



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:14 AM UTC

PDB ID : 7RRY / pdb_00007rry
Title : Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with DMERI-20
Authors : Min, J.; Nwachukwu, J.C.; Min, C.K.; Njeri, J.W.; Srinivasan, S.; Rangarajan, E.S.; Nettles, C.C.; Yan, S.; Houtman, R.; Griffin, P.R.; Izard, T.; Katzenellenbogen, B.S.; Katzenellenbogen, J.A.; Nettles, K.W.
Deposited on : 2021-08-10
Resolution : 1.87 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](#) ①) 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

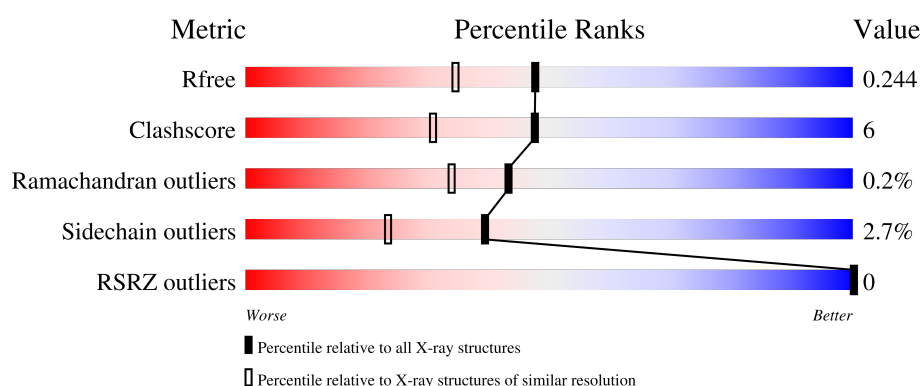
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	257	 81% 10% 9%
1	B	257	 75% 10% 14%
1	C	257	 77% 11% 12%
1	D	257	 71% 9% 19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7470 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.

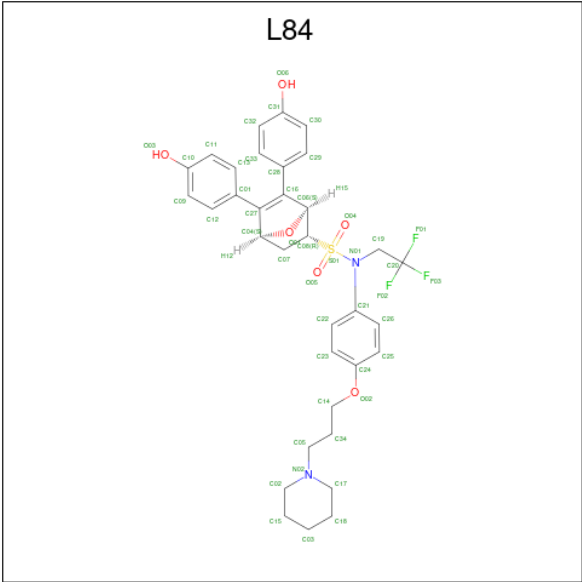
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	2	0
			1843	1176	321	329	17			
1	B	221	Total	C	N	O	S	0	2	0
			1758	1128	304	310	16			
1	C	227	Total	C	N	O	S	0	4	0
			1834	1173	321	323	17			
1	D	209	Total	C	N	O	S	0	0	0
			1639	1050	280	293	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	SER	LEU	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	UNP P03372
B	372	SER	LEU	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372
C	372	SER	LEU	engineered mutation	UNP P03372
C	536	SER	LEU	engineered mutation	UNP P03372
D	372	SER	LEU	engineered mutation	UNP P03372
D	536	SER	LEU	engineered mutation	UNP P03372

- Molecule 2 is (1S,2R,4S,5S,6S)-5,6-bis(4-hydroxyphenyl)-N-{4-[3-(piperidin-1-yl)propoxy]phenyl}-N-(2,2,2-trifluoroethyl)-7-oxabicyclo[2.2.1]heptane-2-sulfonamide (CCD ID: L84) (formula: C₃₄H₃₇F₃N₂O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			46	34	3	2	6	1		
2	B	1	Total	C	F	N	O	S	0	0
			37	26	3	1	6	1		
2	C	1	Total	C	F	N	O	S	0	0
			46	34	3	2	6	1		
2	D	1	Total	C	F	N	O	S	0	0
			46	34	3	2	6	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	B	55	Total	O	0	0
			55	55		
4	C	65	Total	O	0	0
			65	65		

Continued on next page...

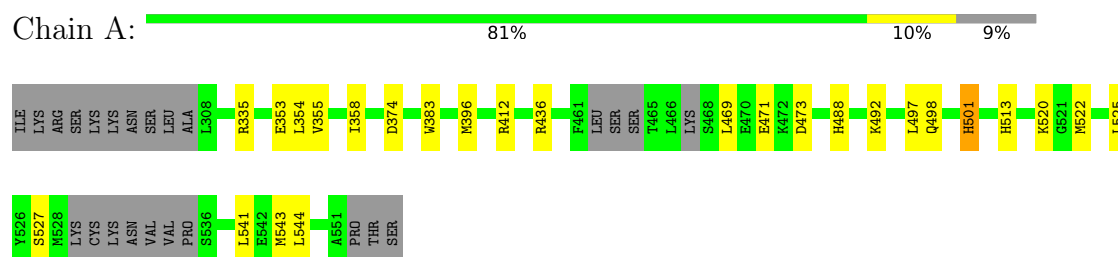
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	45	Total	O	0	0
			45	45		

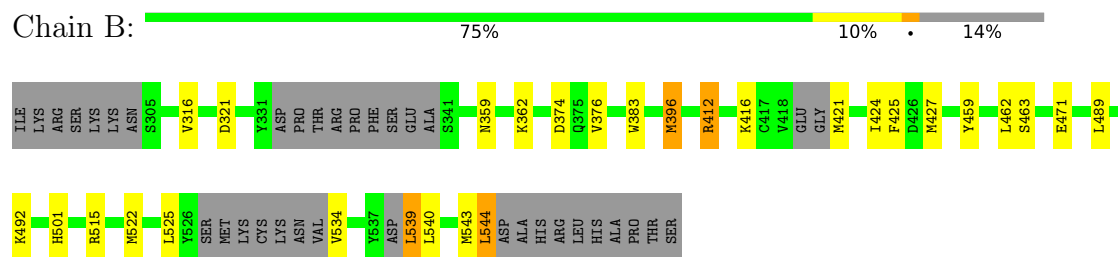
3 Residue-property plots

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.

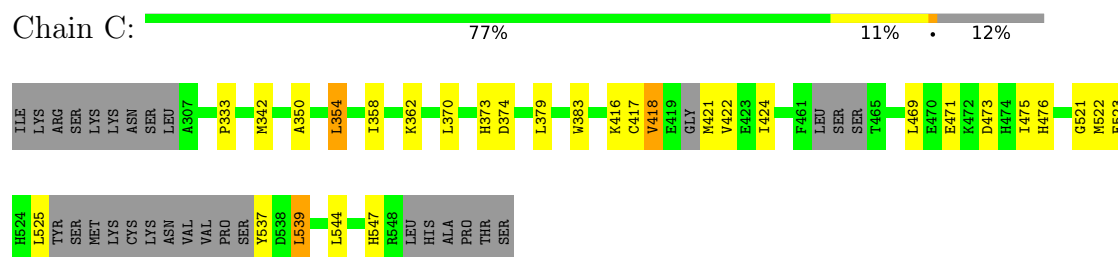
• Molecule 1: Estrogen receptor



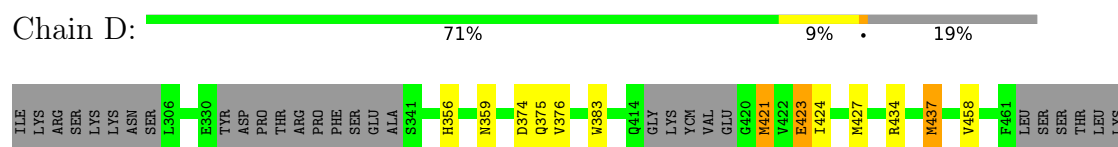
• Molecule 1: Estrogen receptor



• Molecule 1: Estrogen receptor



• Molecule 1: Estrogen receptor



S468	E471	H476	Q498	H501	H516	K520	G521	M522	E523	H524	I525	Y526	SER	MET	LYS	CYS	LYS	ASN	VAL	VAL	P535	D538	L539	L540	LEU	E542	M543	L544	ASP	ALA	HIS	ARG	LEU	HIS	ALA	PRO	THR	SER
------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	-----	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.42Å 59.12Å 93.52Å 86.54° 74.98° 63.19°	Depositor
Resolution (Å)	90.13 – 1.87 90.13 – 1.87	Depositor EDS
% Data completeness (in resolution range)	76.0 (90.13-1.87) 76.4 (90.13-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.207 , 0.236 0.218 , 0.244	Depositor DCC
R_{free} test set	3095 reflections (3.61%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.109 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7470	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.16% 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: YCM, L84, CL

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	1.06	0/1854	1.40	3/2502 (0.1%)
1	B	1.05	0/1770	1.38	8/2385 (0.3%)
1	C	1.05	0/1846	1.38	1/2490 (0.0%)
1	D	1.08	0/1652	1.35	2/2227 (0.1%)
All	All	1.06	0/7122	1.38	14/9604 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	SER	N-CA-C	-10.71	99.57	111.14
1	B	425	PHE	CA-CB-CG	-7.16	106.64	113.80
1	B	359	ASN	CA-CB-CG	-5.69	106.91	112.60
1	D	458	VAL	N-CA-C	5.60	118.05	111.05
1	B	463	SER	N-CA-C	5.51	117.64	110.43
1	D	359	ASN	CA-CB-CG	-5.45	107.15	112.60
1	B	462	LEU	N-CA-C	5.41	116.98	111.14
1	A	412	ARG	N-CA-C	5.34	117.79	111.33
1	B	321	ASP	CA-CB-CG	-5.31	107.29	112.60
1	B	396	MET	N-CA-C	5.28	117.72	111.33
1	C	476	HIS	CB-CA-C	5.23	119.48	110.79
1	A	335	ARG	N-CA-C	-5.13	102.39	110.14
1	B	534	VAL	CA-C-N	5.05	126.15	119.84
1	B	534	VAL	C-N-CA	5.05	126.15	119.84

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	1843	0	1833	21	0
1	B	1758	0	1780	19	0
1	C	1834	0	1831	30	0
1	D	1639	0	1657	19	0
2	A	46	0	0	1	0
2	B	37	0	0	0	0
2	C	46	0	0	0	0
2	D	46	0	0	2	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	54	0	0	2	0
4	B	55	0	0	0	0
4	C	65	0	0	1	0
4	D	45	0	0	1	0
All	All	7470	0	7101	80	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 6.

All (80) 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:C:539:LEU:H	1:C:539:LEU:HD12	1.23	1.04
1:D:374:ASP:OD2	1:D:471:GLU:OE1	1.78	1.01
1:A:501[A]:HIS:NE2	1:B:501:HIS:HE1	1.65	0.94
1:C:539:LEU:H	1:C:539:LEU:CD1	1.93	0.82
1:A:501[A]:HIS:CD2	1:B:501:HIS:CE1	2.69	0.80
1:A:488:HIS:ND1	4:A:701:HOH:O	2.15	0.80
1:D:427:MET:HE1	1:D:516:HIS:CD2	2.20	0.76
1:A:501[A]:HIS:CD2	1:B:501:HIS:HE1	2.03	0.76
1:C:333:PRO:HD2	4:C:739:HOH:O	1.91	0.71
1:A:497:LEU:O	1:A:501[A]:HIS:CD2	2.43	0.70
1:D:421:MET:SD	2:D:601:L84:O04	2.49	0.70
1:A:354:LEU:O	1:A:358:ILE:HD13	1.91	0.70
1:B:412:ARG:HG3	1:B:412:ARG:NH1	2.08	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ARG:HG3	1:B:412:ARG:HH11	1.60	0.67
1:A:396:MET:O	1:A:436:ARG:HD3	1.95	0.66
1:A:501[A]:HIS:NE2	1:B:501:HIS:CE1	2.56	0.65
1:C:539:LEU:HD12	1:C:539:LEU:N	2.05	0.64
1:B:412:ARG:HH11	1:B:412:ARG:CG	2.12	0.63
1:B:376:VAL:CG2	1:B:544:LEU:HD23	2.30	0.61
1:C:418:VAL:O	1:C:421:MET:HB3	2.02	0.58
1:A:525:LEU:C	1:A:525:LEU:HD13	2.30	0.57
1:A:541:LEU:HD21	1:C:373:HIS:CG	2.40	0.57
1:D:376:VAL:HG13	1:D:540:LEU:HB2	1.87	0.57
1:C:525:LEU:C	1:C:525:LEU:HD13	2.29	0.56
1:D:356:HIS:HD2	4:D:743:HOH:O	1.88	0.56
1:D:423:GLU:CD	1:D:524:HIS:HE1	2.14	0.55
1:C:537:TYR:C	1:C:537:TYR:CD1	2.85	0.55
1:D:421:MET:SD	2:D:601:L84:C19	2.96	0.54
1:C:416:LYS:HG2	1:C:422:VAL:HG21	1.90	0.53
1:B:376:VAL:HG22	1:B:544:LEU:HD23	1.92	0.52
1:C:416:LYS:C	1:C:418:VAL:H	2.17	0.51
1:C:370:LEU:HD11	1:C:475:ILE:HD11	1.92	0.51
1:A:520:LYS:NZ	4:A:704:HOH:O	2.43	0.50
1:B:376:VAL:HG23	1:B:544:LEU:HD23	1.93	0.50
1:D:375:GLN:HB3	1:D:544:LEU:HD11	1.94	0.50
1:A:374:ASP:OD2	1:A:471:GLU:OE1	2.30	0.50
1:C:342:MET:HE3	1:C:421:MET:SD	2.52	0.50
1:A:541:LEU:CD2	1:C:373:HIS:ND1	2.76	0.49
1:C:374:ASP:OD2	1:C:471:GLU:OE2	2.31	0.49
1:D:427:MET:HE1	1:D:516:HIS:HD2	1.72	0.48
1:A:541:LEU:HD23	1:C:373:HIS:CE1	2.49	0.48
1:C:416:LYS:C	1:C:418:VAL:N	2.70	0.48
1:B:374:ASP:OD2	1:B:471:GLU:OE1	2.32	0.47
1:C:383:TRP:CZ2	1:C:522:MET:HE1	2.50	0.46
1:C:350:ALA:O	1:C:354:LEU:HD23	2.16	0.46
1:C:539:LEU:CD1	1:C:539:LEU:N	2.71	0.46
1:D:538:ASP:O	1:D:542:GLU:CB	2.63	0.46
1:B:515[B]:ARG:HA	1:B:515[B]:ARG:HD3	1.74	0.45
1:D:476:HIS:CD2	1:D:476:HIS:C	2.94	0.45
1:A:501[A]:HIS:CD2	1:A:501[A]:HIS:N	2.85	0.45
1:C:358:ILE:CD1	1:C:379:LEU:HD13	2.46	0.45
1:D:434:ARG:HD2	1:D:437:MET:HE3	1.98	0.45
1:B:424:ILE:HD13	1:B:427:MET:CE	2.48	0.44
1:A:383:TRP:CZ2	1:A:522:MET:HE1	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:TRP:CZ2	1:B:522:MET:HE1	2.53	0.44
1:C:537:TYR:CD1	1:C:537:TYR:O	2.70	0.44
1:C:537:TYR:O	1:C:537:TYR:CG	2.71	0.44
1:D:423:GLU:OE2	1:D:520:LYS:HE3	2.17	0.44
1:B:376:VAL:HG13	1:B:540:LEU:HB2	1.99	0.43
1:B:539:LEU:CD1	1:B:543:MET:SD	3.07	0.43
1:D:535:PRO:HB3	1:D:539:LEU:HD23	2.01	0.43
1:B:525:LEU:C	1:B:525:LEU:HD13	2.44	0.43
1:D:383:TRP:CZ2	1:D:522:MET:HE1	2.54	0.43
1:D:427:MET:CE	1:D:516:HIS:HD2	2.32	0.43
1:D:423:GLU:HG3	1:D:424:ILE:N	2.34	0.43
1:B:316:VAL:HG21	1:B:489:LEU:HD21	2.01	0.42
1:A:355:VAL:HG22	1:A:543:MET:HE3	2.01	0.42
1:C:416:LYS:HA	1:C:422:VAL:CG2	2.50	0.42
1:C:362:LYS:HG3	1:C:547:HIS:CE1	2.55	0.41
1:D:539:LEU:HD12	1:D:539:LEU:O	2.20	0.41
1:C:424:ILE:HD13	1:C:521:GLY:HA2	2.02	0.41
1:A:513:HIS:HB2	1:B:459:TYR:CD2	2.55	0.41
1:C:350:ALA:O	1:C:354:LEU:CD2	2.69	0.41
1:C:475:ILE:HD13	1:C:475:ILE:HA	1.92	0.41
1:C:523:GLU:HA	1:C:523:GLU:OE1	2.20	0.41
1:A:353:GLU:OE1	2:A:601:L84:O03	2.39	0.40
1:A:541:LEU:HD21	1:C:373:HIS:ND1	2.36	0.40
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.56	0.40
1:A:498:GLN:HA	1:A:501[B]:HIS:CE1	2.57	0.40
1:C:418:VAL:O	1:C:421:MET:CB	2.68	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	225/257 (88%)	223 (99%)	2 (1%)	0	100	100
1	B	211/257 (82%)	209 (99%)	1 (0%)	1 (0%)	24	13
1	C	221/257 (86%)	218 (99%)	2 (1%)	1 (0%)	24	13
1	D	196/257 (76%)	195 (100%)	1 (0%)	0	100	100
All	All	853/1028 (83%)	845 (99%)	6 (1%)	2 (0%)	43	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	416	LYS
1	C	418	VAL

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	196/230 (85%)	190 (97%)	6 (3%)	35	18
1	B	191/230 (83%)	184 (96%)	7 (4%)	30	14
1	C	195/230 (85%)	190 (97%)	5 (3%)	40	24
1	D	178/230 (77%)	175 (98%)	3 (2%)	53	40
All	All	760/920 (83%)	739 (97%)	21 (3%)	39	22

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	469	LEU
1	A	473	ASP
1	A	492	LYS
1	A	501[A]	HIS
1	A	501[B]	HIS
1	A	544	LEU
1	B	362	LYS
1	B	396	MET
1	B	412	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	421	MET
1	B	492	LYS
1	B	539	LEU
1	B	544	LEU
1	C	354	LEU
1	C	469	LEU
1	C	473	ASP
1	C	539	LEU
1	C	544	LEU
1	D	421	MET
1	D	423	GLU
1	D	437	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	474	HIS
1	A	488	HIS
1	A	513	HIS
1	A	519	ASN
1	B	398	HIS
1	B	488	HIS
1	B	501	HIS
1	B	513	HIS
1	B	516	HIS
1	B	519	ASN
1	C	398	HIS
1	C	455	ASN
1	C	474	HIS
1	C	519	ASN
1	C	547	HIS
1	D	356	HIS
1	D	398	HIS
1	D	476	HIS
1	D	488	HIS
1	D	513	HIS
1	D	516	HIS
1	D	519	ASN
1	D	524	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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$
1	YCM	A	417	1	7,9,10	0.47	0	5,10,12	0.65	0
1	YCM	D	381	1	7,9,10	0.41	0	5,10,12	0.39	0
1	YCM	C	417	1	7,9,10	1.21	1 (14%)	5,10,12	1.62	2 (40%)
1	YCM	C	381	1	7,9,10	0.48	0	5,10,12	0.52	0
1	YCM	A	381	1	7,9,10	0.51	0	5,10,12	0.50	0
1	YCM	B	381	1	7,9,10	0.50	0	5,10,12	0.43	0
1	YCM	B	417	1	3,4,10	0.96	0	2,4,12	1.42	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
1	YCM	A	417	1	-	4/6/8/10	-
1	YCM	D	381	1	-	1/6/8/10	-
1	YCM	C	417	1	-	4/6/8/10	-
1	YCM	C	381	1	-	1/6/8/10	-
1	YCM	A	381	1	-	1/6/8/10	-
1	YCM	B	381	1	-	1/6/8/10	-
1	YCM	B	417	1	-	0/1/2/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	417	YCM	CD-SG	-2.28	1.75	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	417	YCM	CE-CD-SG	-2.30	106.56	113.81
1	C	417	YCM	CB-CA-C	-2.15	104.97	110.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	381	YCM	SG-CD-CE-NZ2
1	A	417	YCM	CE-CD-SG-CB
1	A	417	YCM	SG-CD-CE-OZ1
1	A	417	YCM	SG-CD-CE-NZ2
1	B	381	YCM	SG-CD-CE-NZ2
1	C	381	YCM	SG-CD-CE-NZ2
1	C	417	YCM	CA-CB-SG-CD
1	C	417	YCM	CE-CD-SG-CB
1	C	417	YCM	SG-CD-CE-OZ1
1	C	417	YCM	SG-CD-CE-NZ2
1	D	381	YCM	SG-CD-CE-NZ2
1	A	417	YCM	CA-CB-SG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	L84	C	601	-	49,51,51	2.54	18 (36%)	65,75,75	2.95	33 (50%)
2	L84	A	601	-	49,51,51	2.42	14 (28%)	65,75,75	2.61	20 (30%)
2	L84	D	601	-	49,51,51	2.45	17 (34%)	65,75,75	2.47	20 (30%)
2	L84	B	601	-	39,41,51	2.95	18 (46%)	53,63,75	2.93	21 (39%)

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	L84	C	601	-	-	17/34/68/68	0/7/6/6
2	L84	A	601	-	-	13/34/68/68	0/7/6/6
2	L84	D	601	-	-	9/34/68/68	0/7/6/6
2	L84	B	601	-	-	6/27/53/68	0/6/5/6

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	L84	C21-N01	-9.16	1.31	1.44
2	D	601	L84	C21-N01	-8.98	1.32	1.44
2	C	601	L84	C21-N01	-8.68	1.32	1.44
2	A	601	L84	C21-N01	-8.37	1.32	1.44
2	B	601	L84	C28-C16	-6.87	1.35	1.48
2	C	601	L84	C28-C16	-6.74	1.35	1.48
2	B	601	L84	C01-C27	-6.62	1.36	1.48
2	B	601	L84	O04-S01	6.36	1.48	1.43
2	D	601	L84	C01-C27	-6.25	1.36	1.48
2	A	601	L84	C28-C16	-6.01	1.37	1.48
2	D	601	L84	C28-C16	-5.94	1.37	1.48
2	C	601	L84	O04-S01	5.88	1.48	1.43
2	A	601	L84	O04-S01	5.64	1.48	1.43
2	A	601	L84	C01-C27	-5.50	1.38	1.48
2	C	601	L84	C01-C27	-5.48	1.38	1.48
2	D	601	L84	O04-S01	4.46	1.47	1.43
2	C	601	L84	O05-S01	3.51	1.46	1.43
2	A	601	L84	O05-S01	3.42	1.46	1.43
2	A	601	L84	S01-N01	3.41	1.74	1.67
2	B	601	L84	O05-S01	3.29	1.46	1.43
2	D	601	L84	O05-S01	3.20	1.46	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	L84	S01-N01	3.12	1.73	1.67
2	B	601	L84	C33-C28	-3.05	1.34	1.39
2	C	601	L84	C33-C28	-2.96	1.34	1.39
2	D	601	L84	S01-N01	2.96	1.73	1.67
2	B	601	L84	C11-C13	-2.92	1.34	1.38
2	B	601	L84	C29-C28	-2.84	1.35	1.39
2	B	601	L84	C30-C29	-2.77	1.34	1.38
2	B	601	L84	O01-C06	-2.76	1.40	1.43
2	A	601	L84	C04-C27	2.74	1.55	1.52
2	C	601	L84	C30-C29	-2.74	1.34	1.38
2	D	601	L84	C11-C10	-2.68	1.34	1.39
2	B	601	L84	C33-C32	-2.66	1.34	1.38
2	C	601	L84	C06-C16	2.63	1.53	1.50
2	D	601	L84	C29-C28	-2.62	1.35	1.39
2	A	601	L84	C06-C16	2.61	1.53	1.50
2	C	601	L84	O01-C06	-2.59	1.40	1.43
2	D	601	L84	C11-C13	-2.55	1.34	1.38
2	B	601	L84	C32-C31	-2.52	1.34	1.39
2	C	601	L84	C09-C10	-2.51	1.34	1.39
2	A	601	L84	C33-C32	-2.49	1.34	1.38
2	C	601	L84	C33-C32	-2.45	1.34	1.38
2	A	601	L84	C30-C29	-2.43	1.34	1.38
2	A	601	L84	C33-C28	-2.40	1.35	1.39
2	C	601	L84	C30-C31	-2.39	1.34	1.39
2	D	601	L84	C33-C28	-2.37	1.35	1.39
2	B	601	L84	C25-C24	-2.35	1.34	1.39
2	C	601	L84	C11-C13	-2.33	1.35	1.38
2	C	601	L84	C04-C27	2.32	1.55	1.52
2	C	601	L84	C13-C01	-2.31	1.35	1.39
2	D	601	L84	C32-C31	-2.30	1.34	1.39
2	D	601	L84	O01-C04	-2.29	1.39	1.44
2	B	601	L84	C12-C01	-2.28	1.36	1.39
2	A	601	L84	C30-C31	-2.25	1.34	1.39
2	D	601	L84	O01-C06	-2.24	1.40	1.43
2	C	601	L84	C29-C28	-2.24	1.36	1.39
2	D	601	L84	C25-C26	-2.22	1.35	1.38
2	B	601	L84	C09-C10	-2.21	1.34	1.39
2	A	601	L84	C09-C10	-2.19	1.34	1.39
2	D	601	L84	C30-C29	-2.19	1.35	1.38
2	B	601	L84	C11-C10	-2.17	1.34	1.39
2	A	601	L84	C11-C13	-2.15	1.35	1.38
2	D	601	L84	C13-C01	-2.13	1.36	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	L84	C25-C26	-2.12	1.35	1.38
2	B	601	L84	S01-N01	2.12	1.71	1.67
2	D	601	L84	C30-C31	-2.11	1.35	1.39
2	C	601	L84	C25-C24	-2.07	1.34	1.38

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	L84	C20-C19-N01	14.09	125.83	112.14
2	A	601	L84	C20-C19-N01	12.10	123.89	112.14
2	B	601	L84	C20-C19-N01	10.32	122.17	112.14
2	D	601	L84	C20-C19-N01	9.30	121.18	112.14
2	B	601	L84	O05-S01-N01	-8.05	97.78	107.39
2	C	601	L84	O05-S01-N01	-7.60	98.31	107.39
2	D	601	L84	O04-S01-C08	7.14	116.49	107.79
2	B	601	L84	O04-S01-N01	-6.99	99.04	107.39
2	A	601	L84	O05-S01-N01	-6.22	99.96	107.39
2	C	601	L84	C26-C21-N01	6.16	129.13	120.15
2	B	601	L84	O04-S01-C08	6.13	115.25	107.79
2	A	601	L84	C26-C21-N01	5.63	128.36	120.15
2	D	601	L84	O05-S01-N01	-5.53	100.78	107.39
2	B	601	L84	C19-N01-C21	5.14	124.37	117.63
2	D	601	L84	C25-C24-C23	-4.71	113.28	120.16
2	A	601	L84	O04-S01-C08	4.68	113.50	107.79
2	C	601	L84	C25-C24-C23	-4.61	113.44	120.16
2	D	601	L84	O04-S01-N01	-4.55	101.95	107.39
2	D	601	L84	C26-C21-N01	4.39	126.55	120.15
2	C	601	L84	O04-S01-C08	4.34	113.07	107.79
2	A	601	L84	C25-C24-C23	-4.18	114.07	120.16
2	C	601	L84	C26-C21-C22	-3.91	111.71	119.18
2	B	601	L84	O05-S01-C08	3.89	112.53	107.79
2	B	601	L84	C26-C21-N01	3.86	125.77	120.15
2	B	601	L84	C04-C07-C08	-3.82	97.24	100.61
2	A	601	L84	C26-C21-C22	-3.79	111.96	119.18
2	D	601	L84	C04-C07-C08	-3.76	97.29	100.61
2	D	601	L84	C26-C21-C22	-3.71	112.10	119.18
2	C	601	L84	C12-C01-C13	-3.66	113.91	118.57
2	C	601	L84	O01-C04-C27	3.62	107.03	101.99
2	A	601	L84	C26-C25-C24	3.62	123.86	119.73
2	C	601	L84	C04-C07-C08	-3.58	97.45	100.61
2	A	601	L84	C12-C01-C13	-3.57	114.03	118.57
2	D	601	L84	C26-C25-C24	3.53	123.76	119.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	L84	C26-C25-C24	3.50	123.73	119.73
2	A	601	L84	C23-C22-C21	3.49	124.72	120.30
2	B	601	L84	C26-C21-C22	-3.31	112.86	119.18
2	B	601	L84	C25-C26-C21	3.27	124.44	120.30
2	C	601	L84	C23-C22-C21	3.19	124.34	120.30
2	A	601	L84	C33-C28-C29	-3.10	114.62	118.57
2	C	601	L84	O05-S01-O04	3.04	121.47	119.17
2	B	601	L84	C25-C24-C23	-3.04	114.93	119.77
2	C	601	L84	O05-S01-C08	3.03	111.48	107.79
2	D	601	L84	C25-C26-C21	2.98	124.08	120.30
2	C	601	L84	C25-C26-C21	2.98	124.08	120.30
2	A	601	L84	C11-C13-C01	2.97	123.97	120.80
2	C	601	L84	O04-S01-N01	-2.94	103.88	107.39
2	C	601	L84	F03-C20-C19	2.90	117.51	112.04
2	D	601	L84	C23-C22-C21	2.87	123.93	120.30
2	D	601	L84	C33-C28-C16	2.81	124.55	120.91
2	B	601	L84	C12-C01-C13	-2.79	115.02	118.57
2	A	601	L84	C04-C07-C08	-2.74	98.19	100.61
2	D	601	L84	C22-C23-C24	2.71	122.82	119.73
2	D	601	L84	C33-C28-C29	-2.71	115.13	118.57
2	A	601	L84	C30-C29-C28	2.68	123.66	120.80
2	A	601	L84	C33-C28-C16	2.66	124.35	120.91
2	D	601	L84	C12-C01-C13	-2.64	115.20	118.57
2	B	601	L84	C22-C23-C24	2.64	122.67	119.88
2	C	601	L84	C33-C28-C29	-2.64	115.22	118.57
2	A	601	L84	C25-C26-C21	2.63	123.64	120.30
2	C	601	L84	C22-C23-C24	2.57	122.66	119.73
2	D	601	L84	C19-N01-C21	2.54	120.96	117.63
2	A	601	L84	O01-C04-C27	2.52	105.50	101.99
2	D	601	L84	C12-C01-C27	2.49	124.14	120.91
2	C	601	L84	C01-C27-C16	2.48	135.23	128.81
2	A	601	L84	O01-C04-C07	-2.44	99.97	104.73
2	C	601	L84	C09-C12-C01	2.40	123.36	120.80
2	A	601	L84	C28-C16-C27	2.34	134.87	128.81
2	B	601	L84	C01-C27-C16	2.33	134.85	128.81
2	C	601	L84	C14-O02-C24	-2.32	111.89	117.93
2	D	601	L84	C28-C16-C27	2.26	134.65	128.81
2	B	601	L84	C11-C13-C01	2.23	123.18	120.80
2	B	601	L84	C12-C01-C27	2.23	123.80	120.91
2	C	601	L84	C02-N02-C17	2.23	113.64	108.84
2	C	601	L84	C33-C28-C16	2.21	123.77	120.91
2	D	601	L84	O01-C04-C07	-2.20	100.42	104.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	L84	C12-C01-C27	2.20	123.76	120.91
2	B	601	L84	C12-C09-C10	2.20	122.20	119.88
2	B	601	L84	C33-C28-C29	-2.19	115.78	118.57
2	C	601	L84	C11-C13-C01	2.18	123.13	120.80
2	A	601	L84	C13-C01-C27	2.14	123.68	120.91
2	B	601	L84	C26-C25-C24	2.14	122.14	119.88
2	C	601	L84	C15-C02-N02	2.13	114.61	111.30
2	C	601	L84	C04-C27-C16	-2.11	102.53	106.97
2	B	601	L84	C32-C33-C28	2.11	123.06	120.80
2	C	601	L84	C32-C33-C28	2.09	123.03	120.80
2	C	601	L84	C28-C16-C27	2.08	134.20	128.81
2	B	601	L84	C23-C22-C21	2.08	122.94	120.30
2	C	601	L84	O01-C04-C07	-2.06	100.71	104.73
2	C	601	L84	C11-C10-C09	-2.06	116.49	119.77
2	D	601	L84	C11-C13-C01	2.05	122.99	120.80
2	C	601	L84	C30-C29-C28	2.05	122.99	120.80
2	A	601	L84	C15-C02-N02	2.01	114.41	111.30
2	C	601	L84	C13-C11-C10	2.00	122.00	119.88

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	L84	C20-C19-N01-C21
2	A	601	L84	C20-C19-N01-S01
2	A	601	L84	C21-N01-S01-O05
2	A	601	L84	C19-N01-S01-O04
2	A	601	L84	C19-N01-S01-O05
2	B	601	L84	C20-C19-N01-C21
2	B	601	L84	C21-N01-S01-O05
2	B	601	L84	C19-N01-S01-O04
2	B	601	L84	C19-N01-S01-O05
2	C	601	L84	N02-C05-C34-C14
2	C	601	L84	C20-C19-N01-C21
2	C	601	L84	C20-C19-N01-S01
2	C	601	L84	C21-N01-S01-O05
2	C	601	L84	C19-N01-S01-O04
2	C	601	L84	C19-N01-S01-O05
2	D	601	L84	C21-N01-S01-O05
2	D	601	L84	C19-N01-S01-O04
2	D	601	L84	C19-N01-S01-O05
2	C	601	L84	C34-C05-N02-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	601	L84	O02-C14-C34-C05
2	D	601	L84	C26-C21-N01-S01
2	A	601	L84	O02-C14-C34-C05
2	C	601	L84	C34-C05-N02-C02
2	A	601	L84	N01-C19-C20-F01
2	A	601	L84	N01-C19-C20-F02
2	A	601	L84	N01-C19-C20-F03
2	C	601	L84	N01-C19-C20-F01
2	D	601	L84	N01-C19-C20-F02
2	D	601	L84	N01-C19-C20-F03
2	A	601	L84	C26-C21-N01-S01
2	A	601	L84	C19-N01-S01-C08
2	B	601	L84	C19-N01-S01-C08
2	C	601	L84	C19-N01-S01-C08
2	D	601	L84	C19-N01-S01-C08
2	C	601	L84	C26-C21-N01-S01
2	A	601	L84	N02-C05-C34-C14
2	C	601	L84	N01-C19-C20-F02
2	D	601	L84	N01-C19-C20-F01
2	C	601	L84	N01-C19-C20-F03
2	B	601	L84	C20-C19-N01-S01
2	C	601	L84	C06-C16-C28-C29
2	C	601	L84	C06-C16-C28-C33
2	C	601	L84	C06-C08-S01-O05
2	C	601	L84	C07-C08-S01-O05
2	A	601	L84	C34-C05-N02-C02

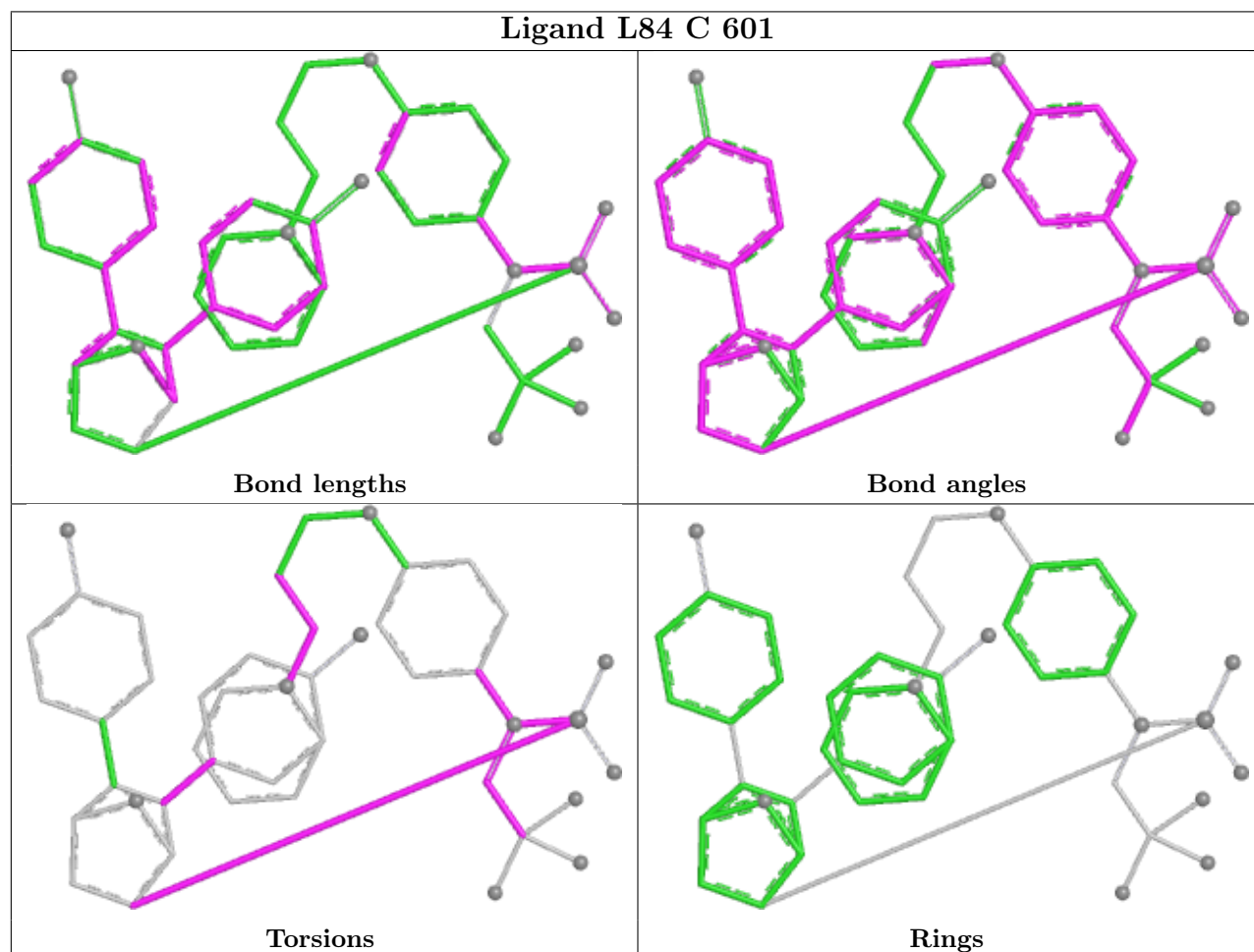
There are no ring outliers.

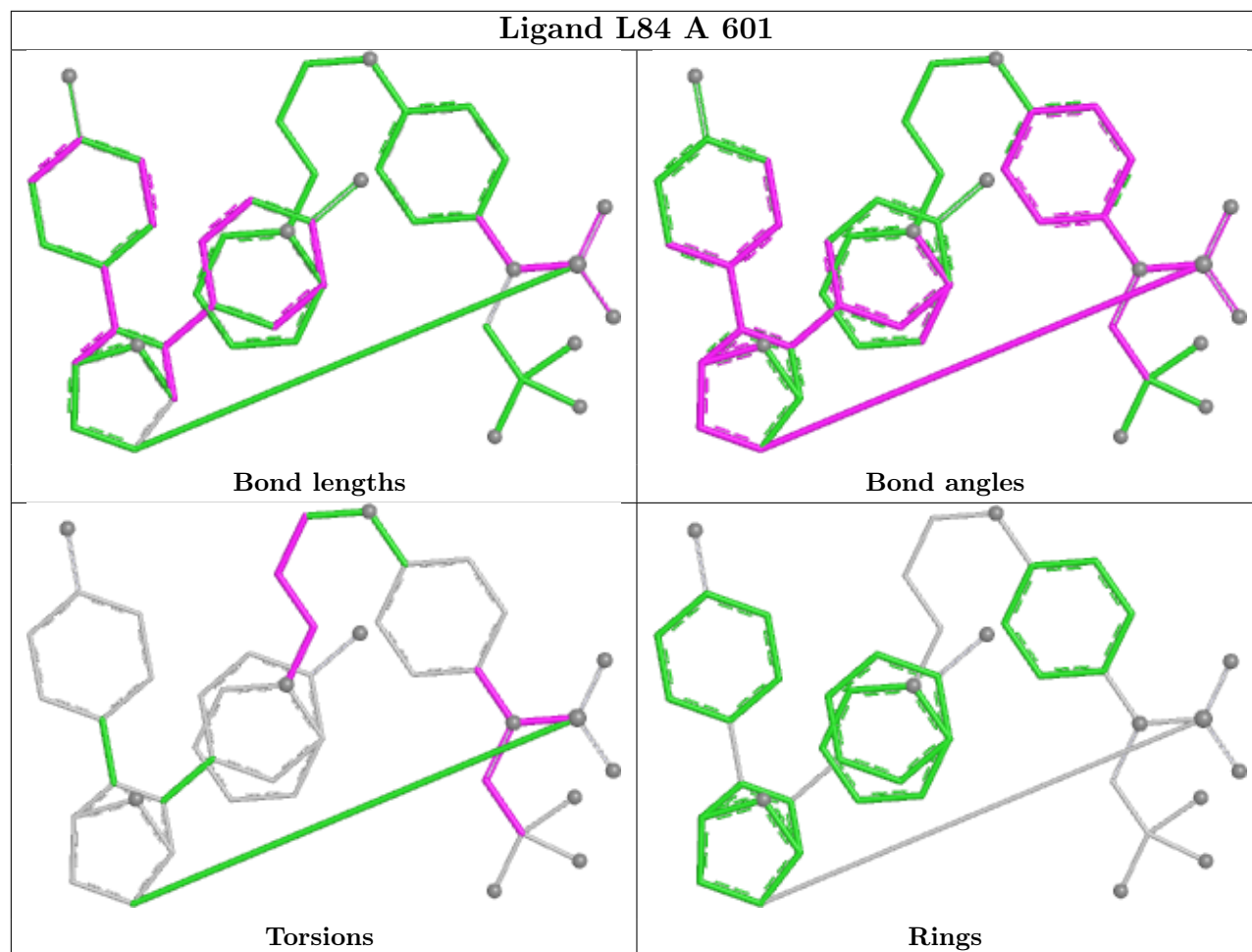
2 monomers are involved in 3 short contacts:

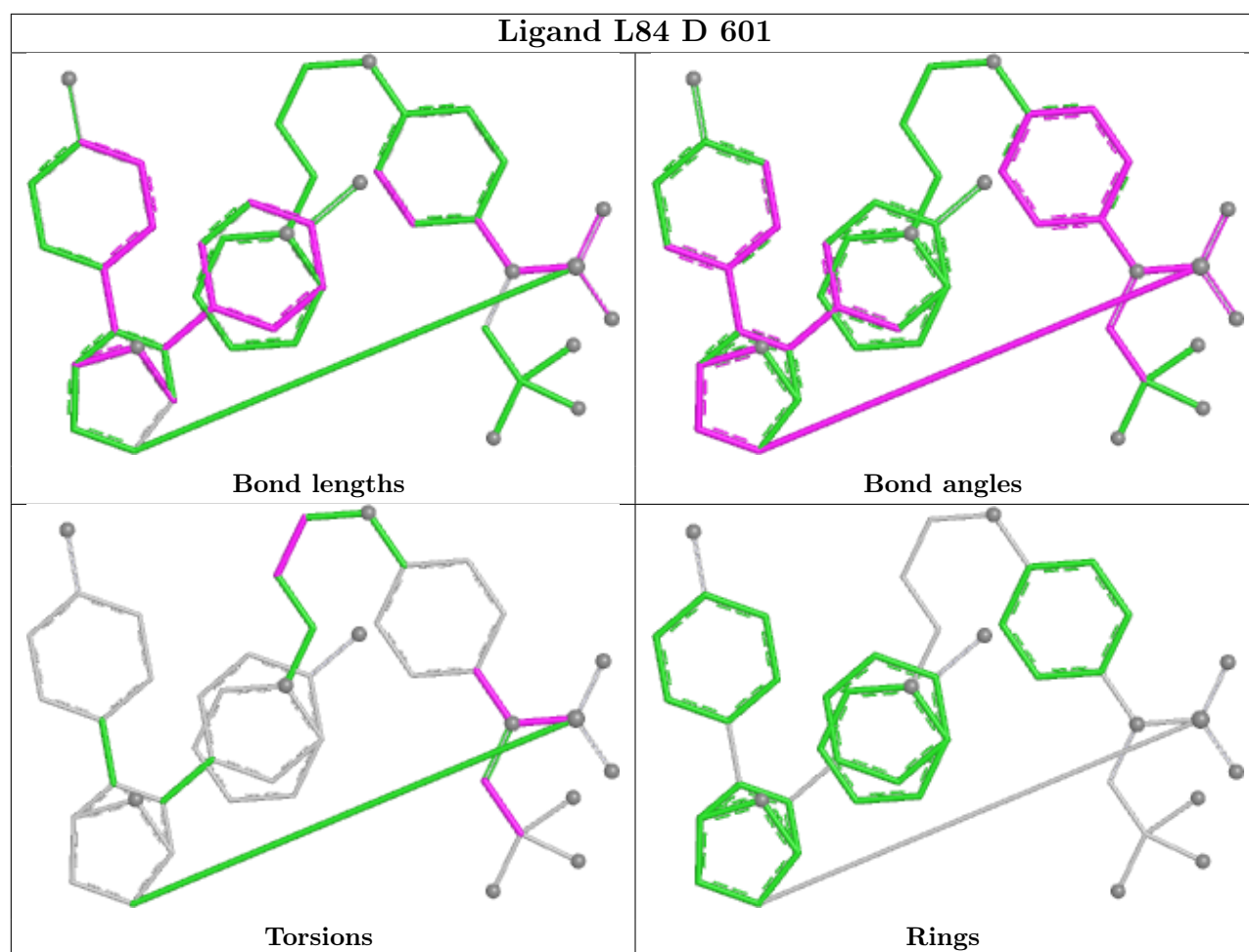
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	L84	1	0
2	D	601	L84	2	0

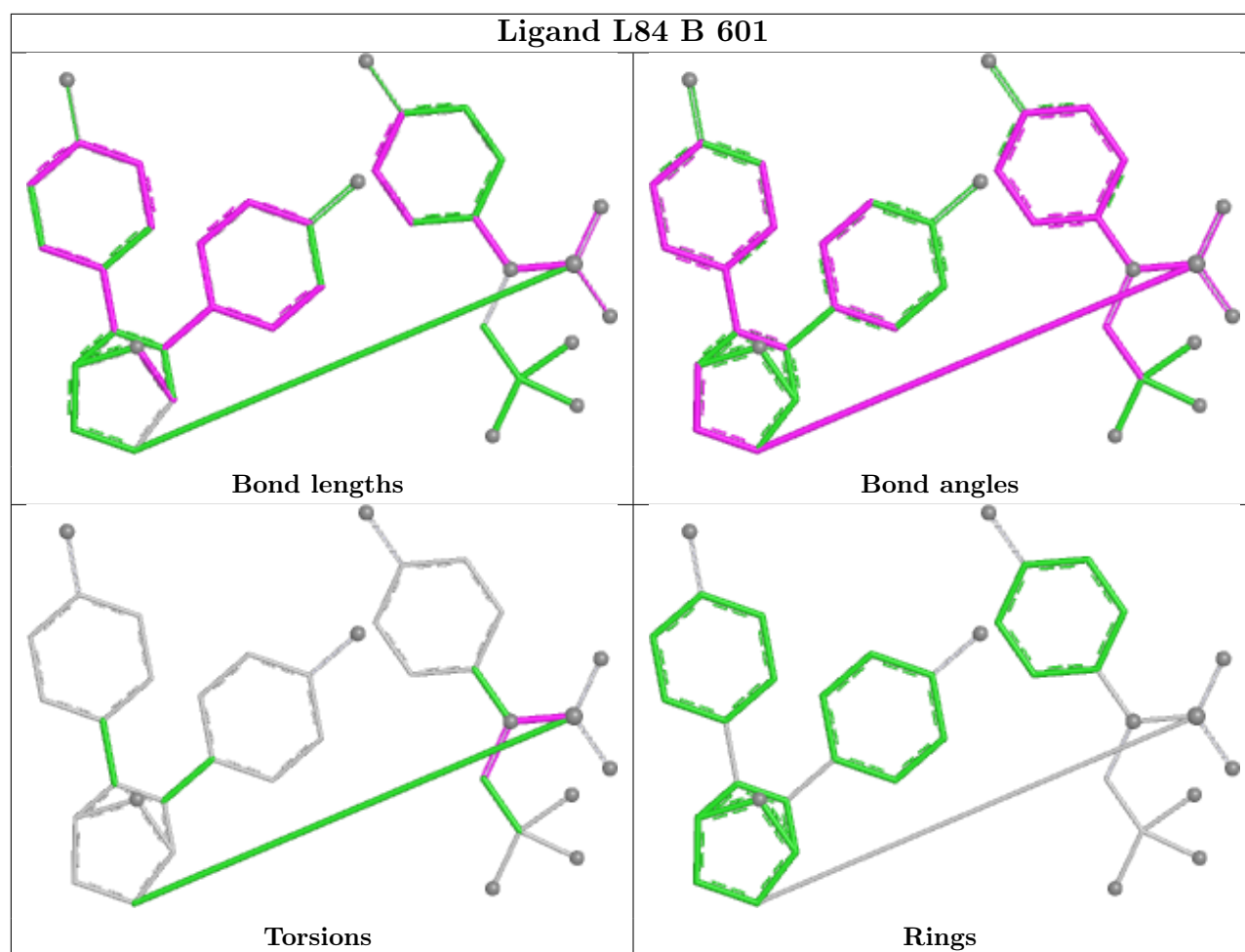
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	231/257 (89%)	-1.20	0 100 100	16, 44, 75, 110	2 (0%)
1	B	219/257 (85%)	-1.24	0 100 100	15, 40, 78, 97	2 (0%)
1	C	225/257 (87%)	-1.26	0 100 100	14, 39, 70, 97	4 (1%)
1	D	208/257 (80%)	-1.19	0 100 100	24, 39, 75, 94	0
All	All	883/1028 (85%)	-1.22	0 100 100	14, 41, 75, 110	8 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	YCM	B	417	5/11	0.96	0.07	97,101,102,104	0
1	YCM	A	417	10/11	0.98	0.05	77,85,91,92	0
1	YCM	A	381	10/11	0.99	0.04	27,32,64,76	0
1	YCM	C	417	10/11	0.99	0.04	70,74,82,88	0
1	YCM	C	381	10/11	1.00	0.03	25,30,51,58	0
1	YCM	B	381	10/11	1.00	0.03	27,32,64,73	0
1	YCM	D	381	10/11	1.00	0.04	34,39,68,69	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

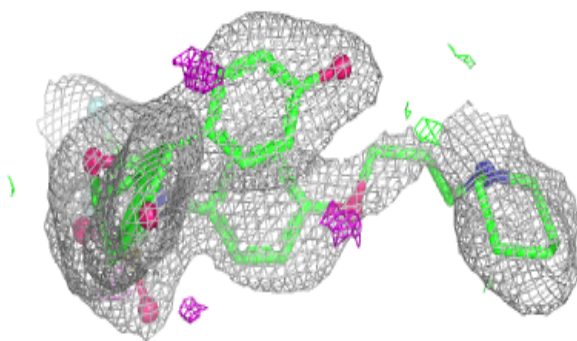
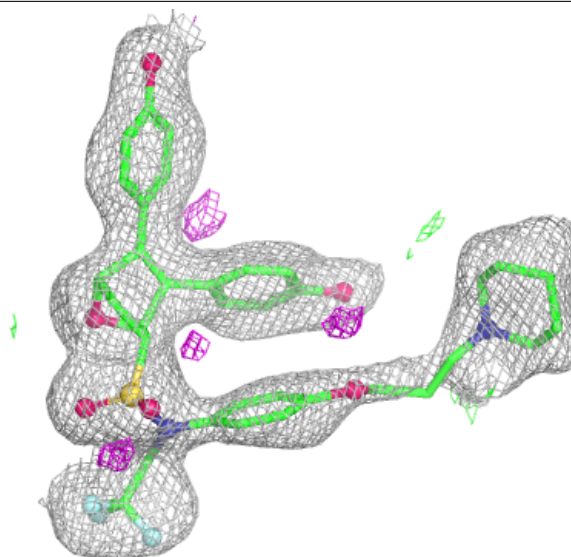
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	L84	C	601	46/46	0.98	0.06	24,49,81,88	0
2	L84	B	601	37/46	0.99	0.03	30,39,77,85	0
2	L84	A	601	46/46	0.99	0.04	23,46,84,92	0
2	L84	D	601	46/46	0.99	0.04	27,50,91,101	0
3	CL	B	602	1/1	1.00	0.02	34,34,34,34	0
3	CL	C	602	1/1	1.00	0.01	34,34,34,34	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.

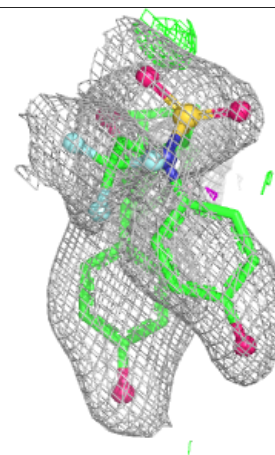
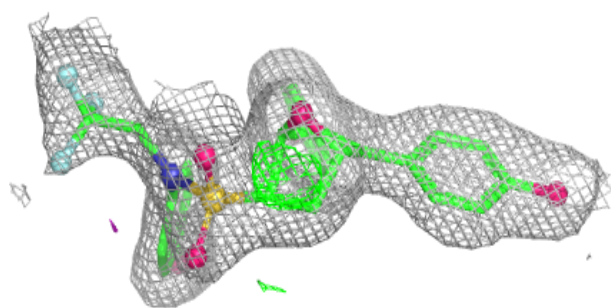
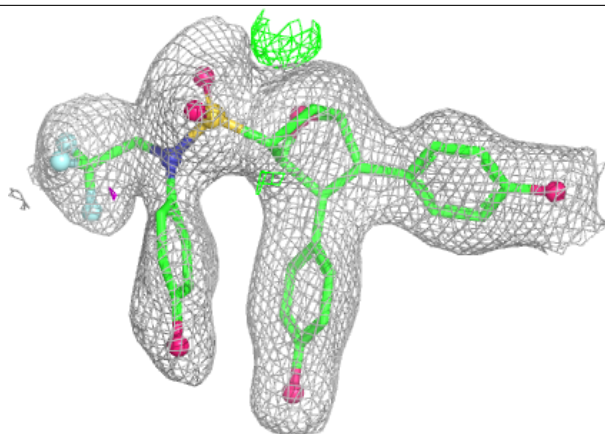
Electron density around L84 C 601:

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



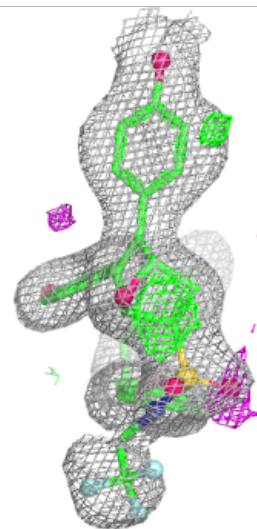
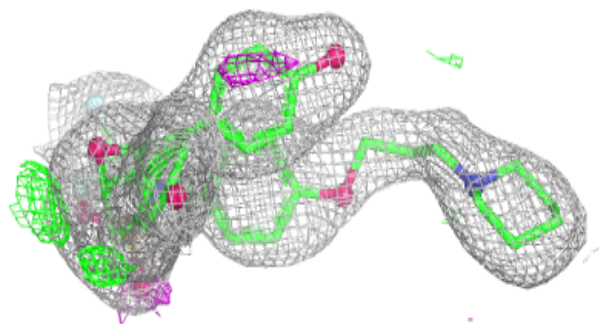
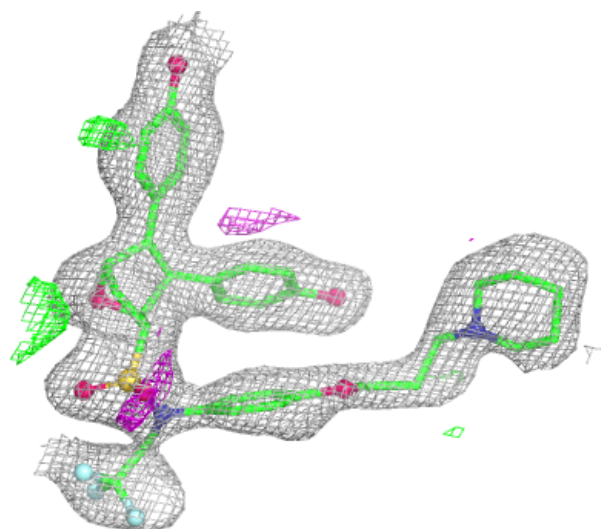
Electron density around L84 B 601:

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



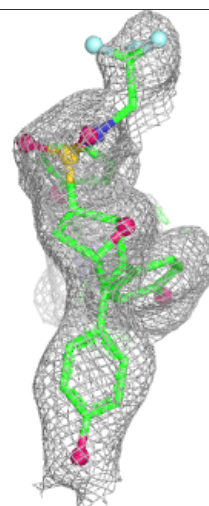
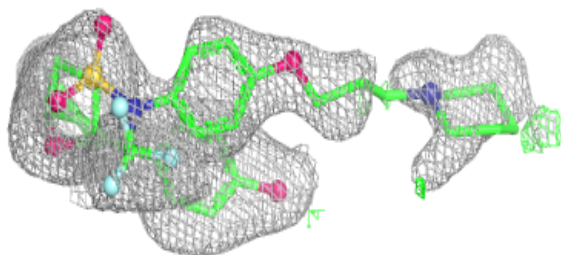
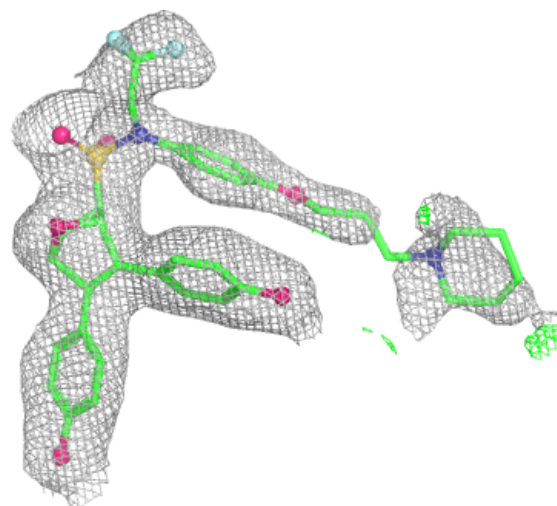
Electron density around L84 A 601:

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



Electron density around L84 D 601:

$2mF_o-DF_c$ (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.