



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 03:15 PM UTC

PDB ID : 8PHW / pdb_00008phw
EMDB ID : EMD-17677
Title : Human OATP1B1
Authors : Ciuta, A.-D.; Nosol, K.; Kowal, J.; Mukherjee, S.; Ramirez, A.S.; Stieger, B.; Kossiakoff, A.A.; Locher, K.P.
Deposited on : 2023-06-20
Resolution : 3.60 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

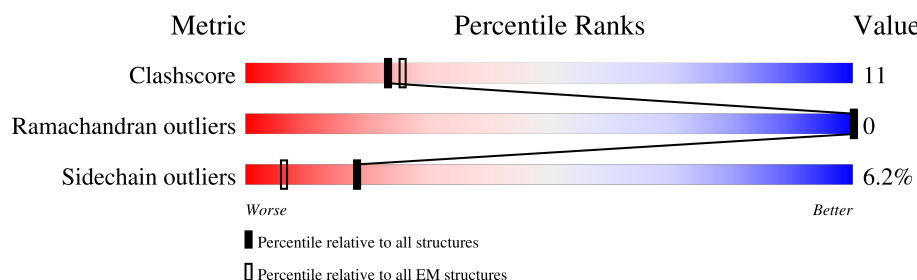
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	691	
2	H	230	
3	L	215	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5359 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Solute carrier organic anion transporter family member 1B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	454	Total	C	N	O	S	0	0
			3528	2342	546	611	29		

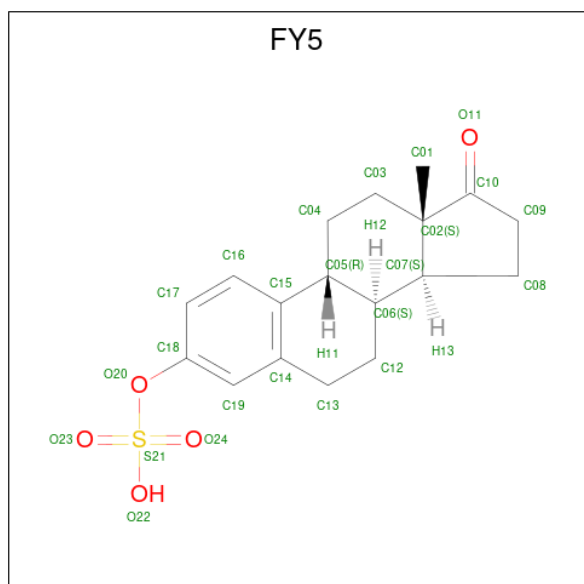
- Molecule 2 is a protein called Fab18 (heavy chain, variable region).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	128	Total	C	N	O	S	0	0
			972	611	168	190	3		

- Molecule 3 is a protein called Fab18 (light chain, variable region).

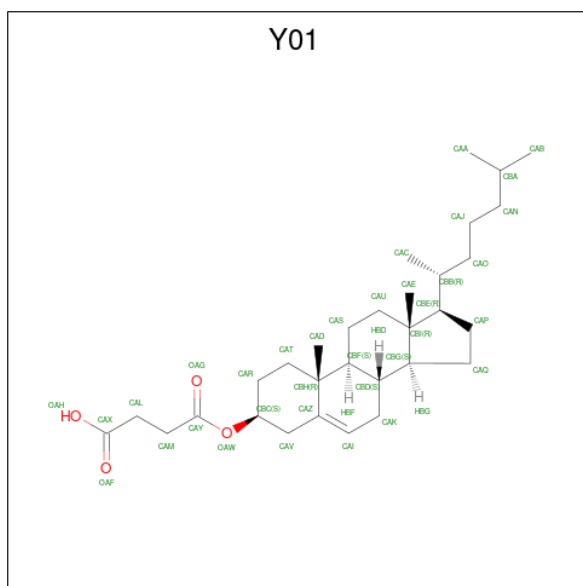
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	107	Total	C	N	O	S	0	0
			800	498	133	166	3		

- Molecule 4 is estrone 3-sulfate (CCD ID: FY5) (formula: $C_{18}H_{22}O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	S	0
			24	18	5	1	

- Molecule 5 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).

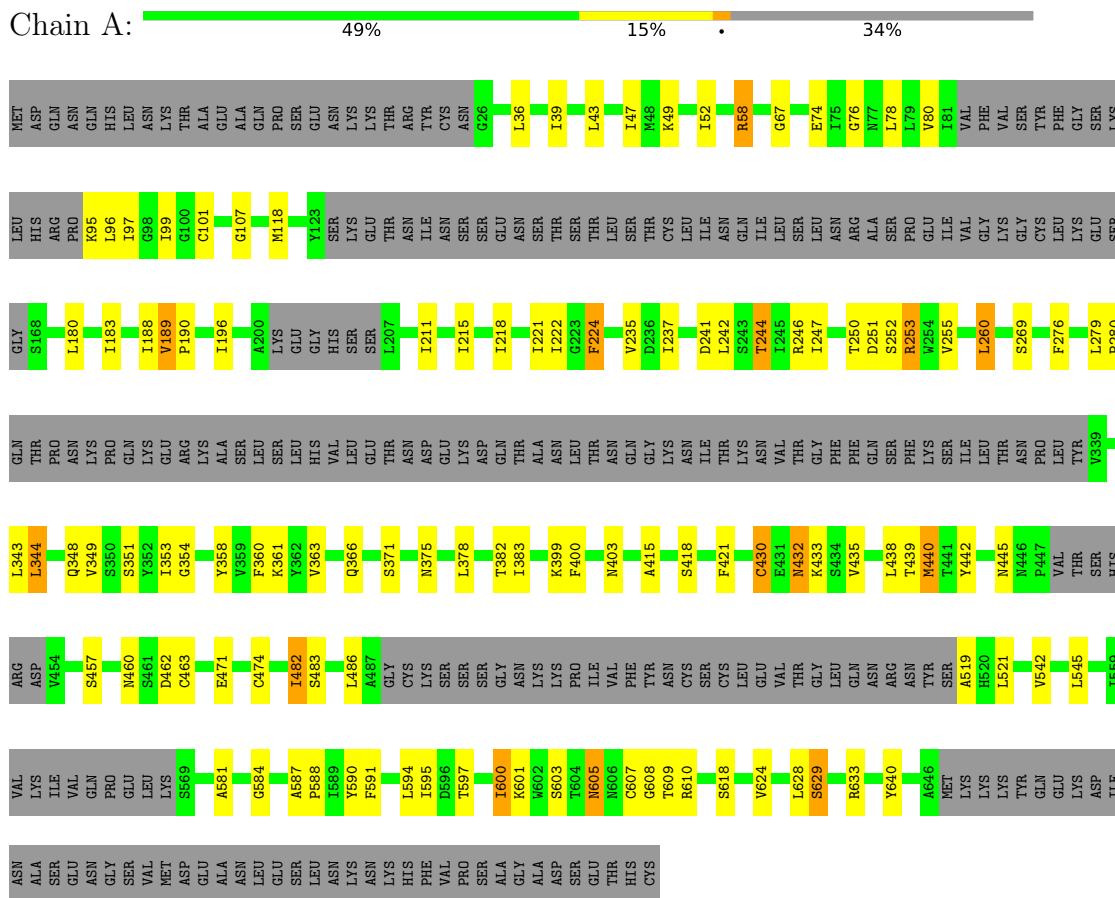


Mol	Chain	Residues	Atoms			AltConf
5	H	1	Total	C	O	0
			35	31	4	

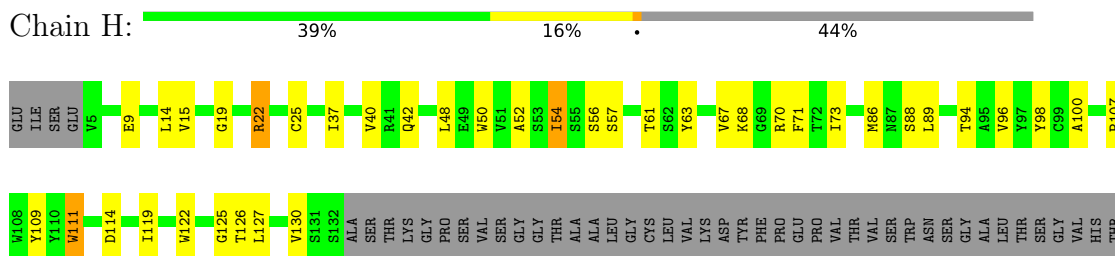
3 Residue-property plots

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. 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. 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: Solute carrier organic anion transporter family member 1B1

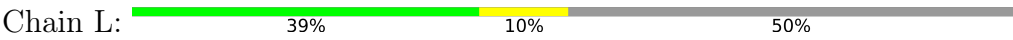


- Molecule 2: Fab18 (heavy chain, variable region)



PHE	PRO	ALA	LEU	GLN	SER	SER	GLY	TYR	SER	LEU	SER	SER	VAL	VAL	THR	THR	PRO	PRO	SER	SER	LEU	GLY	THR	GLN	THR	THR	TYR	ILE	CYS	ASN	VAL	ASN	HIS	LYS	PRO	SER	ASN	THR	LYS	VAL	ASP	LYS	LYS	VAL	GLU	PRO	LYS	SER	CYS	ASP	LYS	THR	HIS	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 3: Fab18 (light chain, variable region)



S1	D2	I3	Q4	Q7	S8	P9	G17	V20	T21	I22	T23	Q39	S54	T75	S78	L79	D83	F94	A85	T86	Y87	Q90	L96	F99	G102	T103	K104	V105	E106	I107	LYS	ARG	THR	VAL	ALA	ALA	PRO	SER	VAL	PHE	ILE	PHE	PRO	PRO	LEU	SER	ASP	SER
----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLN	LEU	LYS	GLY	THR	ALA	SER	VAL	VAL	ALA	CYS	LEU	LEU	ASN	ASN	PHE	TYR	PRO	ARG	GLU	ALA	LYS	VAL	GLN	TRP	LYS	VAL	ASP	ASN	ASN	ALA	LEU	GLN	SER	GLY	ASN	SER	GLN	GLU	SER	VAL	THR	GLU	THR	GLN	ASP	SER	THR	LYS	ASP	SER	THR	THR	TYR	SER	LEU	SER	SER	THR	LEU	THR	LEU	SER	ASP	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ALA	ASP	TYR	GLU	LYS	HIS	LYS	VAL	TYR	ALA	CYS	GLU	VAL	THR	HIS	GLN	GLY	LEU	SER	SER	PRO	VAL	THR	LYS	SER	PHE	ASN	ARG	GLY	GLU	CYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.5	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

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: FY5, Y01

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	0.21	0/3613	0.44	0/4891
2	H	0.23	0/998	0.43	0/1356
3	L	0.26	0/815	0.46	0/1105
All	All	0.22	0/5426	0.44	0/7352

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 [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	3528	0	3578	70	0
2	H	972	0	915	36	0
3	L	800	0	785	11	0
4	A	24	0	0	0	0
5	H	35	0	49	11	0
All	All	5359	0	5327	117	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 11.

All (117) 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:H:109:TYR:CE1	5:H:301:Y01:HAC1	1.84	1.12
2:H:109:TYR:HE1	5:H:301:Y01:HAC1	1.31	0.88
1:A:438:LEU:HD23	1:A:600:ILE:HB	1.68	0.75
2:H:70:ARG:NH2	2:H:88:SER:O	2.25	0.70
1:A:43:LEU:O	1:A:47:ILE:HG12	1.92	0.70
1:A:474:CYS:O	1:A:519:ALA:N	2.25	0.69
1:A:80:VAL:HG21	1:A:183:ILE:HA	1.73	0.69
1:A:432:ASN:ND2	1:A:433:LYS:O	2.27	0.68
1:A:67:GLY:HA2	1:A:588:PRO:HB2	1.75	0.67
3:L:2:ASP:O	3:L:4:GLN:NE2	2.30	0.64
1:A:366:GLN:NE2	1:A:430:CYS:O	2.32	0.62
1:A:442:TYR:CG	1:A:457:SER:HB2	2.35	0.62
2:H:109:TYR:CE1	5:H:301:Y01:CAC	2.74	0.60
2:H:109:TYR:HE1	5:H:301:Y01:HAE2	1.65	0.60
2:H:54:ILE:HG23	2:H:73:ILE:HG12	1.83	0.59
1:A:237:ILE:HG13	1:A:242:LEU:HD11	1.84	0.58
1:A:246:ARG:HH11	1:A:521:LEU:HD21	1.69	0.57
1:A:101:CYS:O	1:A:269:SER:OG	2.21	0.57
1:A:435:VAL:HG12	1:A:438:LEU:HD13	1.85	0.57
2:H:50:TRP:NE1	2:H:52:ALA:O	2.37	0.57
1:A:587:ALA:HA	1:A:590:TYR:CZ	2.40	0.56
1:A:360:PHE:HA	1:A:363:VAL:HG22	1.88	0.56
1:A:218:ILE:HG22	1:A:222:ILE:HD11	1.86	0.56
2:H:109:TYR:CD1	5:H:301:Y01:HAU2	2.40	0.56
1:A:597:THR:HG22	1:A:597:THR:O	2.06	0.56
2:H:63:TYR:HB2	2:H:68:LYS:HG3	1.87	0.56
3:L:83:ASP:OD1	3:L:87:TYR:OH	2.23	0.55
1:A:58:ARG:HE	1:A:235:VAL:HG21	1.72	0.54
1:A:629:SER:O	1:A:633:ARG:HG2	2.07	0.54
1:A:358:TYR:HD2	1:A:361:LYS:HD2	1.73	0.54
1:A:440:MET:HG2	1:A:445:ASN:HA	1.91	0.53
1:A:605:ASN:OD1	1:A:605:ASN:N	2.42	0.53
1:A:189:VAL:HG13	1:A:190:PRO:HD3	1.90	0.53
1:A:594:LEU:HD12	1:A:628:LEU:HD12	1.90	0.52
1:A:78:LEU:HD21	1:A:581:ALA:HB2	1.92	0.52
2:H:109:TYR:CE1	5:H:301:Y01:HAU2	2.44	0.52
2:H:109:TYR:CE1	5:H:301:Y01:HAE2	2.44	0.51
1:A:251:ASP:OD1	1:A:252:SER:N	2.33	0.51
1:A:403:ASN:N	1:A:403:ASN:OD1	2.42	0.51
1:A:415:ALA:O	1:A:418:SER:OG	2.22	0.51
1:A:74:GLU:HG2	1:A:584:GLY:HA3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:THR:HB	2:H:63:TYR:HE1	1.77	0.50
2:H:89:LEU:O	2:H:130:VAL:HG11	2.12	0.50
1:A:241:ASP:O	1:A:244:THR:OG1	2.29	0.50
2:H:86:MET:HB2	2:H:89:LEU:HD21	1.93	0.50
1:A:442:TYR:CD1	1:A:457:SER:HB2	2.47	0.49
1:A:97:ILE:HG13	1:A:188:ILE:HA	1.95	0.49
1:A:382:THR:HG22	1:A:542:VAL:HG22	1.94	0.49
2:H:54:ILE:HG12	2:H:73:ILE:HD11	1.95	0.49
1:A:358:TYR:CD2	1:A:361:LYS:HD2	2.48	0.48
2:H:109:TYR:CZ	5:H:301:Y01:HAC1	2.44	0.48
1:A:96:LEU:HD12	1:A:99:ILE:HD12	1.95	0.48
3:L:7:GLN:OE1	3:L:103:THR:N	2.47	0.48
1:A:276:PHE:HA	1:A:279:LEU:HB2	1.95	0.47
1:A:439:THR:OG1	1:A:440:MET:N	2.47	0.47
2:H:22:ARG:HE	2:H:22:ARG:HB2	1.49	0.47
2:H:119:ILE:HG22	2:H:122:TRP:NE1	2.29	0.47
2:H:100:ALA:HB1	2:H:119:ILE:HG23	1.97	0.46
1:A:349:VAL:O	1:A:353:ILE:HG22	2.16	0.46
5:H:301:Y01:HAV1	5:H:301:Y01:OAG	2.15	0.46
1:A:438:LEU:HB3	1:A:600:ILE:HG21	1.96	0.46
1:A:471:GLU:O	1:A:483:SER:HA	2.15	0.46
3:L:17:GLY:HA2	3:L:78:SER:HB3	1.98	0.46
1:A:260:LEU:HD12	1:A:260:LEU:HA	1.75	0.46
1:A:482:ILE:HD13	1:A:601:LYS:HZ3	1.80	0.46
1:A:371:SER:O	1:A:375:ASN:ND2	2.39	0.46
2:H:56:SER:OG	2:H:57:SER:N	2.49	0.46
1:A:36:LEU:HD23	1:A:39:ILE:HD12	1.97	0.46
1:A:348:GLN:O	1:A:351:SER:OG	2.31	0.46
2:H:48:LEU:HD12	3:L:99:PHE:CE2	2.51	0.45
1:A:399:LYS:HG3	1:A:400:PHE:CE2	2.52	0.45
1:A:107:GLY:HA2	1:A:180:LEU:HD23	1.98	0.45
5:H:301:Y01:OAG	5:H:301:Y01:HAR2	2.15	0.45
2:H:67:VAL:HB	2:H:71:PHE:HE1	1.81	0.45
1:A:610:ARG:HA	1:A:610:ARG:HD3	1.81	0.45
2:H:9:GLU:CD	2:H:125:GLY:HA2	2.41	0.45
2:H:89:LEU:HB2	2:H:130:VAL:HG21	1.97	0.45
3:L:39:GLN:O	3:L:85:ALA:HB1	2.17	0.45
2:H:42:GLN:HB2	2:H:48:LEU:HD22	1.99	0.44
1:A:460:ASN:ND2	1:A:486:LEU:O	2.49	0.44
1:A:76:GLY:O	1:A:80:VAL:HG23	2.18	0.44
1:A:49:LYS:O	1:A:52:ILE:HG22	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:127:LEU:HD12	2:H:127:LEU:H	1.83	0.44
2:H:9:GLU:OE2	2:H:126:THR:N	2.39	0.43
2:H:111:TRP:CH2	3:L:54:SER:HB2	2.54	0.43
1:A:58:ARG:NH1	1:A:118:MET:HE1	2.32	0.43
1:A:180:LEU:HD12	1:A:183:ILE:HD12	1.99	0.43
2:H:40:VAL:HG23	2:H:98:TYR:HB2	2.00	0.43
3:L:8:SER:HB2	3:L:9:PRO:HD3	1.99	0.43
1:A:211:ILE:O	1:A:215:ILE:HG12	2.19	0.43
3:L:7:GLN:NE2	3:L:102:GLY:H	2.16	0.43
1:A:224:PHE:HD1	1:A:224:PHE:HA	1.68	0.42
1:A:460:ASN:N	1:A:460:ASN:OD1	2.52	0.42
2:H:107:PRO:HG2	2:H:111:TRP:HZ3	1.84	0.42
1:A:594:LEU:HB3	1:A:624:VAL:HG11	2.01	0.42
3:L:20:VAL:O	3:L:75:THR:HA	2.19	0.42
2:H:109:TYR:OH	5:H:301:Y01:HAC3	2.18	0.42
1:A:218:ILE:O	1:A:221:ILE:HG12	2.20	0.42
3:L:22:ILE:HG23	3:L:103:THR:HG21	2.01	0.42
1:A:399:LYS:HG3	1:A:400:PHE:CZ	2.54	0.42
1:A:462:ASP:OD1	1:A:463:CYS:N	2.53	0.42
1:A:545:LEU:HD13	1:A:545:LEU:HA	1.86	0.41
1:A:608:GLY:O	1:A:609:THR:C	2.63	0.41
2:H:19:GLY:O	2:H:88:SER:N	2.35	0.41
1:A:378:LEU:O	1:A:383:ILE:HG12	2.20	0.41
1:A:605:ASN:C	1:A:607:CYS:H	2.28	0.41
2:H:15:VAL:O	2:H:130:VAL:HG13	2.20	0.41
2:H:61:THR:HB	2:H:63:TYR:CE1	2.55	0.41
1:A:196:ILE:HD13	1:A:196:ILE:HA	1.93	0.41
1:A:344:LEU:HD21	1:A:640:TYR:CZ	2.56	0.41
1:A:597:THR:O	1:A:597:THR:CG2	2.68	0.41
2:H:70:ARG:HH22	2:H:89:LEU:HA	1.86	0.41
2:H:119:ILE:HG22	2:H:122:TRP:HE1	1.86	0.41
1:A:247:ILE:HD12	1:A:253:ARG:NH1	2.37	0.40
1:A:354:GLY:HA3	1:A:591:PHE:CE2	2.56	0.40
1:A:279:LEU:HB3	1:A:280:PRO:HD3	2.04	0.40
1:A:591:PHE:O	1:A:595:ILE:HG12	2.22	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 PDB entries followed by that with respect to all EM entries.

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	438/691 (63%)	413 (94%)	25 (6%)	0	100	100
2	H	126/230 (55%)	110 (87%)	16 (13%)	0	100	100
3	L	105/215 (49%)	96 (91%)	9 (9%)	0	100	100
All	All	669/1136 (59%)	619 (92%)	50 (8%)	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 PDB entries followed by that with respect to all EM entries.

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	386/602 (64%)	365 (95%)	21 (5%)	20	47
2	H	102/191 (53%)	93 (91%)	9 (9%)	9	33
3	L	93/190 (49%)	87 (94%)	6 (6%)	15	43
All	All	581/983 (59%)	545 (94%)	36 (6%)	18	44

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ARG
1	A	95	LYS
1	A	189	VAL
1	A	224	PHE
1	A	244	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	250	THR
1	A	253	ARG
1	A	255	VAL
1	A	260	LEU
1	A	343	LEU
1	A	344	LEU
1	A	421	PHE
1	A	430	CYS
1	A	432	ASN
1	A	440	MET
1	A	482	ILE
1	A	600	ILE
1	A	603	SER
1	A	605	ASN
1	A	618	SER
1	A	629	SER
2	H	14	LEU
2	H	22	ARG
2	H	25	CYS
2	H	37	ILE
2	H	54	ILE
2	H	94	THR
2	H	96	VAL
2	H	111	TRP
2	H	114	ASP
3	L	20	VAL
3	L	23	THR
3	L	79	LEU
3	L	90	GLN
3	L	96	LEU
3	L	105	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	541	GLN
1	A	617	ASN
2	H	42	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 ⓘ

2 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	FY5	A	701	-	27,27,27	0.44	0	41,43,43	1.11	4 (9%)
5	Y01	H	301	-	38,38,38	0.46	0	57,57,57	0.49	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
4	FY5	A	701	-	-	0/5/45/45	0/4/4/4
5	Y01	H	301	-	-	4/19/77/77	0/4/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	FY5	C02-C07-C06	2.59	115.86	113.13
4	A	701	FY5	C12-C06-C07	2.07	115.52	112.08
4	A	701	FY5	C04-C05-C15	2.07	116.92	113.84
4	A	701	FY5	C09-C08-C07	-2.02	99.94	103.00

There are no chirality outliers.

All (4) torsion outliers are listed below:

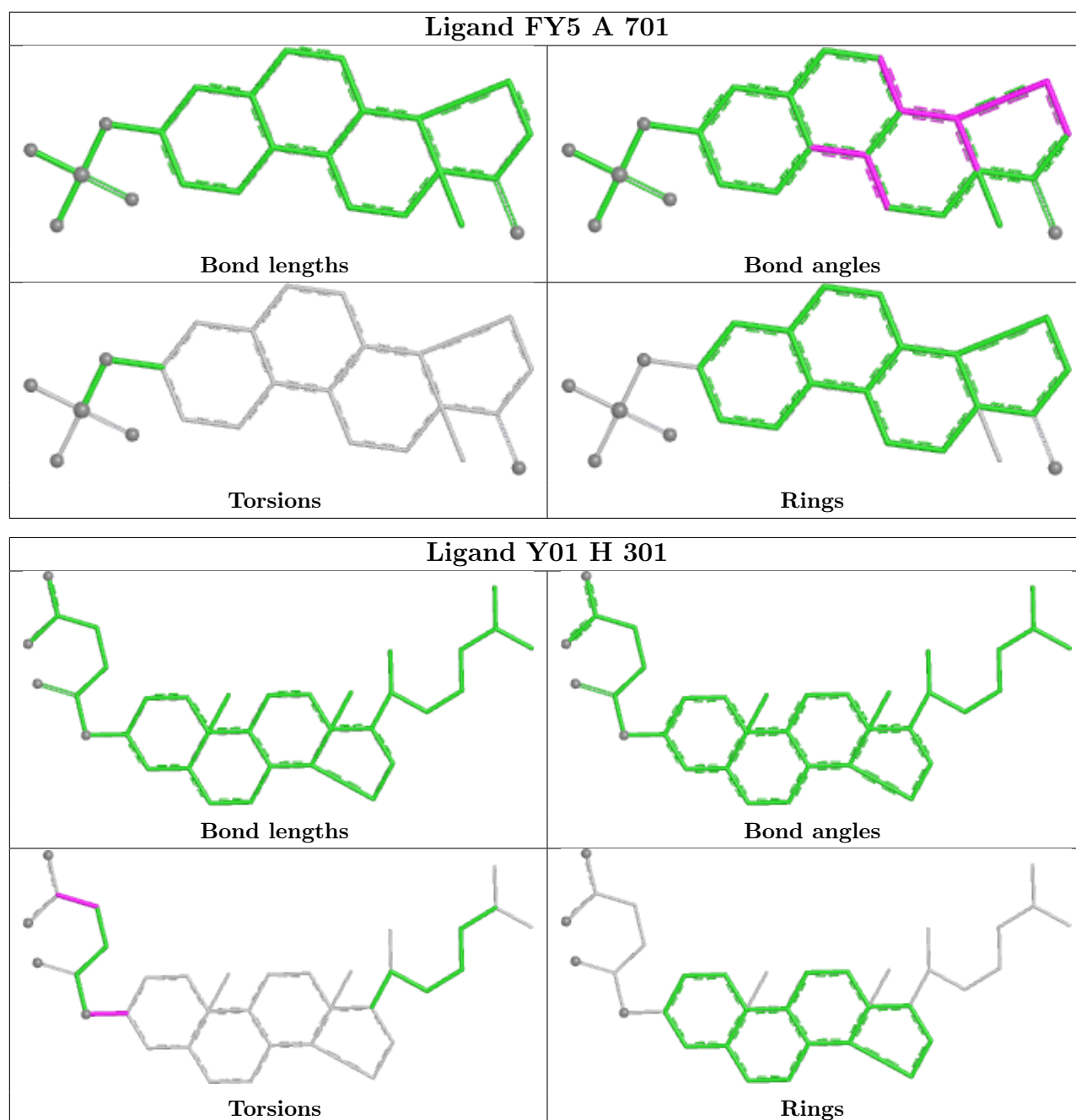
Mol	Chain	Res	Type	Atoms
5	H	301	Y01	CAR-CBC-OAW-CAY
5	H	301	Y01	CAV-CBC-OAW-CAY
5	H	301	Y01	CAM-CAL-CAX-OAH
5	H	301	Y01	CAM-CAL-CAX-OAF

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	301	Y01	11	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.