



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:48 AM UTC

PDB ID : 7Q0M / pdb_00007q0m
Title : Crystal structure of the peptide transporter YePEPT-K314A in complex with LZNV at 2.66 Å
Authors : Jeckelmann, J.M.; Stauffer, M.; Ilgue, H.; Fotiadis, D.
Deposited on : 2021-10-15
Resolution : 2.54 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

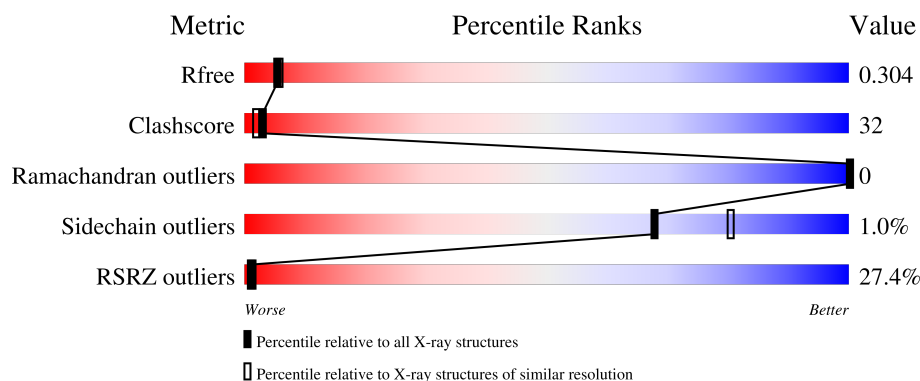
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	519	25% 54% 38% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3827 atoms, of which 71 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.

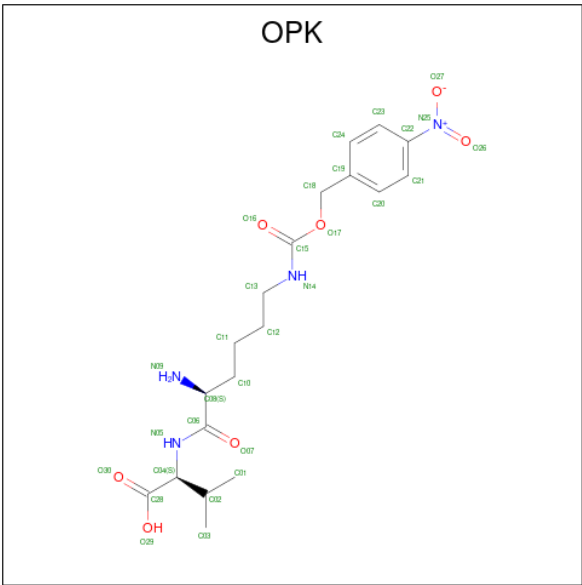
- Molecule 1 is a protein called Peptide transporter YePEPT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3692	2462	597	604	29			

There are 9 discrepancies between the modelled and reference sequences:

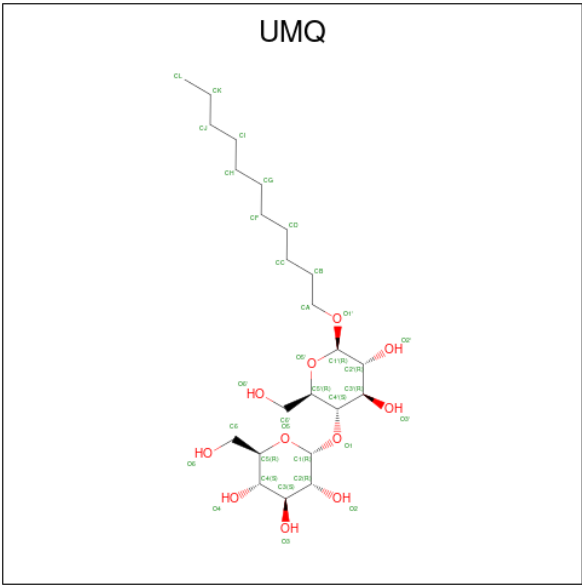
Chain	Residue	Modelled	Actual	Comment	Reference
A	314	ALA	LYS	engineered mutation	UNP A0A2R9TD79
A	512	LEU	-	expression tag	UNP A0A2R9TD79
A	513	GLU	-	expression tag	UNP A0A2R9TD79
A	514	LEU	-	expression tag	UNP A0A2R9TD79
A	515	GLU	-	expression tag	UNP A0A2R9TD79
A	516	VAL	-	expression tag	UNP A0A2R9TD79
A	517	LEU	-	expression tag	UNP A0A2R9TD79
A	518	PHE	-	expression tag	UNP A0A2R9TD79
A	519	GLN	-	expression tag	UNP A0A2R9TD79

- Molecule 2 is (2 {S})-2-[[2 {S})-2-azanyl-6-[(4-nitrophenyl)methoxycarbonylamino]hexanoyl]amino]-3-methyl-butanoic acid (CCD ID: OPK) (formula: C₁₉H₂₈N₄O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			57	19	27	4	7		

- Molecule 3 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: $C_{23}H_{44}O_{11}$).

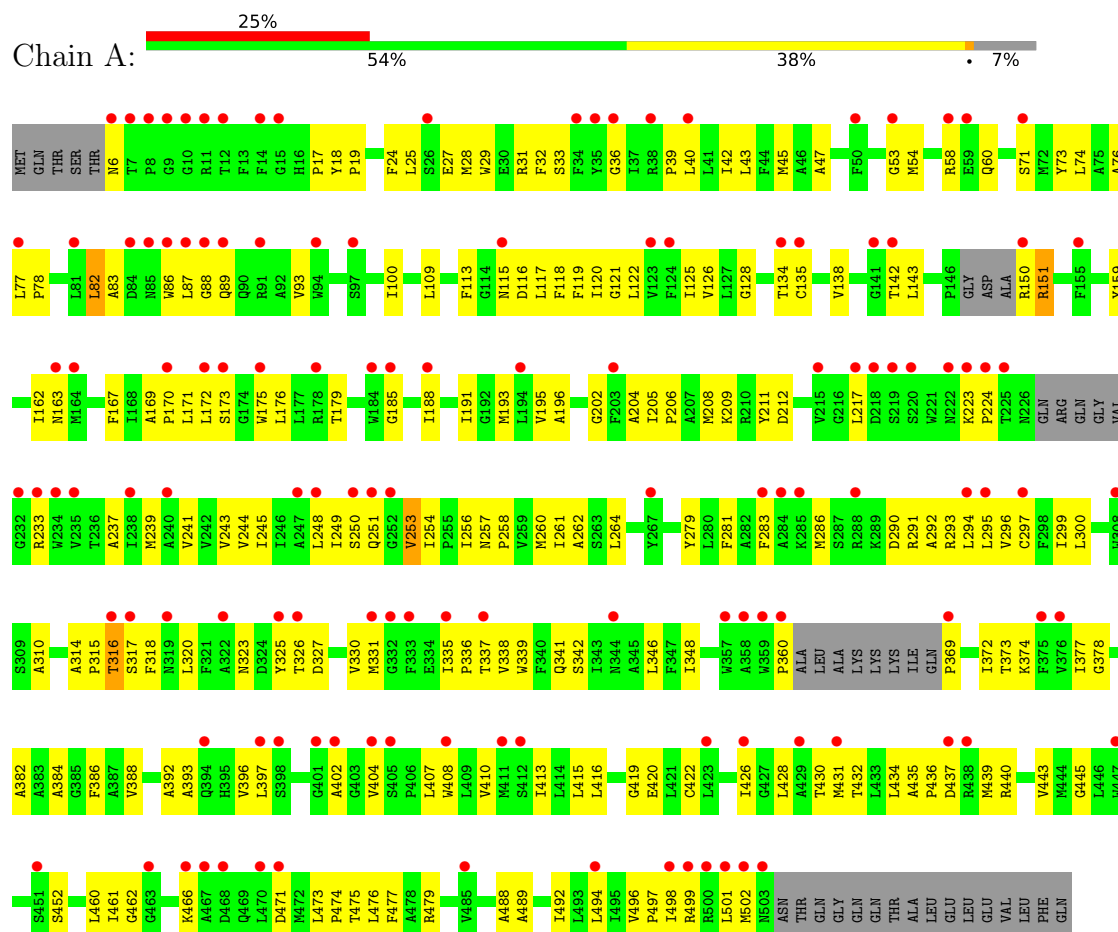


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	78	23	44	11	0	0

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: Peptide transporter YePEPT



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.40Å 100.37Å 103.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.96 – 2.54 24.96 – 2.54	Depositor EDS
% Data completeness (in resolution range)	79.7 (24.96-2.54) 74.3 (24.96-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.91 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.267 , 0.291 0.280 , 0.304	Depositor DCC
R_{free} test set	1227 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	74.2	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3827	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: OPK, UMQ

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	0.53	0/3793	0.82	4/5156 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	316	THR	N-CA-C	7.72	123.20	112.93
1	A	316	THR	CB-CA-C	-6.18	100.38	110.08
1	A	253	VAL	N-CA-CB	-5.37	107.23	111.64
1	A	24	PHE	CA-CB-CG	5.36	119.16	113.80

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	3692	0	3803	236	0
2	A	30	27	0	4	0
3	A	34	44	44	19	0
All	All	3756	71	3847	241	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 32.

All (241) 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:360:PRO:HB3	3:A:702:UMQ:O2	1.16	1.26
1:A:437:ASP:OD1	1:A:440:ARG:NH1	1.82	1.13
1:A:54:MET:HE1	1:A:119:PHE:CZ	1.90	1.05
1:A:374:LYS:NZ	3:A:702:UMQ:H6'2	1.73	1.01
1:A:83:ALA:HA	1:A:87:LEU:HB2	1.43	1.00
1:A:169:ALA:HB3	1:A:170:PRO:HD3	1.45	0.99
1:A:150:ARG:CD	1:A:151:ARG:HE	1.75	0.98
1:A:360:PRO:CB	3:A:702:UMQ:O2	2.12	0.93
1:A:374:LYS:HZ3	3:A:702:UMQ:H6'2	1.34	0.86
1:A:237:ALA:O	1:A:241:VAL:HG23	1.76	0.86
1:A:212:ASP:HB2	1:A:217:LEU:HD12	1.58	0.86
1:A:461:ILE:HG23	1:A:476:LEU:HD11	1.58	0.86
1:A:248:LEU:HD23	1:A:251:GLN:OE1	1.76	0.84
1:A:360:PRO:HB3	3:A:702:UMQ:HO21	1.41	0.83
1:A:47:ALA:HB3	1:A:53:GLY:HA3	1.60	0.82
1:A:150:ARG:CD	1:A:151:ARG:HH11	1.93	0.82
1:A:150:ARG:HD2	1:A:151:ARG:HH11	1.45	0.81
1:A:100:ILE:HG22	1:A:193:MET:HG2	1.64	0.79
1:A:40:LEU:HD23	1:A:338:VAL:HG11	1.63	0.79
1:A:58:ARG:HD2	1:A:466:LYS:HG2	1.66	0.78
1:A:150:ARG:HD2	1:A:151:ARG:HE	1.46	0.78
1:A:295:LEU:O	1:A:299:ILE:HG12	1.85	0.77
1:A:325:TYR:HB3	1:A:396:VAL:HG21	1.68	0.76
1:A:150:ARG:HD2	1:A:151:ARG:NH1	2.02	0.75
1:A:54:MET:HE1	1:A:119:PHE:HZ	1.50	0.74
1:A:396:VAL:HB	1:A:404:VAL:CG2	2.17	0.74
1:A:393:ALA:HB1	1:A:473:LEU:HD22	1.69	0.73
3:A:702:UMQ:O5	3:A:702:UMQ:O3'	2.05	0.73
1:A:382:ALA:HA	1:A:416:LEU:HD23	1.72	0.72
1:A:428:LEU:O	1:A:432:THR:HG23	1.90	0.71
1:A:150:ARG:CD	1:A:151:ARG:NE	2.53	0.71
1:A:416:LEU:HD12	2:A:701:OPK:C23	2.20	0.71
1:A:150:ARG:HD2	1:A:151:ARG:NE	2.04	0.71
1:A:256:ILE:HG23	1:A:261:ILE:CD1	2.21	0.70
1:A:118:PHE:CE1	1:A:122:LEU:HD11	2.26	0.70
1:A:249:ILE:HG22	1:A:254:ILE:HG13	1.74	0.70
1:A:310:ALA:HB1	1:A:386:PHE:CE1	2.28	0.69
1:A:499:ARG:HA	1:A:502:MET:HG2	1.75	0.69
1:A:54:MET:HE3	1:A:115:ASN:ND2	2.07	0.69
1:A:150:ARG:HG3	1:A:151:ARG:N	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ILE:O	1:A:253:VAL:N	2.23	0.68
1:A:256:ILE:HG23	1:A:261:ILE:HD11	1.75	0.68
1:A:372:ILE:HD11	1:A:498:ILE:HG21	1.76	0.68
1:A:316:THR:O	1:A:320:LEU:HG	1.94	0.68
1:A:314:ALA:HB2	2:A:701:OPK:C20	2.25	0.66
1:A:82:LEU:HD22	1:A:87:LEU:HG	1.77	0.66
1:A:109:LEU:HB2	1:A:117:LEU:HD23	1.76	0.66
3:A:702:UMQ:O2	3:A:702:UMQ:H4'1	1.94	0.65
1:A:205:ILE:O	1:A:209:LYS:HG3	1.97	0.65
1:A:169:ALA:HB3	1:A:170:PRO:CD	2.25	0.65
1:A:150:ARG:HG3	1:A:151:ARG:HG3	1.78	0.65
1:A:348:ILE:HD11	1:A:420:GLU:OE1	1.98	0.64
1:A:396:VAL:HG23	1:A:402:ALA:O	1.96	0.64
1:A:89:GLN:OE1	1:A:138:VAL:HB	1.98	0.64
1:A:396:VAL:HB	1:A:404:VAL:HG21	1.79	0.63
1:A:374:LYS:HZ3	3:A:702:UMQ:C6'	2.10	0.63
1:A:208:MET:HE3	1:A:217:LEU:HD13	1.80	0.62
1:A:54:MET:HE1	1:A:119:PHE:CE2	2.34	0.62
1:A:122:LEU:O	1:A:126:VAL:HG23	2.00	0.62
1:A:323:ASN:OD1	1:A:337:THR:HG21	2.00	0.62
1:A:374:LYS:NZ	3:A:702:UMQ:C6'	2.56	0.61
1:A:18:TYR:N	1:A:19:PRO:HD2	2.14	0.61
1:A:318:PHE:HE2	1:A:413:ILE:HD11	1.65	0.61
1:A:374:LYS:CD	3:A:702:UMQ:H6'2	2.30	0.61
1:A:150:ARG:HD2	1:A:151:ARG:CZ	2.31	0.61
1:A:150:ARG:HG3	1:A:151:ARG:H	1.65	0.60
1:A:100:ILE:HG13	1:A:128:GLY:HA3	1.82	0.60
1:A:54:MET:HE3	1:A:115:ASN:CG	2.26	0.60
1:A:293:ARG:HG2	1:A:501:LEU:HD21	1.82	0.60
1:A:60:GLN:OE1	1:A:258:PRO:HD2	2.02	0.60
1:A:416:LEU:HD12	2:A:701:OPK:C24	2.32	0.60
1:A:294:LEU:HD12	1:A:439:MET:SD	2.42	0.59
1:A:47:ALA:HB3	1:A:53:GLY:CA	2.33	0.58
1:A:374:LYS:CE	3:A:702:UMQ:H6'2	2.33	0.58
1:A:260:MET:O	1:A:264:LEU:HG	2.03	0.58
1:A:77:LEU:HD21	1:A:445:GLY:HA2	1.84	0.58
1:A:392:ALA:HB2	1:A:408:TRP:CD2	2.38	0.58
1:A:323:ASN:HA	1:A:337:THR:HG22	1.86	0.58
1:A:416:LEU:CD1	2:A:701:OPK:C23	2.83	0.57
1:A:473:LEU:HB3	1:A:474:PRO:HD3	1.86	0.57
1:A:150:ARG:CD	1:A:151:ARG:NH1	2.64	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:CD2	1:A:338:VAL:HG11	2.34	0.57
1:A:169:ALA:CB	1:A:170:PRO:HD3	2.29	0.57
1:A:323:ASN:HA	1:A:337:THR:CG2	2.34	0.56
1:A:211:TYR:CD2	1:A:217:LEU:HD21	2.39	0.56
1:A:473:LEU:HD21	1:A:477:PHE:CE2	2.40	0.56
1:A:374:LYS:HD3	3:A:702:UMQ:H6'2	1.85	0.56
1:A:175:TRP:HE3	1:A:176:LEU:HD12	1.69	0.56
1:A:32:PHE:CE1	1:A:169:ALA:HA	2.41	0.56
1:A:407:LEU:HD23	1:A:410:VAL:HG21	1.86	0.56
1:A:150:ARG:HH11	1:A:151:ARG:NH1	2.04	0.56
1:A:436:PRO:HD2	1:A:439:MET:SD	2.46	0.55
1:A:249:ILE:CG2	1:A:254:ILE:HG13	2.37	0.55
1:A:205:ILE:HG22	1:A:209:LYS:HE3	1.89	0.55
1:A:208:MET:O	1:A:217:LEU:CD1	2.55	0.55
1:A:116:ASP:O	1:A:120:ILE:HG13	2.08	0.54
1:A:473:LEU:HD21	1:A:477:PHE:HE2	1.72	0.54
1:A:360:PRO:HG3	3:A:702:UMQ:H31	1.90	0.54
1:A:378:GLY:HA2	1:A:419:GLY:HA2	1.89	0.54
1:A:426:ILE:HG13	1:A:430:THR:OG1	2.07	0.54
1:A:150:ARG:CG	1:A:151:ARG:HE	2.21	0.54
1:A:202:GLY:O	1:A:206:PRO:HG2	2.08	0.54
1:A:396:VAL:HB	1:A:404:VAL:HG23	1.90	0.53
1:A:73:TYR:HB2	1:A:452:SER:HB3	1.91	0.53
1:A:109:LEU:CB	1:A:117:LEU:HD23	2.39	0.53
1:A:297:CYS:SG	1:A:435:ALA:HA	2.48	0.53
1:A:83:ALA:O	1:A:88:GLY:N	2.39	0.53
1:A:40:LEU:HD11	1:A:173:SER:OG	2.09	0.53
1:A:317:SER:HB3	1:A:462:GLY:HA2	1.90	0.53
1:A:489:ALA:HA	1:A:492:ILE:HD12	1.89	0.53
1:A:330:VAL:HG12	1:A:331:MET:HG2	1.91	0.53
3:A:702:UMQ:HO21	3:A:702:UMQ:H4'1	1.72	0.53
1:A:29:TRP:HB2	1:A:196:ALA:HB2	1.91	0.52
1:A:150:ARG:HD3	1:A:151:ARG:HE	1.68	0.52
1:A:262:ALA:HB3	1:A:460:LEU:HD21	1.92	0.52
1:A:172:LEU:HG	1:A:188:ILE:HG12	1.92	0.52
1:A:292:ALA:O	1:A:296:VAL:HG23	2.09	0.52
1:A:18:TYR:N	1:A:19:PRO:CD	2.73	0.52
1:A:45:MET:HG2	1:A:54:MET:SD	2.50	0.52
3:A:702:UMQ:HO3'	3:A:702:UMQ:C5	2.23	0.51
1:A:436:PRO:HG2	1:A:439:MET:HG2	1.93	0.51
1:A:326:THR:HG22	1:A:327:ASP:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:VAL:N	1:A:497:PRO:HD2	2.26	0.51
1:A:19:PRO:HG2	1:A:143:LEU:CD2	2.41	0.51
1:A:83:ALA:CA	1:A:87:LEU:HB2	2.30	0.50
1:A:121:GLY:O	1:A:125:ILE:HG13	2.11	0.50
1:A:212:ASP:HB2	1:A:217:LEU:CD1	2.35	0.50
1:A:74:LEU:O	1:A:78:PRO:HD2	2.11	0.50
1:A:150:ARG:CG	1:A:151:ARG:H	2.25	0.50
1:A:17:PRO:C	1:A:19:PRO:HD2	2.36	0.50
1:A:372:ILE:CD1	1:A:498:ILE:HG21	2.41	0.50
1:A:25:LEU:HA	1:A:28:MET:HE2	1.93	0.49
1:A:281:PHE:CE1	1:A:291:ARG:HB3	2.47	0.49
1:A:323:ASN:CB	1:A:337:THR:HG21	2.42	0.49
1:A:431:MET:HG2	1:A:443:VAL:HG13	1.94	0.49
1:A:211:TYR:HD2	1:A:217:LEU:HD21	1.76	0.49
1:A:281:PHE:HE1	1:A:291:ARG:HB3	1.77	0.49
1:A:388:VAL:HG13	1:A:408:TRP:CE3	2.48	0.49
1:A:77:LEU:HD21	1:A:445:GLY:CA	2.43	0.49
1:A:241:VAL:O	1:A:244:VAL:HG22	2.12	0.49
1:A:33:SER:HB2	1:A:193:MET:HB2	1.93	0.49
1:A:150:ARG:CG	1:A:151:ARG:N	2.76	0.49
1:A:86:TRP:HZ2	1:A:233:ARG:HG3	1.78	0.49
1:A:223:LYS:HG3	1:A:224:PRO:HD2	1.95	0.48
1:A:488:ALA:O	1:A:492:ILE:HG13	2.13	0.48
1:A:150:ARG:NH1	1:A:151:ARG:HH11	2.11	0.48
1:A:47:ALA:CB	1:A:53:GLY:HA3	2.39	0.48
1:A:257:ASN:O	1:A:261:ILE:HG13	2.13	0.48
1:A:440:ARG:HA	1:A:443:VAL:HG23	1.94	0.48
1:A:296:VAL:HG11	1:A:434:LEU:HD13	1.95	0.48
1:A:393:ALA:O	1:A:396:VAL:HG12	2.12	0.48
1:A:36:GLY:HA2	1:A:169:ALA:HB1	1.94	0.48
1:A:374:LYS:HZ2	3:A:702:UMQ:H6'2	1.70	0.48
1:A:397:LEU:CD1	1:A:471:ASP:HA	2.44	0.48
3:A:702:UMQ:O6	3:A:702:UMQ:O4	2.23	0.48
1:A:32:PHE:O	1:A:36:GLY:N	2.46	0.47
1:A:78:PRO:O	1:A:82:LEU:HB2	2.15	0.47
1:A:336:PRO:HD2	1:A:339:TRP:CD2	2.49	0.47
1:A:185:GLY:O	1:A:188:ILE:HG22	2.14	0.47
1:A:204:ALA:O	1:A:208:MET:HG2	2.13	0.47
1:A:27:GLU:OE1	1:A:27:GLU:HA	2.14	0.47
1:A:256:ILE:HG23	1:A:261:ILE:HD12	1.94	0.47
1:A:245:ILE:O	1:A:249:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:HB3	1:A:431:MET:HE2	1.97	0.46
1:A:45:MET:HA	1:A:54:MET:HB2	1.96	0.46
1:A:159:TYR:OH	1:A:420:GLU:OE2	2.32	0.46
1:A:248:LEU:HD23	1:A:251:GLN:CD	2.41	0.46
1:A:250:SER:HB3	1:A:256:ILE:CD1	2.44	0.46
1:A:318:PHE:CE2	1:A:413:ILE:HD11	2.47	0.46
1:A:39:PRO:HB3	1:A:341:GLN:HG3	1.98	0.46
1:A:316:THR:O	1:A:320:LEU:CG	2.63	0.46
1:A:393:ALA:CB	1:A:473:LEU:HD22	2.43	0.46
1:A:249:ILE:HG23	1:A:253:VAL:HB	1.97	0.46
1:A:374:LYS:HD3	3:A:702:UMQ:C6'	2.45	0.46
1:A:150:ARG:HH11	1:A:151:ARG:HH11	1.61	0.46
1:A:286:MET:HB3	1:A:290:ASP:CB	2.46	0.46
1:A:71:SER:OG	1:A:126:VAL:HG11	2.16	0.46
1:A:208:MET:O	1:A:217:LEU:HD11	2.15	0.46
1:A:208:MET:O	1:A:217:LEU:HD12	2.16	0.46
1:A:286:MET:HB3	1:A:290:ASP:HB3	1.97	0.46
1:A:293:ARG:HB3	1:A:434:LEU:O	2.15	0.46
1:A:29:TRP:CB	1:A:196:ALA:HB2	2.45	0.46
1:A:241:VAL:HA	1:A:244:VAL:HG22	1.98	0.46
1:A:475:THR:HG22	1:A:479:ARG:HD2	1.98	0.46
1:A:31:ARG:HG3	1:A:162:ILE:HG12	1.97	0.45
1:A:83:ALA:HA	1:A:87:LEU:CB	2.29	0.45
1:A:314:ALA:HB3	1:A:315:PRO:HD3	1.98	0.45
1:A:382:ALA:HA	1:A:416:LEU:CD2	2.44	0.45
1:A:314:ALA:N	1:A:315:PRO:HD2	2.31	0.45
1:A:113:PHE:HB2	1:A:117:LEU:HD22	1.97	0.45
1:A:167:PHE:CE1	1:A:346:LEU:HB2	2.52	0.45
1:A:76:ALA:HB1	1:A:134:THR:HG21	1.99	0.45
1:A:77:LEU:HB2	1:A:78:PRO:CD	2.47	0.45
1:A:250:SER:HB3	1:A:256:ILE:HD11	1.97	0.45
1:A:392:ALA:HB2	1:A:408:TRP:CG	2.52	0.45
1:A:396:VAL:HG22	1:A:396:VAL:O	2.17	0.45
1:A:159:TYR:O	1:A:162:ILE:HB	2.17	0.44
1:A:249:ILE:CG2	1:A:253:VAL:HB	2.48	0.44
1:A:384:ALA:CB	1:A:415:LEU:HD13	2.47	0.44
1:A:150:ARG:NH1	1:A:151:ARG:NH1	2.66	0.44
1:A:175:TRP:CE2	1:A:179:THR:HG21	2.53	0.44
1:A:279:TYR:HA	1:A:283:PHE:HD2	1.82	0.44
1:A:223:LYS:CG	1:A:224:PRO:HD2	2.48	0.43
1:A:300:LEU:CB	1:A:431:MET:HE2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLN:OE1	1:A:135:CYS:HA	2.18	0.43
1:A:191:ILE:O	1:A:195:VAL:HG23	2.18	0.43
1:A:407:LEU:HD23	1:A:407:LEU:HA	1.83	0.43
1:A:36:GLY:CA	1:A:169:ALA:HB1	2.49	0.43
1:A:76:ALA:HB1	1:A:134:THR:CG2	2.49	0.43
1:A:43:LEU:O	1:A:47:ALA:HB2	2.19	0.43
1:A:473:LEU:O	1:A:476:LEU:HB3	2.19	0.43
1:A:393:ALA:HA	1:A:396:VAL:HG12	2.01	0.43
1:A:19:PRO:HB2	1:A:208:MET:SD	2.58	0.43
1:A:170:PRO:HB2	1:A:342:SER:OG	2.19	0.43
1:A:89:GLN:O	1:A:93:VAL:HG23	2.18	0.42
1:A:392:ALA:HB2	1:A:408:TRP:CE3	2.54	0.42
1:A:82:LEU:HD23	1:A:86:TRP:HB3	2.01	0.42
1:A:42:ILE:HG23	1:A:43:LEU:N	2.34	0.42
1:A:244:VAL:HG23	1:A:245:ILE:N	2.35	0.42
1:A:373:THR:O	1:A:377:ILE:HG13	2.20	0.42
1:A:397:LEU:HD12	1:A:471:ASP:HA	2.00	0.42
1:A:422:CYS:SG	3:A:702:UMQ:HC1	2.60	0.42
1:A:489:ALA:O	1:A:492:ILE:HB	2.19	0.42
1:A:431:MET:HE3	1:A:431:MET:HB2	1.71	0.41
1:A:171:LEU:HA	1:A:339:TRP:CD1	2.55	0.41
1:A:239:MET:O	1:A:243:VAL:HG23	2.20	0.41
1:A:314:ALA:HB3	1:A:315:PRO:CD	2.49	0.41
1:A:19:PRO:HG2	1:A:143:LEU:HD21	2.01	0.41
1:A:138:VAL:O	1:A:142:THR:HG23	2.20	0.41
1:A:19:PRO:HG2	1:A:143:LEU:HD22	2.02	0.41
1:A:83:ALA:C	1:A:88:GLY:H	2.26	0.41
1:A:369:PRO:HB2	1:A:374:LYS:HE3	2.03	0.41
1:A:473:LEU:HD23	1:A:473:LEU:C	2.46	0.41
1:A:118:PHE:HE1	1:A:122:LEU:HD11	1.78	0.41
1:A:330:VAL:HG21	1:A:335:ILE:HD11	2.03	0.41
1:A:431:MET:O	1:A:435:ALA:HB2	2.21	0.41
1:A:323:ASN:HA	1:A:337:THR:HG21	2.04	0.40
1:A:494:LEU:O	1:A:498:ILE:HG13	2.21	0.40
1:A:29:TRP:O	1:A:32:PHE:HB3	2.22	0.40
1:A:33:SER:CB	1:A:193:MET:HB2	2.51	0.40
1:A:314:ALA:HA	1:A:318:PHE:HB3	2.04	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	474/519 (91%)	465 (98%)	9 (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	382/412 (93%)	378 (99%)	4 (1%)	68	80

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

Mol	Chain	Res	Type
1	A	6	ASN
1	A	82	LEU
1	A	151	ARG
1	A	163	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	90	GLN
1	A	341	GLN
1	A	464	HIS

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	$\# Z > 2$
2	OPK	A	701	-	30,30,30	2.04	6 (20%)	37,39,39	2.35	13 (35%)
3	UMQ	A	702	-	35,35,35	0.66	0	46,46,46	0.83	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	OPK	A	701	-	-	11/31/33/33	0/1/1/1
3	UMQ	A	702	-	-	13/20/60/60	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	OPK	C04-C28	4.69	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	OPK	O17-C15	4.44	1.44	1.35
2	A	701	OPK	C04-N05	4.34	1.54	1.45
2	A	701	OPK	C15-N14	3.37	1.41	1.34
2	A	701	OPK	C06-N05	2.41	1.39	1.34
2	A	701	OPK	C01-C02	2.24	1.60	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	OPK	O17-C15-N14	8.31	124.32	110.62
2	A	701	OPK	O17-C15-O16	-4.32	115.98	124.26
2	A	701	OPK	C18-O17-C15	4.24	125.47	115.93
2	A	701	OPK	O16-C15-N14	-3.48	119.69	124.93
2	A	701	OPK	C08-C06-N05	3.43	120.85	116.21
2	A	701	OPK	C18-C19-C20	2.91	127.36	120.64
2	A	701	OPK	C01-C02-C04	2.69	118.54	111.16
2	A	701	OPK	C21-C22-N25	2.56	121.58	119.34
2	A	701	OPK	C02-C04-C28	2.45	116.42	111.04
2	A	701	OPK	O17-C18-C19	2.37	115.14	109.40
2	A	701	OPK	C04-N05-C06	2.16	127.25	121.90
2	A	701	OPK	C12-C13-N14	2.12	118.13	112.20
2	A	701	OPK	C10-C08-C06	2.03	114.90	110.76

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	OPK	C06-C08-C10-C11
2	A	701	OPK	N09-C08-C10-C11
2	A	701	OPK	O16-C15-N14-C13
2	A	701	OPK	O17-C15-N14-C13
2	A	701	OPK	N14-C15-O17-C18
2	A	701	OPK	O16-C15-O17-C18
3	A	702	UMQ	C2-C1-O1-C4'
3	A	702	UMQ	O5'-C1'-O1'-CA
3	A	702	UMQ	O1'-CA-CB-CC
3	A	702	UMQ	O5-C5-C6-O6
3	A	702	UMQ	C2'-C1'-O1'-CA
3	A	702	UMQ	O5'-C5'-C6'-O6'
3	A	702	UMQ	CF-CG-CH-CI
3	A	702	UMQ	CA-CB-CC-CD
3	A	702	UMQ	CG-CH-CI-CJ

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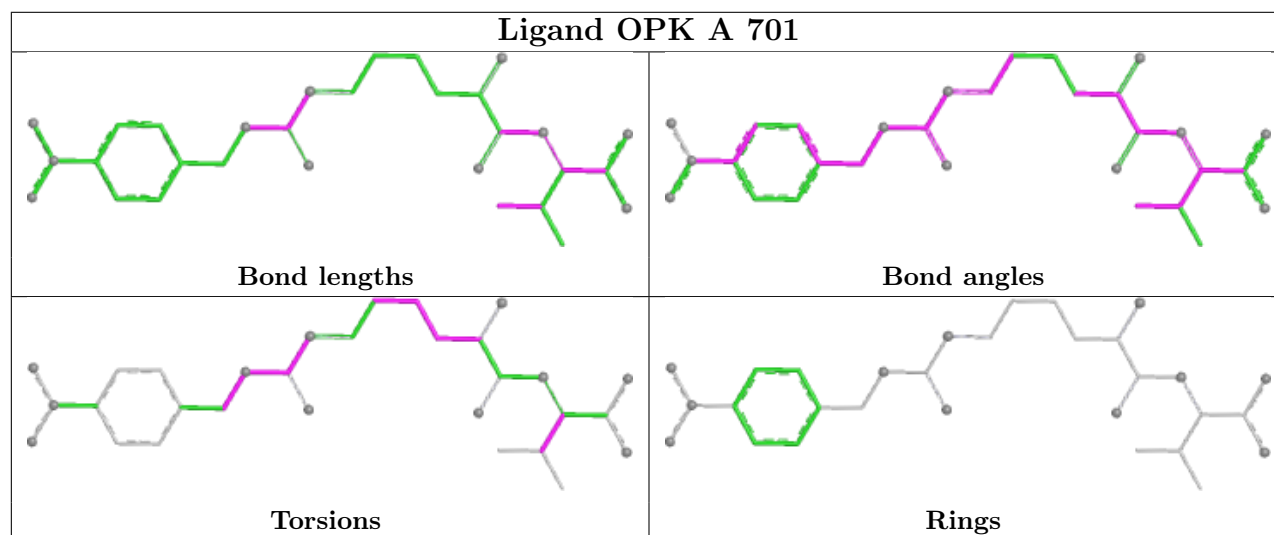
Mol	Chain	Res	Type	Atoms
2	A	701	OPK	C08-C10-C11-C12
2	A	701	OPK	C10-C11-C12-C13
3	A	702	UMQ	C5'-C4'-O1-C1
3	A	702	UMQ	C3'-C4'-O1-C1
2	A	701	OPK	C01-C02-C04-N05
2	A	701	OPK	C03-C02-C04-N05
2	A	701	OPK	C19-C18-O17-C15
3	A	702	UMQ	O5-C1-O1-C4'
3	A	702	UMQ	CD-CF-CG-CH

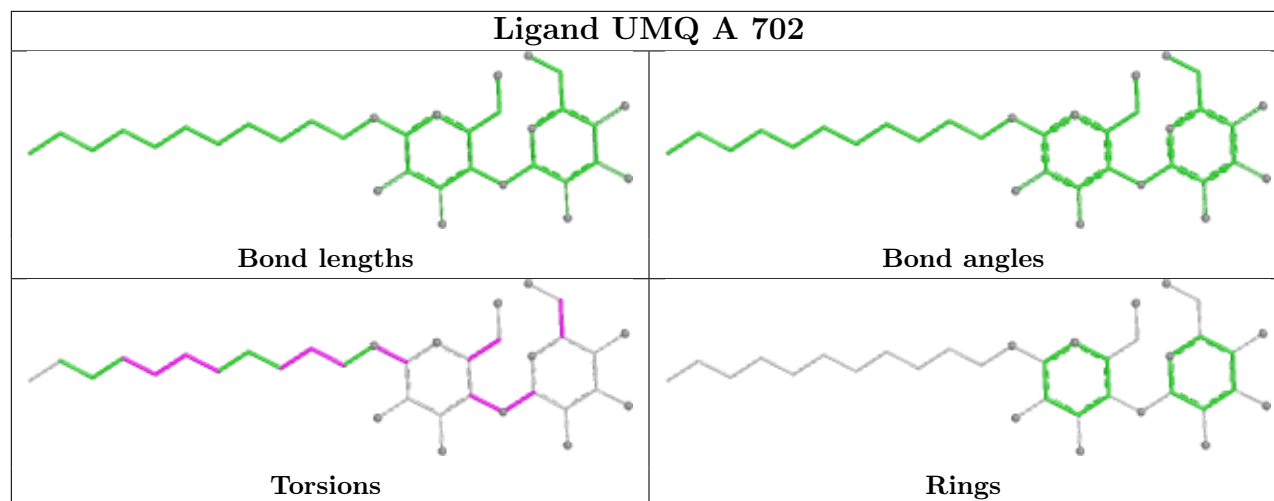
There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	OPK	4	0
3	A	702	UMQ	19	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	482/519 (92%)	1.44	132 (27%) 1 1	56, 88, 144, 216	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	VAL	6.3
1	A	225	THR	6.1
1	A	325	TYR	6.0
1	A	234	TRP	5.7
1	A	10	GLY	5.7
1	A	85	ASN	5.6
1	A	86	TRP	5.5
1	A	220	SER	5.4
1	A	333	PHE	5.3
1	A	332	GLY	5.2
1	A	218	ASP	5.1
1	A	8	PRO	4.8
1	A	172	LEU	4.7
1	A	217	LEU	4.7
1	A	224	PRO	4.7
1	A	219	SER	4.6
1	A	357	TRP	4.6
1	A	247	ALA	4.5
1	A	423	LEU	4.4
1	A	97	SER	4.3
1	A	81	LEU	4.2
1	A	502	MET	4.1
1	A	284	ALA	4.1
1	A	223	LYS	4.0
1	A	9	GLY	4.0
1	A	471	ASP	3.9
1	A	397	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	402	ALA	3.8
1	A	50	PHE	3.8
1	A	251	GLN	3.8
1	A	285	LYS	3.7
1	A	447	TRP	3.7
1	A	398	SER	3.7
1	A	501	LEU	3.6
1	A	503	ASN	3.6
1	A	359	TRP	3.6
1	A	87	LEU	3.6
1	A	500	ARG	3.6
1	A	15	GLY	3.6
1	A	248	LEU	3.5
1	A	14	PHE	3.5
1	A	468	ASP	3.5
1	A	203	PHE	3.5
1	A	12	THR	3.4
1	A	404	VAL	3.3
1	A	185	GLY	3.3
1	A	84	ASP	3.3
1	A	222	ASN	3.3
1	A	141	GLY	3.3
1	A	250	SER	3.2
1	A	175	TRP	3.2
1	A	466	LYS	3.2
1	A	337	THR	3.2
1	A	360	PRO	3.2
1	A	163	ASN	3.2
1	A	467	ALA	3.1
1	A	295	LEU	3.1
1	A	408	TRP	3.1
1	A	71	SER	3.1
1	A	88	GLY	3.0
1	A	188	ILE	3.0
1	A	426	ILE	2.9
1	A	411	MET	2.9
1	A	53	GLY	2.9
1	A	35	TYR	2.9
1	A	7	THR	2.8
1	A	232	GLY	2.8
1	A	401	GLY	2.8
1	A	238	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	498	ILE	2.7
1	A	405	SER	2.7
1	A	451	SER	2.7
1	A	369	PRO	2.7
1	A	438	ARG	2.7
1	A	240	ALA	2.7
1	A	437	ASP	2.6
1	A	319	ASN	2.6
1	A	331	MET	2.6
1	A	6	ASN	2.6
1	A	34	PHE	2.6
1	A	40	LEU	2.6
1	A	494	LEU	2.6
1	A	344	ASN	2.6
1	A	115	ASN	2.6
1	A	173	SER	2.6
1	A	499	ARG	2.5
1	A	184	TRP	2.5
1	A	124	PHE	2.5
1	A	215	VAL	2.5
1	A	150	ARG	2.5
1	A	142	THR	2.5
1	A	11	ARG	2.5
1	A	164	MET	2.5
1	A	470	LEU	2.4
1	A	89	GLN	2.4
1	A	283	PHE	2.4
1	A	77	LEU	2.4
1	A	252	GLY	2.4
1	A	394	GLN	2.4
1	A	91	ARG	2.3
1	A	412	SER	2.3
1	A	59	GLU	2.3
1	A	358	ALA	2.3
1	A	233	ARG	2.3
1	A	288	ARG	2.3
1	A	94	TRP	2.3
1	A	322	ALA	2.2
1	A	463	GLY	2.2
1	A	155	PHE	2.2
1	A	58	ARG	2.2
1	A	326	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	38	ARG	2.2
1	A	485	VAL	2.2
1	A	431	MET	2.2
1	A	194	LEU	2.2
1	A	317	SER	2.1
1	A	375	PHE	2.1
1	A	335	ILE	2.1
1	A	178	ARG	2.1
1	A	135	CYS	2.1
1	A	134	THR	2.1
1	A	316	THR	2.1
1	A	170	PRO	2.1
1	A	376	VAL	2.1
1	A	36	GLY	2.1
1	A	26	SER	2.1
1	A	297	CYS	2.1
1	A	308	TRP	2.0
1	A	267	TYR	2.0
1	A	123	VAL	2.0
1	A	294	LEU	2.0
1	A	429	ALA	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](#)

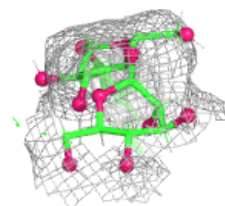
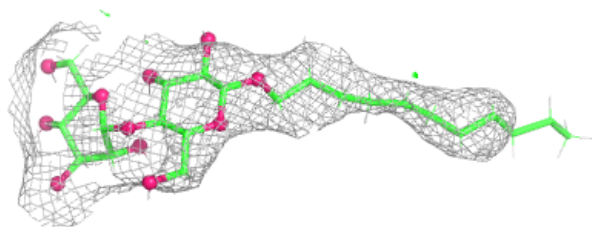
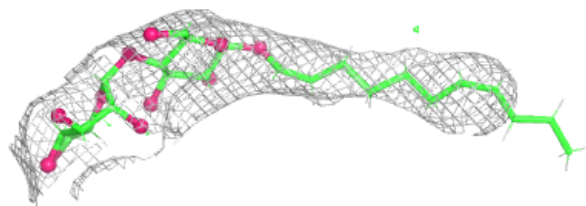
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	UMQ	A	702	34/34	0.67	0.16	105,136,162,167	0
2	OPK	A	701	30/30	0.81	0.21	83,110,143,148	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.

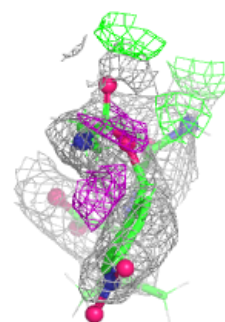
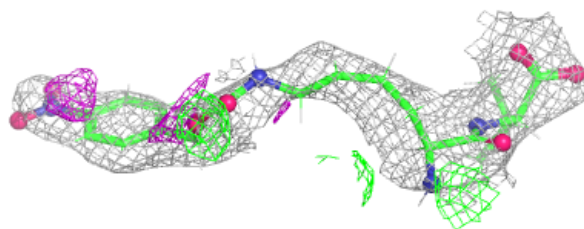
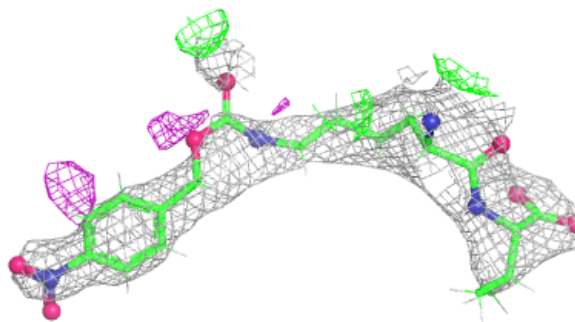
Electron density around UMQ A 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OPK A 701:

$2mF_o-DF_c$ (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.