



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:19 PM EDT

PDB ID : 6YG9 / pdb_00006yg9
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 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

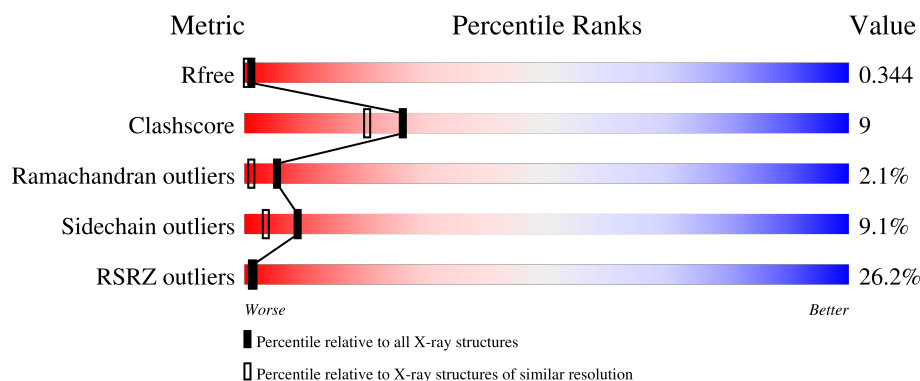
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 $\leq 5\%$. 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	25% 71% 22% ...

2 Entry composition [i](#)

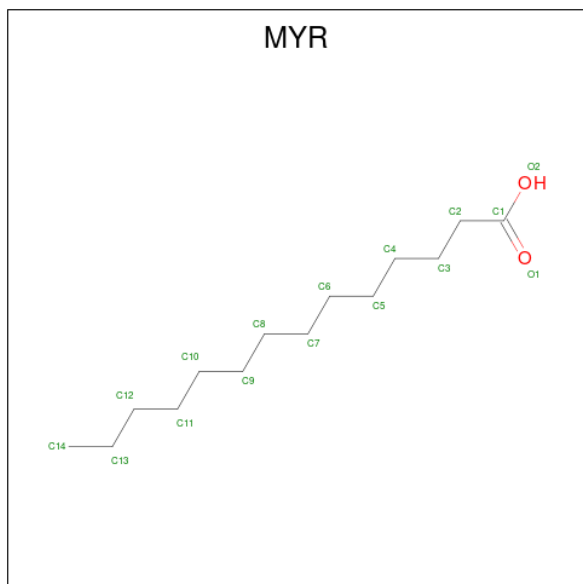
There are 4 unique types of molecules in this entry. The entry contains 5303 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



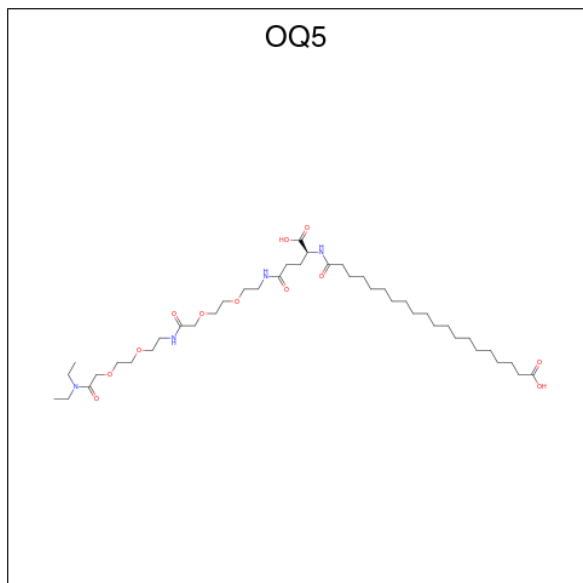
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	12	2		
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			12	10	2		
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			16	14	2		

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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-(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 (CCD ID: OQ5) (formula: C₄₁H₇₆N₄O₁₂) (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

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



4 Data and refinement statistics

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 58.51 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.2 (58.51-1.89) 96.2 (58.51-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	2791 reflections (5.02%)	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)	0.36 , 80.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	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.*

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: 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	0.89	1/4581 (0.0%)	1.47	30/6180 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	ASN	CA-C	5.01	1.59	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	GLU	CA-C-N	8.51	137.32	122.09
1	A	368	GLU	C-N-CA	8.51	137.32	122.09
1	A	353	TYR	CA-C-N	6.71	129.16	120.44
1	A	353	TYR	C-N-CA	6.71	129.16	120.44
1	A	13	ASP	CA-CB-CG	6.67	119.27	112.60
1	A	369	CYS	N-CA-C	-6.34	105.67	113.41
1	A	31	LEU	CA-C-N	6.24	130.68	120.63
1	A	31	LEU	C-N-CA	6.24	130.68	120.63
1	A	428	ARG	CA-C-N	6.16	128.44	120.44
1	A	428	ARG	C-N-CA	6.16	128.44	120.44
1	A	458	ASN	CA-C-N	5.89	128.17	120.28
1	A	458	ASN	C-N-CA	5.89	128.17	120.28
1	A	122	VAL	N-CA-CB	5.77	119.24	110.58
1	A	38	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	276	LYS	CA-C-N	5.61	128.05	120.65
1	A	276	LYS	C-N-CA	5.61	128.05	120.65
1	A	511	ALA	CA-C-N	5.36	128.20	120.38
1	A	511	ALA	C-N-CA	5.36	128.20	120.38
1	A	102	PHE	CA-C-N	5.34	127.44	120.28
1	A	102	PHE	C-N-CA	5.34	127.44	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	533	VAL	N-CA-C	-5.22	107.33	111.81
1	A	256	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	375	ASP	N-CA-C	-5.20	106.09	112.90
1	A	327	LEU	CA-C-N	5.17	125.69	120.00
1	A	327	LEU	C-N-CA	5.17	125.69	120.00
1	A	54	VAL	N-CA-C	-5.15	105.69	110.53
1	A	394	LEU	N-CA-C	-5.12	107.69	114.04
1	A	366	PRO	CA-C-N	5.10	131.29	121.54
1	A	366	PRO	C-N-CA	5.10	131.29	121.54
1	A	56	ASP	N-CA-C	5.06	115.81	107.20

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:18:ASN:HD21	1:A:159:LYS:HZ3	1.51	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:37:GLU:H	1:A:37:GLU:CD	2.15	0.55
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:THR:HA	1:A:530:VAL:HG11	1.98	0.46
1:A:541:LYS:HD3	1:A:541:LYS:HA	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:72:ASP:O	1:A:76:THR:HG23	2.16	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: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: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:416:PRO:O	1:A:534:LYS:HE2	2.20	0.41
1:A:426:VAL:HG11	2:A:605:MYR:H102	2.02	0.41
1:A:525:LYS:HB3	2:A:602:MYR:H32	2.02	0.41
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.61	0.41
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%)	5 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%)	443 (91%)	44 (9%)	9 3

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	37	GLU
1	A	41	LYS
1	A	74	LEU
1	A	79	THR
1	A	83	THR
1	A	94	GLN
1	A	109	ASN
1	A	116	VAL
1	A	122	VAL
1	A	136	LYS
1	A	167	GLU
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	310	VAL
1	A	314	ASP
1	A	347	LEU
1	A	380	LEU
1	A	382	GLU
1	A	389	LYS
1	A	390	GLN
1	A	410	ARG
1	A	432	LYS
1	A	440	HIS
1	A	444	LYS
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
1	A	515	THR
1	A	516	LEU
1	A	529	LEU
1	A	534	LYS
1	A	536	LYS
1	A	540	THR
1	A	541	LYS

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Mol	Chain	Res	Type
1	A	576	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	61	ASN
1	A	94	GLN
1	A	105	HIS
1	A	130	ASN
1	A	170	GLN
1	A	196	GLN
1	A	204	GLN
1	A	390	GLN
1	A	391	ASN
1	A	397	GLN
1	A	458	ASN
1	A	503	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](#)

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](#)

7 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	$\# Z > 2$
2	MYR	A	602	-	15,15,15	0.56	0	15,15,15	0.91	1 (6%)
2	MYR	A	603	-	11,11,15	0.62	0	11,11,15	1.06	0
2	MYR	A	601	-	13,13,15	0.48	0	13,13,15	0.92	0
2	MYR	A	606	-	15,15,15	0.54	0	15,15,15	0.88	0
2	MYR	A	605	-	15,15,15	0.54	0	15,15,15	0.82	0
3	OQ5	A	607	-	56,56,56	0.54	2 (3%)	63,63,63	0.70	2 (3%)
2	MYR	A	604	-	12,12,15	0.61	0	12,12,15	0.91	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYR	A	602	-	-	10/13/13/13	-
2	MYR	A	603	-	-	8/9/9/13	-
2	MYR	A	601	-	-	9/11/11/13	-
2	MYR	A	606	-	-	10/13/13/13	-
2	MYR	A	605	-	-	9/13/13/13	-
3	OQ5	A	607	-	-	30/64/64/64	-
2	MYR	A	604	-	-	7/10/10/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	607	OQ5	O26-C25	-2.63	1.22	1.30
3	A	607	OQ5	O27-C25	2.57	1.29	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	607	OQ5	O26-C25-C21	3.31	124.70	113.51
3	A	607	OQ5	O27-C25-C21	-3.23	111.82	122.26
2	A	602	MYR	O2-C1-C2	2.23	121.06	114.00

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	607	OQ5	C22-C21-C25-O26
3	A	607	OQ5	C21-C22-C23-C24
3	A	607	OQ5	C2-C1-N20-C21
3	A	607	OQ5	O18-C1-N20-C21
3	A	607	OQ5	N20-C21-C22-C23
2	A	603	MYR	C1-C2-C3-C4
2	A	604	MYR	C7-C8-C9-C10
3	A	607	OQ5	C10-C11-C12-C13
2	A	605	MYR	C11-C10-C9-C8
2	A	602	MYR	C7-C8-C9-C10
2	A	606	MYR	C11-C10-C9-C8
2	A	602	MYR	C5-C6-C7-C8
2	A	605	MYR	C10-C11-C12-C13
3	A	607	OQ5	C22-C21-C25-O27
2	A	606	MYR	C2-C3-C4-C5
2	A	604	MYR	C5-C6-C7-C8
2	A	603	MYR	C3-C4-C5-C6
2	A	603	MYR	C6-C7-C8-C9
3	A	607	OQ5	C3-C19-C4-C5
2	A	604	MYR	C6-C7-C8-C9
2	A	601	MYR	C2-C3-C4-C5
2	A	601	MYR	C3-C4-C5-C6
2	A	606	MYR	C9-C10-C11-C12
2	A	603	MYR	C2-C3-C4-C5
2	A	601	MYR	C6-C7-C8-C9
2	A	606	MYR	C10-C11-C12-C13
2	A	602	MYR	C4-C5-C6-C7
2	A	601	MYR	C11-C10-C9-C8
3	A	607	OQ5	C9-C10-C11-C12
2	A	601	MYR	C7-C8-C9-C10
3	A	607	OQ5	C19-C4-C5-C6
2	A	601	MYR	C1-C2-C3-C4
2	A	605	MYR	C3-C4-C5-C6
2	A	601	MYR	C5-C6-C7-C8
3	A	607	OQ5	C4-C5-C6-C7
3	A	607	OQ5	C7-C8-C9-C10
3	A	607	OQ5	O45-C46-C47-O48
2	A	605	MYR	C5-C6-C7-C8
3	A	607	OQ5	O45-C46-C47-N49
2	A	606	MYR	C11-C12-C13-C14
3	A	607	OQ5	C4-C19-C3-C2
2	A	604	MYR	C4-C5-C6-C7

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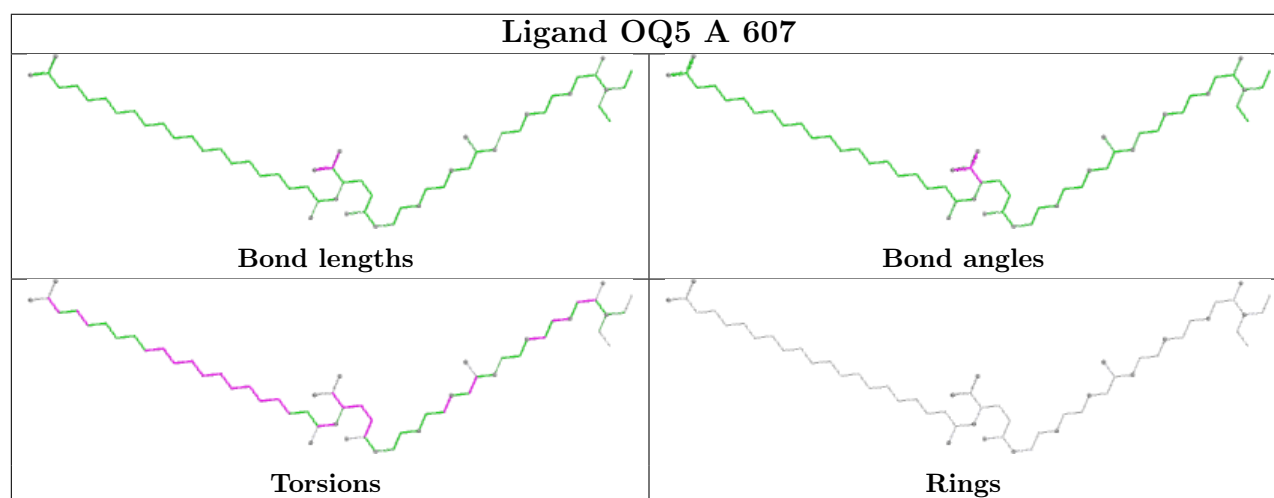
Mol	Chain	Res	Type	Atoms
3	A	607	OQ5	O35-C36-C37-O38
2	A	605	MYR	C11-C12-C13-C14
3	A	607	OQ5	C44-C43-O42-C41
2	A	602	MYR	C9-C10-C11-C12
3	A	607	OQ5	C43-C44-O45-C46
3	A	607	OQ5	N20-C21-C25-O26
2	A	602	MYR	C10-C11-C12-C13
3	A	607	OQ5	O35-C36-C37-N39
2	A	606	MYR	C7-C8-C9-C10
3	A	607	OQ5	C25-C21-C22-C23
2	A	602	MYR	C6-C7-C8-C9
3	A	607	OQ5	C11-C10-C9-C8
2	A	602	MYR	C11-C12-C13-C14
3	A	607	OQ5	C33-C34-O35-C36
2	A	604	MYR	C3-C4-C5-C6
2	A	605	MYR	C9-C10-C11-C12
2	A	601	MYR	O1-C1-C2-C3
2	A	605	MYR	O1-C1-C2-C3
2	A	601	MYR	O2-C1-C2-C3
2	A	606	MYR	O1-C1-C2-C3
3	A	607	OQ5	N20-C21-C25-O27
2	A	605	MYR	C2-C3-C4-C5
2	A	606	MYR	O2-C1-C2-C3
2	A	604	MYR	O1-C1-C2-C3
2	A	604	MYR	O2-C1-C2-C3
2	A	606	MYR	C1-C2-C3-C4
2	A	603	MYR	O1-C1-C2-C3
2	A	602	MYR	C2-C3-C4-C5
2	A	605	MYR	O2-C1-C2-C3
2	A	606	MYR	C5-C6-C7-C8
3	A	607	OQ5	C5-C6-C7-C8
3	A	607	OQ5	C6-C7-C8-C9
2	A	603	MYR	O2-C1-C2-C3
2	A	603	MYR	C4-C5-C6-C7
3	A	607	OQ5	C17-C50-C51-O53
3	A	607	OQ5	C17-C50-C51-O52
3	A	607	OQ5	C22-C23-C24-O29
2	A	602	MYR	O2-C1-C2-C3
2	A	603	MYR	C5-C6-C7-C8
3	A	607	OQ5	C15-C16-C17-C50
2	A	602	MYR	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	MYR	1	0
2	A	601	MYR	2	0
2	A	606	MYR	1	0
2	A	605	MYR	7	0
2	A	604	MYR	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	568/585 (97%)	1.48	149 (26%) 1 1	11, 34, 62, 81	2 (0%)

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	7.2
1	A	462	VAL	7.0
1	A	578	ALA	6.6
1	A	581	ALA	6.3
1	A	493	VAL	6.2
1	A	502	PHE	5.9
1	A	566	THR	5.6
1	A	568	PHE	5.5
1	A	498	VAL	5.2
1	A	511	ALA	5.1
1	A	575	LEU	4.9
1	A	569	ALA	4.9
1	A	567	CYS	4.8
1	A	538	LYS	4.8
1	A	577	ALA	4.7
1	A	540	THR	4.7
1	A	179	LEU	4.7
1	A	582	ALA	4.6
1	A	544	LEU	4.5
1	A	372	LYS	4.5
1	A	370	TYR	4.5
1	A	527	THR	4.4
1	A	546	ALA	4.4
1	A	528	ALA	4.4
1	A	497	TYR	4.4
1	A	509	PHE	4.1
1	A	360	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	386	ASN	4.1
1	A	172	ALA	4.0
1	A	539	ALA	4.0
1	A	533	VAL	4.0
1	A	516	LEU	3.8
1	A	550	ASP	3.8
1	A	409	VAL	3.8
1	A	371	ALA	3.8
1	A	547	VAL	3.8
1	A	362	ALA	3.7
1	A	584	GLY	3.6
1	A	576	VAL	3.5
1	A	507	PHE	3.4
1	A	583	LEU	3.4
1	A	299	PRO	3.4
1	A	572	GLY	3.4
1	A	460	LEU	3.4
1	A	552	ALA	3.3
1	A	423	LEU	3.3
1	A	481	LEU	3.3
1	A	503	ASN	3.3
1	A	517	SER	3.3
1	A	513	ILE	3.2
1	A	579	SER	3.2
1	A	334	TYR	3.2
1	A	466	LYS	3.2
1	A	573	LYS	3.2
1	A	548	MET	3.1
1	A	543	GLN	3.1
1	A	551	PHE	3.1
1	A	367	HIS	3.1
1	A	395	PHE	3.1
1	A	303	PRO	3.1
1	A	305	LEU	3.1
1	A	398	LEU	3.1
1	A	514	CYS	3.1
1	A	180	PRO	3.1
1	A	468	PRO	3.1
1	A	512	ASP	3.0
1	A	116	VAL	3.0
1	A	369	CYS	3.0
1	A	458	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	211	PHE	3.0
1	A	310	VAL	2.9
1	A	530	VAL	2.9
1	A	432	LYS	2.9
1	A	506	THR	2.9
1	A	171	ALA	2.9
1	A	377	PHE	2.9
1	A	535	HIS	2.9
1	A	463	LEU	2.9
1	A	110	PRO	2.8
1	A	455	VAL	2.8
1	A	374	PHE	2.8
1	A	177	CYS	2.8
1	A	412	THR	2.8
1	A	574	LYS	2.7
1	A	523	ILE	2.7
1	A	206	PHE	2.7
1	A	496	THR	2.7
1	A	397	GLN	2.7
1	A	104	GLN	2.6
1	A	394	LEU	2.6
1	A	532	LEU	2.6
1	A	545	LYS	2.6
1	A	366	PRO	2.5
1	A	465	GLU	2.5
1	A	373	VAL	2.5
1	A	452	TYR	2.5
1	A	443	ALA	2.5
1	A	504	ALA	2.5
1	A	459	GLN	2.5
1	A	205	LYS	2.5
1	A	49	PHE	2.5
1	A	542	GLU	2.5
1	A	301	ASP	2.5
1	A	414	LYS	2.5
1	A	499	PRO	2.5
1	A	536	LYS	2.4
1	A	173	ASP	2.4
1	A	309	PHE	2.4
1	A	413	LYS	2.4
1	A	419	SER	2.4
1	A	464	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	178	LEU	2.3
1	A	302	LEU	2.3
1	A	529	LEU	2.3
1	A	109	ASN	2.3
1	A	203	LEU	2.3
1	A	306	ALA	2.3
1	A	381	VAL	2.3
1	A	415	VAL	2.3
1	A	380	LEU	2.3
1	A	194	ALA	2.3
1	A	293	VAL	2.3
1	A	82[A]	GLU	2.2
1	A	441	PRO	2.2
1	A	183	ASP	2.2
1	A	185	LEU	2.2
1	A	457	LEU	2.2
1	A	390	GLN	2.2
1	A	549	ASP	2.2
1	A	117	ARG	2.2
1	A	355	THR	2.2
1	A	168	CYS	2.2
1	A	134	PHE	2.2
1	A	388	ILE	2.2
1	A	482	VAL	2.2
1	A	204	GLN	2.1
1	A	474	THR	2.1
1	A	357	LEU	2.1
1	A	537	PRO	2.1
1	A	501	GLU	2.1
1	A	312	SER	2.1
1	A	508	THR	2.1
1	A	456	VAL	2.1
1	A	156	PHE	2.1
1	A	108	ASP	2.1
1	A	262	LYS	2.0
1	A	424	VAL	2.0
1	A	111	ASN	2.0
1	A	418	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

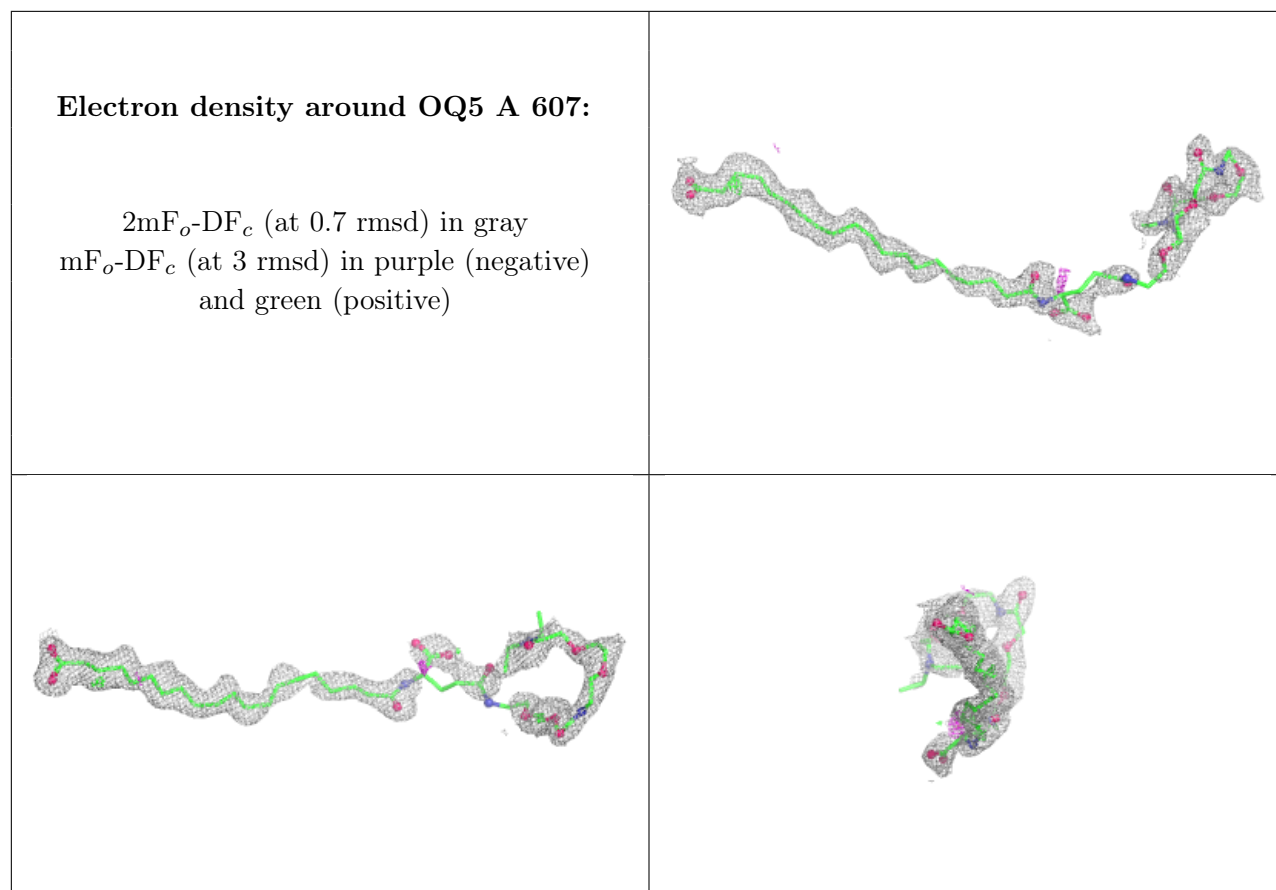
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
2	MYR	A	601	14/16	0.77	0.16	28,38,41,41	0
2	MYR	A	603	12/16	0.78	0.16	27,31,47,48	0
2	MYR	A	602	16/16	0.80	0.16	35,41,52,54	0
3	OQ5	A	607	57/57	0.81	0.17	17,49,63,63	57
2	MYR	A	604	13/16	0.82	0.18	34,39,40,40	0
2	MYR	A	605	16/16	0.83	0.18	37,45,56,57	0
2	MYR	A	606	16/16	0.85	0.14	31,35,46,47	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 ⓘ

There are no such residues in this entry.