Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2021 – 04:09 PM GMT

PDB ID	:	6YG9
Title	:	CRYSTAL STRUCTURE OF HUMAN SERUM ALBUMIN (HSA) IN COMPLEX WITH GN-07.
Authors	:	Schreuder, H.A.; Liesum, A.
Deposited on	:	2020-03-27
Resolution	:	1.89 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:

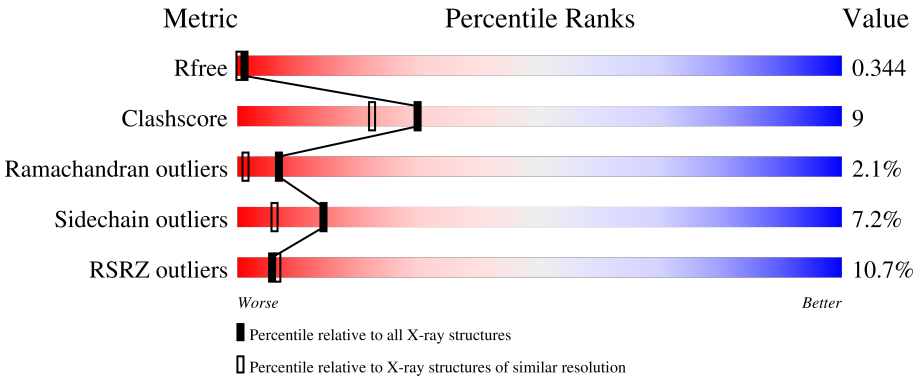
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	585	10% 74% 21%

2 Entry composition

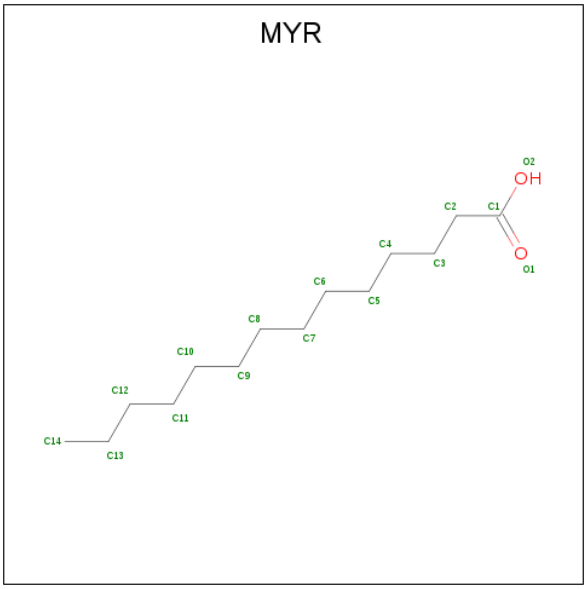
There are 4 unique types of molecules in this entry. The entry contains 5303 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	2	0
			4497	2839	764	857	37			

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	12	2		
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			12	10	2		
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			16	14	2		

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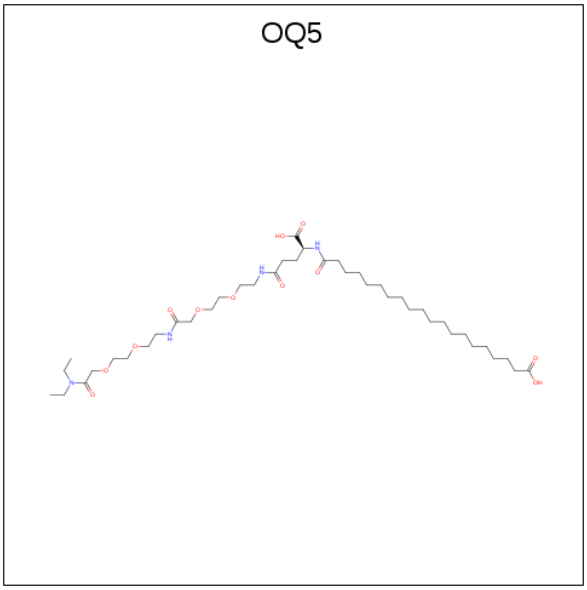
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	14	2		

- Molecule 3 is 20-[[(2 {S})-5-[2-[2-[2-[2-[2-[2-(diethylamino)-2-oxidanylidene-ethoxy]ethoxy]ethylamino]-2-oxidanylidene-ethoxy]ethoxy]ethylamino]-1-oxidanyl-1,5-bis(oxidanylidene)pentan-2-yl]amino]-20-oxidanylidene-icosanoic acid (three-letter code: OQ5) (formula: $C_{41}H_{76}N_4O_{12}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			57	41	4	12		

- Molecule 4 is water.

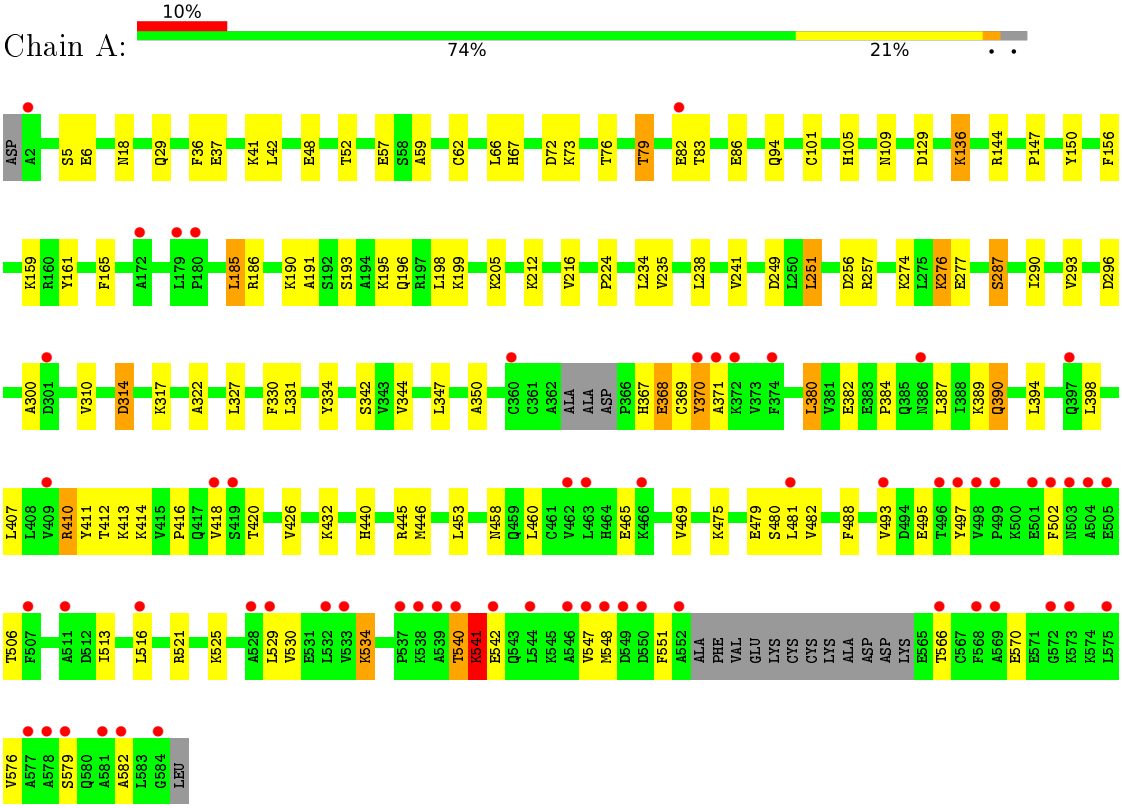
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	662	Total	O	0	0
			662	662		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Serum albumin

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	197.72Å 38.14Å 95.37Å 90.00° 105.88° 90.00°	Depositor
Resolution (Å)	58.51 – 1.89 58.50 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.2 (58.51-1.89) 96.3 (58.50-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 1.90Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.239 , 0.313 0.258 , 0.344	Depositor DCC
R_{free} test set	2690 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 88.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5303	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: OQ5, MYR

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	0.51	0/4581	0.71	1/6180 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	368	GLU	C-N-CA	6.25	137.32	121.70

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	4497	0	4397	84	0
2	A	87	0	135	13	0
3	A	57	0	0	0	0
4	A	662	0	0	13	0
All	All	5303	0	4532	86	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 9.

All (86) 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)
1:A:330:PHE:HB2	4:A:713:HOH:O	1.84	0.77
1:A:241:VAL:HG22	1:A:256:ASP:HB3	1.68	0.74
1:A:460:LEU:HD11	2:A:605:MYR:H132	1.69	0.73
1:A:453:LEU:HD11	2:A:604:MYR:H82	1.70	0.73
1:A:234:LEU:HD12	4:A:1132:HOH:O	1.91	0.71
1:A:416:PRO:HA	4:A:890:HOH:O	1.92	0.68
1:A:276:LYS:HG2	1:A:277:GLU:N	2.10	0.67
1:A:387:LEU:HD23	2:A:604:MYR:H62	1.76	0.67
1:A:18:ASN:HD21	1:A:159:LYS:NZ	1.94	0.65
1:A:165:PHE:CE2	2:A:601:MYR:H81	2.32	0.65
1:A:165:PHE:HE2	2:A:601:MYR:H81	1.62	0.64
1:A:66:LEU:HD12	1:A:251:LEU:HD21	1.80	0.64
1:A:101:CYS:O	1:A:105:HIS:HD2	1.81	0.63
1:A:344:VAL:HG23	1:A:482:VAL:HA	1.81	0.63
1:A:6:GLU:HB3	1:A:66:LEU:HG	1.81	0.63
1:A:502:PHE:HZ	1:A:576:VAL:HG13	1.64	0.62
1:A:198:LEU:HD13	1:A:458:ASN:HB2	1.82	0.61
1:A:276:LYS:HG2	1:A:277:GLU:H	1.65	0.61
2:A:605:MYR:H91	2:A:605:MYR:H142	1.82	0.61
1:A:42:LEU:HD22	1:A:73:LYS:HE3	1.83	0.60
1:A:310:VAL:HG13	1:A:371:ALA:HA	1.84	0.60
1:A:48:GLU:O	1:A:52:THR:HG23	2.04	0.58
1:A:238:LEU:HD12	4:A:1136:HOH:O	2.05	0.57
1:A:370:TYR:HD1	1:A:371:ALA:H	1.50	0.57
1:A:407:LEU:HD23	1:A:410:ARG:HH12	1.69	0.57
1:A:426:VAL:HG21	1:A:460:LEU:HD13	1.86	0.56
1:A:479:GLU:HG3	1:A:480:SER:H	1.70	0.56
1:A:290:ILE:O	1:A:293:VAL:HG22	2.07	0.55
1:A:418:VAL:HG21	2:A:605:MYR:H131	1.90	0.53
1:A:398:LEU:HD22	4:A:983:HOH:O	2.10	0.52
1:A:488:PHE:HB3	2:A:605:MYR:H62	1.93	0.51
1:A:191:ALA:O	1:A:195:LYS:HG2	2.11	0.51
1:A:37:GLU:CD	1:A:37:GLU:H	2.15	0.50
1:A:18:ASN:HD21	1:A:159:LYS:HZ3	1.56	0.50
1:A:479:GLU:HG3	1:A:480:SER:N	2.27	0.49
1:A:161:TYR:O	1:A:165:PHE:HD2	1.95	0.49
1:A:327:LEU:HB3	2:A:606:MYR:H82	1.94	0.49
1:A:5:SER:HB3	1:A:57:GLU:HG2	1.95	0.49
1:A:412:THR:HG23	4:A:890:HOH:O	2.12	0.48
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.96	0.48
1:A:257:ARG:HH11	1:A:287:SER:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:VAL:CG2	1:A:482:VAL:HA	2.43	0.47
1:A:161:TYR:CZ	1:A:185:LEU:HB3	2.49	0.47
1:A:380:LEU:O	1:A:384:PRO:HD2	2.15	0.47
1:A:540:THR:O	1:A:541:LYS:HB2	2.16	0.46
1:A:150:TYR:H	1:A:196:GLN:HE22	1.64	0.46
1:A:195:LYS:HG3	4:A:828:HOH:O	2.16	0.46
1:A:420:THR:HA	1:A:530:VAL:HG11	1.98	0.46
1:A:541:LYS:HA	1:A:541:LYS:HD3	1.76	0.46
1:A:66:LEU:CD1	1:A:251:LEU:HD21	2.46	0.46
1:A:314:ASP:HB3	1:A:317:LYS:HB3	1.97	0.45
1:A:274:LYS:HD2	1:A:296:ASP:HA	1.98	0.45
1:A:579:SER:HA	1:A:582:ALA:HB3	1.98	0.45
1:A:72:ASP:O	1:A:76:THR:HG23	2.16	0.45
1:A:129:ASP:HB2	4:A:1076:HOH:O	2.17	0.45
1:A:380:LEU:O	1:A:384:PRO:CD	2.65	0.44
1:A:342:SER:HB3	1:A:446:MET:HG2	1.98	0.44
1:A:411:TYR:HB3	2:A:605:MYR:H92	1.99	0.44
1:A:413:LYS:HB3	1:A:493:VAL:HG13	2.00	0.43
1:A:212:LYS:O	1:A:216:VAL:HG23	2.19	0.42
2:A:605:MYR:H91	2:A:605:MYR:C14	2.49	0.42
1:A:216:VAL:HG22	1:A:235:VAL:HG21	2.01	0.42
1:A:416:PRO:HB2	1:A:497:TYR:CE1	2.54	0.42
1:A:445:ARG:HD2	4:A:1048:HOH:O	2.19	0.42
1:A:389:LYS:HA	4:A:834:HOH:O	2.19	0.42
1:A:480:SER:HB2	4:A:722:HOH:O	2.19	0.42
1:A:521:ARG:HG2	1:A:525:LYS:HE2	2.02	0.41
1:A:79:THR:HG22	1:A:82[B]:GLU:HG3	2.03	0.41
1:A:186:ARG:HD2	1:A:190:LYS:HE3	2.02	0.41
1:A:414:LYS:HA	1:A:493:VAL:HA	2.03	0.41
1:A:29:GLN:HG2	1:A:147:PRO:HA	2.02	0.41
1:A:420:THR:HG23	1:A:530:VAL:HB	2.02	0.41
1:A:380:LEU:HD12	1:A:380:LEU:HA	1.97	0.41
1:A:150:TYR:CZ	1:A:257:ARG:HD3	2.56	0.41
1:A:36:PHE:HZ	1:A:136:LYS:HG3	1.85	0.41
1:A:426:VAL:HG11	2:A:605:MYR:H102	2.02	0.41
1:A:67:HIS:HE1	1:A:249:ASP:OD1	2.03	0.41
1:A:331:LEU:HD13	1:A:350:ALA:HB2	2.03	0.41
1:A:390:GLN:NE2	1:A:394:LEU:HD22	2.36	0.41
1:A:525:LYS:HB3	2:A:602:MYR:H32	2.02	0.41
1:A:416:PRO:O	1:A:534:LYS:HE2	2.20	0.41
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLU:HG3	1:A:105:HIS:CE1	2.56	0.40
1:A:368:GLU:HA	4:A:726:HOH:O	2.20	0.40
1:A:394:LEU:HG	4:A:983:HOH:O	2.21	0.40
1:A:196:GLN:HA	1:A:199:LYS:HE2	2.03	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	564/585 (96%)	519 (92%)	33 (6%)	12 (2%)	7 1

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	367	HIS
1	A	370	TYR
1	A	541	LYS
1	A	542	GLU
1	A	547	VAL
1	A	300	ALA
1	A	570	GLU
1	A	322	ALA
1	A	548	MET
1	A	566	THR
1	A	551	PHE

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	487/511 (95%)	452 (93%)	35 (7%)	14 6

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	79	THR
1	A	83	THR
1	A	94	GLN
1	A	136	LYS
1	A	144	ARG
1	A	156	PHE
1	A	185	LEU
1	A	193	SER
1	A	205	LYS
1	A	251	LEU
1	A	276	LYS
1	A	287	SER
1	A	314	ASP
1	A	334	TYR
1	A	347	LEU
1	A	369	CYS
1	A	380	LEU
1	A	382	GLU
1	A	390	GLN
1	A	410	ARG
1	A	432	LYS
1	A	440	HIS
1	A	465	GLU
1	A	469	VAL
1	A	475	LYS
1	A	481	LEU
1	A	495	GLU
1	A	506	THR
1	A	513	ILE

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Mol	Chain	Res	Type
1	A	516	LEU
1	A	529	LEU
1	A	534	LYS
1	A	540	THR
1	A	541	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	67	HIS
1	A	94	GLN
1	A	105	HIS
1	A	196	GLN
1	A	247	HIS
1	A	268	GLN
1	A	391	ASN
1	A	397	GLN
1	A	458	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

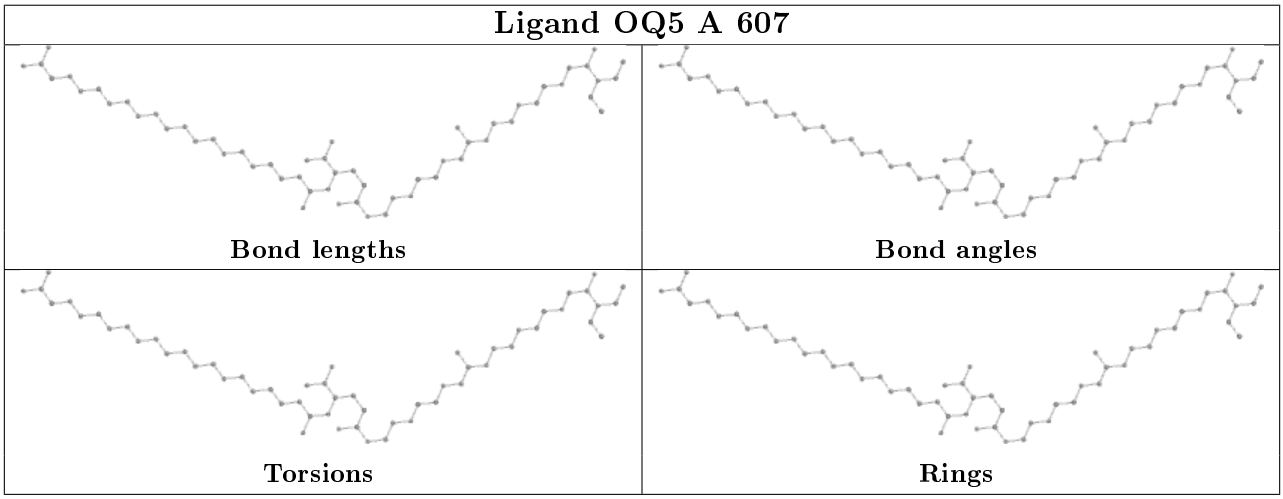
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 OQ5 A 607



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^{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	568/585 (97%)	0.70	61 (10%) 6 6	11, 34, 62, 81	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	581	ALA	8.9
1	A	578	ALA	7.8
1	A	538	LYS	7.7
1	A	493	VAL	7.7
1	A	2	ALA	6.8
1	A	502	PHE	6.7
1	A	498	VAL	6.5
1	A	548	MET	6.0
1	A	516	LEU	5.4
1	A	503	ASN	5.1
1	A	511	ALA	5.0
1	A	577	ALA	5.0
1	A	462	VAL	4.8
1	A	546	ALA	4.7
1	A	582	ALA	4.7
1	A	539	ALA	4.5
1	A	496	THR	4.0
1	A	528	ALA	4.0
1	A	547	VAL	3.8
1	A	360	CYS	3.7
1	A	568	PHE	3.6
1	A	386	ASN	3.6
1	A	579	SER	3.6
1	A	575	LEU	3.5
1	A	371	ALA	3.5
1	A	499	PRO	3.4
1	A	537	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	505	GLU	3.3
1	A	544	LEU	3.1
1	A	504	ALA	3.1
1	A	540	THR	3.1
1	A	507	PHE	3.0
1	A	418	VAL	3.0
1	A	542	GLU	3.0
1	A	466	LYS	3.0
1	A	550	ASP	2.9
1	A	463	LEU	2.9
1	A	409	VAL	2.8
1	A	372	LYS	2.8
1	A	370	TYR	2.7
1	A	573	LYS	2.6
1	A	301	ASP	2.6
1	A	397	GLN	2.6
1	A	549	ASP	2.6
1	A	552	ALA	2.6
1	A	497	TYR	2.5
1	A	569	ALA	2.4
1	A	572	GLY	2.4
1	A	584	GLY	2.4
1	A	481	LEU	2.4
1	A	172	ALA	2.3
1	A	501	GLU	2.3
1	A	566	THR	2.3
1	A	179	LEU	2.3
1	A	532	LEU	2.3
1	A	533	VAL	2.2
1	A	529	LEU	2.1
1	A	374	PHE	2.1
1	A	419	SER	2.1
1	A	82[A]	GLU	2.0
1	A	180	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

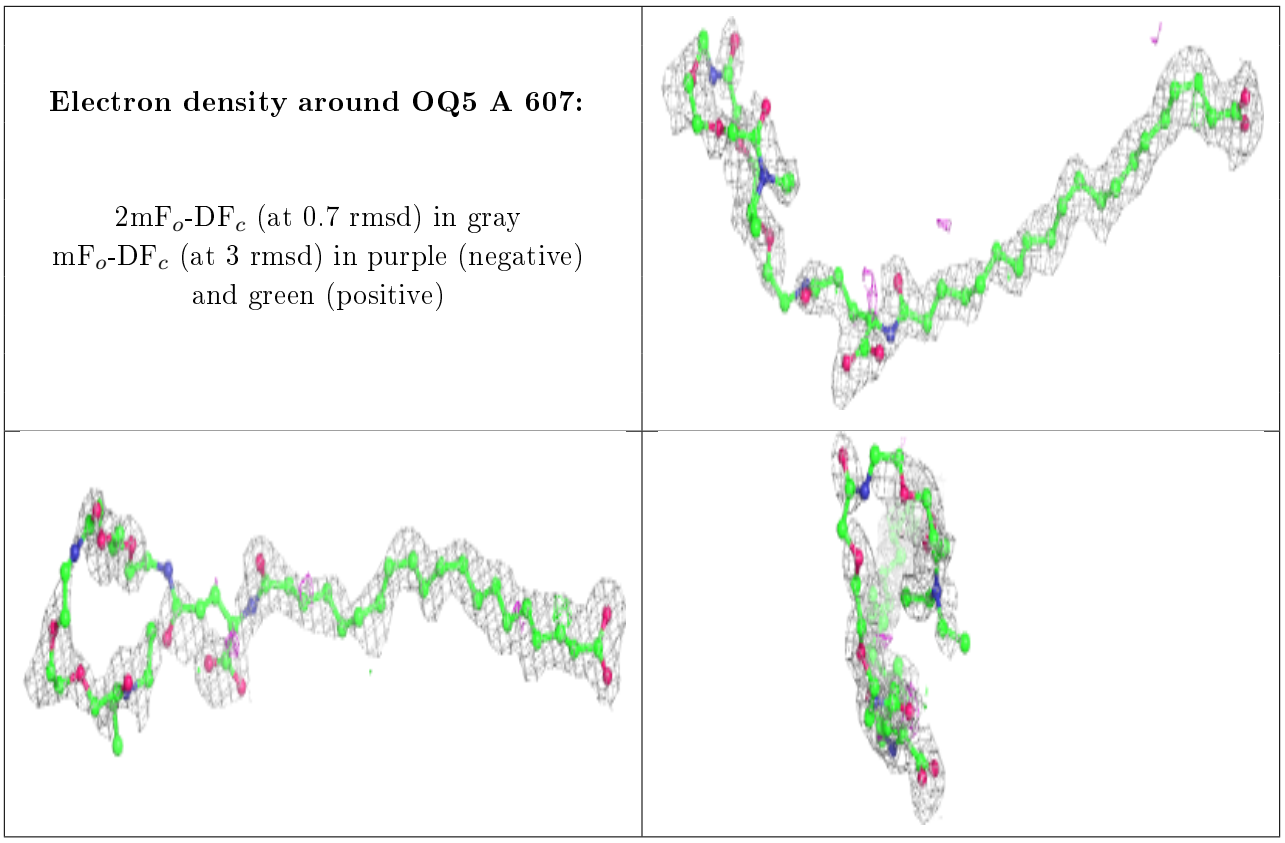
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	MYR	A	603	12/16	0.68	0.24	27,31,47,48	0
2	MYR	A	601	14/16	0.75	0.17	28,38,41,41	0
3	OQ5	A	607	57/57	0.75	0.28	17,49,63,63	57
2	MYR	A	602	16/16	0.82	0.14	35,41,52,54	0
2	MYR	A	604	13/16	0.84	0.17	34,39,40,40	0
2	MYR	A	606	16/16	0.86	0.13	31,35,46,47	0
2	MYR	A	605	16/16	0.86	0.18	37,45,56,57	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 OQ5 A 607:

$2mF_o$-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

There are no such residues in this entry.