



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:58 PM UTC

PDB ID : 7RS2 / pdb_00007rs2
Title : Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with DMERI-23
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 : 1.72 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

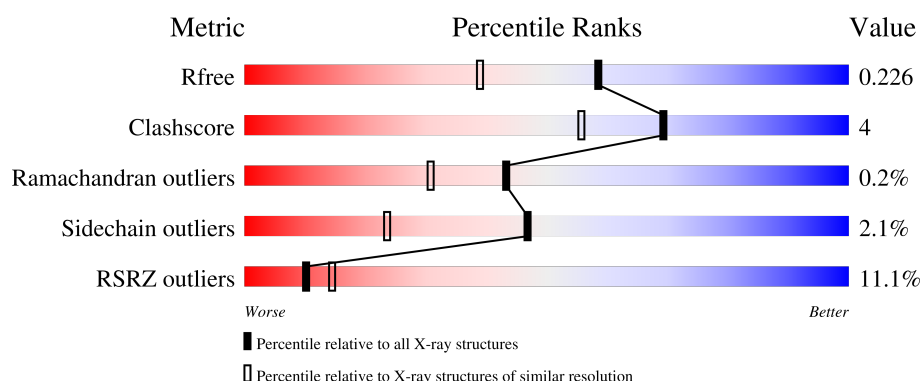
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	260	10% 86% 7% • 6%
1	B	260	7% 83% 5% 12%
1	C	260	14% 87% 7% • 5%
1	D	260	9% 82% 7% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8126 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.

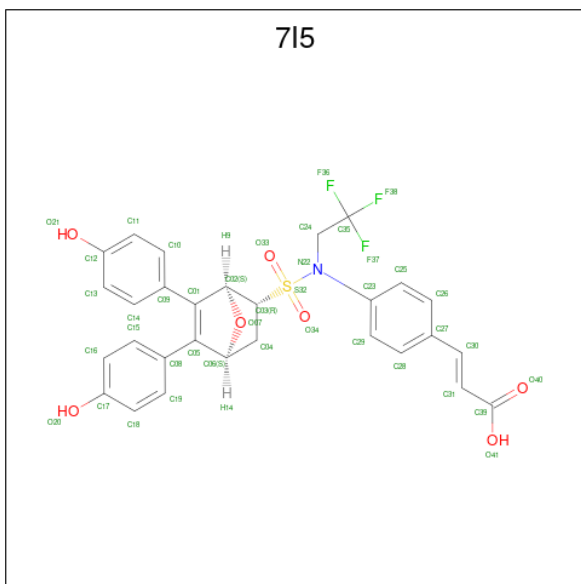
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	1	0
			1962	1252	335	358	17			
1	B	230	Total	C	N	O	S	0	0	0
			1842	1178	314	331	19			
1	C	247	Total	C	N	O	S	0	1	0
			1964	1252	337	359	16			
1	D	234	Total	C	N	O	S	0	0	0
			1865	1191	318	337	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	295	SER	-	expression tag	UNP P03372
A	296	ASN	-	expression tag	UNP P03372
A	297	ALA	-	expression tag	UNP P03372
A	372	SER	LEU	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	UNP P03372
B	295	SER	-	expression tag	UNP P03372
B	296	ASN	-	expression tag	UNP P03372
B	297	ALA	-	expression tag	UNP P03372
B	372	SER	LEU	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372
C	295	SER	-	expression tag	UNP P03372
C	296	ASN	-	expression tag	UNP P03372
C	297	ALA	-	expression tag	UNP P03372
C	372	SER	LEU	engineered mutation	UNP P03372
C	536	SER	LEU	engineered mutation	UNP P03372
D	295	SER	-	expression tag	UNP P03372
D	296	ASN	-	expression tag	UNP P03372
D	297	ALA	-	expression tag	UNP P03372
D	372	SER	LEU	engineered mutation	UNP P03372
D	536	SER	LEU	engineered mutation	UNP P03372

- Molecule 2 is (2E)-3-(4-{[(1S,2R,4S,5S,6S)-5,6-bis(4-hydroxyphenyl)-7-oxabicyclo[2.2.1]heptane-2-sulfonyl](2,2,2-trifluoroethyl)amino}phenyl)prop-2-enoic acid (CCD ID: 7I5) (formula: C₂₉H₂₄F₃NO₇S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 33	C 26	N 1	O 5	S 1	0	0	
2	B	1	Total 41	C 29	F 3	N 1	O 7	S 1	0	0
2	C	1	Total 33	C 26	N 1	O 5	S 1	0	0	
2	D	1	Total 41	C 29	F 3	N 1	O 7	S 1	0	0

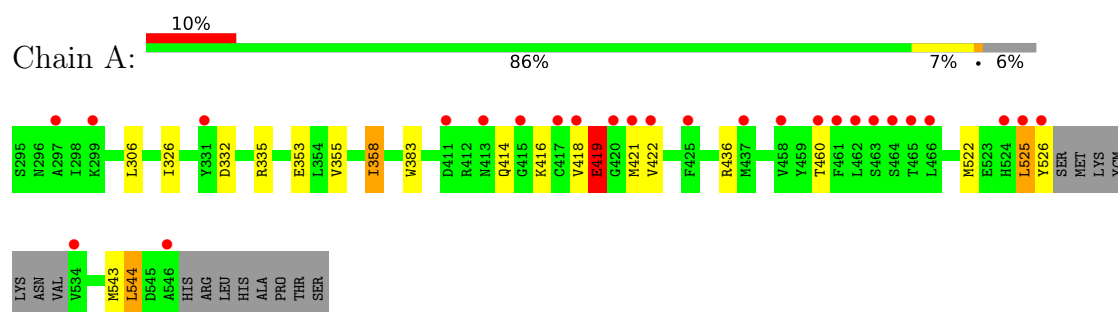
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	112	Total O 112 112	0	0
3	B	82	Total O 82 82	0	0
3	C	75	Total O 75 75	0	0
3	D	76	Total O 76 76	0	0

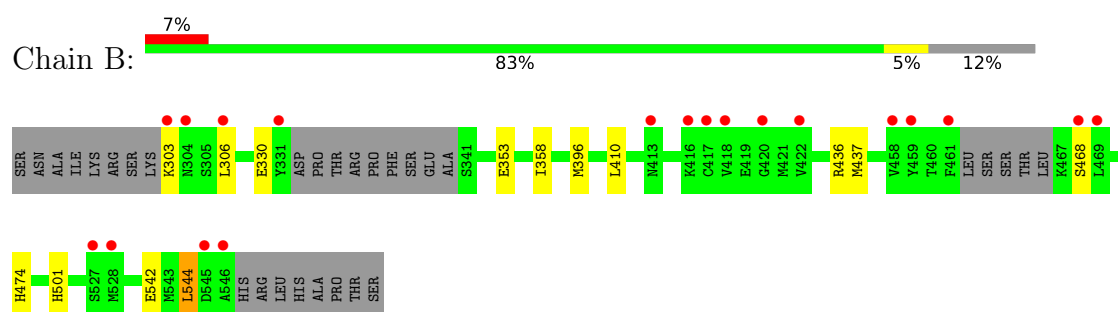
3 Residue-property plots [i](#)

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.

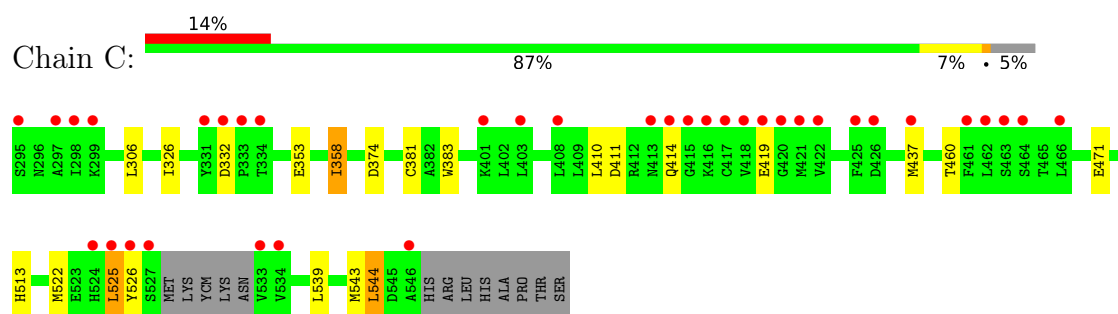
• Molecule 1: Estrogen receptor



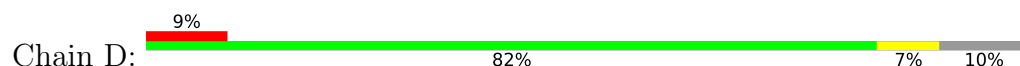
• Molecule 1: Estrogen receptor

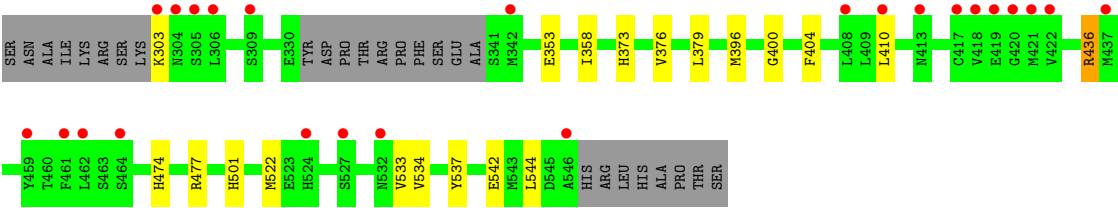


• Molecule 1: Estrogen receptor



• Molecule 1: Estrogen receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.86Å 58.76Å 93.70Å 86.45° 75.11° 62.82°	Depositor
Resolution (Å)	90.36 – 1.72 90.36 – 1.72	Depositor EDS
% Data completeness (in resolution range)	72.8 (90.36-1.72) 72.8 (90.36-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.194 , 0.221 0.203 , 0.226	Depositor DCC
R_{free} test set	3761 reflections (3.48%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.107 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8126	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.71% 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: YCM, 7I5

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	1.05	0/1986	1.33	0/2680
1	B	1.01	0/1851	1.37	3/2492 (0.1%)
1	C	1.04	1/1988 (0.1%)	1.34	0/2684
1	D	1.03	1/1874 (0.1%)	1.37	2/2525 (0.1%)
All	All	1.03	2/7699 (0.0%)	1.35	5/10381 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	501	HIS	CE1-NE2	5.47	1.38	1.32
1	C	513	HIS	CE1-NE2	5.40	1.38	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	542	GLU	CB-CG-CD	6.08	122.94	112.60
1	B	501	HIS	CA-CB-CG	5.50	119.30	113.80
1	D	501	HIS	CA-CB-CG	5.42	119.22	113.80
1	B	501	HIS	CB-CA-C	5.36	119.96	110.85
1	D	542	GLU	CB-CG-CD	5.19	121.42	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	460	THR	Peptide
1	C	460	THR	Peptide

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	1962	0	2006	23	0
1	B	1842	0	1889	7	0
1	C	1964	0	1995	11	0
1	D	1865	0	1920	14	0
2	A	33	0	0	3	0
2	B	41	0	0	1	0
2	C	33	0	0	1	0
2	D	41	0	0	3	0
3	A	112	0	0	0	1
3	B	82	0	0	1	1
3	C	75	0	0	1	0
3	D	76	0	0	3	0
All	All	8126	0	7810	55	1

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 4.

All (55) 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:D:533:VAL:HG11	2:D:601:7I5:O21	1.78	0.82
1:D:533:VAL:CG1	2:D:601:7I5:O21	2.34	0.74
1:A:416:LYS:HG2	1:A:422:VAL:HG21	1.69	0.73
1:C:411:ASP:H	1:C:414:GLN:HE21	1.35	0.73
1:B:330:GLU:OE2	3:B:701:HOH:O	2.10	0.69
1:A:525:LEU:HD12	2:A:601:7I5:C27	2.24	0.67
1:A:355:VAL:HA	1:A:543:MET:CE	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:LEU:HD13	1:C:526:TYR:N	2.13	0.64
1:A:525:LEU:C	1:A:525:LEU:CD2	2.71	0.63
1:A:525:LEU:HD12	2:A:601:7I5:C30	2.32	0.58
1:A:526:TYR:C	1:A:526:TYR:CD1	2.82	0.58
1:D:400:GLY:O	3:D:701:HOH:O	2.17	0.58
1:D:477:ARG:NH2	3:D:702:HOH:O	2.37	0.57
1:A:525:LEU:C	1:A:525:LEU:HD23	2.30	0.57
1:C:525:LEU:HD13	1:C:525:LEU:C	2.31	0.56
1:A:418:VAL:HG11	1:A:421:MET:HE3	1.90	0.53
1:A:335:ARG:NH1	1:A:414:GLN:HE22	2.06	0.52
1:A:525:LEU:HD23	1:A:525:LEU:O	2.10	0.52
1:D:353:GLU:OE1	2:D:601:7I5:O20	2.29	0.51
1:B:353:GLU:OE1	2:B:601:7I5:O20	2.29	0.50
1:D:373:HIS:HD2	1:D:537:TYR:OH	1.94	0.50
1:C:381:YCM:HD3	3:C:710:HOH:O	2.12	0.50
1:D:376:VAL:HG22	1:D:544:LEU:HD12	1.94	0.50
1:A:525:LEU:HD22	1:A:526:TYR:CD2	2.48	0.49
1:A:526:TYR:C	1:A:526:TYR:HD1	2.20	0.49
1:C:410:LEU:HA	1:C:414:GLN:NE2	2.28	0.49
1:A:355:VAL:HA	1:A:543:MET:HE1	1.96	0.48
1:B:358:ILE:HG23	1:B:544:LEU:HD13	1.95	0.48
1:A:355:VAL:HA	1:A:543:MET:HE2	1.96	0.48
1:C:539:LEU:CD1	1:C:543:MET:HE2	2.44	0.48
1:A:353:GLU:OE1	2:A:601:7I5:O20	2.31	0.47
1:D:477:ARG:NH2	3:D:703:HOH:O	2.47	0.47
1:B:410:LEU:HD12	1:B:410:LEU:N	2.30	0.46
1:A:306:LEU:HD22	1:A:306:LEU:N	2.32	0.45
1:C:539:LEU:HG	1:C:543:MET:CE	2.46	0.45
1:C:353:GLU:OE1	2:C:601:7I5:O20	2.34	0.45
1:A:383:TRP:CZ2	1:A:522:MET:HE1	2.52	0.45
1:C:383:TRP:CZ2	1:C:522:MET:HE1	2.51	0.45
1:D:404:PHE:CE2	1:D:410:LEU:HD12	2.52	0.44
1:D:376:VAL:CG2	1:D:544:LEU:HD12	2.48	0.43
1:A:418:VAL:HG11	1:A:421:MET:CE	2.48	0.43
1:A:525:LEU:HD22	1:A:526:TYR:HB3	2.00	0.43
1:C:358:ILE:HG23	1:C:544:LEU:HD13	2.00	0.43
1:A:358:ILE:HG23	1:A:544:LEU:HD13	2.00	0.42
1:B:303:LYS:HG3	1:B:474:HIS:ND1	2.34	0.42
1:A:416:LYS:HA	1:A:422:VAL:CG2	2.50	0.42
1:A:418:VAL:HG12	1:A:419:GLU:HG2	2.01	0.42
1:D:522:MET:HE1	1:D:534:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:VAL:HG22	1:A:543:MET:HE3	2.02	0.41
1:D:396:MET:HE3	1:D:436:ARG:HA	2.03	0.41
1:C:374:ASP:OD2	1:C:471:GLU:OE1	2.39	0.41
1:D:358:ILE:HD12	1:D:379:LEU:HD13	2.04	0.40
1:B:396:MET:HE3	1:B:436:ARG:HA	2.03	0.40
1:B:437:MET:HE3	1:B:437:MET:HB3	1.85	0.40
1:D:303:LYS:HG3	1:D:474:HIS:ND1	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:786:HOH:O	3:B:701:HOH:O[1_565]	1.67	0.53

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	241/260 (93%)	238 (99%)	2 (1%)	1 (0%)	30	16
1	B	222/260 (85%)	219 (99%)	3 (1%)	0	100	100
1	C	243/260 (94%)	240 (99%)	2 (1%)	1 (0%)	30	16
1	D	228/260 (88%)	225 (99%)	3 (1%)	0	100	100
All	All	934/1040 (90%)	922 (99%)	10 (1%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	419	GLU
1	C	419	GLU

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	220/232 (95%)	213 (97%)	7 (3%)	34	11
1	B	205/232 (88%)	202 (98%)	3 (2%)	57	36
1	C	218/232 (94%)	211 (97%)	7 (3%)	34	11
1	D	209/232 (90%)	208 (100%)	1 (0%)	81	71
All	All	852/928 (92%)	834 (98%)	18 (2%)	47	23

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	326	ILE
1	A	332	ASP
1	A	358	ILE
1	A	419	GLU
1	A	436	ARG
1	A	525	LEU
1	A	544	LEU
1	B	306	LEU
1	B	468	SER
1	B	544	LEU
1	C	306	LEU
1	C	326	ILE
1	C	332	ASP
1	C	358	ILE
1	C	437	MET
1	C	525	LEU
1	C	544	LEU
1	D	436	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	455	ASN

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Mol	Chain	Res	Type
1	A	513	HIS
1	A	519	ASN
1	B	359	ASN
1	B	398	HIS
1	B	488	HIS
1	B	516	HIS
1	B	519	ASN
1	C	359	ASN
1	C	398	HIS
1	C	513	HIS
1	C	519	ASN
1	D	373	HIS
1	D	455	ASN
1	D	488	HIS
1	D	519	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	B	381	1	7,9,10	0.60	0	5,10,12	0.57	0
1	YCM	A	381	1	7,9,10	0.46	0	5,10,12	0.29	0
1	YCM	C	381	1	7,9,10	0.49	0	5,10,12	0.40	0
1	YCM	B	530	1	7,9,10	0.48	0	5,10,12	0.46	0
1	YCM	D	530	1	7,9,10	0.50	0	5,10,12	0.57	0
1	YCM	D	381	1	7,9,10	0.60	0	5,10,12	0.46	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	B	381	1	-	1/6/8/10	-
1	YCM	A	381	1	-	2/6/8/10	-
1	YCM	C	381	1	-	2/6/8/10	-
1	YCM	B	530	1	-	1/6/8/10	-
1	YCM	D	530	1	-	0/6/8/10	-
1	YCM	D	381	1	-	1/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	381	YCM	CE-CD-SG-CB
1	A	381	YCM	SG-CD-CE-NZ2
1	B	381	YCM	SG-CD-CE-NZ2
1	C	381	YCM	CE-CD-SG-CB
1	C	381	YCM	SG-CD-CE-NZ2
1	D	381	YCM	SG-CD-CE-NZ2
1	B	530	YCM	SG-CD-CE-NZ2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	381	YCM	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	7I5	B	601	-	43,45,45	2.84	24 (55%)	58,68,68	2.42	19 (32%)
2	7I5	A	601	-	35,37,45	3.19	23 (65%)	46,56,68	2.87	14 (30%)
2	7I5	D	601	-	43,45,45	3.14	21 (48%)	58,68,68	2.41	17 (29%)
2	7I5	C	601	-	35,37,45	3.33	25 (71%)	46,56,68	2.96	15 (32%)

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	7I5	B	601	-	-	4/32/58/58	0/6/5/5
2	7I5	A	601	-	-	4/22/48/58	0/6/5/5
2	7I5	D	601	-	-	7/32/58/58	0/6/5/5
2	7I5	C	601	-	-	6/22/48/58	0/6/5/5

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	7I5	C02-C01	8.33	1.59	1.50
2	D	601	7I5	C02-C01	8.02	1.59	1.50
2	C	601	7I5	C02-C01	7.63	1.59	1.50
2	B	601	7I5	C02-C01	7.52	1.58	1.50
2	C	601	7I5	C30-C27	6.47	1.70	1.51
2	D	601	7I5	C23-N22	6.11	1.53	1.44
2	C	601	7I5	C25-C26	6.03	1.48	1.38
2	A	601	7I5	C30-C27	5.90	1.68	1.51
2	D	601	7I5	C19-C08	5.49	1.47	1.39
2	A	601	7I5	C25-C26	5.41	1.47	1.38
2	D	601	7I5	C29-C28	5.36	1.47	1.38
2	D	601	7I5	O07-C02	5.34	1.51	1.43
2	D	601	7I5	C27-C30	5.23	1.62	1.47
2	D	601	7I5	C14-C09	5.21	1.47	1.39
2	C	601	7I5	S32-N22	5.11	1.78	1.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	7I5	C27-C30	5.08	1.61	1.47
2	D	601	7I5	C31-C39	5.05	1.61	1.48
2	A	601	7I5	O07-C02	4.70	1.50	1.43
2	C	601	7I5	C14-C09	4.70	1.46	1.39
2	B	601	7I5	C06-C05	4.44	1.58	1.52
2	B	601	7I5	C29-C28	4.40	1.45	1.38
2	C	601	7I5	C29-C28	4.39	1.45	1.38
2	D	601	7I5	C28-C27	4.38	1.48	1.39
2	B	601	7I5	C28-C27	4.34	1.48	1.39
2	B	601	7I5	C31-C39	4.33	1.59	1.48
2	B	601	7I5	O07-C02	4.30	1.49	1.43
2	D	601	7I5	C09-C01	4.24	1.56	1.48
2	D	601	7I5	C06-C05	4.21	1.57	1.52
2	B	601	7I5	C13-C12	4.13	1.46	1.39
2	C	601	7I5	C13-C12	4.11	1.46	1.39
2	A	601	7I5	C24-N22	4.09	1.54	1.47
2	A	601	7I5	S32-N22	4.00	1.75	1.67
2	C	601	7I5	C24-N22	3.97	1.54	1.47
2	B	601	7I5	C14-C09	3.94	1.45	1.39
2	A	601	7I5	C13-C12	3.90	1.46	1.39
2	B	601	7I5	C19-C08	3.89	1.45	1.39
2	C	601	7I5	C16-C15	3.75	1.44	1.38
2	B	601	7I5	C09-C01	3.73	1.55	1.48
2	B	601	7I5	C18-C17	3.58	1.45	1.39
2	A	601	7I5	C19-C08	3.52	1.44	1.39
2	B	601	7I5	C11-C10	3.52	1.44	1.38
2	C	601	7I5	C19-C08	3.44	1.44	1.39
2	C	601	7I5	C29-C23	3.42	1.45	1.39
2	A	601	7I5	C29-C28	3.37	1.44	1.38
2	B	601	7I5	C25-C26	3.36	1.44	1.38
2	C	601	7I5	C18-C17	3.36	1.45	1.39
2	A	601	7I5	C10-C09	3.35	1.44	1.39
2	A	601	7I5	C06-C05	3.33	1.56	1.52
2	D	601	7I5	C11-C10	3.30	1.44	1.38
2	C	601	7I5	C09-C01	3.30	1.54	1.48
2	A	601	7I5	C03-S32	3.30	1.84	1.77
2	C	601	7I5	C28-C27	3.30	1.46	1.38
2	C	601	7I5	C25-C23	3.25	1.45	1.39
2	D	601	7I5	C13-C12	3.21	1.45	1.39
2	A	601	7I5	C18-C17	3.14	1.44	1.39
2	B	601	7I5	C23-N22	3.06	1.49	1.44
2	D	601	7I5	C25-C26	3.04	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	7I5	C14-C09	3.03	1.44	1.39
2	C	601	7I5	C15-C08	3.00	1.44	1.39
2	C	601	7I5	C11-C10	2.96	1.43	1.38
2	A	601	7I5	C29-C23	2.93	1.44	1.39
2	D	601	7I5	C18-C17	2.92	1.44	1.39
2	C	601	7I5	C06-C05	2.88	1.55	1.52
2	A	601	7I5	C16-C15	2.88	1.43	1.38
2	A	601	7I5	C09-C01	2.84	1.53	1.48
2	D	601	7I5	C29-C23	2.78	1.44	1.39
2	D	601	7I5	C14-C13	2.75	1.43	1.38
2	A	601	7I5	C28-C27	2.73	1.45	1.38
2	D	601	7I5	C03-S32	2.71	1.83	1.77
2	C	601	7I5	O07-C02	2.70	1.47	1.43
2	B	601	7I5	C29-C23	2.65	1.44	1.39
2	D	601	7I5	C19-C18	2.59	1.43	1.38
2	A	601	7I5	C15-C08	2.46	1.43	1.39
2	C	601	7I5	C10-C09	2.44	1.43	1.39
2	C	601	7I5	C14-C13	2.43	1.42	1.38
2	A	601	7I5	C19-C18	2.39	1.42	1.38
2	A	601	7I5	C25-C23	2.37	1.43	1.39
2	B	601	7I5	C25-C23	2.31	1.43	1.39
2	B	601	7I5	C04-C03	-2.21	1.51	1.54
2	A	601	7I5	C04-C06	2.21	1.57	1.53
2	B	601	7I5	C19-C18	2.21	1.42	1.38
2	B	601	7I5	C15-C08	2.20	1.42	1.39
2	B	601	7I5	C14-C13	2.20	1.42	1.38
2	B	601	7I5	C16-C15	2.19	1.42	1.38
2	B	601	7I5	O41-C39	-2.19	1.24	1.30
2	B	601	7I5	C24-C35	2.13	1.54	1.50
2	D	601	7I5	C16-C15	2.11	1.42	1.38
2	C	601	7I5	C16-C17	2.11	1.42	1.39
2	C	601	7I5	C05-C01	2.10	1.38	1.34
2	C	601	7I5	C26-C27	2.05	1.43	1.38
2	C	601	7I5	C03-S32	2.04	1.82	1.77
2	A	601	7I5	C11-C10	2.04	1.42	1.38
2	D	601	7I5	O41-C39	-2.01	1.25	1.30

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	7I5	O34-S32-O33	-11.81	110.28	119.17
2	A	601	7I5	O34-S32-O33	-10.26	111.45	119.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	7I5	O33-S32-N22	8.29	116.62	107.14
2	D	601	7I5	O34-S32-O33	-7.95	113.18	119.17
2	B	601	7I5	O34-S32-C03	-7.91	98.16	107.79
2	A	601	7I5	O33-S32-N22	7.31	115.50	107.14
2	B	601	7I5	O34-S32-O33	-6.11	114.57	119.17
2	D	601	7I5	C10-C09-C01	5.90	128.56	120.91
2	B	601	7I5	C08-C05-C06	-5.85	110.80	121.26
2	A	601	7I5	O34-S32-N22	5.13	113.01	107.14
2	A	601	7I5	O07-C06-C04	-5.12	94.75	104.73
2	B	601	7I5	O07-C06-C04	-5.11	94.76	104.73
2	B	601	7I5	C10-C09-C01	5.03	127.43	120.91
2	A	601	7I5	O33-S32-C03	-4.98	101.72	107.79
2	C	601	7I5	O07-C06-C04	-4.96	95.05	104.73
2	D	601	7I5	C06-C04-C03	4.84	104.89	100.61
2	D	601	7I5	O07-C06-C04	-4.77	95.42	104.73
2	D	601	7I5	C14-C09-C01	-4.64	114.89	120.91
2	C	601	7I5	C15-C08-C05	4.45	126.67	120.91
2	C	601	7I5	C19-C08-C05	-4.42	115.18	120.91
2	A	601	7I5	C06-C04-C03	4.35	104.46	100.61
2	C	601	7I5	C08-C05-C01	4.15	139.56	128.81
2	D	601	7I5	O34-S32-N22	4.15	112.34	107.39
2	C	601	7I5	O34-S32-N22	4.07	111.80	107.14
2	A	601	7I5	C19-C08-C05	-4.00	115.72	120.91
2	A	601	7I5	C10-C09-C01	3.99	126.08	120.91
2	D	601	7I5	O33-S32-C03	-3.98	102.94	107.79
2	D	601	7I5	C15-C08-C05	3.96	126.04	120.91
2	C	601	7I5	C10-C09-C01	3.93	126.00	120.91
2	B	601	7I5	C06-C04-C03	3.89	104.05	100.61
2	B	601	7I5	C14-C09-C01	-3.88	115.88	120.91
2	B	601	7I5	O33-S32-N22	3.83	111.96	107.39
2	B	601	7I5	F38-C35-C24	3.83	119.25	112.04
2	A	601	7I5	C08-C05-C01	3.77	138.55	128.81
2	A	601	7I5	C15-C08-C05	3.74	125.76	120.91
2	A	601	7I5	C14-C09-C01	-3.73	116.07	120.91
2	C	601	7I5	C06-C04-C03	3.63	103.82	100.61
2	D	601	7I5	O34-S32-C03	-3.62	103.39	107.79
2	D	601	7I5	C19-C08-C05	-3.56	116.29	120.91
2	D	601	7I5	C29-C23-N22	3.56	125.33	120.15
2	C	601	7I5	C14-C09-C01	-3.27	116.67	120.91
2	D	601	7I5	C25-C23-N22	-3.27	115.39	120.15
2	C	601	7I5	C08-C05-C06	-3.26	115.43	121.26
2	A	601	7I5	C08-C05-C06	-3.25	115.44	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	7I5	C08-C05-C01	3.02	136.63	128.81
2	D	601	7I5	F38-C35-C24	3.01	117.70	112.04
2	A	601	7I5	C09-C01-C05	2.99	136.54	128.81
2	C	601	7I5	O33-S32-C03	-2.98	104.16	107.79
2	B	601	7I5	C15-C08-C05	2.77	124.50	120.91
2	D	601	7I5	C15-C16-C17	2.73	122.77	119.88
2	C	601	7I5	C09-C01-C05	2.55	135.41	128.81
2	B	601	7I5	C35-C24-N22	2.51	114.58	112.14
2	C	601	7I5	C09-C01-C02	-2.47	116.66	121.10
2	B	601	7I5	C19-C08-C05	-2.42	117.77	120.91
2	D	601	7I5	C24-N22-C23	2.37	120.73	117.63
2	B	601	7I5	F37-C35-C24	2.36	116.48	112.04
2	D	601	7I5	O07-C06-C05	-2.31	98.77	101.99
2	A	601	7I5	C25-C23-N22	2.30	123.40	120.05
2	B	601	7I5	C13-C14-C09	2.30	123.25	120.80
2	D	601	7I5	C13-C14-C09	2.28	123.23	120.80
2	B	601	7I5	C25-C23-N22	-2.20	116.95	120.15
2	B	601	7I5	C30-C31-C39	2.13	127.85	122.32
2	C	601	7I5	C25-C23-N22	2.12	123.13	120.05
2	B	601	7I5	C09-C01-C05	2.10	134.23	128.81
2	B	601	7I5	C24-N22-C23	2.06	120.34	117.63

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	7I5	C24-N22-S32-C03
2	A	601	7I5	C23-N22-S32-C03
2	A	601	7I5	C24-N22-S32-O33
2	A	601	7I5	C23-N22-S32-O33
2	C	601	7I5	C24-N22-S32-C03
2	C	601	7I5	C23-N22-S32-C03
2	C	601	7I5	C24-N22-S32-O33
2	C	601	7I5	C23-N22-S32-O33
2	D	601	7I5	C02-C03-S32-O33
2	D	601	7I5	C02-C03-S32-O34
2	D	601	7I5	C24-N22-S32-O33
2	C	601	7I5	C25-C23-N22-S32
2	D	601	7I5	C04-C03-S32-O33
2	B	601	7I5	C01-C05-C08-C15
2	C	601	7I5	C29-C23-N22-S32
2	D	601	7I5	C04-C03-S32-O34

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Mol	Chain	Res	Type	Atoms
2	B	601	7I5	C01-C05-C08-C19
2	D	601	7I5	C24-N22-S32-C03
2	B	601	7I5	C24-N22-S32-O33
2	B	601	7I5	C24-N22-S32-O34
2	D	601	7I5	C24-N22-S32-O34

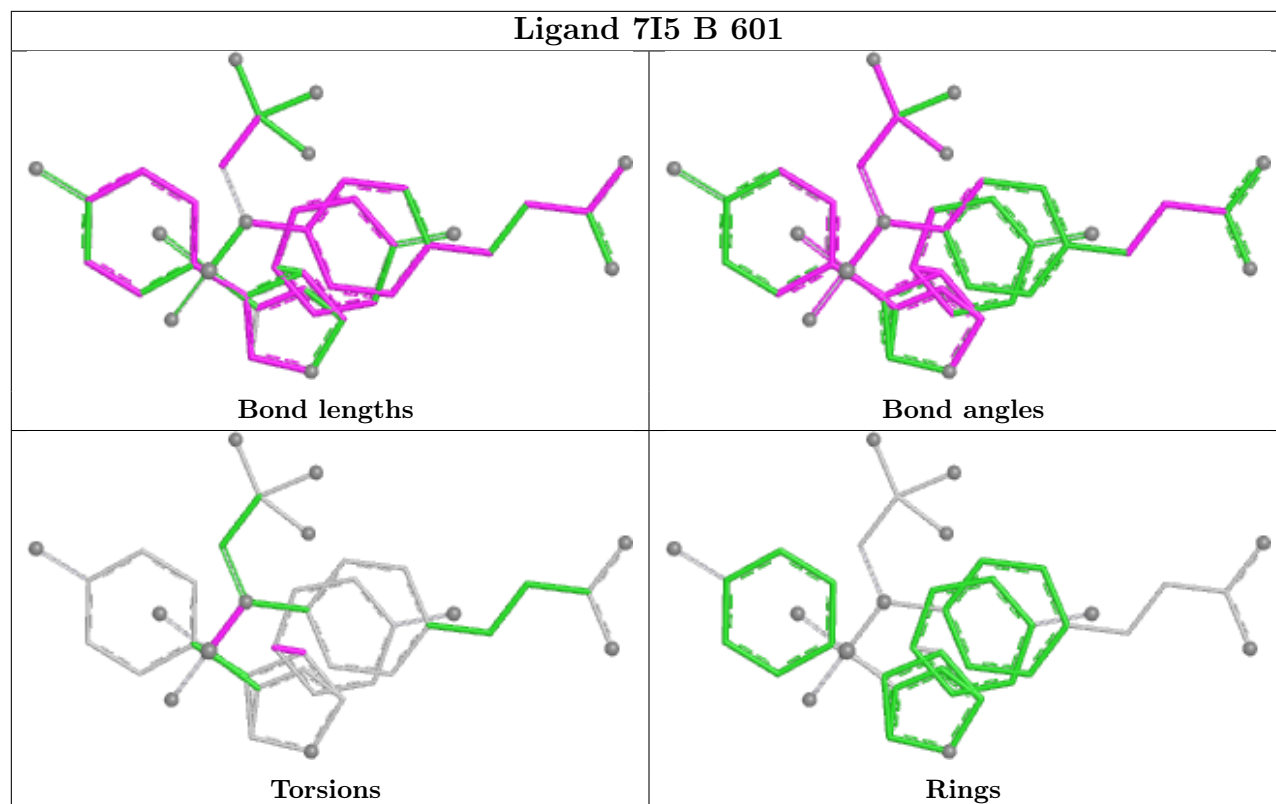
There are no ring outliers.

4 monomers are involved in 8 short contacts:

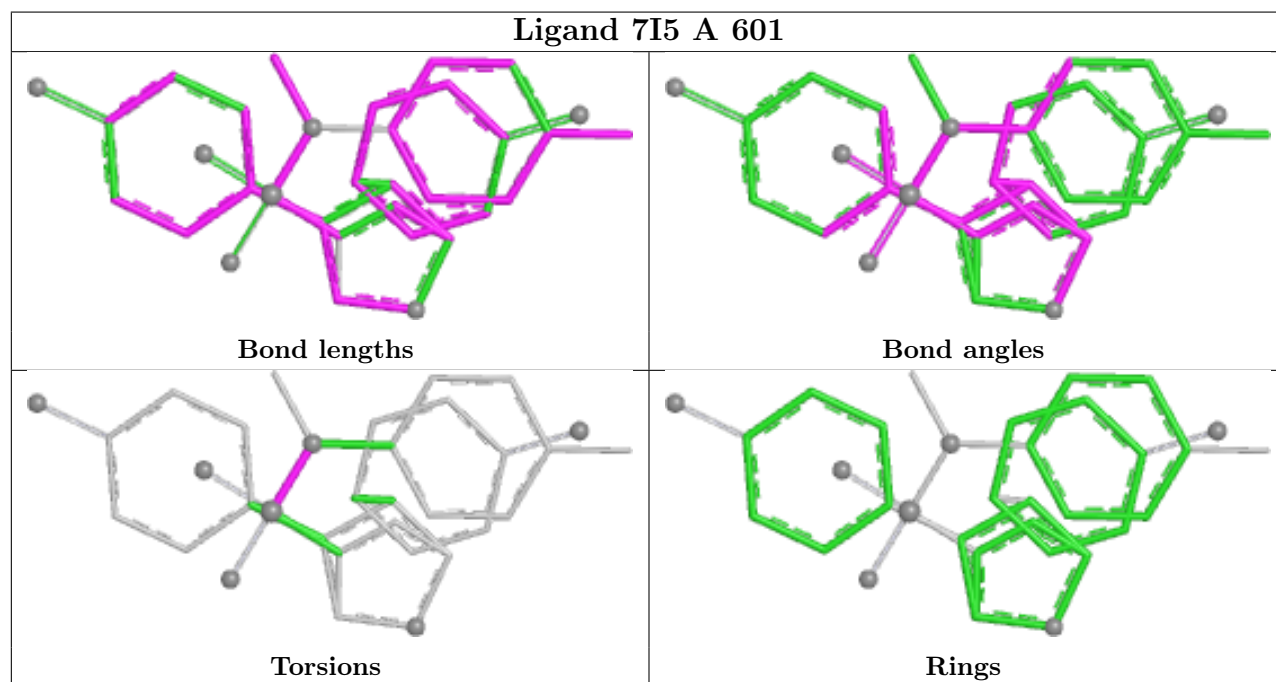
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	7I5	1	0
2	A	601	7I5	3	0
2	D	601	7I5	3	0
2	C	601	7I5	1	0

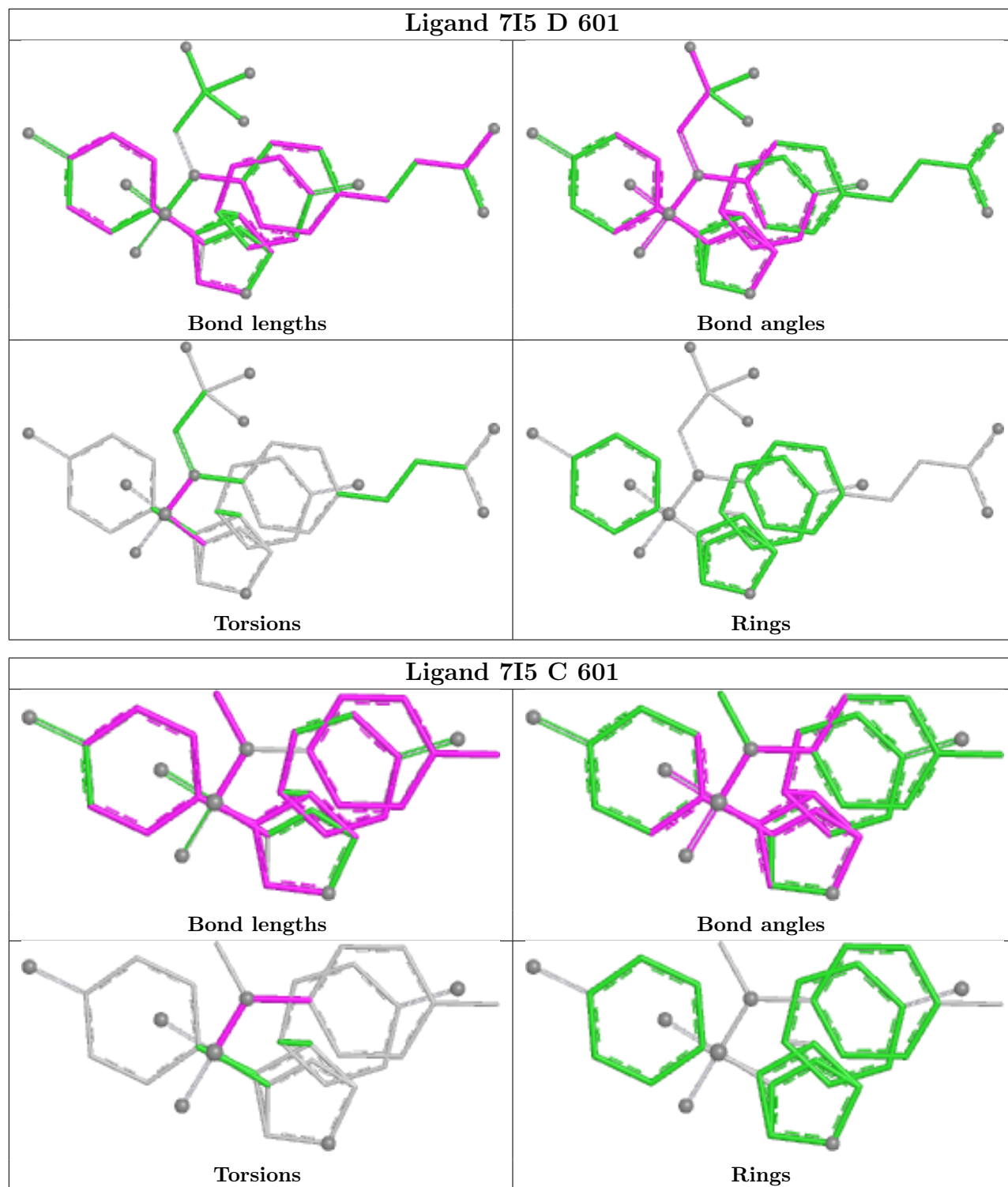
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 7I5 B 601



Ligand 7I5 A 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	244/260 (93%)	0.56	26 (10%) 11 15	14, 25, 62, 84	1 (0%)
1	B	228/260 (87%)	0.60	19 (8%) 17 22	14, 26, 65, 101	0
1	C	246/260 (94%)	0.86	36 (14%) 6 9	16, 29, 67, 100	1 (0%)
1	D	232/260 (89%)	0.64	24 (10%) 12 16	14, 28, 60, 104	0
All	All	950/1040 (91%)	0.67	105 (11%) 10 14	14, 27, 65, 104	2 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	VAL	7.0
1	C	526	TYR	6.2
1	C	533	VAL	6.1
1	D	462	LEU	6.0
1	D	303	LYS	5.8
1	B	546	ALA	5.7
1	C	418	VAL	5.5
1	A	526	TYR	4.7
1	C	421	MET	4.5
1	B	306	LEU	4.2
1	A	420	GLY	4.1
1	C	420	GLY	4.0
1	C	527	SER	4.0
1	D	304	ASN	4.0
1	A	425	PHE	3.9
1	C	524	HIS	3.8
1	B	417	CYS	3.8
1	C	417	CYS	3.8
1	C	525	LEU	3.8
1	B	303	LYS	3.7
1	B	468	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	524	HIS	3.7
1	C	298	ILE	3.6
1	A	546	ALA	3.6
1	C	461	PHE	3.5
1	C	534	VAL	3.5
1	A	534	VAL	3.5
1	B	331	TYR	3.5
1	A	525	LEU	3.5
1	D	461	PHE	3.4
1	A	462	LEU	3.4
1	A	422	VAL	3.4
1	B	418	VAL	3.4
1	C	297	ALA	3.3
1	D	306	LEU	3.3
1	C	413	ASN	3.3
1	C	462	LEU	3.3
1	A	466	LEU	3.3
1	D	418	VAL	3.3
1	D	410	LEU	3.2
1	D	422	VAL	3.2
1	C	332	ASP	3.1
1	C	414	GLN	3.1
1	C	333	PRO	3.1
1	A	463	SER	3.1
1	D	464	SER	3.1
1	A	437	MET	3.1
1	B	459	TYR	3.0
1	B	469	LEU	3.0
1	C	466	LEU	3.0
1	C	419	GLU	3.0
1	D	546	ALA	3.0
1	C	463	SER	3.0
1	A	464	SER	3.0
1	B	461	PHE	3.0
1	A	421	MET	2.9
1	C	334	THR	2.9
1	C	425	PHE	2.8
1	C	299	LYS	2.8
1	A	461	PHE	2.8
1	C	546	ALA	2.8
1	D	437	MET	2.8
1	B	422	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	408	LEU	2.7
1	C	331	TYR	2.7
1	B	545	ASP	2.7
1	A	417	CYS	2.7
1	D	459	TYR	2.7
1	C	464	SER	2.6
1	A	458	VAL	2.6
1	B	458	VAL	2.6
1	A	460	THR	2.5
1	B	304	ASN	2.5
1	C	422	VAL	2.5
1	D	420	GLY	2.4
1	C	437	MET	2.4
1	C	408	LEU	2.4
1	A	465	THR	2.4
1	D	421	MET	2.4
1	B	420	GLY	2.3
1	D	417	CYS	2.3
1	D	419	GLU	2.3
1	C	415	GLY	2.3
1	C	403	LEU	2.3
1	A	413	ASN	2.3
1	A	299	LYS	2.3
1	D	527	SER	2.2
1	D	309	SER	2.2
1	A	411	ASP	2.2
1	C	426	ASP	2.2
1	B	413	ASN	2.2
1	D	413	ASN	2.2
1	B	528	MET	2.1
1	A	415	GLY	2.1
1	C	401	LYS	2.1
1	C	295	SER	2.1
1	D	532	ASN	2.1
1	B	527	SER	2.1
1	D	305	SER	2.1
1	A	297	ALA	2.1
1	B	416	LYS	2.1
1	D	342	MET	2.1
1	D	524	HIS	2.1
1	C	416	LYS	2.1
1	A	331	TYR	2.0

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	530	10/11	0.90	0.12	28,38,48,48	0
1	YCM	D	530	10/11	0.90	0.14	37,44,72,74	0
1	YCM	C	381	10/11	0.93	0.14	17,21,60,78	0
1	YCM	D	381	10/11	0.95	0.09	20,23,39,39	0
1	YCM	B	381	10/11	0.95	0.11	22,26,70,75	0
1	YCM	A	381	10/11	0.96	0.10	16,21,56,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

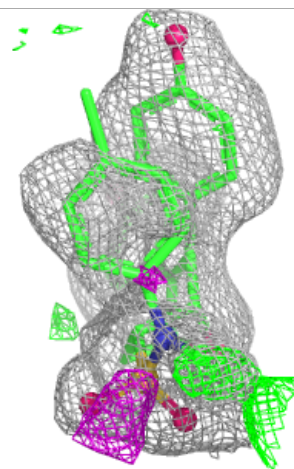
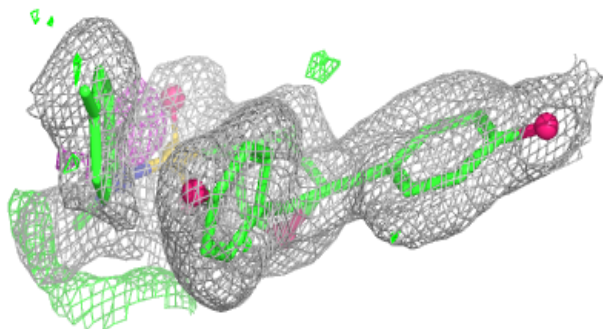
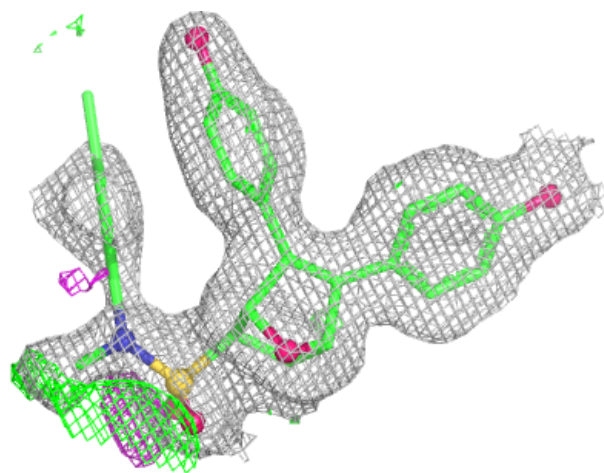
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	7I5	C	601	33/41	0.92	0.12	16,26,67,83	0
2	7I5	A	601	33/41	0.93	0.11	15,25,51,65	0
2	7I5	D	601	41/41	0.93	0.11	20,34,57,81	0
2	7I5	B	601	41/41	0.94	0.09	15,32,48,63	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.

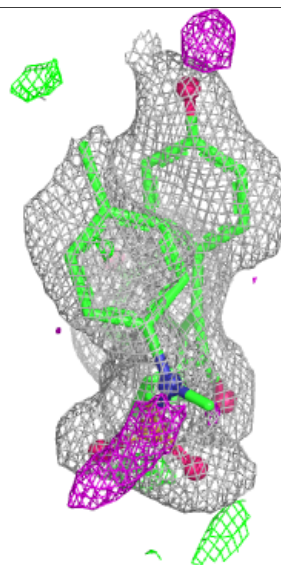
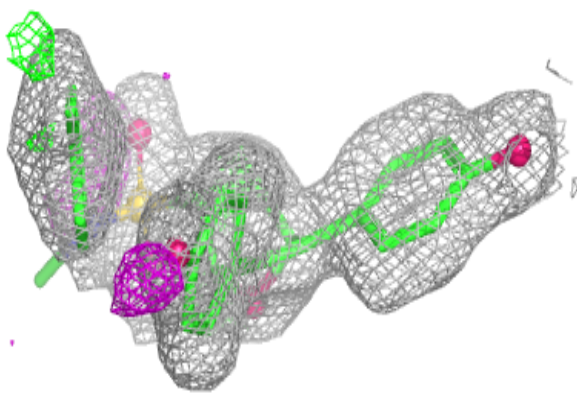
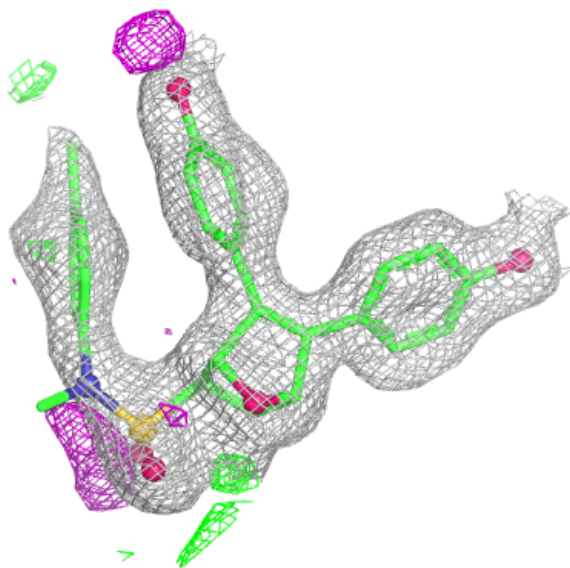
Electron density around 7I5 C 601:

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



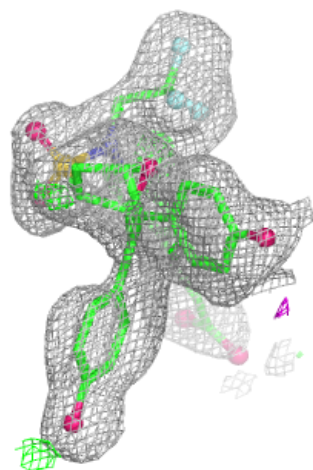
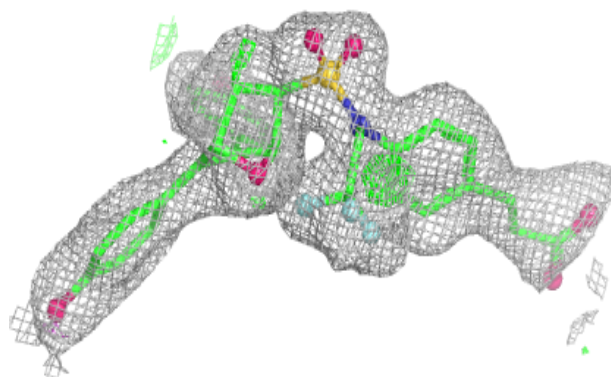
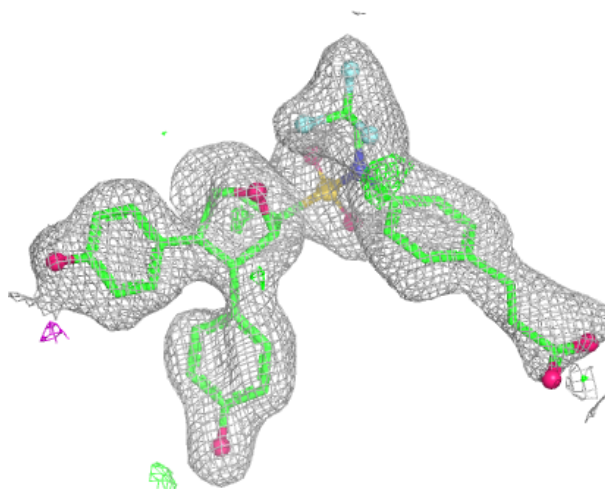
Electron density around 7I5 A 601:

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



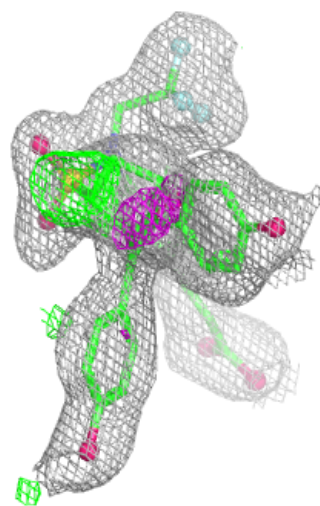
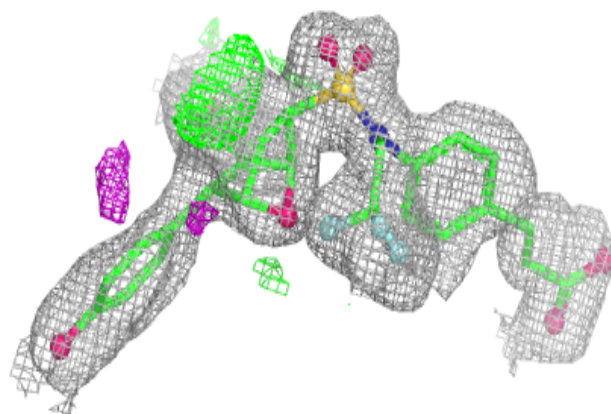
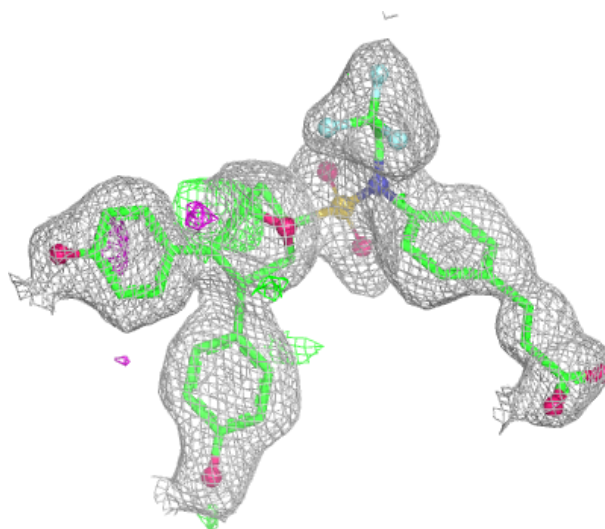
Electron density around 7I5 D 601:

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



Electron density around 7I5 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.