



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:30 pm BST

PDB ID : 6QIO
Title : Ternary complex of FcRn ectodomain, FcRn binding optimised human serum albumin and the human growth hormone derivative somapacitan
Authors : Johansson, E.
Deposited on : 2019-01-21
Resolution : 1.95 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

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	:	2.11
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)	:	2.11

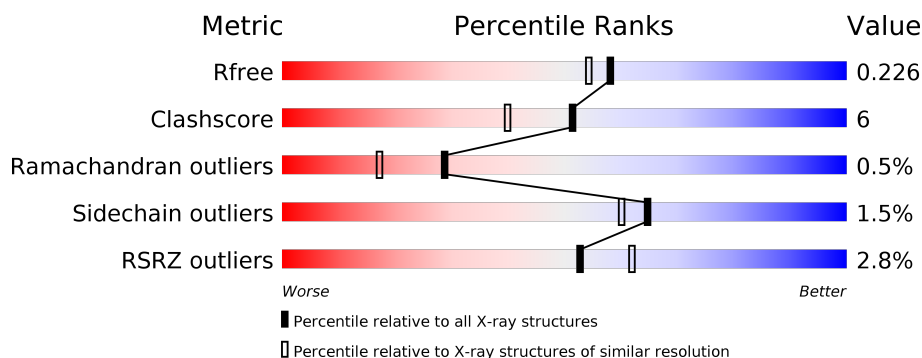
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	585	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
2	B	274	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>••</div> </div> </div>
3	C	105	<div> <div></div> <div> <div></div> <div>88%</div> <div>8%</div> <div>5%</div> </div> </div>
4	D	191	<div> <div>•</div> <div> <div></div> <div>99%</div> </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16235 atoms, of which 7578 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 Serum albumin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	583	9318	2958	4626	793	899	42	0	20	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	418	MET	VAL	engineered mutation	UNP P02768
A	420	ALA	THR	engineered mutation	UNP P02768
A	505	GLY	GLU	engineered mutation	UNP P02768
A	547	ALA	VAL	engineered mutation	UNP P02768

- Molecule 2 is a protein called IgG receptor FcRn large subunit p51.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	267	4178	1361	2042	369	398	8	0	10	0

- Molecule 3 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	100	1651	537	807	144	160	3	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	100	HIS	-	expression tag	UNP P61769
C	101	HIS	-	expression tag	UNP P61769
C	102	HIS	-	expression tag	UNP P61769
C	103	HIS	-	expression tag	UNP P61769
C	104	HIS	-	expression tag	UNP P61769
C	105	HIS	-	expression tag	UNP P61769

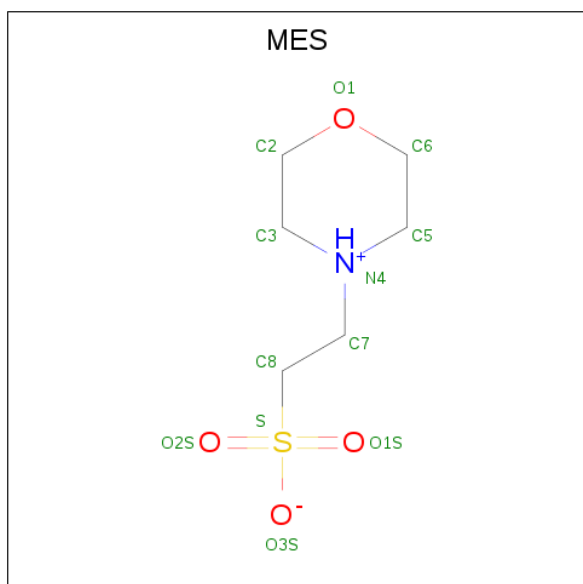
- Molecule 4 is a protein called Somatotropin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S		
4	D	1	9	3	3	1	1	1	9	0

There is a discrepancy between the modelled and reference sequences:

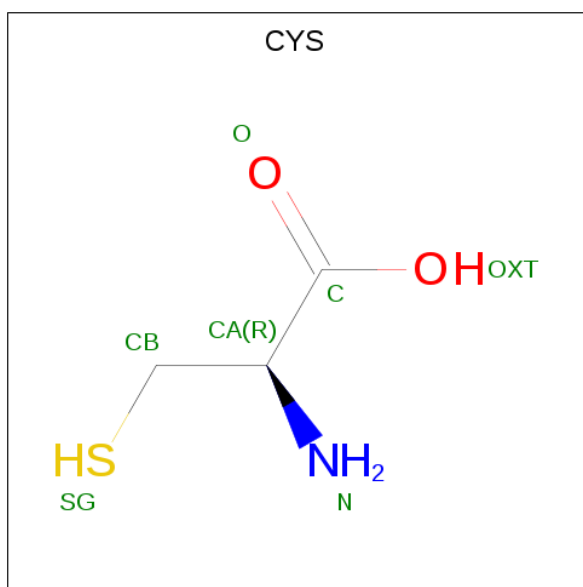
Chain	Residue	Modelled	Actual	Comment	Reference
D	149	CYS	LEU	engineered mutation	UNP P01241

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



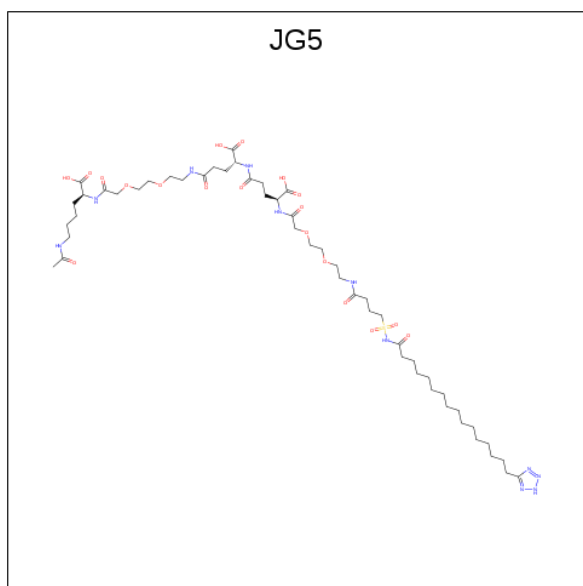
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O	S	
5	A	1	25	6	13	1	4	1	0

- Molecule 6 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	S	
			10	3	3	1	2	1	

- Molecule 7 is (2S)-6-acetamido-2-[[2-[2-[2-[[4-carboxy-4-[(4S)-4-carboxy-4-[[2-[2-[2-[4-[16-(1H-tetrazol-5-yl)hexadecanoylsulfamoyl]butanoylamino]ethoxy]ethoxy]acetyl]amino]butanoyl]amino]butanoyl]amino]ethoxy]ethoxy]acetyl]amino]hexanoic acid (three-letter code: JG5) (formula: C₅₁H₈₉N₁₁O₁₉S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	H	N	O	S	
			166	51	84	11	19	1	

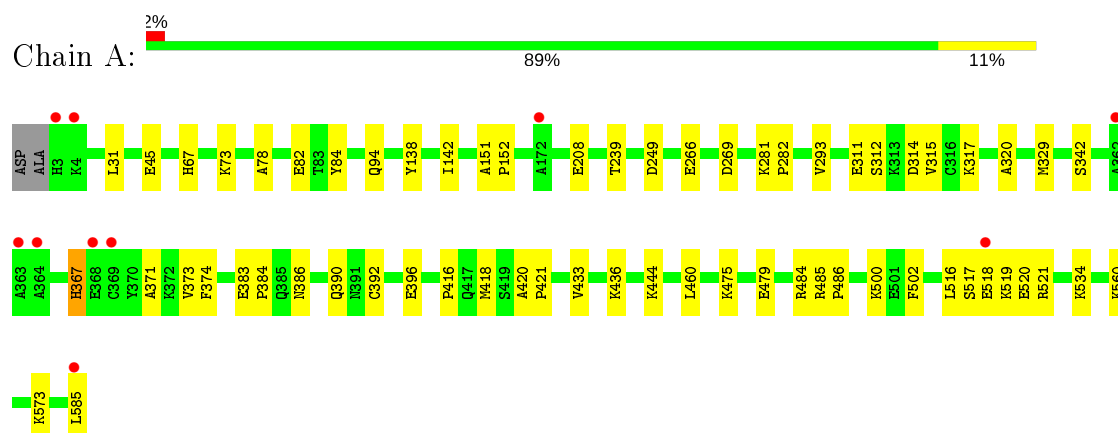
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	530	Total 530	O 530	0	0
8	B	225	Total 225	O 225	0	0
8	C	120	Total 120	O 120	0	0
8	D	3	Total 3	O 3	0	0

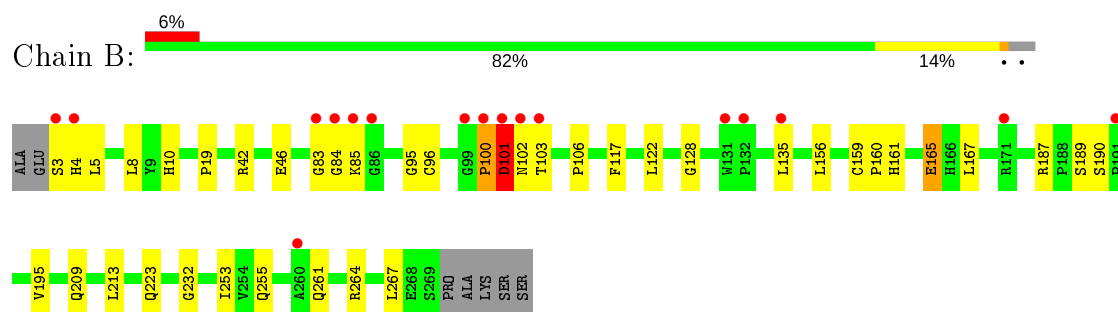
3 Residue-property plots [i](#)

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.

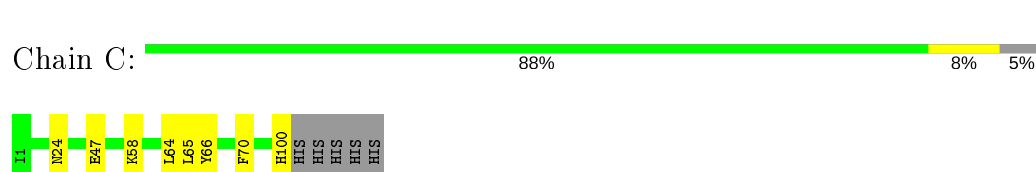
- Molecule 1: Serum albumin



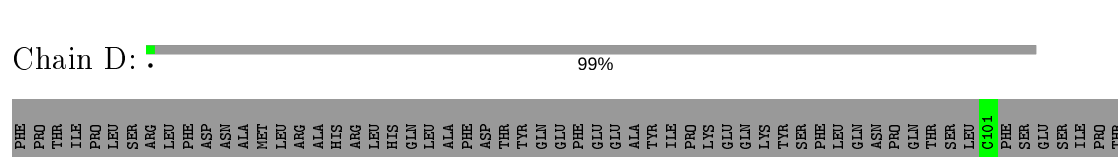
- Molecule 2: IgG receptor FcRn large subunit p51



- Molecule 3: Beta-2-microglobulin



- Molecule 4: Somatotropin



PRO	SER	ASN	ARG	LEU	MET	GLY	THR	GLN	GLY	LYS	SER	ASN	LEU	GLU	LEU	GLY	ARG	ILE	SER	LEU	LEU	ILE	ILE	GLN	SER	TRP	LEU	GLU	PRO	VAL	GLN	HIS	ASN	PHE	LEU	ASP	ARG	ALA	SER	VAL	PHE	LEU	LYS	ALA	ASN	SER	CYS	VAL	TYR	GLY	ALA	SER	PHE	ASP	ASN	VAL	MET	VAL	TYR	ASP	LYS	ASP	LEU	LYS	VAL	GLU	THR	PHE	LEU	ARG	ILE	GLY	VAL																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
ILE	GLN	THR	LEU	SER	VAL	GLY	ARG	LEU	GLY	ASP	GLY	SER	PRO	ARG	THR	GLY	GLN	ILE	PHE	LYS	GLN	THR	TYR	SER	LYS	PHE	ASP	THR	ASN	SER	HIS	ASN	ASP	ASP	ALA	SER	LEU	LEU	LYS	ASN	TYR	SER	GLY	LEU	LEU	TYR	GLY	CYS	THR	PHE	ARG	LYS	ASP	ASN	VAL	MET	ASP	LYS	VAL	LEU	GLU	THR	LYS	PHE	LEU	ARG	ILE	GLY	VAL																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.29Å 108.12Å 159.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.85 – 1.95 48.85 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.85-1.95) 99.7 (48.85-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.182 , 0.226 0.182 , 0.226	Depositor DCC
R_{free} test set	4763 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16235	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: JG5, MES

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	0.55	1/4892 (0.0%)	0.68	2/6592 (0.0%)
2	B	0.65	2/2227 (0.1%)	0.72	0/3026
3	C	0.57	0/876	0.71	0/1186
4	D	0.22	0/5	0.21	0/5
All	All	0.58	3/8000 (0.0%)	0.70	2/10809 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	96	CYS	CB-SG	-11.61	1.62	1.82
2	B	165	GLU	CG-CD	6.01	1.60	1.51
1	A	329	MET	CG-SD	5.42	1.95	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	329	MET	CB-CG-SD	-5.42	96.13	112.40

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	4692	4626	4492	49	1
2	B	2136	2042	2015	30	0
3	C	844	807	802	5	0
4	D	6	3	3	0	0
5	A	12	13	13	2	0
6	B	7	3	3	0	0
7	D	82	84	0	0	0
8	A	530	0	0	16	0
8	B	225	0	0	13	0
8	C	120	0	0	3	0
8	D	3	0	0	0	0
All	All	8657	7578	7328	85	1

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 (85) 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)
2:B:209:GLN:NE2	2:B:255:GLN:OE1	1.93	1.00
2:B:101:ASP:N	8:B:401:HOH:O	1.99	0.94
1:A:585:LEU:HD21	8:A:1150:HOH:O	1.67	0.94
1:A:516:LEU:O	8:A:701:HOH:O	1.96	0.83
3:C:100:HIS:O	8:C:201:HOH:O	1.97	0.82
1:A:312:SER:O	8:A:703:HOH:O	1.99	0.80
1:A:516:LEU:O	8:A:702:HOH:O	1.98	0.79
2:B:100:PRO:HB2	8:B:401:HOH:O	1.84	0.77
1:A:266:GLU:OE1	8:A:705:HOH:O	2.04	0.76
2:B:128:GLY:N	8:B:404:HOH:O	2.19	0.75
2:B:187:ARG:NE	8:B:406:HOH:O	2.21	0.73
1:A:519:LYS:NZ	8:A:704:HOH:O	2.03	0.72
1:A:293:VAL:O	8:A:706:HOH:O	2.09	0.69
1:A:269:ASP:OD1	8:A:707:HOH:O	2.11	0.68
2:B:19:PRO:O	8:B:402:HOH:O	2.12	0.67
2:B:5:LEU:HD23	2:B:167:LEU:HD21	1.77	0.66
1:A:521:ARG:NH2	8:A:713:HOH:O	2.30	0.65
2:B:264:ARG:NH2	8:B:407:HOH:O	2.27	0.64
1:A:517:SER:O	1:A:520:GLU:N	2.29	0.64
1:A:311:GLU:O	8:A:703:HOH:O	2.15	0.63
1:A:45:GLU:OE1	1:A:73:LYS:NZ	2.29	0.61
2:B:106:PRO:HG3	2:B:122:LEU:HD22	1.83	0.60
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:LEU:CD2	2:B:167:LEU:HD21	2.32	0.59
3:C:58:LYS:NZ	8:C:206:HOH:O	2.35	0.59
1:A:396:GLU:O	8:A:708:HOH:O	2.17	0.57
1:A:138:TYR:CE1	1:A:142:ILE:HD11	2.40	0.57
1:A:418:MET:HE1	1:A:460[A]:LEU:HD11	1.87	0.56
2:B:103:THR:HG23	8:B:401:HOH:O	2.06	0.55
2:B:135:LEU:HD22	8:B:481:HOH:O	2.07	0.54
1:A:392:CYS:O	1:A:396:GLU:HG2	2.07	0.54
1:A:420:ALA:HB3	1:A:421:PRO:HD3	1.88	0.54
2:B:102:ASN:N	8:B:405:HOH:O	2.40	0.54
2:B:122:LEU:HD23	2:B:156:LEU:HD21	1.90	0.53
1:A:31:LEU:HD11	1:A:78:ALA:HB2	1.92	0.51
2:B:103:THR:CG2	8:B:401:HOH:O	2.58	0.51
2:B:232:GLY:HA3	8:B:579:HOH:O	2.10	0.50
2:B:128:GLY:CA	8:B:404:HOH:O	2.58	0.50
2:B:253:ILE:HD13	2:B:264:ARG:HA	1.94	0.50
1:A:518:GLU:HA	1:A:521:ARG:HB2	1.93	0.49
1:A:418:MET:CE	1:A:460[A]:LEU:HD11	2.43	0.48
2:B:42:ARG:NE	2:B:46:GLU:OE2	2.47	0.48
1:A:585:LEU:HD22	1:A:585:LEU:N	2.28	0.48
2:B:8:LEU:HD23	2:B:95:GLY:HA3	1.95	0.47
1:A:67:HIS:NE2	1:A:249:ASP:OD1	2.45	0.47
1:A:367:HIS:O	1:A:371:ALA:HB2	2.14	0.47
1:A:518:GLU:HG2	8:A:702:HOH:O	2.16	0.46
3:C:47:GLU:OE1	8:C:202:HOH:O	2.21	0.46
1:A:433:VAL:HG11	5:A:601:MES:C6	2.47	0.45
2:B:159:CYS:HB3	2:B:160:PRO:CD	2.47	0.45
1:A:82:GLU:OE1	1:A:82:GLU:N	2.44	0.45
1:A:433:VAL:HG11	5:A:601:MES:H61	1.99	0.44
2:B:3:SER:OG	2:B:4:HIS:N	2.50	0.44
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.82	0.44
1:A:314:ASP:O	1:A:317:LYS:N	2.50	0.44
2:B:122:LEU:HD23	2:B:156:LEU:CD2	2.48	0.44
3:C:24:ASN:HB3	3:C:65:LEU:HD11	1.99	0.44
1:A:84:TYR:HA	8:A:1046:HOH:O	2.16	0.44
1:A:281:LYS:HB3	1:A:282:PRO:HD2	1.99	0.43
2:B:161:HIS:O	2:B:165:GLU:HG3	2.18	0.43
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.54	0.43
1:A:500:LYS:NZ	8:A:742:HOH:O	2.51	0.43
1:A:367:HIS:ND1	1:A:367:HIS:O	2.50	0.43
1:A:475:LYS:HE2	1:A:479:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:PRO:O	1:A:534:LYS:HE2	2.19	0.43
1:A:485:ARG:HB3	1:A:486:PRO:HD3	2.01	0.43
2:B:100:PRO:O	2:B:102:ASN:N	2.51	0.42
2:B:189[A]:SER:HB2	2:B:195:VAL:HG23	2.00	0.42
3:C:64:LEU:HD21	3:C:66:TYR:HE1	1.84	0.42
2:B:213:LEU:HD11	2:B:253:ILE:HG13	2.00	0.42
1:A:320:ALA:HB2	8:A:743:HOH:O	2.20	0.41
2:B:135:LEU:HD23	2:B:135:LEU:C	2.41	0.41
1:A:585:LEU:CD2	1:A:585:LEU:N	2.84	0.41
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.98	0.41
1:A:386:ASN:O	1:A:390:GLN:HG3	2.21	0.41
1:A:314:ASP:O	1:A:315:VAL:C	2.59	0.41
2:B:189[B]:SER:HB2	2:B:195:VAL:HG23	2.02	0.41
1:A:208[B]:GLU:HG3	1:A:239:THR:HG21	2.02	0.40
2:B:159:CYS:HB3	2:B:160:PRO:HD3	2.03	0.40
1:A:418:MET:CE	1:A:460[A]:LEU:CD1	2.99	0.40
1:A:560:LYS:HG3	8:A:717:HOH:O	2.20	0.40
1:A:151:ALA:N	1:A:152:PRO:HD2	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLN:OE1	1:A:444:LYS:NZ[3_554]	2.05	0.15

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	603/585 (103%)	590 (98%)	13 (2%)	0	100	100
2	B	275/274 (100%)	263 (96%)	7 (2%)	5 (2%)	8	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
All	All	978/964 (102%)	952 (97%)	21 (2%)	5 (0%)	29	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	100	PRO
2	B	85	LYS
2	B	101	ASP
2	B	84	GLY
2	B	83	GLY

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	528/508 (104%)	523 (99%)	5 (1%)	78	77
2	B	228/226 (101%)	220 (96%)	8 (4%)	36	24
3	C	97/100 (97%)	96 (99%)	1 (1%)	76	74
4	D	1/176 (1%)	1 (100%)	0	100	100
All	All	854/1010 (85%)	840 (98%)	14 (2%)	65	58

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	SER
1	A	367	HIS
1	A	436[A]	LYS
1	A	436[B]	LYS
1	A	573	LYS
2	B	10	HIS
2	B	101	ASP
2	B	117	PHE
2	B	190[A]	SER

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Mol	Chain	Res	Type
2	B	190[B]	SER
2	B	223	GLN
2	B	261	GLN
2	B	267	LEU
3	C	70	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	209	GLN
2	B	248	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 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	$\# Z > 2$
5	MES	A	601	-	12,12,12	2.21	1 (8%)	14,16,16	2.10	2 (14%)
7	JG5	D	301	4	73,82,82	2.64	24 (32%)	77,99,99	1.67	12 (15%)

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
5	MES	A	601	-	-	6/6/14/14	0/1/1/1
7	JG5	D	301	4	-	33/82/94/94	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	301	JG5	C62-N64	7.73	1.50	1.34
7	D	301	JG5	C46-N48	7.25	1.49	1.34
5	A	601	MES	C8-S	-7.17	1.67	1.77
7	D	301	JG5	C30-N32	7.01	1.49	1.33
7	D	301	JG5	C40-N42	6.88	1.48	1.34
7	D	301	JG5	C52-N54	6.09	1.47	1.33
7	D	301	JG5	C21-N23	4.93	1.48	1.38
7	D	301	JG5	C71-N70	4.65	1.47	1.34
7	D	301	JG5	S24-N23	4.32	1.72	1.63
7	D	301	JG5	N11-N12	3.91	1.39	1.32
7	D	301	JG5	C09-N10	3.87	1.36	1.33
7	D	301	JG5	C50-C49	3.77	1.58	1.53
7	D	301	JG5	C61-C62	3.35	1.57	1.51
7	D	301	JG5	C29-C30	3.13	1.57	1.51
7	D	301	JG5	C08-C09	3.00	1.54	1.50
7	D	301	JG5	C45-C46	2.96	1.57	1.51
7	D	301	JG5	O26-S24	2.91	1.47	1.43
7	D	301	JG5	O25-S24	2.80	1.47	1.43
7	D	301	JG5	O22-C21	-2.65	1.17	1.23
7	D	301	JG5	O41-C40	-2.63	1.17	1.23
7	D	301	JG5	C49-N48	2.56	1.50	1.46
7	D	301	JG5	O63-C62	-2.42	1.18	1.23
7	D	301	JG5	C39-C40	2.38	1.55	1.51
7	D	301	JG5	C20-C21	2.26	1.55	1.51
7	D	301	JG5	C28-C27	2.21	1.59	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	301	JG5	O26-S24-O25	-8.16	107.53	119.35
5	A	601	MES	O1S-S-C8	5.86	113.97	106.92
7	D	301	JG5	N10-N11-N12	-4.91	106.33	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	MES	C5-N4-C3	3.63	117.01	108.83
7	D	301	JG5	C28-C27-S24	-3.53	104.93	113.70
7	D	301	JG5	C61-C62-N64	3.23	121.99	116.37
7	D	301	JG5	C09-N10-N11	2.72	107.08	104.33
7	D	301	JG5	O63-C62-N64	-2.42	118.86	122.95
7	D	301	JG5	C21-N23-S24	-2.40	120.19	124.32
7	D	301	JG5	O38-C39-C40	-2.27	107.50	112.38
7	D	301	JG5	C39-C40-N42	2.25	120.28	116.37
7	D	301	JG5	C73-C71-N70	2.17	119.93	116.09
7	D	301	JG5	C51-C52-N54	2.08	119.92	116.42
7	D	301	JG5	O26-S24-C27	2.03	111.11	107.86

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	301	JG5	C06-C07-C08-C09
7	D	301	JG5	C28-C27-S24-N23
7	D	301	JG5	C28-C27-S24-O25
7	D	301	JG5	C28-C27-S24-O26
7	D	301	JG5	C81-C49-C50-C51
7	D	301	JG5	C50-C49-N48-C46
7	D	301	JG5	C81-C49-N48-C46
7	D	301	JG5	C61-C62-N64-C65
7	D	301	JG5	C21-N23-S24-O25
7	D	301	JG5	C21-N23-S24-O26
5	A	601	MES	C8-C7-N4-C3
5	A	601	MES	N4-C7-C8-S
5	A	601	MES	C7-C8-S-O2S
7	D	301	JG5	C18-C19-C20-C21
7	D	301	JG5	C66-C67-C68-C69
7	D	301	JG5	O63-C62-N64-C65
7	D	301	JG5	O35-C36-C37-O38
7	D	301	JG5	N48-C49-C50-C51
7	D	301	JG5	C17-C18-C19-C20
7	D	301	JG5	O38-C39-C40-N42
7	D	301	JG5	C43-C44-C45-C46
7	D	301	JG5	C02-C03-C04-C05
7	D	301	JG5	C05-C06-C07-C08
7	D	301	JG5	C01-C02-C03-C04
7	D	301	JG5	O38-C39-C40-O41
7	D	301	JG5	C04-C05-C06-C07

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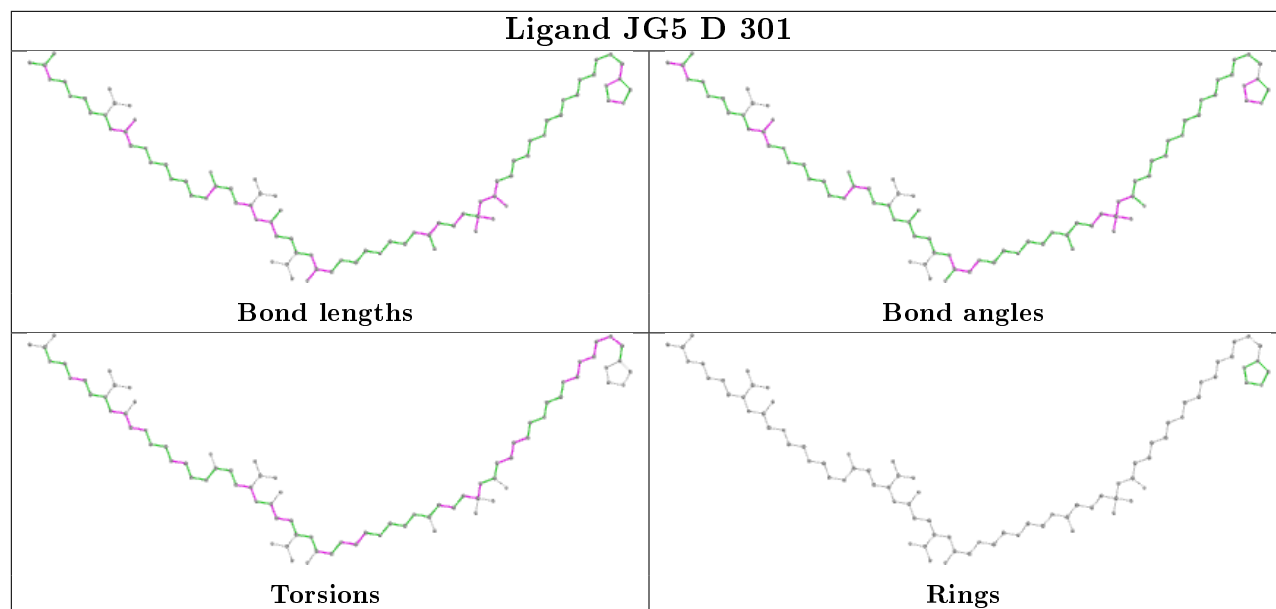
Mol	Chain	Res	Type	Atoms
7	D	301	JG5	C16-C17-C18-C19
5	A	601	MES	C8-C7-N4-C5
7	D	301	JG5	C03-C04-C05-C06
5	A	601	MES	C7-C8-S-O1S
7	D	301	JG5	O60-C61-C62-N64
7	D	301	JG5	O60-C61-C62-O63
7	D	301	JG5	C27-C28-C29-C30
5	A	601	MES	C7-C8-S-O3S
7	D	301	JG5	C36-C37-O38-C39
7	D	301	JG5	C62-C61-O60-C59
7	D	301	JG5	C44-C45-C46-O47
7	D	301	JG5	C55-C56-O57-C58
7	D	301	JG5	C44-C45-C46-N48

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	MES	2	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 than 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	583/585 (99%)	0.03	10 (1%) 70 77	18, 32, 58, 82	0
2	B	267/274 (97%)	0.34	17 (6%) 19 28	17, 29, 64, 109	0
3	C	100/105 (95%)	0.02	0 100 100	20, 29, 51, 68	0
4	D	0/191	-	-	-	-
All	All	950/1155 (82%)	0.12	27 (2%) 53 62	17, 31, 58, 109	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3	SER	8.9
2	B	102	ASN	8.1
2	B	99	GLY	7.7
2	B	101	ASP	7.5
2	B	4	HIS	6.5
1	A	364	ALA	6.0
2	B	100	PRO	5.7
2	B	84	GLY	4.8
2	B	103	THR	4.8
1	A	3	HIS	4.3
2	B	85	LYS	4.0
2	B	135	LEU	3.5
1	A	4	LYS	3.1
1	A	363	ALA	3.1
2	B	131	TRP	3.0
1	A	172	ALA	2.8
1	A	362	ALA	2.6
2	B	171	ARG	2.6
2	B	83	GLY	2.5
1	A	585	LEU	2.5
2	B	191	PRO	2.4
2	B	260	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	86	GLY	2.2
1	A	369	CYS	2.2
1	A	368	GLU	2.2
1	A	518	GLU	2.1
2	B	132	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

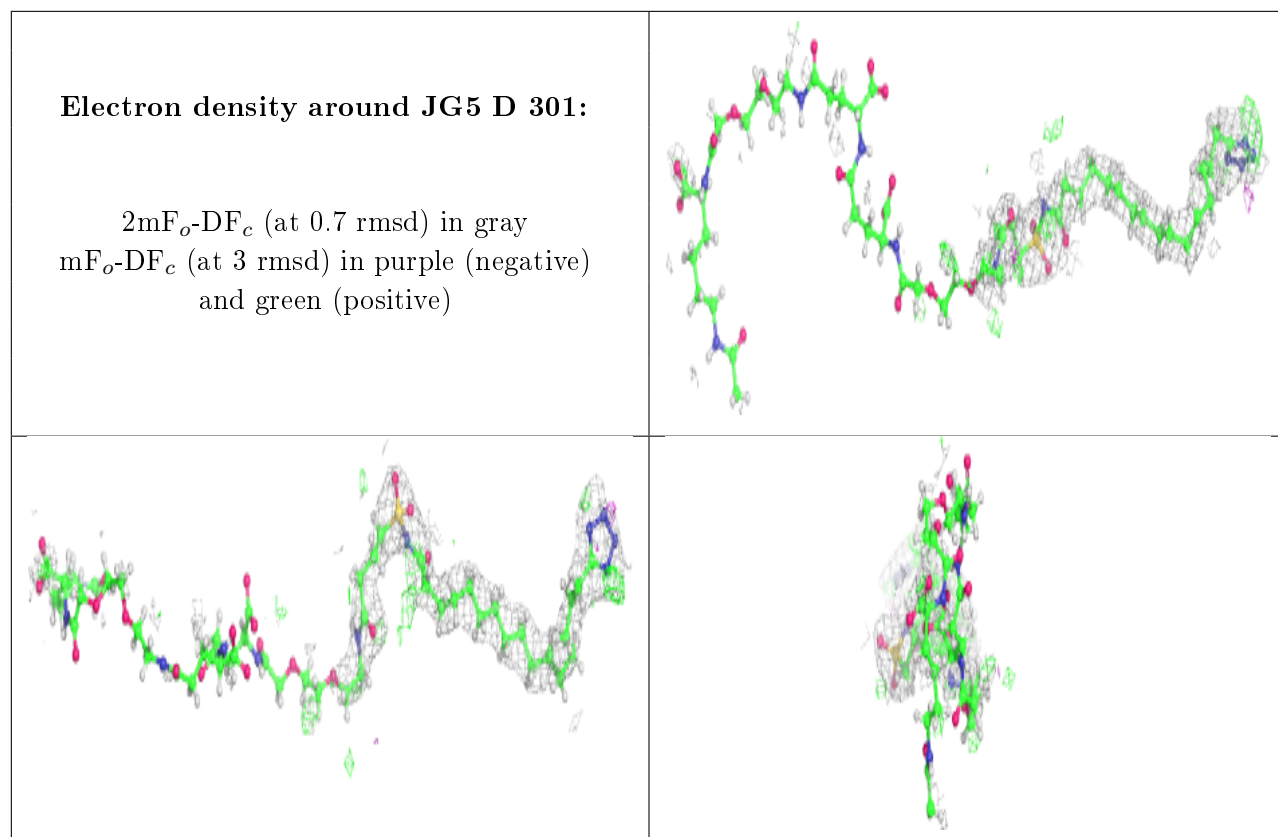
There are no carbohydrates in this entry.

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. 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
5	MES	A	601	12/12	0.83	0.34	48,79,103,105	0
7	JG5	D	301	82/82	0.90	0.15	23,30,74,89	90
6	CYS	B	301	7/7	0.91	0.20	33,52,63,69	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.