



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 04:00 AM UTC

PDB ID : 6QIO / pdb_00006qio
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

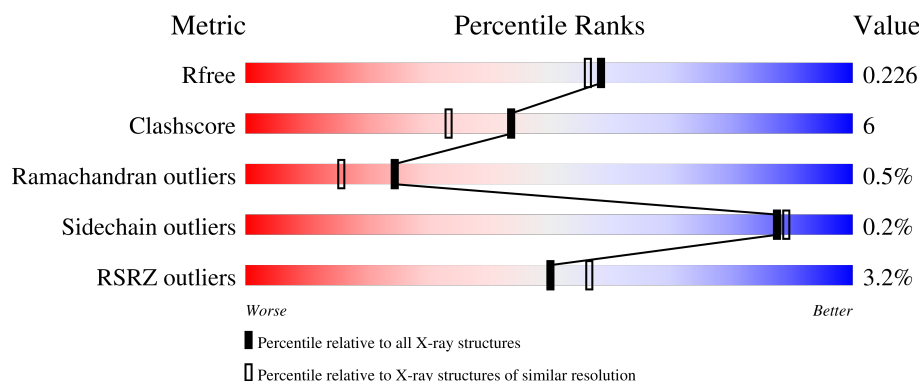
1 Overall quality at a glance

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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 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 $\leq 5\%$. 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	3% 89% 10%
2	B	274	4% 83% 14% ••
3	C	105	% 89% 7% 5%

2 Entry composition

There are 7 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
1	A	583	Total	C	H	N	O	S	0	20	0
			9318	2958	4626	793	899	42			

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
2	B	267	Total	C	H	N	O	S	0	10	0
			4178	1361	2042	369	398	8			

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

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

There are 6 discrepancies between the modelled and reference sequences:

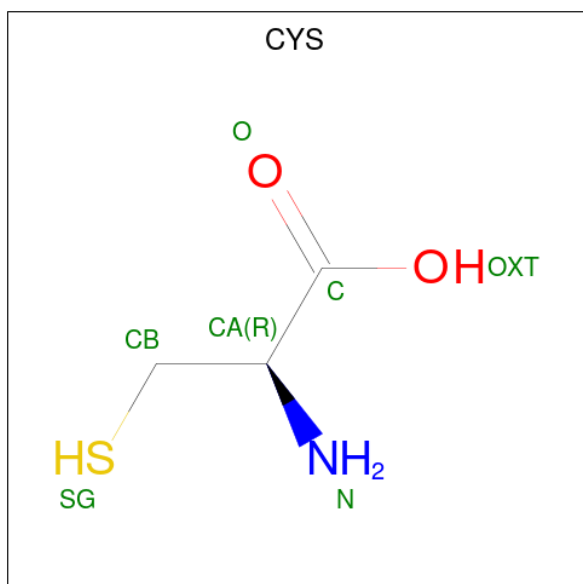
Chain	Residue	Modelled	Actual	Comment	Reference
C	100	HIS	-	expression tag	UNP P61769
C	101	HIS	-	expression tag	UNP P61769
C	102	HIS	-	expression tag	UNP P61769
C	103	HIS	-	expression tag	UNP P61769
C	104	HIS	-	expression tag	UNP P61769
C	105	HIS	-	expression tag	UNP P61769

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 5 is CYSTEINE (CCD ID: CYS) (formula: $C_3H_7NO_2S$).



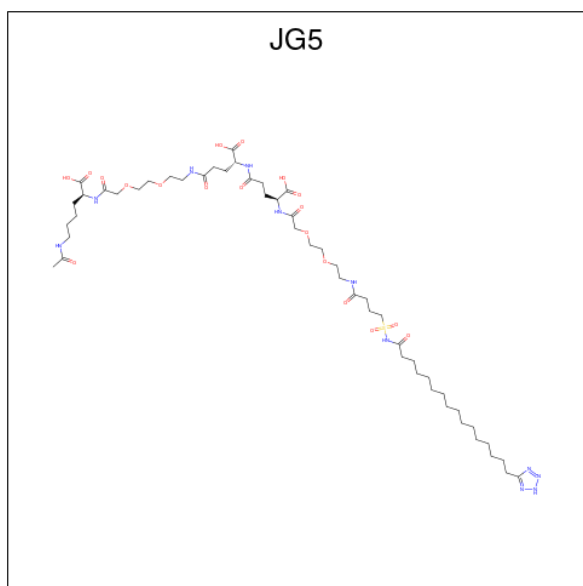
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	S	9	0
			9	3	3	1	1	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	S	0	0
			10	3	3	1	2	1		

- Molecule 6 is Somapacitan (CCD ID: JG5) (formula: $C_{51}H_{89}N_{11}O_{19}S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	S	90	0
			166	51	84	11	19	1		

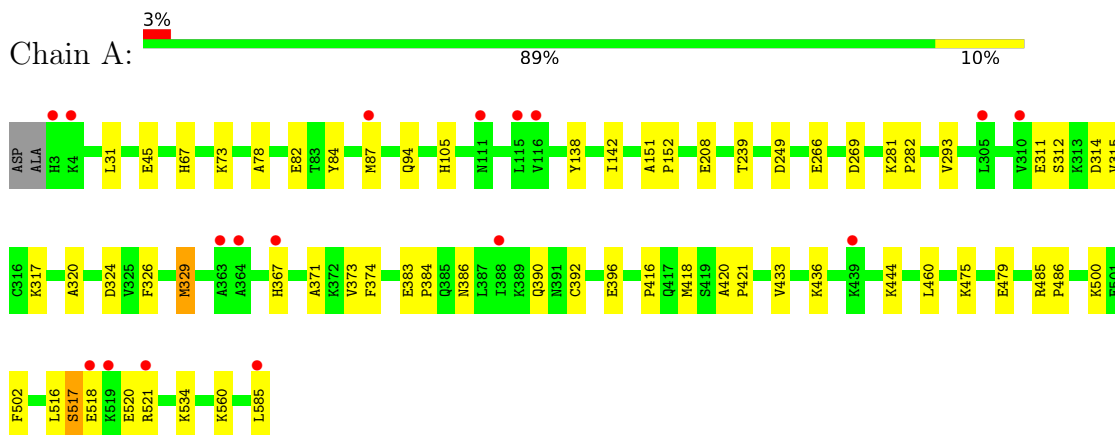
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	533	Total	O	0	0
			533	533		
7	B	225	Total	O	0	0
			225	225		
7	C	120	Total	O	0	0
			120	120		

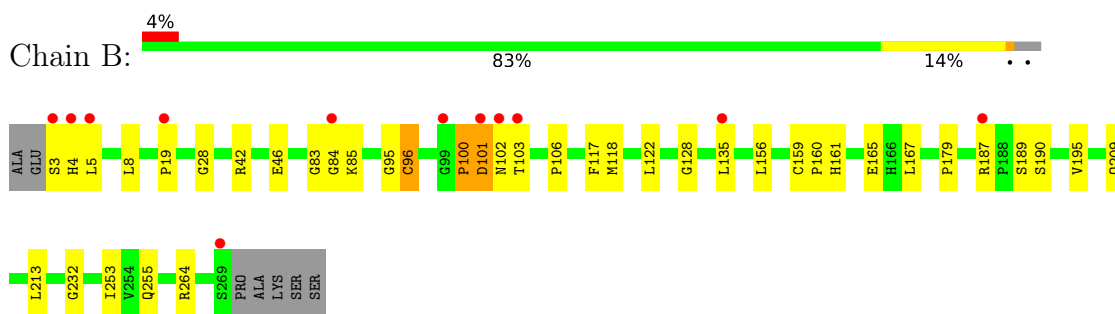
3 Residue-property plots

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.

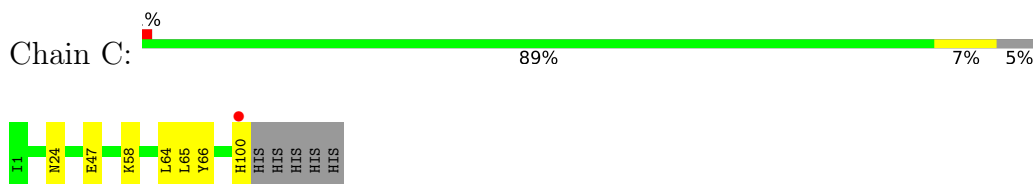
- Molecule 1: Serum albumin



- Molecule 2: IgG receptor FcRn large subunit p51



- Molecule 3: Beta-2-microglobulin



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) 99.6 (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 0.184 , 0.226	Depositor DCC
R_{free} test set	4775 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)	0.37 , 41.3	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 [i](#)

5.1 Standard geometry [i](#)

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	0.50	1/4892 (0.0%)	0.64	3/6592 (0.0%)
2	B	0.59	2/2227 (0.1%)	0.70	2/3026 (0.1%)
3	C	0.48	0/876	0.64	0/1186
All	All	0.53	3/7995 (0.0%)	0.66	5/10804 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	28	GLY	CA-C	7.36	1.57	1.52
1	A	329	MET	CG-SD	5.80	1.95	1.80
2	B	96	CYS	CB-SG	-5.68	1.62	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	179	PRO	N-CA-CB	5.83	106.25	103.22
1	A	329	MET	CB-CG-SD	-5.52	96.13	112.70
2	B	179	PRO	O-C-N	-5.38	118.62	121.15
1	A	517	SER	CA-C-N	-5.04	112.24	122.31
1	A	517	SER	C-N-CA	-5.04	112.24	122.31

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	4692	4626	4492	54	1
2	B	2136	2042	2015	32	0
3	C	844	807	802	5	0
4	A	12	13	13	2	0
5	A	6	3	3	0	0
5	B	7	3	3	0	0
6	A	82	84	0	0	0
7	A	533	0	0	15	0
7	B	225	0	0	13	0
7	C	120	0	0	3	0
All	All	8657	7578	7328	92	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 (92) 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	7:B:401:HOH:O	1.99	0.94
1:A:585:LEU:HD21	7:A:1152:HOH:O	1.67	0.94
1:A:516:LEU:O	7:A:701:HOH:O	1.96	0.83
3:C:100:HIS:O	7:C:201:HOH:O	1.97	0.82
1:A:312:SER:O	7:A:703:HOH:O	1.99	0.80
1:A:516:LEU:O	7:A:702:HOH:O	1.98	0.79
2:B:100:PRO:HB2	7:B:401:HOH:O	1.84	0.77
1:A:266:GLU:OE1	7:A:705:HOH:O	2.04	0.76
2:B:128:GLY:N	7:B:404:HOH:O	2.19	0.75
2:B:187:ARG:NE	7:B:406:HOH:O	2.21	0.73
1:A:293:VAL:O	7:A:706:HOH:O	2.09	0.69
2:B:117:PHE:CZ	2:B:118:MET:HE2	2.28	0.69
1:A:269:ASP:OD1	7:A:707:HOH:O	2.11	0.68
2:B:19:PRO:O	7: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	7:A:713:HOH:O	2.30	0.65
2:B:264:ARG:NH2	7: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	7:A:703:HOH:O	2.15	0.63
1:A:418:MET:HE1	1:A:460[A]:LEU:CD1	2.28	0.63
1:A:45:GLU:OE1	1:A:73:LYS:NZ	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:MET:HE1	1:A:460[A]:LEU:HD11	1.82	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
2:B:5:LEU:CD2	2:B:167:LEU:HD21	2.32	0.59
3:C:58:LYS:NZ	7:C:206:HOH:O	2.35	0.59
1:A:396:GLU:O	7:A:708:HOH:O	2.17	0.57
1:A:138:TYR:CE1	1:A:142:ILE:HD11	2.40	0.57
2:B:103:THR:HG23	7:B:401:HOH:O	2.06	0.55
2:B:135:LEU:HD22	7: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	7: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	7:B:401:HOH:O	2.58	0.51
2:B:232:GLY:HA3	7:B:579:HOH:O	2.10	0.50
2:B:128:GLY:CA	7: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
1:A:87:MET:HE2	1:A:105:HIS:CB	2.44	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:326:PHE:HA	1:A:329:MET:HE3	1.97	0.46
1:A:418:MET:HE1	1:A:460[A]:LEU:HD13	1.98	0.46
2:B:135:LEU:C	2:B:135:LEU:HD23	2.41	0.46
1:A:518:GLU:HG2	7:A:702:HOH:O	2.16	0.46
3:C:47:GLU:OE1	7:C:202:HOH:O	2.21	0.46
1:A:314:ASP:O	1:A:315:VAL:C	2.59	0.45
1:A:433:VAL:HG11	4: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	4: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TYR:HA	7:A:1048: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	7:A:743:HOH:O	2.51	0.43
1:A:367:HIS:O	1:A:367:HIS:ND1	2.50	0.43
1:A:416:PRO:O	1:A:534:LYS:HE2	2.19	0.43
1:A:475:LYS:HE2	1:A:479:GLU:OE2	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	7:A:744:HOH:O	2.20	0.41
2:B:96:CYS:SG	2:B:159:CYS:C	3.03	0.41
1:A:585:LEU:N	1:A:585:LEU:CD2	2.84	0.41
1:A:87:MET:HE2	1:A:105:HIS:HB2	2.02	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
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	7: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 ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	603/585 (103%)	590 (98%)	13 (2%)	0	100	100
2	B	275/274 (100%)	263 (96%)	7 (2%)	5 (2%)	6	1
3	C	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
All	All	978/964 (102%)	952 (97%)	21 (2%)	5 (0%)	24	16

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%)	526 (100%)	2 (0%)	84	85
2	B	228/226 (101%)	226 (99%)	2 (1%)	70	70
3	C	97/100 (97%)	97 (100%)	0	100	100
All	All	853/834 (102%)	849 (100%)	4 (0%)	87	82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	436[A]	LYS
1	A	436[B]	LYS
2	B	190[A]	SER
2	B	190[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
2	B	149	ASN
2	B	209	GLN
2	B	248	HIS
2	B	255	GLN
3	C	100	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	MES	A	601	-	12,12,12	2.27	1 (8%)	15,16,16	1.89	2 (13%)
6	JG5	A	603	5	82,82,82	2.50	23 (28%)	93,99,99	1.53	11 (11%)
5	CYS	A	602	6	4,5,6	0.61	0	1,5,7	0.05	0
5	CYS	B	301	2	5,6,6	1.35	0	3,7,7	2.72	2 (66%)

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	MES	A	601	-	-	6/6/14/14	0/1/1/1
6	JG5	A	603	5	-	39/94/94/94	0/1/1/1
5	CYS	A	602	6	-	0/1/4/6	-
5	CYS	B	301	2	-	4/6/6/6	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	JG5	C62-N64	7.78	1.50	1.34
4	A	601	MES	C8-S	-7.33	1.67	1.77
6	A	603	JG5	C46-N48	7.30	1.49	1.34
6	A	603	JG5	C40-N42	6.93	1.48	1.34
6	A	603	JG5	C30-N32	6.72	1.49	1.33
6	A	603	JG5	C52-N54	5.84	1.47	1.33
6	A	603	JG5	N12-N11	5.10	1.39	1.31
6	A	603	JG5	C71-N70	5.00	1.47	1.34
6	A	603	JG5	S24-N23	4.53	1.72	1.63
6	A	603	JG5	C08-C09	4.09	1.54	1.49
6	A	603	JG5	C21-N23	3.42	1.48	1.39
6	A	603	JG5	C61-C62	3.38	1.57	1.51
6	A	603	JG5	O26-S24	3.02	1.47	1.43
6	A	603	JG5	C29-C30	2.98	1.57	1.51
6	A	603	JG5	N12-N13	2.97	1.37	1.33
6	A	603	JG5	O25-S24	2.90	1.47	1.43
6	A	603	JG5	C45-C46	2.82	1.57	1.51
6	A	603	JG5	O22-C21	-2.71	1.17	1.23
6	A	603	JG5	O41-C40	-2.69	1.17	1.23
6	A	603	JG5	O63-C62	-2.48	1.18	1.23
6	A	603	JG5	C39-C40	2.40	1.55	1.51
6	A	603	JG5	C20-C21	2.15	1.55	1.51
6	A	603	JG5	C28-C27	2.14	1.59	1.52
6	A	603	JG5	C50-C49	2.03	1.58	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	JG5	O26-S24-O25	-8.44	107.53	119.34
4	A	601	MES	O1S-S-C8	4.79	113.97	106.73
5	B	301	CYS	OXT-C-O	-3.88	115.28	124.08
4	A	601	MES	C5-N4-C3	3.79	117.01	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	JG5	C28-C27-S24	-3.61	104.93	113.74
6	A	603	JG5	C61-C62-N64	3.23	121.99	116.41
6	A	603	JG5	O63-C62-N64	-2.41	118.86	122.95
6	A	603	JG5	O38-C39-C40	-2.37	107.50	112.41
6	A	603	JG5	C39-C40-N42	2.24	120.28	116.41
6	A	603	JG5	C73-C71-N70	2.23	119.93	116.12
6	A	603	JG5	O26-S24-C27	2.05	111.11	107.86
5	B	301	CYS	CA-CB-SG	2.04	118.77	114.40
6	A	603	JG5	C69-N70-C71	-2.04	119.55	122.56
6	A	603	JG5	O25-S24-N23	2.04	112.73	106.48
6	A	603	JG5	O82-C81-O83	-2.03	119.47	124.08

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	MES	C8-C7-N4-C3
4	A	601	MES	N4-C7-C8-S
4	A	601	MES	C7-C8-S-O2S
5	B	301	CYS	O-C-CA-N
5	B	301	CYS	N-CA-CB-SG
5	B	301	CYS	C-CA-CB-SG
6	A	603	JG5	C27-C28-C29-C30
6	A	603	JG5	C28-C27-S24-N23
6	A	603	JG5	C28-C27-S24-O25
6	A	603	JG5	C28-C27-S24-O26
6	A	603	JG5	C61-C62-N64-C65
6	A	603	JG5	C18-C19-C20-C21
6	A	603	JG5	C66-C67-C68-C69
6	A	603	JG5	O63-C62-N64-C65
6	A	603	JG5	O35-C36-C37-O38
6	A	603	JG5	N48-C49-C50-C51
6	A	603	JG5	C81-C49-C50-C51
5	B	301	CYS	OXT-C-CA-N
6	A	603	JG5	O38-C39-C40-N42
6	A	603	JG5	C43-C44-C45-C46
6	A	603	JG5	C17-C18-C19-C20
6	A	603	JG5	C02-C03-C04-C05
6	A	603	JG5	O38-C39-C40-O41
6	A	603	JG5	C05-C06-C07-C08
6	A	603	JG5	C01-C02-C03-C04
4	A	601	MES	C8-C7-N4-C5

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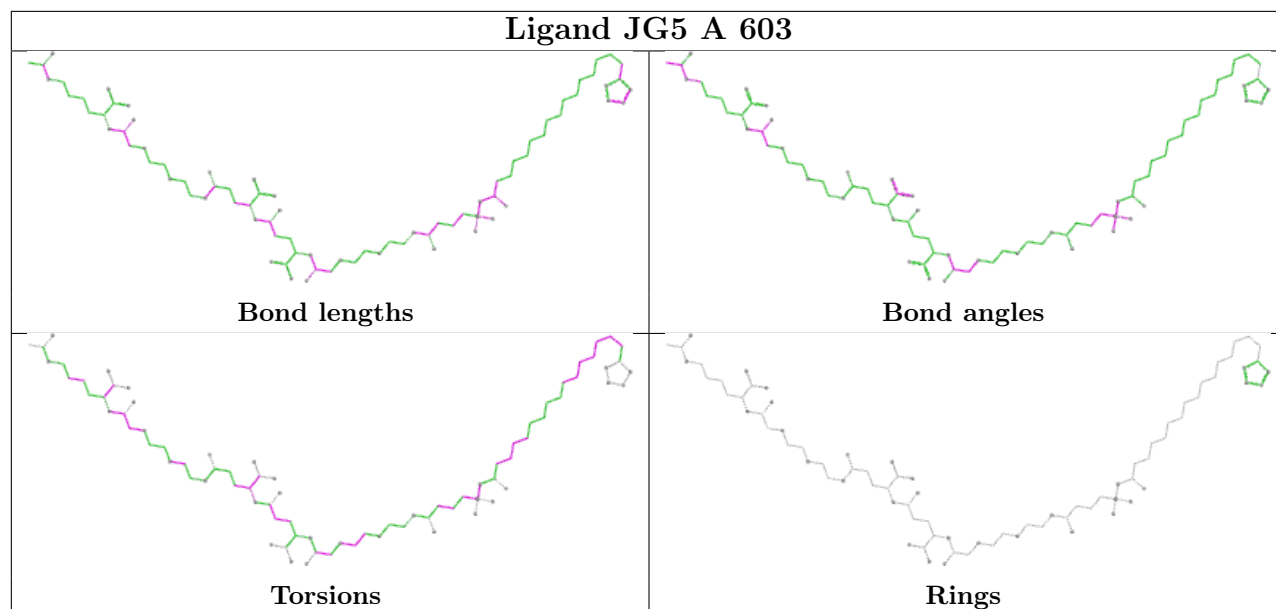
Mol	Chain	Res	Type	Atoms
6	A	603	JG5	C06-C07-C08-C09
6	A	603	JG5	C16-C17-C18-C19
6	A	603	JG5	C81-C49-N48-C46
6	A	603	JG5	C04-C05-C06-C07
6	A	603	JG5	N48-C49-C81-O82
6	A	603	JG5	N48-C49-C81-O83
6	A	603	JG5	C03-C04-C05-C06
6	A	603	JG5	C21-N23-S24-O25
6	A	603	JG5	C50-C49-C81-O82
4	A	601	MES	C7-C8-S-O1S
6	A	603	JG5	C50-C49-C81-O83
6	A	603	JG5	O60-C61-C62-N64
4	A	601	MES	C7-C8-S-O3S
6	A	603	JG5	O60-C61-C62-O63
6	A	603	JG5	C66-C65-C78-O80
6	A	603	JG5	C50-C49-N48-C46
6	A	603	JG5	C66-C65-C78-O79
6	A	603	JG5	C62-C61-O60-C59
6	A	603	JG5	C36-C37-O38-C39
6	A	603	JG5	C21-N23-S24-O26
6	A	603	JG5	C44-C45-C46-O47
6	A	603	JG5	C55-C56-O57-C58
6	A	603	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
4	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%)	-0.13	17 (2%) 53 60	7, 35, 65, 92	8 (1%)
2	B	267/274 (97%)	-0.08	12 (4%) 38 44	15, 32, 71, 119	5 (1%)
3	C	100/105 (95%)	-0.19	1 (1%) 79 84	13, 32, 59, 80	1 (1%)
All	All	950/964 (98%)	-0.12	30 (3%) 50 56	7, 34, 66, 119	14 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	100	HIS	4.1
2	B	99	GLY	3.8
1	A	518	GLU	3.5
1	A	3	HIS	3.3
2	B	269	SER	3.1
1	A	116	VAL	3.0
1	A	585	LEU	2.8
2	B	103	THR	2.8
2	B	3	SER	2.8
1	A	364	ALA	2.8
2	B	101	ASP	2.8
2	B	4	HIS	2.7
1	A	111	ASN	2.7
2	B	5	LEU	2.6
2	B	135	LEU	2.5
1	A	367	HIS	2.4
2	B	84	GLY	2.4
1	A	115	LEU	2.3
2	B	102	ASN	2.3
1	A	87	MET	2.3
2	B	19	PRO	2.2
1	A	4	LYS	2.2
1	A	363	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	521	ARG	2.2
1	A	305	LEU	2.1
1	A	439	LYS	2.0
1	A	310	VAL	2.0
1	A	519	LYS	2.0
1	A	388	ILE	2.0
2	B	187	ARG	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

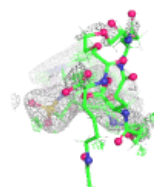
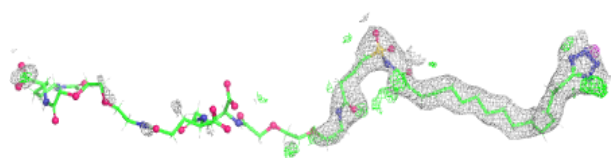
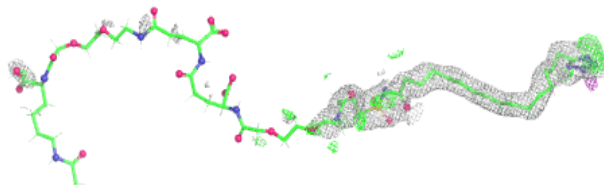
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MES	A	601	12/12	0.86	0.17	48,79,103,105	0
5	CYS	A	602	6/7	-	-	23,23,28,28	9
6	JG5	A	603	82/82	0.88	0.15	23,30,74,89	90
5	CYS	B	301	7/7	0.94	0.14	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.

Electron density around JG5 A 603:

$2mF_o-DF_c$ (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.