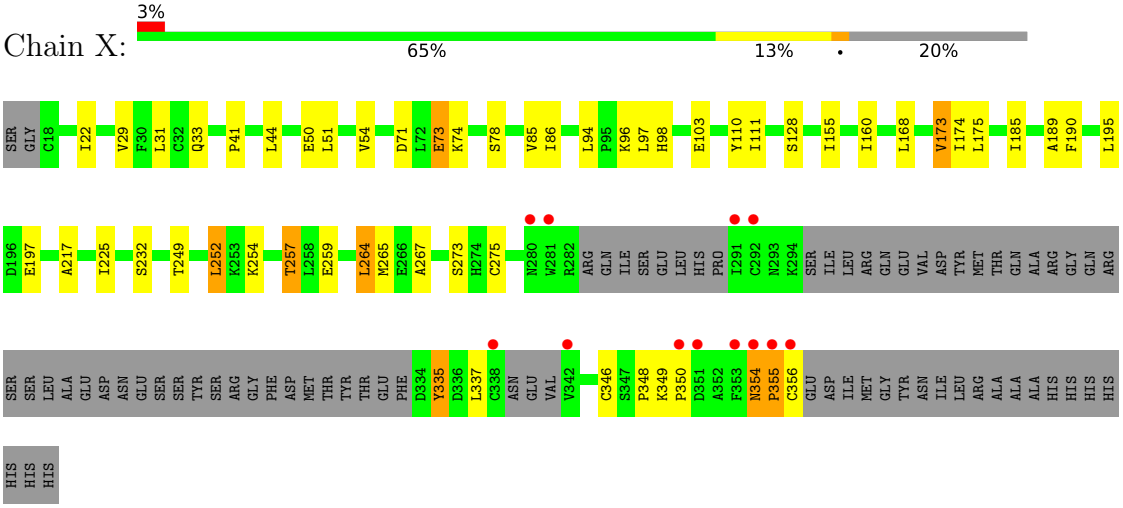
• Molecule 2: Follitropin subunit beta

Chain H:



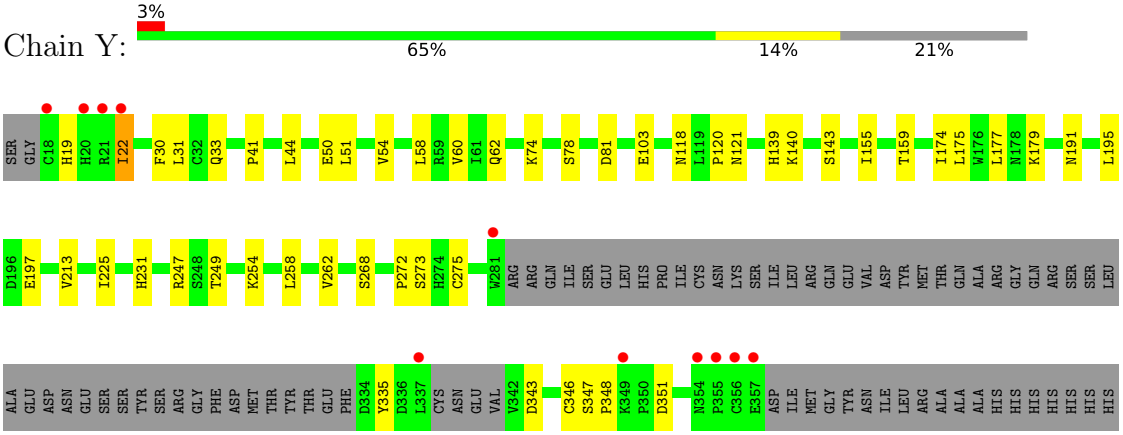
• Molecule 3: Follicle-stimulating hormone receptor

Chain X:



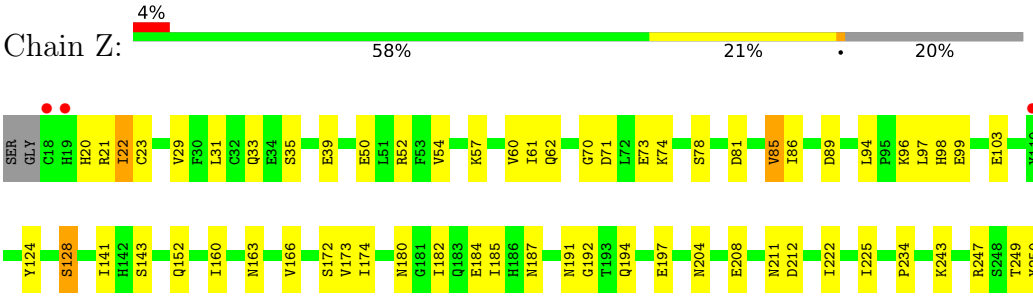
• Molecule 3: Follicle-stimulating hormone receptor

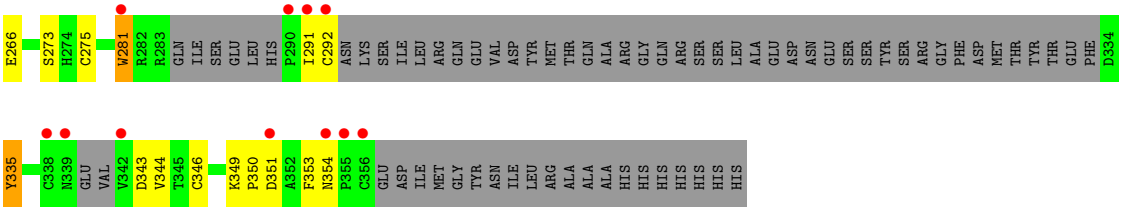
Chain Y:



• Molecule 3: Follicle-stimulating hormone receptor

Chain Z:




E266
S273
H274
C275
W281
R282
R283
GLN
ILE
SER
GLU
LEU
HIS
P290
I291
C292
ASN
LYS
SER
ILE
LEU
ARG
GLN
GLU
VAL
ASP
TYR
MET
THR
GLN
ALA
ARG
GLY
GLN
ARG
SER
SER
LEU
ALA
GLU
ASP
ASN
GLU
SER
SER
TYR
SER
ARG
GLY
PHE
ASP
MET
THR
TYR
THR
GLU
PHE
D334
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C338
N339
GLU
VAL
V342
D343
V344
T345
C346
K349
P350
D351
A352
F353
N354
P355
C356
GLU
ASP
ILE
MET
GLY
TYR
ASN
ILE
LEU
ARG
ALA
ALA
ALA
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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.71 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.5.0066, BUSTER 2.11.5	Depositor
R, R_{free}	0.174 , 0.237 0.192 , 0.256	Depositor DCC
R_{free} test set	2233 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, EDO, TYS, JEF

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

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.

The worst 5 of 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

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%)	17	48
2	H	106/111 (96%)	101 (95%)	3 (3%)	2 (2%)	8	28
3	X	280/361 (78%)	244 (87%)	32 (11%)	4 (1%)	11	36
3	Y	277/361 (77%)	246 (89%)	30 (11%)	1 (0%)	34	66
3	Z	281/361 (78%)	241 (86%)	38 (14%)	2 (1%)	22	54
All	All	1416/1722 (82%)	1277 (90%)	129 (9%)	10 (1%)	22	54

5 of 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

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	80/90 (89%)	72 (90%)	8 (10%)	7 23
1	D	81/90 (90%)	77 (95%)	4 (5%)	25 57
1	G	80/90 (89%)	76 (95%)	4 (5%)	24 57
2	B	97/99 (98%)	84 (87%)	13 (13%)	4 11
2	E	96/99 (97%)	86 (90%)	10 (10%)	7 21
2	H	96/99 (97%)	88 (92%)	8 (8%)	11 32
3	X	256/328 (78%)	245 (96%)	11 (4%)	29 62
3	Y	257/328 (78%)	238 (93%)	19 (7%)	13 38
3	Z	263/328 (80%)	241 (92%)	22 (8%)	11 31
All	All	1306/1551 (84%)	1207 (92%)	99 (8%)	13 36

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Y	213	VAL
2	H	46	LYS
3	Y	254	LYS
1	G	7	CYS
2	H	92	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	Z	93	ASN
3	Z	118	ASN
3	Z	251	ASN
3	Z	163	ASN
3	Y	251	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	2.91	5 (33%)	18,22,24	2.11	10 (55%)
3	TYS	Z	335	3	15,16,17	3.07	9 (60%)	18,22,24	1.53	2 (11%)
3	TYS	Y	335	3	15,16,17	3.38	8 (53%)	18,22,24	2.14	7 (38%)

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	-	8/10/11/13	0/1/1/1
3	TYS	Z	335	3	-	3/10/11/13	0/1/1/1
3	TYS	Y	335	3	-	4/10/11/13	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	335	TYS	OH-S	-8.94	1.44	1.58
3	X	335	TYS	OH-S	-8.37	1.45	1.58
3	Z	335	TYS	OH-S	-8.27	1.45	1.58
3	Y	335	TYS	CE1-CZ	5.13	1.48	1.38
3	Z	335	TYS	CE1-CZ	3.88	1.46	1.38

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	335	TYS	OH-CZ-CE1	4.99	128.45	118.64
3	X	335	TYS	O2-S-O1	4.49	130.23	112.22
3	Z	335	TYS	O2-S-O1	3.89	127.81	112.22
3	Y	335	TYS	OH-CZ-CE2	-3.87	111.03	118.64
3	X	335	TYS	OH-CZ-CE2	3.35	125.23	118.64

There are no chirality outliers.

5 of 15 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	CZ-OH-S-O3
3	Y	335	TYS	CA-CB-CG-CD2

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	Y	402	3	14,14,15	0.30	0	17,19,21	0.66	0
5	EDO	B	204	-	3,3,3	0.68	0	2,2,2	0.16	0
4	NAG	A	202	1	14,14,15	0.29	0	17,19,21	0.74	0
4	NAG	E	201	2	14,14,15	0.31	0	17,19,21	0.72	1 (5%)
5	EDO	X	401	-	3,3,3	0.77	0	2,2,2	0.13	0
4	NAG	G	201	1	14,14,15	0.30	0	17,19,21	1.85	3 (17%)
4	NAG	B	202	2	14,14,15	0.37	0	17,19,21	0.71	0
6	JEF	Z	401	-	6,7,40	1.13	1 (16%)	6,7,48	1.77	1 (16%)
4	NAG	A	201	1	14,14,15	0.27	0	17,19,21	2.19	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	B	203	-	3,3,3	0.79	0	2,2,2	0.05	0
4	NAG	Z	402	3	14,14,15	0.27	0	17,19,21	0.47	0
4	NAG	D	201	1	14,14,15	0.27	0	17,19,21	1.63	3 (17%)
5	EDO	Y	401	-	3,3,3	0.68	0	2,2,2	0.29	0
5	EDO	X	402	-	3,3,3	0.66	0	2,2,2	0.24	0
4	NAG	E	202	2	14,14,15	0.30	0	17,19,21	0.83	2 (11%)
4	NAG	G	202	1	14,14,15	0.28	0	17,19,21	0.48	0
4	NAG	X	403	3	14,14,15	0.28	0	17,19,21	0.61	0
4	NAG	H	202	2	14,14,15	0.28	0	17,19,21	0.49	0
4	NAG	D	202	1	14,14,15	0.29	0	17,19,21	0.71	1 (5%)
4	NAG	H	201	2	14,14,15	0.30	0	17,19,21	0.70	1 (5%)
4	NAG	B	201	2	14,14,15	0.32	0	17,19,21	1.15	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	402	3	-	0/6/23/26	0/1/1/1
5	EDO	B	204	-	-	0/1/1/1	-
4	NAG	A	202	1	-	2/6/23/26	0/1/1/1
4	NAG	E	201	2	-	2/6/23/26	0/1/1/1
5	EDO	X	401	-	-	1/1/1/1	-
4	NAG	G	201	1	-	1/6/23/26	0/1/1/1
4	NAG	B	202	2	-	1/6/23/26	0/1/1/1
6	JEF	Z	401	-	-	2/6/6/46	-
4	NAG	A	201	1	-	2/6/23/26	0/1/1/1
5	EDO	B	203	-	-	1/1/1/1	-
4	NAG	Z	402	3	-	0/6/23/26	0/1/1/1
4	NAG	D	201	1	-	1/6/23/26	0/1/1/1
5	EDO	Y	401	-	-	0/1/1/1	-
5	EDO	X	402	-	-	0/1/1/1	-
4	NAG	E	202	2	-	0/6/23/26	0/1/1/1
4	NAG	G	202	1	-	0/6/23/26	0/1/1/1
4	NAG	X	403	3	-	0/6/23/26	0/1/1/1
4	NAG	H	202	2	-	0/6/23/26	0/1/1/1
4	NAG	D	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	B	201	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	401	JEF	C10-C11	2.09	1.55	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	201	NAG	O5-C1-C2	-6.23	101.44	111.29
4	G	201	NAG	C1-C2-N2	5.47	119.84	110.49
4	A	201	NAG	C1-C2-N2	5.06	119.14	110.49
4	D	201	NAG	O5-C1-C2	-4.58	104.06	111.29
4	G	201	NAG	O5-C1-C2	-4.38	104.37	111.29

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	Z	401	JEF	O5-C10-C11-O4
4	B	201	NAG	C1-C2-N2-C7
4	G	201	NAG	C1-C2-N2-C7
4	E	201	NAG	O5-C5-C6-O6
4	A	201	NAG	C1-C2-N2-C7

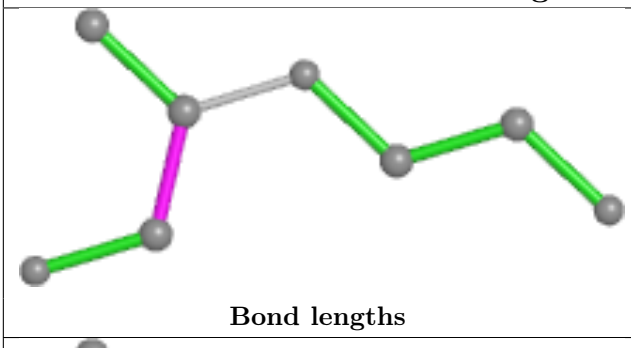
There are no ring outliers.

2 monomers are involved in 2 short contacts:

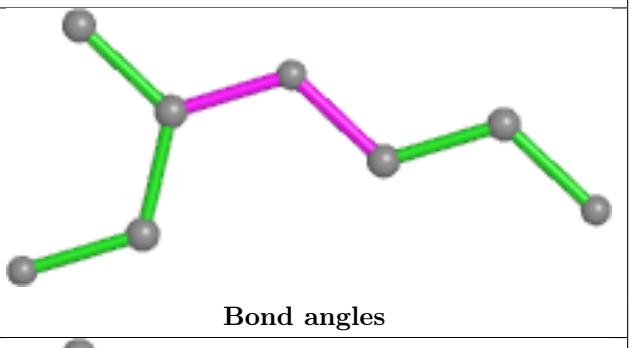
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	202	NAG	1	0
4	G	202	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

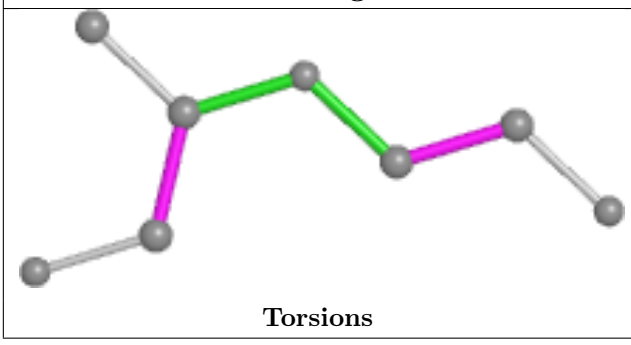
Ligand JEF Z 401



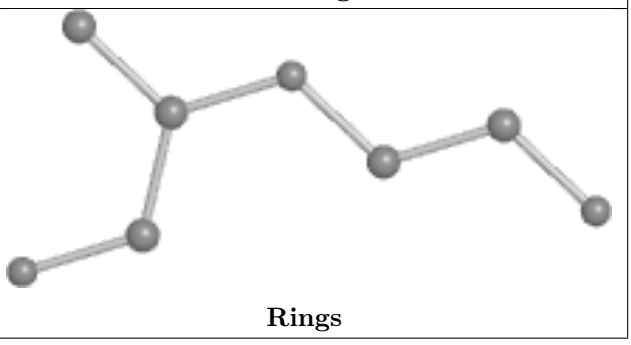
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	88/102 (86%)	-0.48	2 (2%)	60	58	40, 67, 114, 147	0
1	D	89/102 (87%)	-0.43	3 (3%)	45	40	41, 67, 121, 159	0
1	G	88/102 (86%)	-0.47	1 (1%)	80	80	48, 71, 114, 145	0
2	B	109/111 (98%)	-0.40	3 (2%)	53	49	43, 72, 126, 162	0
2	E	108/111 (97%)	-0.44	1 (0%)	84	84	48, 75, 116, 158	0
2	H	108/111 (97%)	-0.32	2 (1%)	66	65	49, 76, 126, 152	0
3	X	288/361 (79%)	-0.19	12 (4%)	36	32	41, 86, 140, 210	0
3	Y	283/361 (78%)	-0.23	11 (3%)	39	35	44, 86, 144, 187	0
3	Z	289/361 (80%)	-0.11	14 (4%)	30	27	42, 92, 143, 195	0
All	All	1450/1722 (84%)	-0.27	49 (3%)	45	40	40, 82, 139, 210	0

The worst 5 of 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	4.9

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TYS	Z	335	16/17	0.84	0.29	105,114,138,139	0
3	TYS	Y	335	16/17	0.89	0.24	114,125,145,147	0
3	TYS	X	335	16/17	0.90	0.26	107,121,139,141	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

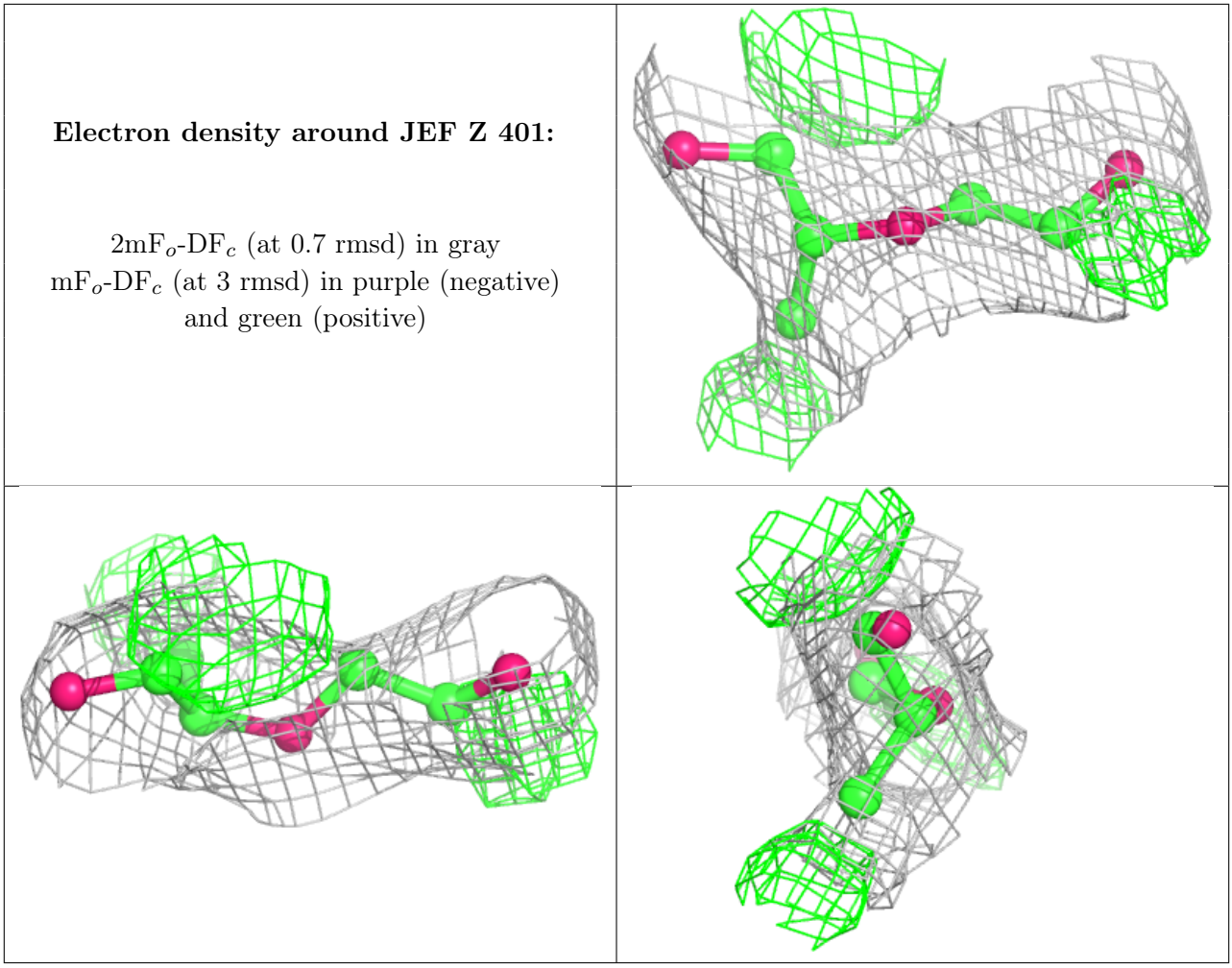
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	E	202	14/15	0.70	0.46	144,150,159,164	0
4	NAG	H	201	14/15	0.70	0.41	140,145,153,154	0
6	JEF	Z	401	8/41	0.71	0.26	108,114,116,117	0
4	NAG	H	202	14/15	0.72	0.38	135,143,151,154	0
4	NAG	E	201	14/15	0.78	0.30	145,152,158,163	0
5	EDO	B	204	4/4	0.79	0.36	109,109,110,110	0
5	EDO	B	203	4/4	0.80	0.22	76,77,78,79	0
4	NAG	B	202	14/15	0.81	0.40	162,171,176,179	0
5	EDO	X	401	4/4	0.82	0.30	66,67,68,68	0
4	NAG	B	201	14/15	0.82	0.41	126,136,146,146	0
4	NAG	X	403	14/15	0.85	0.24	109,117,127,127	0
5	EDO	Y	401	4/4	0.87	0.17	74,76,77,77	0
5	EDO	X	402	4/4	0.90	0.14	97,98,99,99	0
4	NAG	D	201	14/15	0.92	0.14	71,76,80,83	0
4	NAG	Z	402	14/15	0.92	0.21	103,118,123,124	0
4	NAG	G	201	14/15	0.93	0.13	69,79,88,92	0
4	NAG	Y	402	14/15	0.93	0.26	106,118,125,127	0
4	NAG	D	202	14/15	0.94	0.15	75,78,86,87	0
4	NAG	A	201	14/15	0.95	0.13	70,77,86,89	0
4	NAG	G	202	14/15	0.96	0.13	85,88,95,98	0
4	NAG	A	202	14/15	0.98	0.12	72,78,86,92	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around JEF Z 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.