



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 06:26 AM UTC

PDB ID : 7JYE / pdb_00007jye
Title : Human Liver Receptor Homolog-1 in Complex with 9ChoP and a Fragment of Tif2
Authors : D'Agostino, E.H.; Mays, S.G.; Ortlund, E.A.
Deposited on : 2020-08-30
Resolution : 2.55 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

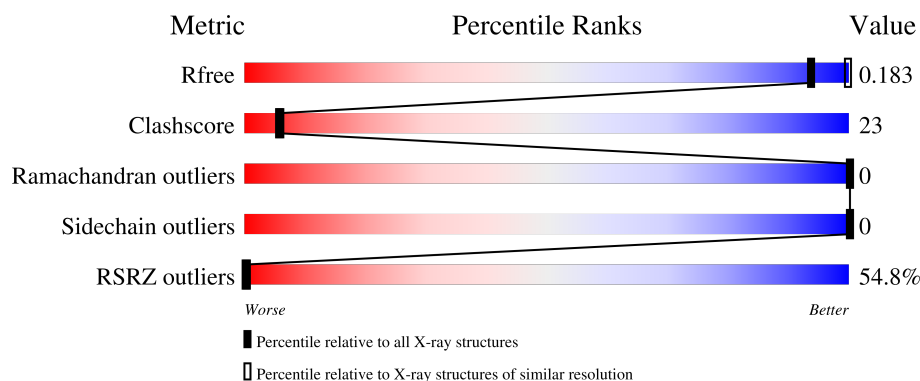
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	246	54% 50%48%
2	C	12	42% 50%33%17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2174 atoms, of which 52 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 Nuclear receptor subfamily 5 group A member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	1	0
			1976	1265	334	364	13			

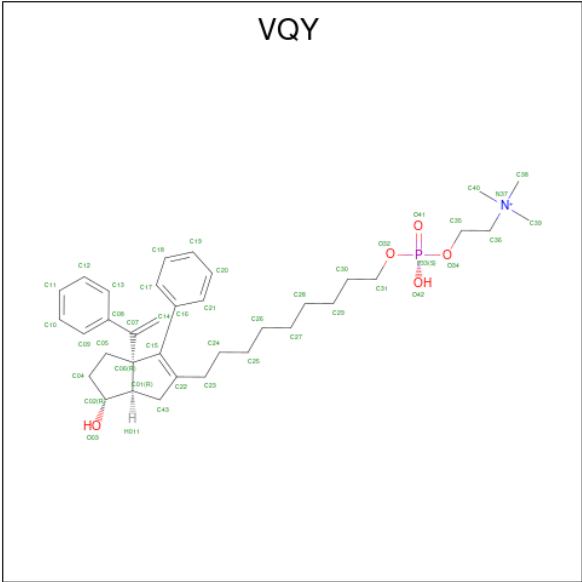
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	SER	-	expression tag	UNP O00482
A	297	ASN	-	expression tag	UNP O00482
A	298	ALA	-	expression tag	UNP O00482

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			85	56	15	14			

- Molecule 3 is 9-[(3 {a} {R},6 {R},6 {a} {R})-6-oxidanyl-3-phenyl-3 {a}-(1-phenyleth enyl)-4,5,6,6 {a}-tetrahydro-1 {H}-pentalen-2-yl]nonyl 2-(trimethyl- l^4 -azanyl)ethyl hydrogen phosphate (CCD ID: VQY) (formula: $C_{36}H_{53}NO_5P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	H	N	O	P	0	0
			95	36	52	1	5	1		

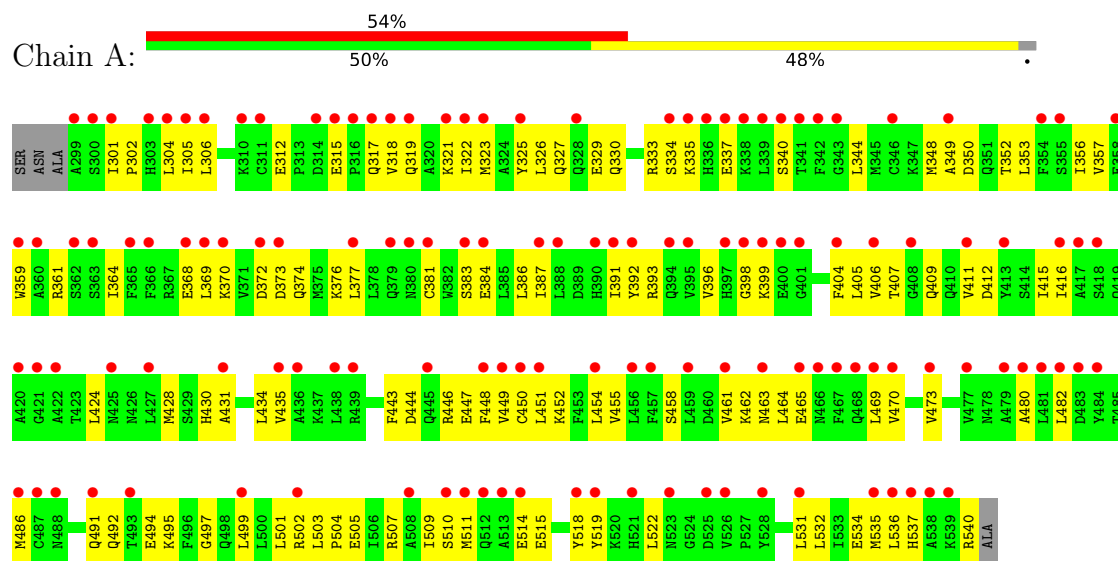
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	C	1	Total	O	0	0
			1	1		

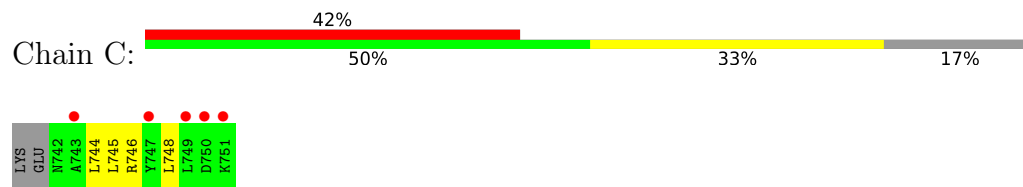
3 Residue-property plots [i](#)

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: Nuclear receptor subfamily 5 group A member 2



- Molecule 2: Nuclear receptor coactivator 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.24Å 89.24Å 106.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.51 – 2.55 35.51 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.51-2.55) 100.0 (35.51-2.55)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	107.23 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.12-2829-000	Depositor
R, R_{free}	0.159 , 0.187 0.161 , 0.183	Depositor DCC
R_{free} test set	818 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 245.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.428 for -h,-k,l	Xtriage
Reported twinning fraction	0.480 for -h,-k,l	Depositor
Outliers	0 of 16427 reflections	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	2174	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: VQY

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	0.07	0/2012	0.20	0/2716
2	C	0.06	0/85	0.19	0/113
All	All	0.07	0/2097	0.20	0/2829

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1976	0	1988	94	0
2	C	85	0	93	3	0
3	A	43	52	0	0	0
4	A	17	0	0	0	0
4	C	1	0	0	1	0
All	All	2122	52	2081	96	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 23.

All (96) 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:534:GLU:HA	1:A:537:HIS:HB3	1.66	0.77
1:A:391:ILE:HG23	1:A:435:VAL:HG22	1.68	0.76
1:A:458:SER:HB3	1:A:461:VAL:HG23	1.69	0.75
1:A:318:VAL:HA	1:A:321:LYS:HD2	1.70	0.74
1:A:511:MET:HE2	1:A:511:MET:HA	1.72	0.71
1:A:497:GLY:O	1:A:501:LEU:HD13	1.92	0.69
1:A:335:LYS:HE2	1:A:335:LYS:N	2.08	0.68
1:A:333:ARG:HB3	1:A:337:GLU:HB2	1.77	0.67
1:A:317:GLN:O	1:A:321:LYS:HG3	1.94	0.67
1:A:411:VAL:HG21	1:A:416:ILE:HG13	1.76	0.66
1:A:319:GLN:HG2	1:A:406:VAL:O	1.96	0.66
1:A:323:MET:SD	1:A:409:GLN:NE2	2.54	0.66
1:A:326:LEU:HD11	1:A:348:MET:HG2	1.78	0.65
1:A:531:LEU:HD12	1:A:532:LEU:N	2.12	0.65
1:A:350:ASP:HA	1:A:353:LEU:HD12	1.79	0.65
1:A:377:LEU:HD23	1:A:461:VAL:HG21	1.78	0.64
1:A:507:ARG:O	1:A:510:SER:OG	2.14	0.64
1:A:348:MET:HE1	1:A:405:LEU:HD13	1.79	0.63
1:A:330:GLN:OE1	1:A:333:ARG:NH2	2.24	0.62
1:A:325:TYR:O	1:A:329:GLU:HG2	2.00	0.62
1:A:302:PRO:HD2	1:A:305:ILE:HD12	1.82	0.61
1:A:357:VAL:O	1:A:361:ARG:HG3	1.99	0.61
1:A:333:ARG:HD2	1:A:337:GLU:HB3	1.84	0.60
1:A:495:LYS:O	1:A:499:LEU:HG	2.01	0.59
1:A:398:GLY:HA2	1:A:404:PHE:CD1	2.38	0.58
1:A:448:PHE:CZ	1:A:452:LYS:HD2	2.39	0.58
1:A:515:GLU:OE2	1:A:540:ARG:NE	2.37	0.57
1:A:534:GLU:OE1	2:C:744:LEU:HB3	2.05	0.56
1:A:373:ASP:OD2	1:A:465:GLU:HB3	2.06	0.55
1:A:503:LEU:HB2	1:A:504:PRO:HD3	1.89	0.55
1:A:335:LYS:HE2	1:A:335:LYS:H	1.71	0.55
1:A:398:GLY:O	1:A:399:LYS:HD3	2.06	0.55
1:A:318:VAL:HA	1:A:321:LYS:CD	2.36	0.54
1:A:443:PHE:CZ	1:A:448:PHE:HA	2.43	0.54
1:A:370:LYS:O	1:A:374:GLN:HG3	2.07	0.54
1:A:301:ILE:HG22	1:A:306:LEU:HG	1.91	0.53
1:A:334:SER:OG	1:A:337:GLU:OE1	2.19	0.53
1:A:370:LYS:HE2	1:A:465:GLU:CB	2.38	0.53
1:A:491:GLN:HG3	1:A:492:GLN:OE1	2.07	0.53
1:A:514:GLU:HG3	1:A:536:LEU:HD21	1.90	0.53
1:A:315:GLU:HA	1:A:318:VAL:HG12	1.89	0.53
1:A:501:LEU:HB3	1:A:502:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LYS:O	1:A:463:ASN:HB2	2.07	0.52
1:A:531:LEU:O	1:A:535:MET:HG2	2.10	0.52
1:A:312:GLU:OE2	1:A:449:VAL:HG12	2.09	0.52
1:A:364:ILE:O	1:A:368:GLU:HG3	2.09	0.52
1:A:377:LEU:CD2	1:A:461:VAL:HG21	2.39	0.52
1:A:518:TYR:HB2	1:A:536:LEU:HD22	1.92	0.52
1:A:369:LEU:O	1:A:374:GLN:NE2	2.36	0.51
1:A:482:LEU:HD12	1:A:486:MET:HG3	1.92	0.51
1:A:304:LEU:HD23	1:A:480:ALA:HB2	1.92	0.50
1:A:407:THR:OG1	1:A:409:GLN:HG3	2.11	0.50
1:A:317:GLN:HG3	1:A:321:LYS:HE3	1.94	0.50
1:A:448:PHE:CE2	1:A:452:LYS:HD2	2.46	0.50
1:A:322:ILE:HD12	1:A:406:VAL:HG22	1.94	0.50
1:A:372:ASP:O	1:A:376:LYS:HG3	2.11	0.50
1:A:322:ILE:HD12	1:A:406:VAL:CG2	2.41	0.50
1:A:519:TYR:OH	1:A:540:ARG:NH2	2.45	0.49
2:C:745:LEU:HA	2:C:748:LEU:HD12	1.94	0.49
1:A:359:TRP:CZ2	1:A:452:LYS:HE2	2.47	0.49
1:A:511:MET:HE2	1:A:511:MET:CA	2.43	0.49
1:A:431:ALA:O	1:A:435:VAL:HG23	2.13	0.49
1:A:430:HIS:ND1	1:A:509:ILE:HD11	2.28	0.48
1:A:325:TYR:CD2	1:A:326:LEU:HD23	2.48	0.48
1:A:383:SER:O	1:A:387:ILE:HG12	2.13	0.48
1:A:412:ASP:HB3	1:A:415:ILE:HG12	1.94	0.48
1:A:381:CYS:HB2	1:A:455:VAL:HG12	1.95	0.48
1:A:323:MET:HB2	1:A:407:THR:HB	1.96	0.48
1:A:384:GLU:OE1	1:A:507:ARG:HD3	2.13	0.48
1:A:494:GLU:OE1	1:A:494:GLU:N	2.44	0.48
1:A:317:GLN:HG3	1:A:318:VAL:N	2.31	0.46
1:A:340:SER:O	1:A:344:LEU:HG	2.15	0.46
1:A:352:THR:O	1:A:356:ILE:HG13	2.16	0.46
1:A:392:TYR:O	1:A:396:VAL:HG23	2.16	0.46
1:A:450:CYS:O	1:A:454:LEU:HG	2.16	0.45
1:A:443:PHE:HZ	1:A:448:PHE:HA	1.79	0.45
1:A:424:LEU:O	1:A:428:MET:HG3	2.16	0.45
1:A:518:TYR:CE2	1:A:522:LEU:HD11	2.52	0.45
1:A:451:LEU:O	1:A:455:VAL:HG23	2.17	0.45
1:A:469:LEU:O	1:A:473:VAL:HG23	2.17	0.44
1:A:446:ARG:O	1:A:449:VAL:HG22	2.17	0.44
2:C:746:ARG:NH2	4:C:801:HOH:O	2.50	0.44
1:A:322:ILE:HG22	1:A:407:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LYS:HE2	1:A:465:GLU:HB2	2.00	0.44
1:A:323:MET:O	1:A:327:GLN:HG3	2.19	0.43
1:A:469:LEU:C	1:A:469:LEU:HD23	2.43	0.43
1:A:518:TYR:O	1:A:522:LEU:HG	2.19	0.43
1:A:537:HIS:ND1	1:A:537:HIS:O	2.52	0.43
1:A:444:ASP:CG	1:A:447:GLU:HG3	2.44	0.42
1:A:393:ARG:CZ	1:A:393:ARG:HB2	2.50	0.42
1:A:348:MET:CE	1:A:405:LEU:HD13	2.49	0.42
1:A:444:ASP:OD1	1:A:447:GLU:HG3	2.20	0.41
1:A:349:ALA:HB1	1:A:386:LEU:HD21	2.01	0.41
1:A:434:LEU:HD21	1:A:505:GLU:OE1	2.21	0.41
1:A:464:LEU:HD13	1:A:470:VAL:HG21	2.02	0.41
1:A:315:GLU:O	1:A:319:GLN:HG3	2.21	0.40

There are no symmetry-related clashes.

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	241/246 (98%)	236 (98%)	5 (2%)	0	100	100
2	C	8/12 (67%)	7 (88%)	1 (12%)	0	100	100
All	All	249/258 (96%)	243 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	219/220 (100%)	219 (100%)	0	100	100
2	C	9/11 (82%)	9 (100%)	0	100	100
All	All	228/231 (99%)	228 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	442	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	VQY	A	601	-	43,46,46	1.99	8 (18%)	47,65,65	0.87	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	VQY	A	601	-	-	21/36/66/66	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	VQY	C22-C15	7.42	1.43	1.34
3	A	601	VQY	C06-C01	-5.57	1.47	1.55
3	A	601	VQY	O03-C02	-3.24	1.36	1.43
3	A	601	VQY	C23-C22	2.95	1.61	1.51
3	A	601	VQY	C16-C15	2.69	1.53	1.48
3	A	601	VQY	P33-O34	2.66	1.69	1.59
3	A	601	VQY	P33-O32	2.15	1.67	1.59
3	A	601	VQY	C19-C18	2.14	1.43	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	VQY	C43-C22-C15	-4.49	107.63	112.29

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	VQY	C01-C06-C07-C08
3	A	601	VQY	C01-C06-C07-C14
3	A	601	VQY	C05-C06-C07-C14
3	A	601	VQY	C15-C22-C23-C24
3	A	601	VQY	C43-C22-C23-C24
3	A	601	VQY	O34-C35-C36-N37
3	A	601	VQY	C31-O32-P33-O34
3	A	601	VQY	C31-O32-P33-O41
3	A	601	VQY	C31-O32-P33-O42
3	A	601	VQY	C35-O34-P33-O32
3	A	601	VQY	C35-O34-P33-O41
3	A	601	VQY	C35-O34-P33-O42
3	A	601	VQY	C22-C23-C24-C25
3	A	601	VQY	C26-C27-C28-C29

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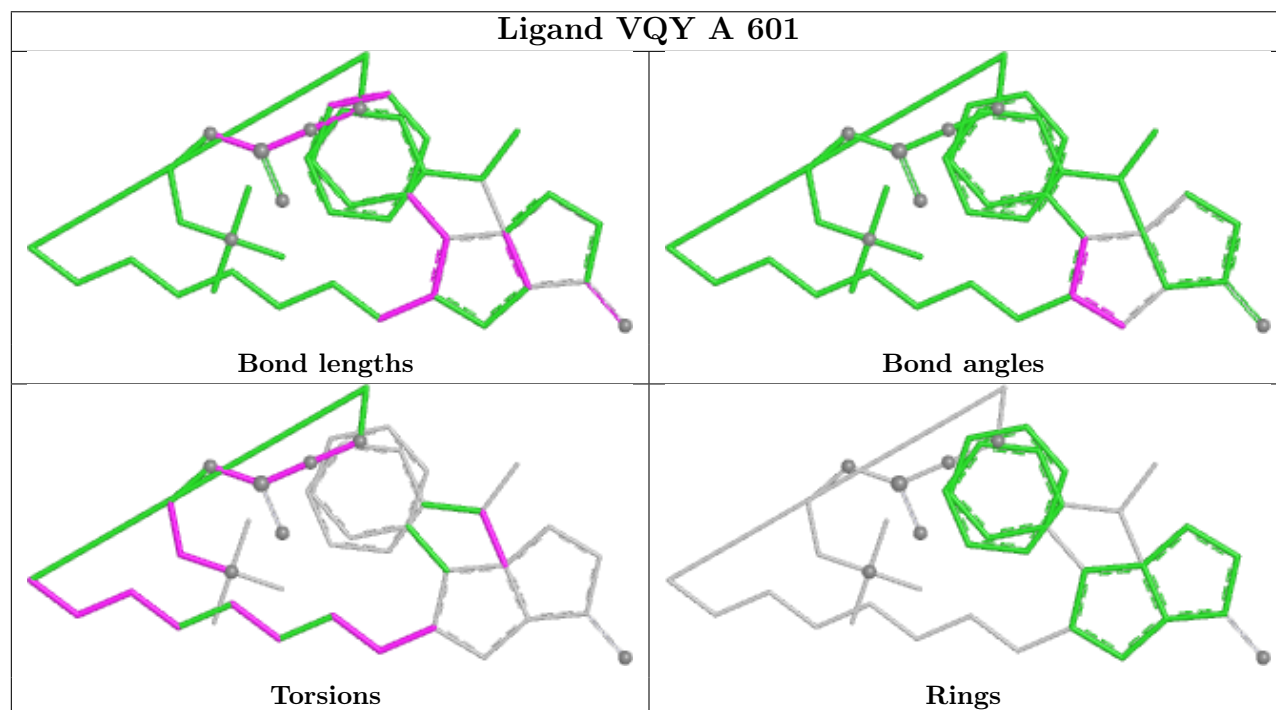
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Mol	Chain	Res	Type	Atoms
3	A	601	VQY	C28-C29-C30-C31
3	A	601	VQY	C24-C25-C26-C27
3	A	601	VQY	C27-C28-C29-C30
3	A	601	VQY	C05-C06-C07-C08
3	A	601	VQY	C15-C06-C07-C14
3	A	601	VQY	C35-C36-N37-C39
3	A	601	VQY	C35-C36-N37-C40

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 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	242/246 (98%)	2.25	133 (54%) 0 0	24, 56, 105, 158	1 (0%)
2	C	10/12 (83%)	2.82	5 (50%) 0 0	59, 90, 123, 156	0
All	All	252/258 (97%)	2.27	138 (54%) 0 0	24, 57, 111, 158	1 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	LYS	7.0
2	C	750	ASP	5.5
1	A	369	LEU	5.3
1	A	397	HIS	5.1
1	A	493	THR	4.9
1	A	523	ASN	4.6
1	A	323	MET	4.5
1	A	379	GLN	4.3
1	A	325	TYR	4.3
1	A	384	GLU	4.3
2	C	743	ALA	4.3
1	A	335	LYS	4.1
1	A	459	LEU	4.0
1	A	400	GLU	3.9
1	A	538	ALA	3.8
1	A	401	GLY	3.8
1	A	531	LEU	3.8
1	A	339	LEU	3.8
1	A	481	LEU	3.8
1	A	368	GLU	3.7
1	A	416	ILE	3.7
1	A	363	SER	3.7
1	A	322	ILE	3.7
1	A	467	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	747	TYR	3.7
1	A	422	ALA	3.6
1	A	450	CYS	3.6
1	A	372	ASP	3.6
1	A	514	GLU	3.6
1	A	513	ALA	3.6
1	A	383	SER	3.5
1	A	421	GLY	3.5
1	A	406	VAL	3.5
1	A	355	SER	3.5
1	A	536	LEU	3.5
1	A	539	LYS	3.5
1	A	537	HIS	3.5
1	A	511	MET	3.4
1	A	305	ILE	3.4
1	A	300	SER	3.4
1	A	303	HIS	3.4
1	A	404	PHE	3.3
2	C	751	LYS	3.3
1	A	358	GLU	3.3
1	A	328	GLN	3.3
1	A	491	GLN	3.3
2	C	749	LEU	3.3
1	A	304	LEU	3.3
1	A	535	MET	3.3
1	A	395	VAL	3.2
1	A	362	SER	3.2
1	A	463	ASN	3.2
1	A	317	GLN	3.2
1	A	528	TYR	3.2
1	A	381	CYS	3.1
1	A	417	ALA	3.1
1	A	340	SER	3.1
1	A	341	THR	3.0
1	A	316	PRO	3.0
1	A	525	ASP	3.0
1	A	461	VAL	3.0
1	A	299	ALA	3.0
1	A	392	TYR	3.0
1	A	521	HIS	3.0
1	A	477	VAL	2.9
1	A	336	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	479	ALA	2.9
1	A	431	ALA	2.9
1	A	508	ALA	2.9
1	A	486	MET	2.9
1	A	306	LEU	2.9
1	A	484	TYR	2.9
1	A	456	LEU	2.8
1	A	301	ILE	2.8
1	A	354	PHE	2.8
1	A	427	LEU	2.8
1	A	314	ASP	2.8
1	A	408	GLY	2.7
1	A	391	ILE	2.7
1	A	343	GLY	2.7
1	A	359	TRP	2.7
1	A	435	VAL	2.7
1	A	519	TYR	2.7
1	A	499	LEU	2.7
1	A	420	ALA	2.7
1	A	468	GLN	2.7
1	A	346	CYS	2.6
1	A	387	ILE	2.6
1	A	380	ASN	2.6
1	A	466	ASN	2.6
1	A	390	HIS	2.6
1	A	473	VAL	2.6
1	A	370	LYS	2.6
1	A	366	PHE	2.5
1	A	399	LYS	2.5
1	A	449	VAL	2.5
1	A	315	GLU	2.5
1	A	483	ASP	2.5
1	A	445	GLN	2.4
1	A	512	GLN	2.4
1	A	470	VAL	2.4
1	A	349	ALA	2.4
1	A	319	GLN	2.4
1	A	451	LEU	2.4
1	A	342	PHE	2.4
1	A	321	LYS	2.4
1	A	337	GLU	2.4
1	A	373	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	448	PHE	2.4
1	A	360	ALA	2.4
1	A	418	SER	2.3
1	A	510	SER	2.3
1	A	318	VAL	2.3
1	A	526	VAL	2.3
1	A	413	TYR	2.3
1	A	487	CYS	2.3
1	A	438	LEU	2.3
1	A	365	PHE	2.3
1	A	480	ALA	2.2
1	A	310	LYS	2.2
1	A	488	ASN	2.2
1	A	425	ASN	2.2
1	A	436	ALA	2.2
1	A	394	GLN	2.2
1	A	398	GLY	2.2
1	A	457	PHE	2.2
1	A	469	LEU	2.1
1	A	482	LEU	2.1
1	A	311	CYS	2.1
1	A	502	ARG	2.1
1	A	439	ARG	2.1
1	A	518	TYR	2.1
1	A	411	VAL	2.1
1	A	377	LEU	2.1
1	A	454	LEU	2.1
1	A	465	GLU	2.1
1	A	334	SER	2.1
1	A	388	LEU	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](#)

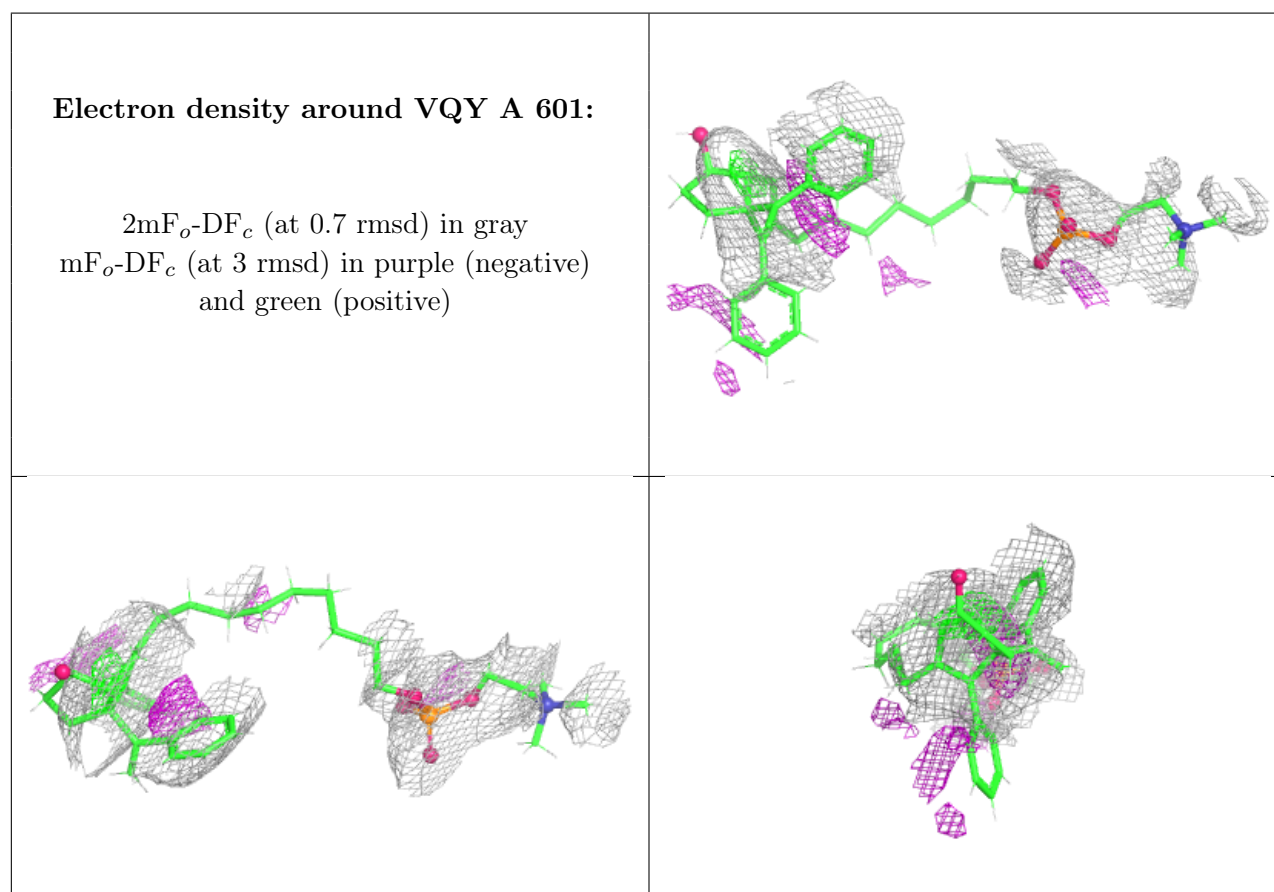
There are no oligosaccharides in this entry.

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
3	VQY	A	601	43/43	0.95	0.22	42,72,114,124	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.