



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:19 PM UTC

PDB ID : 7RS8 / pdb_00007rs8
Title : Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with DMERI-16
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 : 2021-08-11
Resolution : 1.64 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

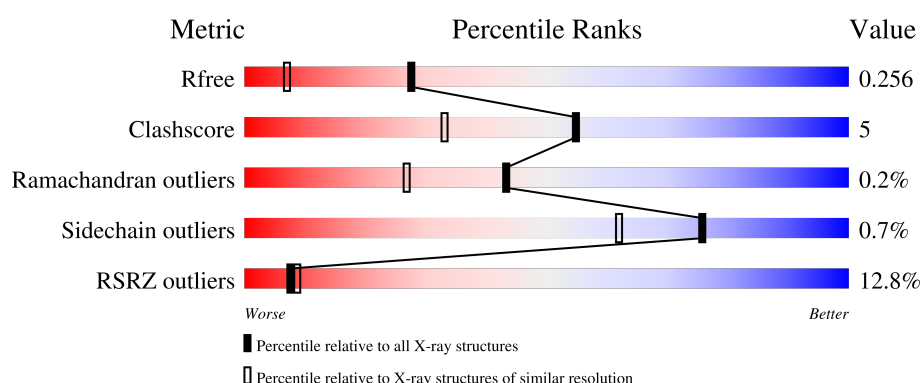
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	13% 77% 11% 11%
1	B	257	11% 82% 6% 12%
1	C	257	10% 81% 8% 11%
2	D	257	11% 75% 9% • 16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8186 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	228	Total	C	N	O	S	0	1	0
			1836	1178	310	332	16			
1	B	227	Total	C	N	O	S	0	2	0
			1831	1172	309	334	16			
1	C	229	Total	C	N	O	S	0	1	0
			1842	1181	310	335	16			

There are 6 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

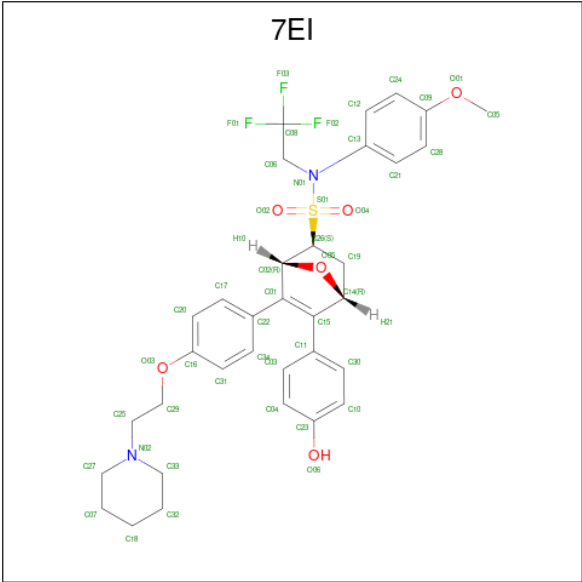
- Molecule 2 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	217	Total	C	N	O	S	0	0	0
			1738	1118	291	312	17			

There are 2 discrepancies between the modelled and reference sequences:

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

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			46	34	3	2	6	1		
3	B	1	Total	C	F	N	O	S	0	1
			88	67	3	4	12	2		
3	C	1	Total	C	F	N	O	S	0	0
			46	34	3	2	6	1		
3	D	1	Total	C	F	N	O	S	0	0
			46	34	3	2	6	1		

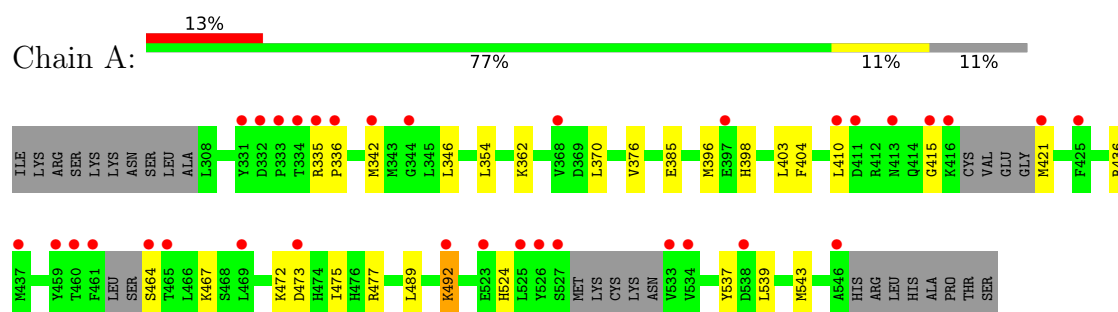
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	190	Total	O	0	0
			190	190		
4	B	176	Total	O	0	0
			176	176		
4	C	187	Total	O	0	0
			187	187		
4	D	160	Total	O	0	0
			160	160		

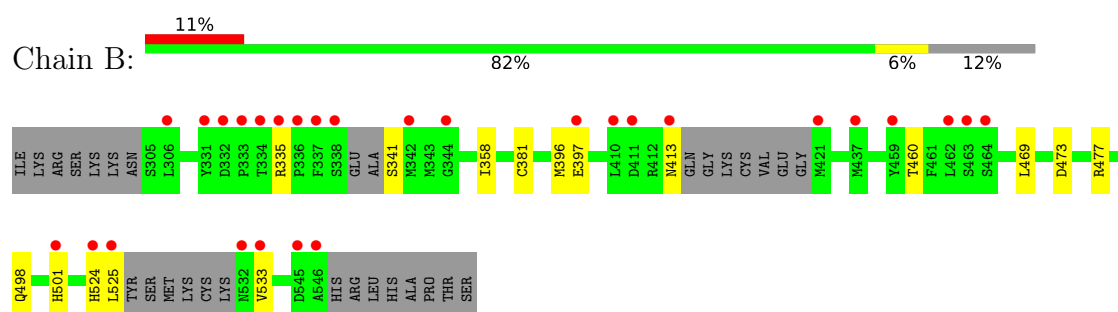
3 Residue-property plots [i](#)

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.

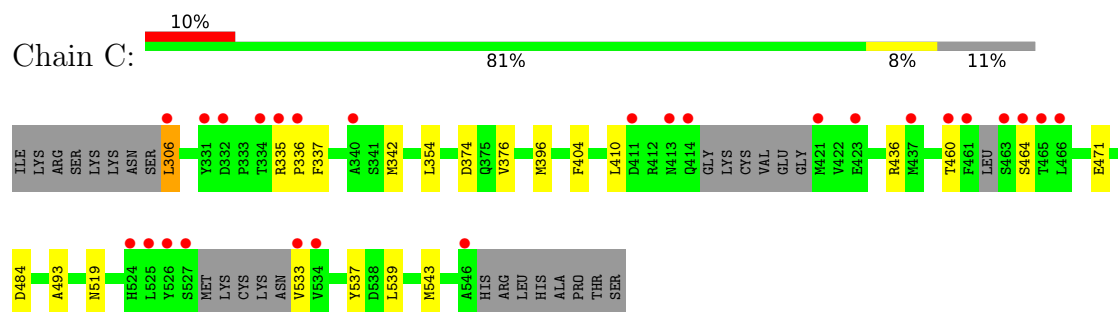
• Molecule 1: Estrogen receptor



• Molecule 1: Estrogen receptor

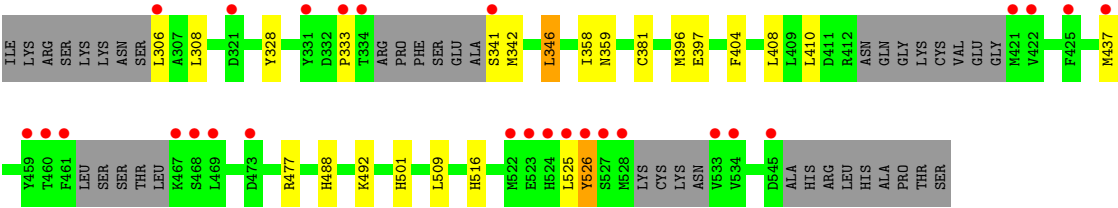


• Molecule 1: Estrogen receptor



• Molecule 2: Estrogen receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.53Å 58.62Å 93.90Å 86.94° 75.26° 62.85°	Depositor
Resolution (Å)	90.57 – 1.64 90.57 – 1.64	Depositor EDS
% Data completeness (in resolution range)	69.0 (90.57-1.64) 69.3 (90.57-1.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.210 , 0.250 0.220 , 0.256	Depositor DCC
R_{free} test set	4122 reflections (3.33%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.107 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8186	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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: 7EI, YCM

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	0.80	0/1858	0.92	0/2508
1	B	0.83	0/1852	0.95	0/2502
1	C	0.85	0/1864	0.93	0/2518
2	D	0.86	0/1768	0.94	1/2386 (0.0%)
All	All	0.84	0/7342	0.93	1/9914 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	359	ASN	CB-CA-C	5.23	120.70	110.67

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	1836	0	1873	24	1
1	B	1831	0	1863	16	1
1	C	1842	0	1870	16	1
2	D	1738	0	1774	18	1
3	A	46	0	0	0	0
3	B	88	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	46	0	0	0	0
3	D	46	0	0	0	0
4	A	190	0	0	5	1
4	B	176	0	0	5	0
4	C	187	0	0	4	0
4	D	160	0	0	3	1
All	All	8186	0	7380	72	3

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 5.

All (72) 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:370:LEU:HD11	1:A:475:ILE:HD11	1.33	1.06
2:D:381:CYS:SG	4:D:850:HOH:O	2.20	0.97
3:B:601[B]:7EI:C12	3:B:601[B]:7EI:O04	2.19	0.85
1:B:525:LEU:HD11	1:B:533:VAL:HG11	1.63	0.80
1:B:381:YCM:NZ2	4:B:701:HOH:O	2.17	0.77
1:C:539:LEU:HG	1:C:543:MET:HE2	1.67	0.76
1:A:342:MET:HE3	1:A:346:LEU:HG	1.66	0.75
2:D:342:MET:O	2:D:346:LEU:HD23	1.87	0.75
1:A:539:LEU:HG	1:A:543:MET:HE2	1.69	0.74
1:C:533:VAL:N	4:C:701:HOH:O	2.20	0.73
1:A:473:ASP:OD2	1:A:477:ARG:CZ	2.38	0.72
1:A:421:MET:HG3	1:A:524:HIS:NE2	2.04	0.72
1:A:467:LYS:NZ	4:A:702:HOH:O	2.26	0.67
1:B:524:HIS:ND1	3:B:601[B]:7EI:C06	2.58	0.67
1:A:489:LEU:O	1:A:492:LYS:HG3	1.94	0.66
1:A:362:LYS:NZ	4:A:703:HOH:O	2.27	0.65
1:B:477:ARG:NH2	4:B:703:HOH:O	2.26	0.65
1:A:385:GLU:OE1	4:A:701:HOH:O	2.14	0.64
1:B:341:SER:N	4:B:704:HOH:O	2.30	0.64
1:C:484:ASP:OD1	2:D:501:HIS:HE1	1.80	0.63
1:A:396:MET:HE1	4:A:721:HOH:O	2.01	0.60
1:B:525:LEU:HD21	1:B:533:VAL:HG11	1.84	0.60
2:D:346:LEU:CD2	2:D:408:LEU:HD21	2.33	0.58
2:D:346:LEU:HD11	2:D:404:PHE:CD2	2.39	0.58
1:B:524:HIS:CE1	3:B:601[B]:7EI:C06	2.89	0.56
2:D:341:SER:N	4:D:703:HOH:O	2.38	0.56
2:D:346:LEU:HD22	2:D:408:LEU:HD21	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LEU:O	1:A:492:LYS:HE3	2.07	0.54
1:C:460:THR:HG21	4:C:745:HOH:O	2.07	0.54
2:D:308:LEU:HD11	2:D:477:ARG:HE	1.73	0.54
1:A:354:LEU:CD2	1:A:543:MET:HE1	2.38	0.53
1:A:370:LEU:CD1	1:A:475:ILE:HD11	2.23	0.53
1:C:396:MET:O	1:C:436:ARG:HD3	2.09	0.53
1:C:306:LEU:N	4:C:707:HOH:O	2.42	0.52
1:A:396:MET:O	1:A:436:ARG:HD3	2.11	0.51
1:B:413:ASN:OD1	1:B:413:ASN:C	2.52	0.51
2:D:404:PHE:CE1	2:D:410:LEU:HD12	2.46	0.51
1:B:525:LEU:HB3	4:B:837:HOH:O	2.11	0.51
1:C:337:PHE:CD2	1:C:342:MET:HE2	2.46	0.50
2:D:525:LEU:O	2:D:526:TYR:HB2	2.12	0.49
2:D:328:TYR:OH	4:D:701:HOH:O	2.20	0.48
1:A:354:LEU:HD23	1:A:543:MET:HE1	1.95	0.48
1:A:473:ASP:OD2	1:A:477:ARG:NH2	2.47	0.48
1:A:421:MET:CG	1:A:524:HIS:NE2	2.77	0.47
1:A:472:LYS:NZ	4:A:705:HOH:O	2.33	0.45
1:C:337:PHE:CD2	1:C:342:MET:CE	2.99	0.45
1:B:335:ARG:CZ	1:B:335:ARG:HB3	2.47	0.45
1:A:342:MET:CE	1:A:346:LEU:HD21	2.47	0.44
1:C:306:LEU:CA	4:C:707:HOH:O	2.66	0.44
1:A:404:PHE:CE2	1:A:410:LEU:HD12	2.53	0.44
1:C:404:PHE:CE2	1:C:410:LEU:HD12	2.53	0.44
2:D:346:LEU:CD1	2:D:404:PHE:CD2	3.01	0.43
1:A:335:ARG:HA	1:A:336:PRO:C	2.43	0.43
1:C:519:ASN:HD21	2:D:516:HIS:HA	1.83	0.43
1:C:335:ARG:HA	1:C:336:PRO:C	2.44	0.43
1:B:473[A]:ASP:OD2	1:B:477:ARG:NH2	2.52	0.42
1:B:469:LEU:HD13	1:C:493:ALA:O	2.20	0.42
1:C:354:LEU:CD2	1:C:543:MET:HE1	2.49	0.42
1:B:498:GLN:HA	1:B:501:HIS:CE1	2.55	0.42
1:C:376:VAL:HG11	1:C:537:TYR:CD2	2.55	0.42
2:D:396:MET:HE2	2:D:397:GLU:OE2	2.20	0.41
2:D:488:HIS:NE2	2:D:492:LYS:HD2	2.35	0.41
1:A:398:HIS:CE1	1:A:403:LEU:HD12	2.55	0.41
2:D:509:LEU:HD23	2:D:509:LEU:HA	1.97	0.41
2:D:346:LEU:HD21	2:D:408:LEU:HD21	2.02	0.41
2:D:437:MET:HE3	2:D:437:MET:HB3	1.88	0.41
1:A:342:MET:HE3	1:A:346:LEU:CG	2.44	0.41
1:A:376:VAL:HG11	1:A:537:TYR:CD2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:THR:HG23	4:B:781:HOH:O	2.22	0.40
1:B:396:MET:HE2	1:B:397:GLU:OE2	2.22	0.40
1:B:525:LEU:CD1	1:B:533:VAL:HG11	2.43	0.40
1:C:374:ASP:OD2	1:C:471:GLU:OE1	2.40	0.40

All (3) 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)
1:A:464:SER:OG	2:D:333:PRO:O[1_566]	1.99	0.21
4:A:877:HOH:O	4:D:851:HOH:O[1_566]	2.05	0.15
1:B:335:ARG:O	1:C:464:SER:OG[1_466]	2.17	0.03

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	220/257 (86%)	218 (99%)	1 (0%)	1 (0%)	24	9
1	B	220/257 (86%)	216 (98%)	4 (2%)	0	100	100
1	C	221/257 (86%)	220 (100%)	1 (0%)	0	100	100
2	D	207/257 (80%)	203 (98%)	3 (1%)	1 (0%)	24	9
All	All	868/1028 (84%)	857 (99%)	9 (1%)	2 (0%)	43	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	526	TYR
1	A	415	GLY

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	206/231 (89%)	205 (100%)	1 (0%)	81	71
1	B	207/231 (90%)	206 (100%)	1 (0%)	81	71
1	C	206/231 (89%)	205 (100%)	1 (0%)	81	71
2	D	196/232 (84%)	193 (98%)	3 (2%)	57	32
All	All	815/925 (88%)	809 (99%)	6 (1%)	76	62

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	492	LYS
1	B	358	ILE
1	C	306	LEU
2	D	306	LEU
2	D	346	LEU
2	D	358	ILE

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	375	GLN
1	A	398	HIS
1	A	474	HIS
1	A	513	HIS
1	A	519	ASN
1	B	356	HIS
1	B	375	GLN
1	B	398	HIS
1	B	488	HIS
1	B	498	GLN
1	B	513	HIS
1	B	519	ASN
1	C	375	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	455	ASN
1	C	513	HIS
1	C	519	ASN
1	C	524	HIS
2	D	359	ASN
2	D	375	GLN
2	D	501	HIS
2	D	513	HIS
2	D	519	ASN
2	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 ⓘ

3 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	C	381	1	7,9,10	0.53	0	5,10,12	0.46	0
1	YCM	B	381	1	7,9,10	0.53	0	5,10,12	0.43	0
1	YCM	A	381	1	7,9,10	0.53	0	5,10,12	0.42	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	C	381	1	-	2/6/8/10	-
1	YCM	B	381	1	-	1/6/8/10	-
1	YCM	A	381	1	-	2/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) 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	CE-CD-SG-CB
1	C	381	YCM	CE-CD-SG-CB
1	C	381	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	B	381	YCM	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
3	7EI	B	601[B]	-	45,47,51	2.29	21 (46%)	58,68,75	3.23	23 (39%)
3	7EI	D	601	-	49,51,51	2.58	15 (30%)	65,75,75	2.34	24 (36%)
3	7EI	C	601	-	49,51,51	2.84	18 (36%)	65,75,75	2.55	20 (30%)
3	7EI	B	601[A]	-	49,51,51	2.71	22 (44%)	65,75,75	2.91	23 (35%)
3	7EI	A	601	-	49,51,51	2.79	18 (36%)	65,75,75	2.21	21 (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
3	7EI	B	601[B]	-	-	9/30/64/69	0/7/6/6
3	7EI	D	601	-	-	9/35/69/69	0/7/6/6
3	7EI	C	601	-	-	5/35/69/69	0/7/6/6
3	7EI	B	601[A]	-	-	8/35/69/69	0/7/6/6
3	7EI	A	601	-	-	7/35/69/69	0/7/6/6

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601[A]	7EI	C13-N01	-11.14	1.29	1.44
3	D	601	7EI	C13-N01	-10.88	1.29	1.44
3	A	601	7EI	C13-N01	-10.85	1.29	1.44
3	C	601	7EI	C13-N01	-10.83	1.29	1.44
3	A	601	7EI	C22-C01	-7.12	1.35	1.48
3	C	601	7EI	C22-C01	-6.88	1.35	1.48
3	C	601	7EI	C11-C15	-6.85	1.35	1.48
3	A	601	7EI	C11-C15	-6.83	1.35	1.48
3	B	601[B]	7EI	C11-C15	-6.72	1.35	1.48
3	D	601	7EI	C22-C01	-6.67	1.36	1.48
3	B	601[A]	7EI	C22-C01	-6.25	1.36	1.48
3	B	601[B]	7EI	C22-C01	-6.20	1.36	1.48
3	B	601[A]	7EI	C11-C15	-6.14	1.37	1.48
3	D	601	7EI	C11-C15	-5.64	1.38	1.48
3	A	601	7EI	O04-S01	5.43	1.48	1.43
3	C	601	7EI	O02-S01	5.01	1.47	1.43
3	C	601	7EI	O04-S01	4.57	1.47	1.43
3	B	601[B]	7EI	O02-S01	4.43	1.47	1.43
3	D	601	7EI	O04-S01	4.40	1.47	1.43
3	B	601[A]	7EI	O02-S01	4.16	1.47	1.43
3	A	601	7EI	O02-S01	3.97	1.46	1.43
3	B	601[A]	7EI	C02-C01	3.93	1.55	1.50
3	B	601[A]	7EI	O04-S01	3.43	1.46	1.43
3	A	601	7EI	C02-C01	3.32	1.54	1.50
3	C	601	7EI	C34-C31	-3.28	1.33	1.38
3	B	601[B]	7EI	O04-S01	3.27	1.46	1.43
3	C	601	7EI	C02-C01	3.19	1.54	1.50
3	C	601	7EI	C20-C17	-3.18	1.33	1.38
3	D	601	7EI	S01-N01	3.16	1.74	1.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	7EI	C34-C22	-3.07	1.34	1.39
3	A	601	7EI	C34-C31	-3.02	1.33	1.38
3	D	601	7EI	C02-C01	2.96	1.53	1.50
3	C	601	7EI	C04-C03	-2.94	1.34	1.38
3	C	601	7EI	C28-C21	-2.88	1.34	1.38
3	A	601	7EI	C34-C22	-2.82	1.35	1.39
3	C	601	7EI	C04-C23	-2.76	1.33	1.39
3	D	601	7EI	C34-C31	-2.73	1.34	1.38
3	B	601[B]	7EI	C28-C21	-2.72	1.34	1.38
3	B	601[A]	7EI	C34-C22	-2.69	1.35	1.39
3	A	601	7EI	C04-C03	-2.66	1.34	1.38
3	A	601	7EI	C20-C17	-2.64	1.34	1.38
3	B	601[B]	7EI	C04-C03	-2.64	1.34	1.38
3	A	601	7EI	C28-C21	-2.62	1.34	1.38
3	B	601[B]	7EI	C30-C11	-2.59	1.35	1.39
3	B	601[B]	7EI	C12-C24	-2.57	1.34	1.38
3	D	601	7EI	C34-C22	-2.53	1.35	1.39
3	A	601	7EI	S01-N01	2.49	1.72	1.67
3	B	601[B]	7EI	C34-C22	-2.49	1.35	1.39
3	B	601[B]	7EI	C03-C11	-2.47	1.35	1.39
3	A	601	7EI	C21-C13	-2.46	1.34	1.39
3	B	601[A]	7EI	C28-C21	-2.46	1.34	1.38
3	C	601	7EI	C17-C22	-2.45	1.35	1.39
3	B	601[B]	7EI	C04-C23	-2.45	1.34	1.39
3	B	601[A]	7EI	C34-C31	-2.44	1.34	1.38
3	D	601	7EI	C04-C23	-2.43	1.34	1.39
3	D	601	7EI	C04-C03	-2.42	1.34	1.38
3	B	601[A]	7EI	C04-C23	-2.41	1.34	1.39
3	D	601	7EI	O02-S01	2.41	1.45	1.43
3	B	601[A]	7EI	C28-C09	-2.37	1.34	1.38
3	D	601	7EI	C20-C17	-2.37	1.35	1.38
3	A	601	7EI	C04-C23	-2.35	1.34	1.39
3	B	601[A]	7EI	C21-C13	-2.34	1.34	1.39
3	B	601[A]	7EI	S01-N01	2.34	1.72	1.67
3	B	601[B]	7EI	C17-C22	-2.34	1.35	1.39
3	C	601	7EI	C28-C09	-2.34	1.34	1.38
3	B	601[A]	7EI	C20-C17	-2.33	1.35	1.38
3	B	601[A]	7EI	C10-C23	-2.33	1.34	1.39
3	A	601	7EI	C14-C15	2.30	1.55	1.52
3	B	601[A]	7EI	C03-C11	-2.30	1.35	1.39
3	B	601[A]	7EI	C30-C11	-2.26	1.36	1.39
3	A	601	7EI	C10-C23	-2.25	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601[B]	7EI	C10-C23	-2.25	1.34	1.39
3	B	601[B]	7EI	C12-C13	-2.24	1.35	1.39
3	B	601[B]	7EI	C20-C17	-2.22	1.35	1.38
3	B	601[A]	7EI	C17-C22	-2.22	1.36	1.39
3	B	601[B]	7EI	C24-C09	-2.20	1.34	1.38
3	B	601[B]	7EI	C30-C10	-2.18	1.35	1.38
3	B	601[A]	7EI	C04-C03	-2.16	1.35	1.38
3	C	601	7EI	C10-C23	-2.15	1.35	1.39
3	C	601	7EI	S01-N01	2.14	1.71	1.67
3	B	601[B]	7EI	C06-N01	2.13	1.51	1.47
3	B	601[B]	7EI	C34-C31	-2.12	1.35	1.38
3	D	601	7EI	C12-C24	-2.12	1.35	1.38
3	B	601[A]	7EI	O05-C02	-2.11	1.40	1.43
3	D	601	7EI	C10-C23	-2.11	1.35	1.39
3	B	601[A]	7EI	C12-C24	-2.11	1.35	1.38
3	C	601	7EI	C20-C16	-2.08	1.34	1.38
3	A	601	7EI	C28-C09	-2.08	1.34	1.38
3	C	601	7EI	C30-C11	-2.05	1.36	1.39
3	B	601[B]	7EI	C28-C09	-2.04	1.34	1.38
3	B	601[B]	7EI	C21-C13	-2.04	1.35	1.39
3	B	601[A]	7EI	C24-C09	-2.04	1.34	1.38
3	A	601	7EI	C17-C22	-2.02	1.36	1.39
3	D	601	7EI	C17-C22	-2.01	1.36	1.39

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601[B]	7EI	O04-S01-N01	-13.68	91.49	107.14
3	B	601[A]	7EI	O02-S01-N01	-13.34	91.45	107.39
3	B	601[B]	7EI	O02-S01-N01	-10.42	95.21	107.14
3	B	601[A]	7EI	O04-S01-N01	-10.28	95.11	107.39
3	D	601	7EI	O02-S01-N01	-9.14	96.48	107.39
3	C	601	7EI	O04-S01-N01	-8.65	97.06	107.39
3	C	601	7EI	O02-S01-N01	-8.32	97.45	107.39
3	B	601[B]	7EI	O04-S01-O02	8.27	125.40	119.17
3	C	601	7EI	O02-S01-C26	7.76	117.24	107.79
3	A	601	7EI	O02-S01-N01	-7.47	98.46	107.39
3	B	601[B]	7EI	O02-S01-C26	6.15	115.28	107.79
3	C	601	7EI	C08-C06-N01	6.09	118.06	112.14
3	A	601	7EI	O04-S01-N01	-5.57	100.74	107.39
3	A	601	7EI	C08-C06-N01	5.53	117.51	112.14
3	D	601	7EI	O04-S01-N01	-5.43	100.90	107.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	7EI	O02-S01-C26	5.38	114.34	107.79
3	B	601[A]	7EI	O04-S01-C26	5.07	113.96	107.79
3	B	601[B]	7EI	C21-C13-N01	4.81	127.06	120.05
3	B	601[A]	7EI	O04-S01-O02	4.70	122.72	119.17
3	B	601[A]	7EI	O02-S01-C26	4.66	113.47	107.79
3	A	601	7EI	O02-S01-C26	4.64	113.44	107.79
3	D	601	7EI	C21-C13-N01	4.22	126.30	120.15
3	B	601[A]	7EI	C21-C13-N01	4.17	126.23	120.15
3	B	601[A]	7EI	C28-C09-C24	-3.96	114.39	120.16
3	D	601	7EI	O04-S01-O02	3.86	122.08	119.17
3	B	601[B]	7EI	C31-C16-C20	-3.86	114.53	120.16
3	A	601	7EI	C28-C09-C24	-3.86	114.53	120.16
3	C	601	7EI	C28-C09-C24	-3.84	114.55	120.16
3	B	601[A]	7EI	C21-C28-C09	3.81	124.09	119.73
3	D	601	7EI	C28-C09-C24	-3.74	114.70	120.16
3	B	601[B]	7EI	O04-S01-C26	3.73	112.33	107.79
3	C	601	7EI	O04-S01-C26	3.67	112.26	107.79
3	B	601[A]	7EI	C31-C16-C20	-3.59	114.92	120.16
3	A	601	7EI	O04-S01-C26	3.51	112.07	107.79
3	B	601[A]	7EI	C30-C11-C03	-3.50	114.11	118.57
3	D	601	7EI	C33-N02-C27	3.49	116.36	108.84
3	D	601	7EI	C08-C06-N01	3.45	115.49	112.14
3	C	601	7EI	C22-C01-C15	3.44	137.70	128.81
3	A	601	7EI	C22-C01-C15	3.28	137.30	128.81
3	B	601[A]	7EI	C34-C22-C17	-3.22	114.47	118.57
3	B	601[B]	7EI	C28-C09-C24	-3.19	115.50	120.16
3	B	601[B]	7EI	C34-C22-C17	-3.17	114.53	118.57
3	D	601	7EI	C30-C11-C03	-3.17	114.53	118.57
3	B	601[B]	7EI	C17-C20-C16	3.17	123.35	119.73
3	C	601	7EI	C21-C28-C09	3.13	123.30	119.73
3	A	601	7EI	C21-C28-C09	3.12	123.29	119.73
3	A	601	7EI	C22-C01-C02	-3.12	115.50	121.10
3	A	601	7EI	C30-C11-C03	-3.04	114.70	118.57
3	D	601	7EI	C31-C16-C20	-3.03	115.74	120.16
3	D	601	7EI	C21-C28-C09	2.90	123.05	119.73
3	D	601	7EI	C07-C27-N02	2.89	115.78	111.30
3	A	601	7EI	C21-C13-N01	2.86	124.31	120.15
3	B	601[B]	7EI	C30-C11-C15	2.83	124.58	120.91
3	B	601[B]	7EI	C21-C28-C09	2.83	122.96	119.73
3	B	601[A]	7EI	C30-C11-C15	2.80	124.53	120.91
3	A	601	7EI	O04-S01-O02	2.78	121.27	119.17
3	C	601	7EI	C22-C01-C02	-2.76	116.13	121.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601[A]	7EI	C17-C20-C16	2.74	122.86	119.73
3	B	601[A]	7EI	C12-C13-C21	-2.72	113.99	119.18
3	C	601	7EI	C30-C11-C03	-2.72	115.11	118.57
3	A	601	7EI	C12-C13-C21	-2.69	114.05	119.18
3	B	601[A]	7EI	C08-C06-N01	2.68	114.74	112.14
3	B	601[A]	7EI	C24-C12-C13	2.67	123.68	120.30
3	B	601[B]	7EI	C22-C01-C02	-2.65	116.33	121.10
3	D	601	7EI	C12-C13-C21	-2.65	114.13	119.18
3	C	601	7EI	O04-S01-O02	2.62	121.15	119.17
3	A	601	7EI	O05-C14-C15	2.62	105.63	101.99
3	C	601	7EI	C12-C13-C21	-2.61	114.19	119.18
3	D	601	7EI	C22-C01-C15	2.60	135.54	128.81
3	B	601[B]	7EI	C22-C01-C15	2.55	135.42	128.81
3	C	601	7EI	O05-C14-C15	2.53	105.51	101.99
3	D	601	7EI	C30-C11-C15	2.52	124.17	120.91
3	D	601	7EI	C24-C12-C13	2.45	123.41	120.30
3	B	601[B]	7EI	C30-C11-C03	-2.45	115.45	118.57
3	D	601	7EI	C17-C20-C16	2.44	122.52	119.73
3	C	601	7EI	C31-C16-C20	-2.43	116.62	120.16
3	A	601	7EI	C31-C16-C20	-2.37	116.70	120.16
3	B	601[B]	7EI	C14-C19-C26	-2.33	98.56	100.61
3	C	601	7EI	C12-C24-C09	2.30	122.36	119.73
3	C	601	7EI	C33-N02-C27	2.30	113.80	108.84
3	B	601[A]	7EI	C34-C31-C16	2.29	122.34	119.73
3	B	601[B]	7EI	C34-C31-C16	2.29	122.34	119.73
3	D	601	7EI	C34-C22-C17	-2.26	115.69	118.57
3	A	601	7EI	C14-C15-C01	-2.25	102.25	106.97
3	C	601	7EI	C21-C13-N01	2.24	123.41	120.15
3	A	601	7EI	C28-C21-C13	2.23	123.12	120.30
3	B	601[B]	7EI	C34-C22-C01	2.22	123.79	120.91
3	B	601[B]	7EI	C11-C15-C14	-2.21	117.31	121.26
3	C	601	7EI	C28-C21-C13	2.20	123.08	120.30
3	B	601[A]	7EI	C31-C34-C22	2.19	123.14	120.80
3	B	601[A]	7EI	C04-C23-C10	-2.17	116.32	119.77
3	A	601	7EI	C24-C12-C13	2.16	123.04	120.30
3	D	601	7EI	C03-C04-C23	2.16	122.16	119.88
3	D	601	7EI	C10-C30-C11	2.16	123.10	120.80
3	C	601	7EI	C32-C33-N02	2.16	114.64	111.30
3	B	601[B]	7EI	O05-C14-C15	2.15	104.99	101.99
3	A	601	7EI	C30-C11-C15	2.15	123.69	120.91
3	C	601	7EI	C30-C11-C15	2.14	123.68	120.91
3	B	601[B]	7EI	C31-C34-C22	2.14	123.08	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601[A]	7EI	C10-C30-C11	2.12	123.07	120.80
3	B	601[B]	7EI	C24-C12-C13	2.11	122.97	120.30
3	D	601	7EI	C29-O03-C16	2.10	123.38	117.93
3	D	601	7EI	O04-S01-C26	2.09	110.34	107.79
3	B	601[A]	7EI	C14-C15-C01	-2.09	102.59	106.97
3	D	601	7EI	O05-C14-C19	-2.09	100.66	104.73
3	B	601[B]	7EI	C12-C13-C21	-2.08	115.20	119.18
3	B	601[A]	7EI	C04-C03-C11	2.04	122.98	120.80
3	A	601	7EI	C10-C30-C11	2.02	122.96	120.80
3	B	601[A]	7EI	C03-C04-C23	2.02	122.02	119.88
3	A	601	7EI	C03-C04-C23	2.01	122.01	119.88
3	D	601	7EI	C12-C24-C09	2.00	122.02	119.73

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601[A]	7EI	C06-N01-S01-O02
3	B	601[A]	7EI	C06-N01-S01-O04
3	B	601[B]	7EI	C21-C13-N01-S01
3	B	601[B]	7EI	C12-C13-N01-S01
3	D	601	7EI	C06-N01-S01-O04
3	B	601[B]	7EI	C24-C09-O01-C05
3	B	601[B]	7EI	C28-C09-O01-C05
3	C	601	7EI	C24-C09-O01-C05
3	C	601	7EI	C28-C09-O01-C05
3	B	601[B]	7EI	C29-C25-N02-C33
3	A	601	7EI	C28-C09-O01-C05
3	A	601	7EI	C24-C09-O01-C05
3	B	601[A]	7EI	C03-C11-C15-C01
3	B	601[A]	7EI	C25-C29-O03-C16
3	D	601	7EI	C25-C29-O03-C16
3	B	601[A]	7EI	C28-C09-O01-C05
3	B	601[A]	7EI	C30-C11-C15-C01
3	B	601[A]	7EI	C24-C09-O01-C05
3	A	601	7EI	C29-C25-N02-C27
3	C	601	7EI	N02-C25-C29-O03
3	D	601	7EI	C28-C09-O01-C05
3	A	601	7EI	C02-C01-C22-C34
3	B	601[B]	7EI	C02-C01-C22-C17
3	B	601[B]	7EI	C02-C01-C22-C34
3	C	601	7EI	C02-C01-C22-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	601[B]	7EI	C06-N01-S01-O04
3	D	601	7EI	C24-C09-O01-C05
3	B	601[B]	7EI	C19-C26-S01-O02
3	A	601	7EI	C02-C01-C22-C17
3	C	601	7EI	C02-C01-C22-C17
3	D	601	7EI	C02-C01-C22-C17
3	B	601[A]	7EI	C06-N01-S01-C26
3	D	601	7EI	C02-C01-C22-C34
3	D	601	7EI	C06-N01-S01-C26
3	A	601	7EI	C06-N01-S01-O04
3	D	601	7EI	C06-N01-S01-O02
3	A	601	7EI	N02-C25-C29-O03
3	D	601	7EI	C15-C01-C22-C34

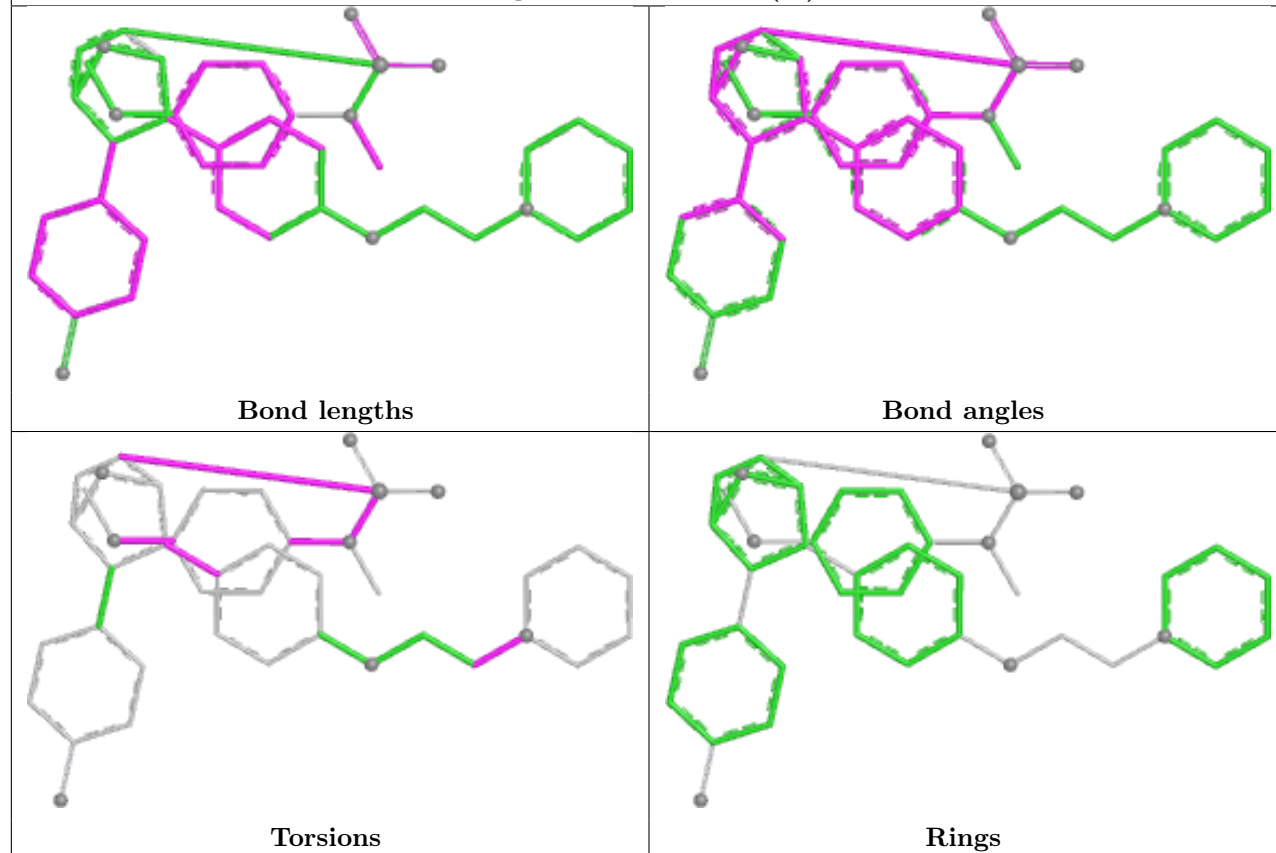
There are no ring outliers.

1 monomer is involved in 3 short contacts:

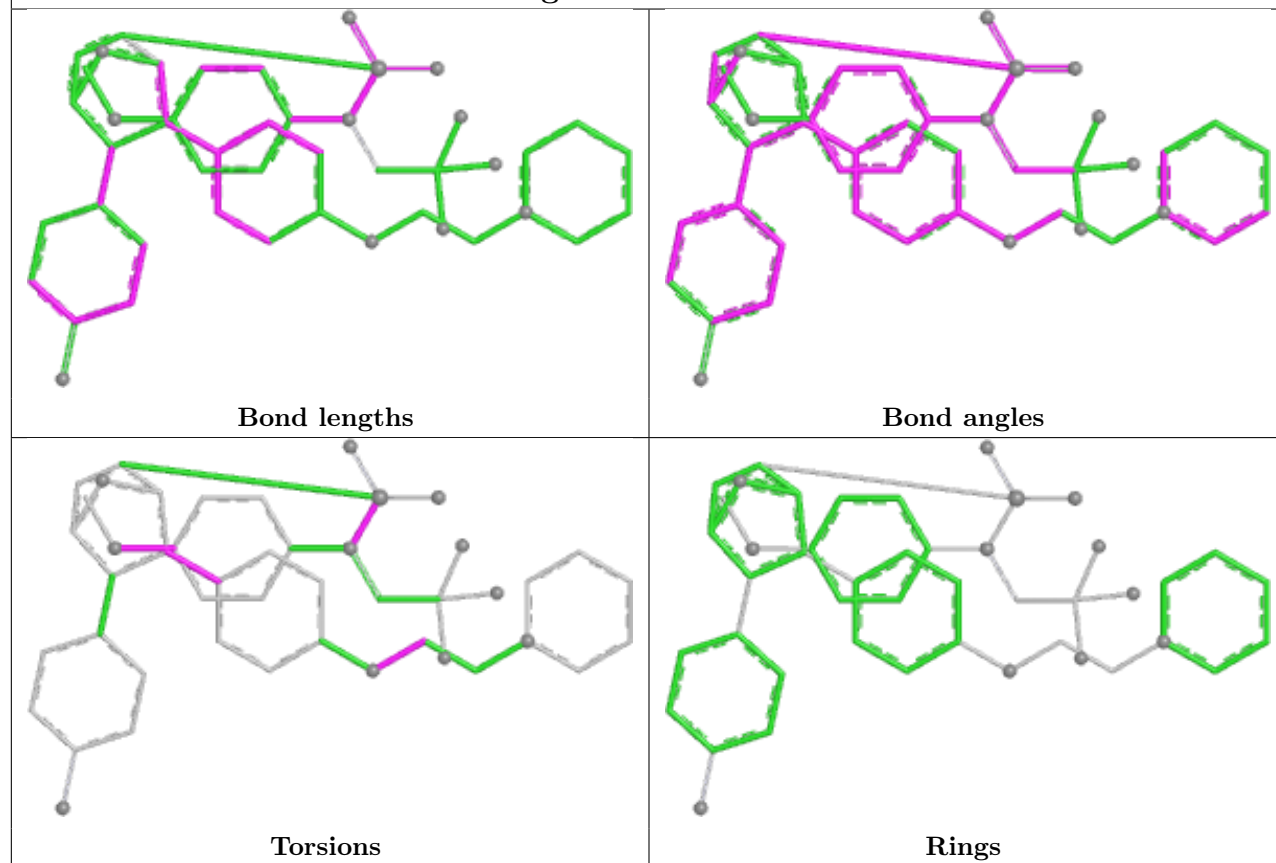
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601[B]	7EI	3	0

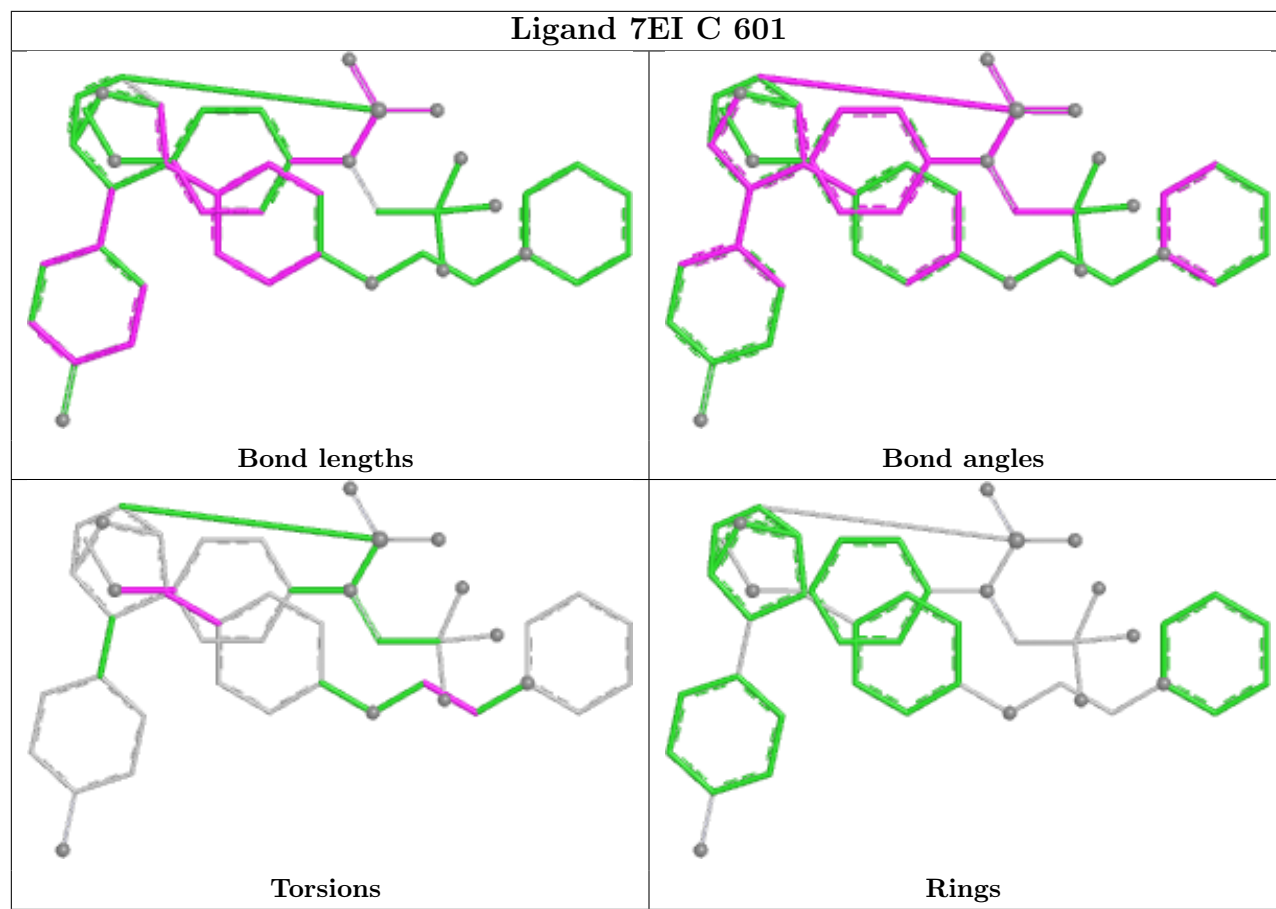
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

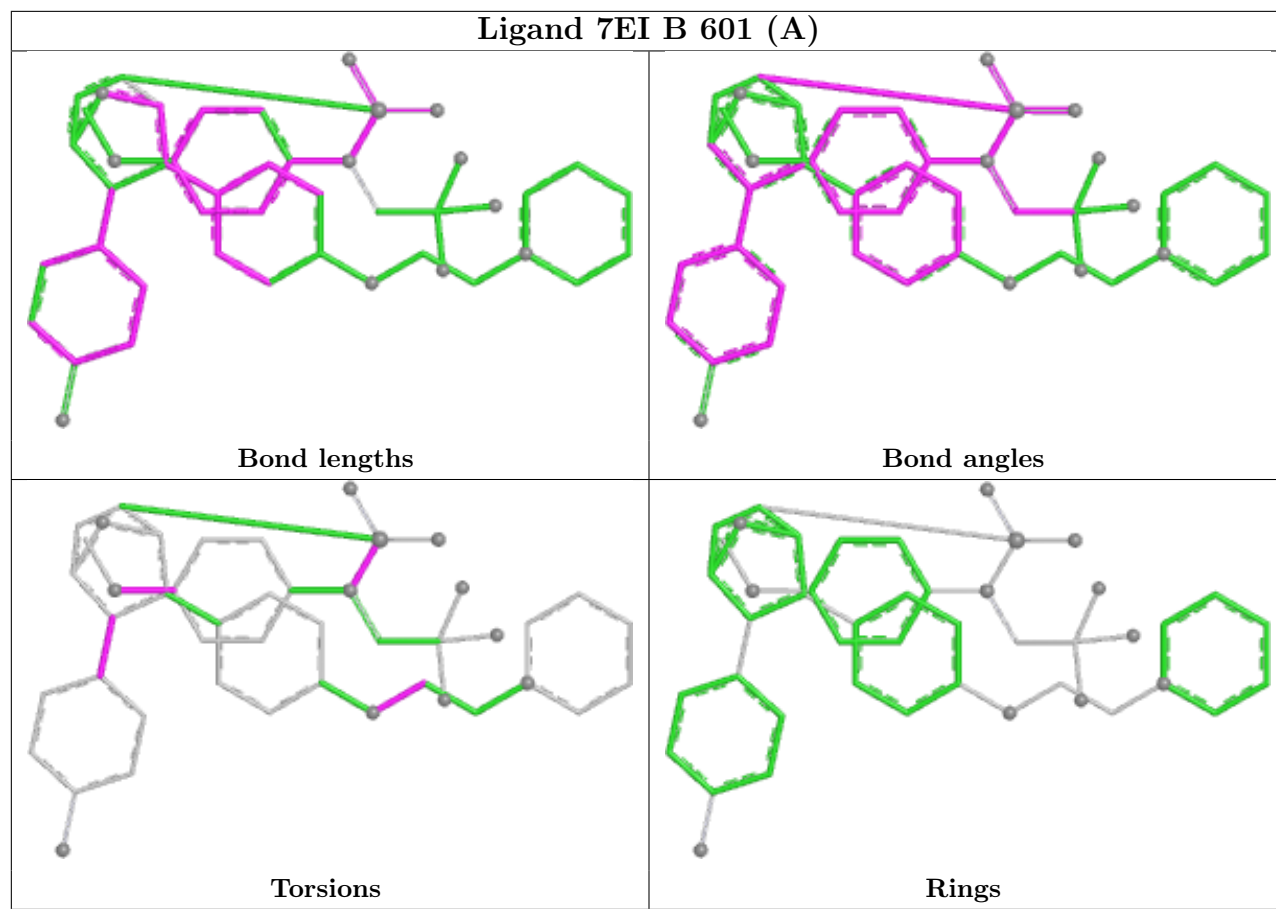
Ligand 7EI B 601 (B)

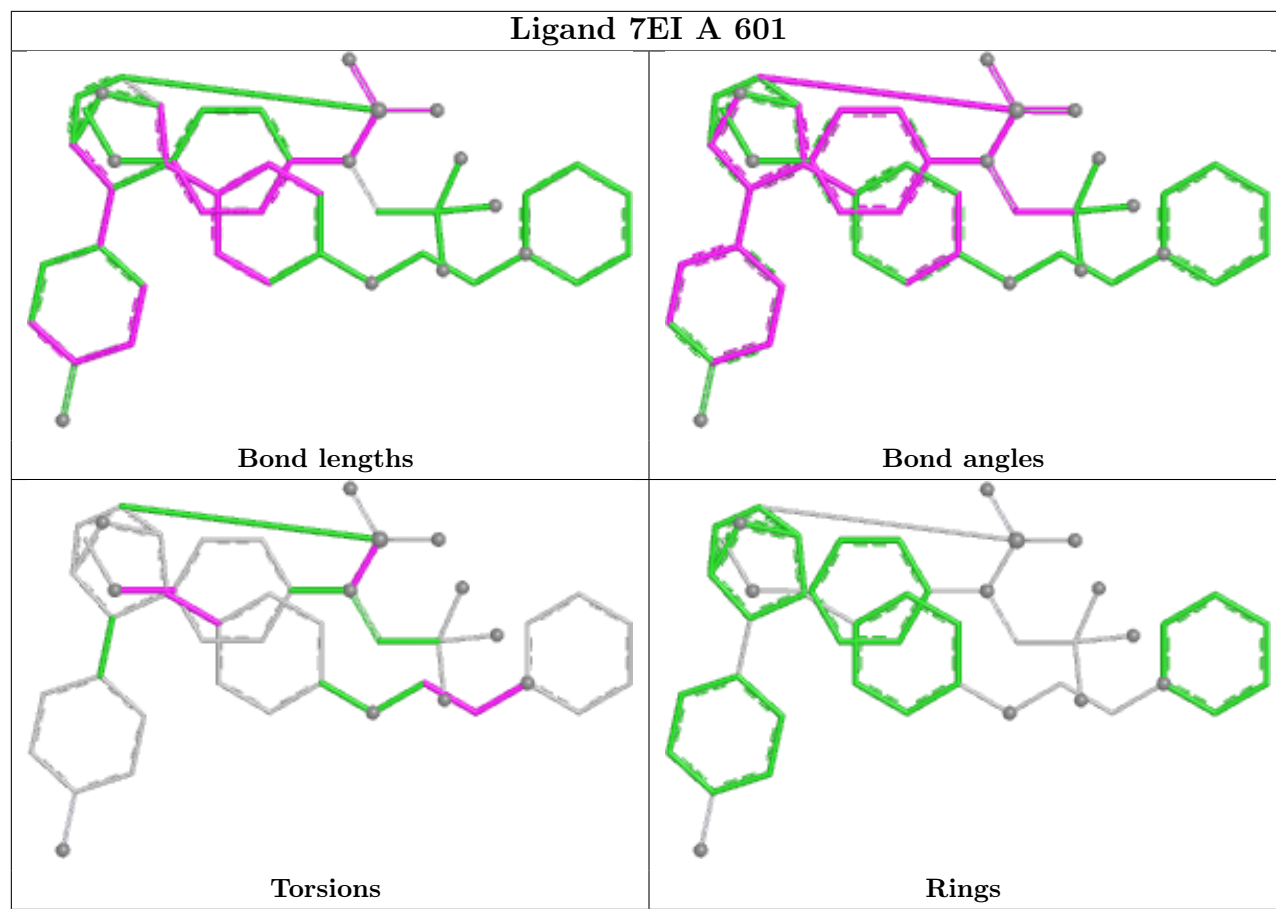


Ligand 7EI D 601









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	227/257 (88%)	0.84	34 (14%) 5 6	7, 26, 50, 76	1 (0%)
1	B	226/257 (87%)	0.82	28 (12%) 8 9	11, 24, 61, 74	2 (0%)
1	C	228/257 (88%)	0.68	26 (11%) 10 11	12, 24, 48, 66	1 (0%)
2	D	217/257 (84%)	0.85	27 (12%) 8 9	13, 24, 57, 85	0
All	All	898/1028 (87%)	0.80	115 (12%) 7 9	7, 25, 55, 85	4 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	533	VAL	5.8
2	D	526	TYR	5.6
1	B	546	ALA	5.5
2	D	421	MET	5.5
1	B	336	PRO	5.4
1	B	525	LEU	5.3
1	A	533	VAL	5.0
2	D	334	THR	4.8
1	A	546	ALA	4.8
1	B	462	LEU	4.7
2	D	306	LEU	4.7
2	D	469	LEU	4.6
1	A	415	GLY	4.5
2	D	525	LEU	4.4
1	B	532	ASN	4.3
1	A	413	ASN	4.3
1	B	533	VAL	4.2
1	B	306	LEU	4.2
2	D	468	SER	4.1
1	B	334	THR	4.0
1	C	533	VAL	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	492	LYS	3.7
1	A	421	MET	3.7
1	C	546	ALA	3.7
1	B	421	MET	3.7
1	A	525	LEU	3.6
1	B	337	PHE	3.5
1	C	306	LEU	3.5
1	C	526	TYR	3.5
2	D	459	TYR	3.5
1	B	335	ARG	3.5
2	D	524	HIS	3.5
1	C	461	PHE	3.4
1	B	464	SER	3.4
2	D	527	SER	3.4
1	B	545	ASP	3.3
1	A	336	PRO	3.3
1	A	334	THR	3.3
1	B	437	MET	3.3
1	C	463	SER	3.3
1	C	437	MET	3.2
1	A	461	PHE	3.2
1	A	416	LYS	3.2
1	A	464	SER	3.2
1	C	464	SER	3.2
1	A	526	TYR	3.1
2	D	545	ASP	3.1
1	C	525	LEU	3.1
2	D	522	MET	3.1
1	C	460	THR	3.1
2	D	331	TYR	3.1
1	B	410	LEU	3.1
1	A	437	MET	3.0
1	C	413	ASN	3.0
1	A	527	SER	3.0
1	A	332	ASP	2.9
1	A	460	THR	2.8
1	C	421	MET	2.8
1	B	331	TYR	2.8
1	C	423	GLU	2.8
2	D	460	THR	2.8
1	B	524	HIS	2.8
2	D	461	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	338	SER	2.7
1	C	334	THR	2.7
1	A	368	VAL	2.7
2	D	333	PRO	2.6
2	D	528	MET	2.6
1	A	425	PHE	2.6
1	B	459	TYR	2.6
2	D	467	LYS	2.6
1	A	331	TYR	2.6
2	D	341	SER	2.5
1	B	463	SER	2.5
2	D	422	VAL	2.5
1	A	344	GLY	2.5
1	B	413	ASN	2.5
1	B	332	ASP	2.5
1	C	527	SER	2.5
1	A	465	THR	2.4
1	B	333	PRO	2.4
1	A	534	VAL	2.4
1	C	411	ASP	2.4
1	A	333	PRO	2.3
1	A	538	ASP	2.3
1	C	332	ASP	2.3
1	B	342	MET	2.3
1	A	411	ASP	2.3
2	D	321	ASP	2.3
1	B	397	GLU	2.3
2	D	473	ASP	2.3
1	C	340	ALA	2.3
1	A	335	ARG	2.3
1	A	397	GLU	2.2
2	D	523	GLU	2.2
1	A	342	MET	2.2
2	D	437	MET	2.2
1	A	410	LEU	2.2
1	B	344	GLY	2.2
2	D	425	PHE	2.2
1	A	459	TYR	2.2
2	D	534	VAL	2.2
1	A	469	LEU	2.2
1	C	465	THR	2.2
1	C	414	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	336	PRO	2.1
1	C	534	VAL	2.1
1	A	473	ASP	2.1
1	C	524	HIS	2.1
1	A	523	GLU	2.1
1	B	411	ASP	2.1
1	C	335	ARG	2.1
1	C	331	TYR	2.1
1	C	466	LEU	2.0
1	B	501	HIS	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	A	381	10/11	0.92	0.11	18,21,32,36	0
1	YCM	B	381	10/11	0.92	0.11	18,20,31,33	0
1	YCM	C	381	10/11	0.92	0.12	19,22,33,35	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

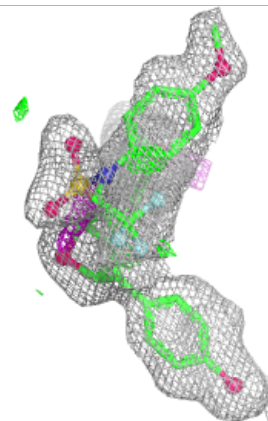
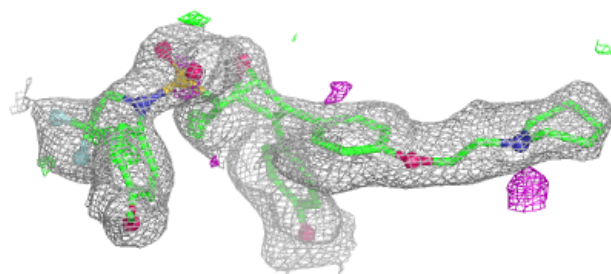
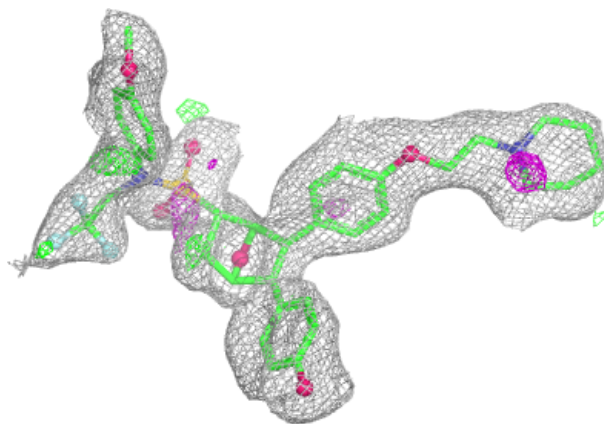
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	7EI	B	601[A]	46/46	0.86	0.13	18,25,30,30	46
3	7EI	B	601[B]	42/46	0.86	0.13	24,32,36,37	42
3	7EI	D	601	46/46	0.90	0.11	23,33,45,47	0
3	7EI	C	601	46/46	0.91	0.10	19,31,42,45	0
3	7EI	A	601	46/46	0.91	0.10	21,31,39,41	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.

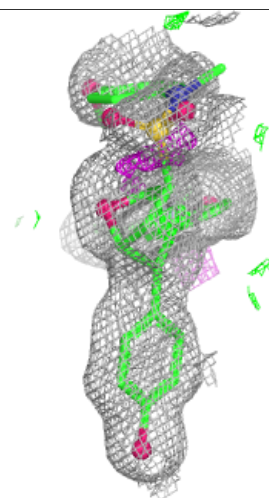
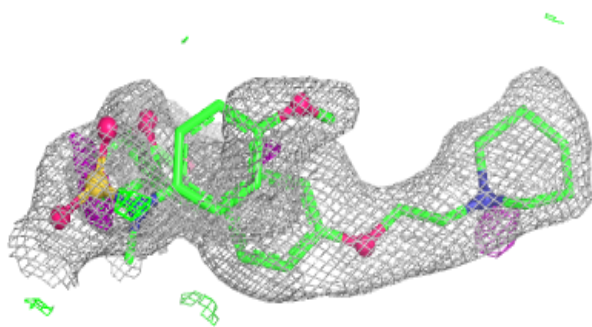
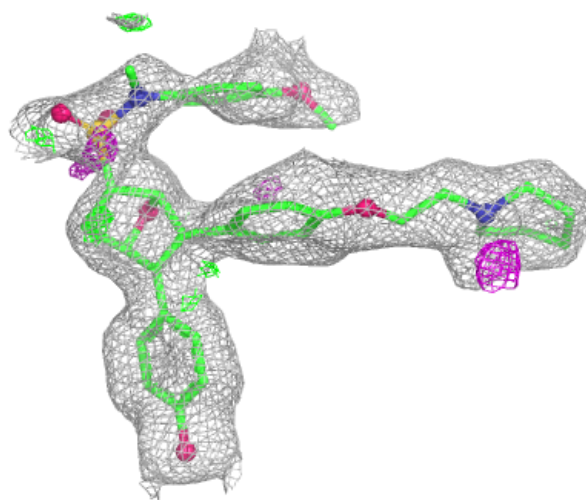
Electron density around 7EI B 601 (A):

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



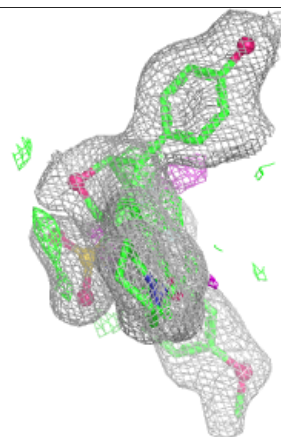
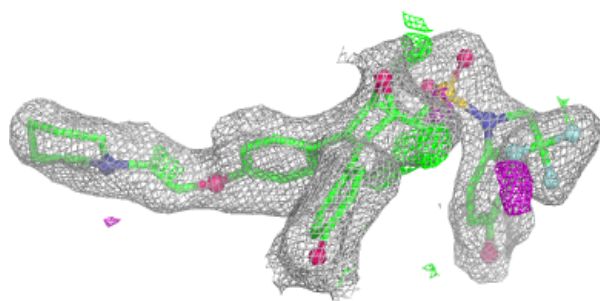
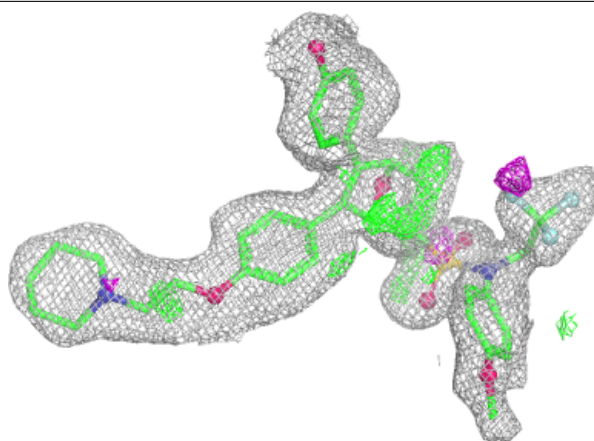
Electron density around 7EI B 601 (B):

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



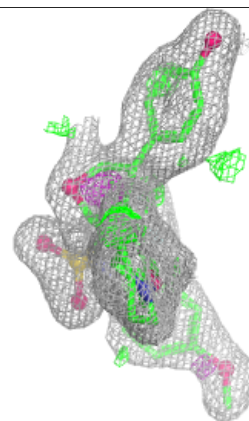
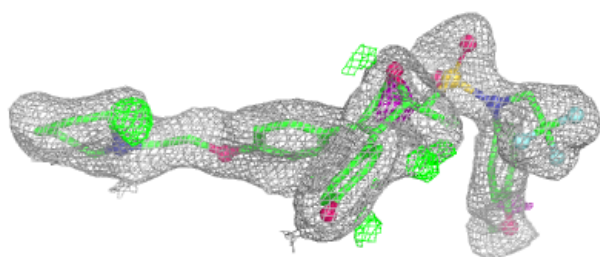
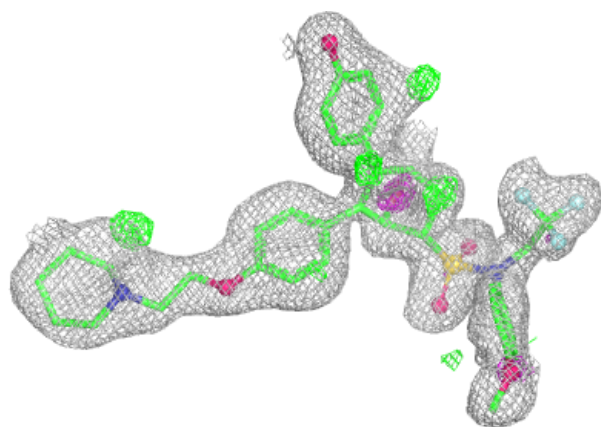
Electron density around 7EI D 601:

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



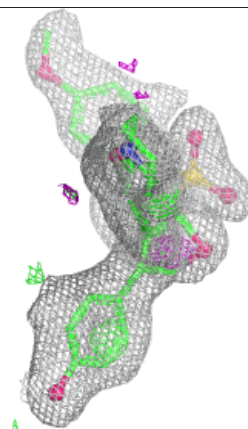
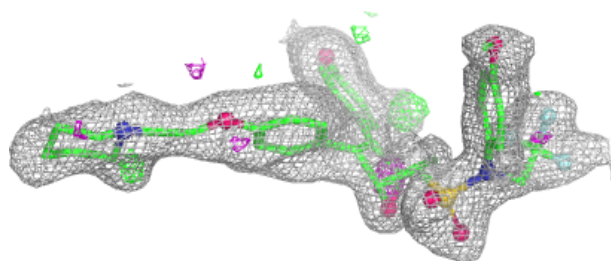
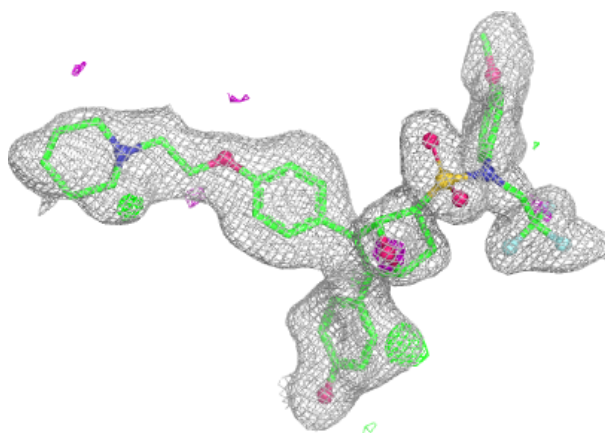
Electron density around 7EI C 601:

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



Electron density around 7EI 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.