



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 06:06 PM EDT

PDB ID : 7RS9
Title : Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with DMERI-25
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 : 1.70 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

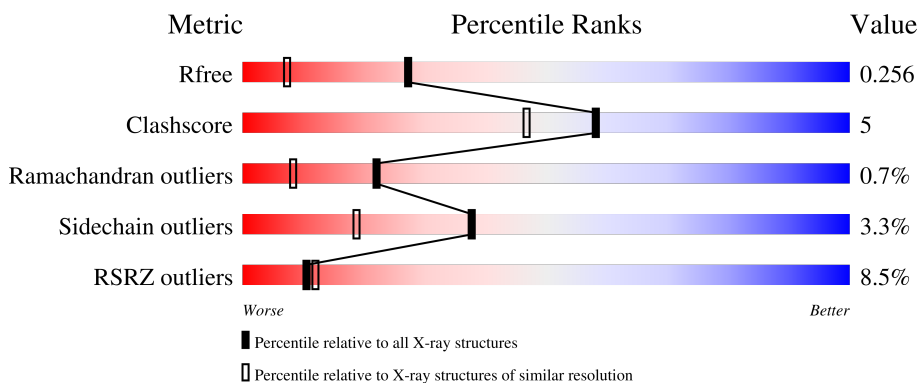
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">11% 82% 11% • 5%</p>
1	B	257	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 77% 10% • 12%</p>
1	C	257	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">8% 79% 12% • 8%</p>
1	D	257	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">7% 78% 9% 13%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7809 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.

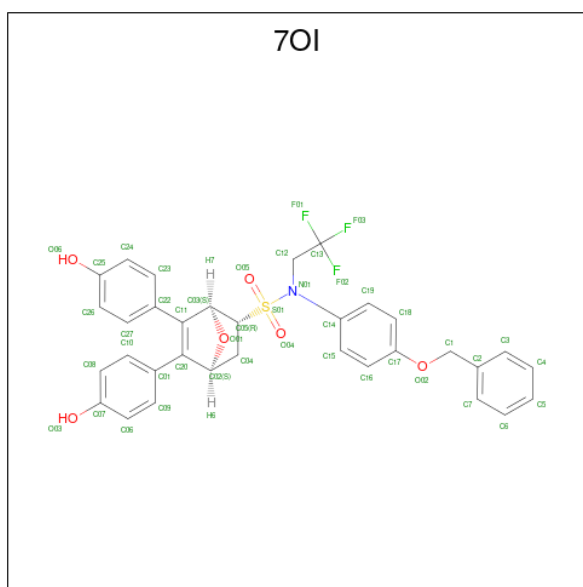
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	1939	1238	329	353	19	0	1	0
1	B	226	1809	1160	306	326	17	0	0	0
1	C	237	1897	1213	319	347	18	0	1	0
1	D	224	1788	1144	304	322	18	0	0	0

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)-N-[4-(benzyloxy)phenyl]-5,6-bis(4-hydroxyphenyl)-N-(2,2,2-trifluoroethyl)-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonamide (three-letter code: 7OI) (formula: C₃₃H₂₈F₃NO₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
			Total	C	F	N	O			S	
2	A	1	Total	36	26	3	1	5	1	0	0
2	B	1	Total	37	26	3	1	6	1	0	0
2	C	1	Total	31	21	3	1	5	1	0	0
2	D	1	Total	37	26	3	1	6	1	0	0

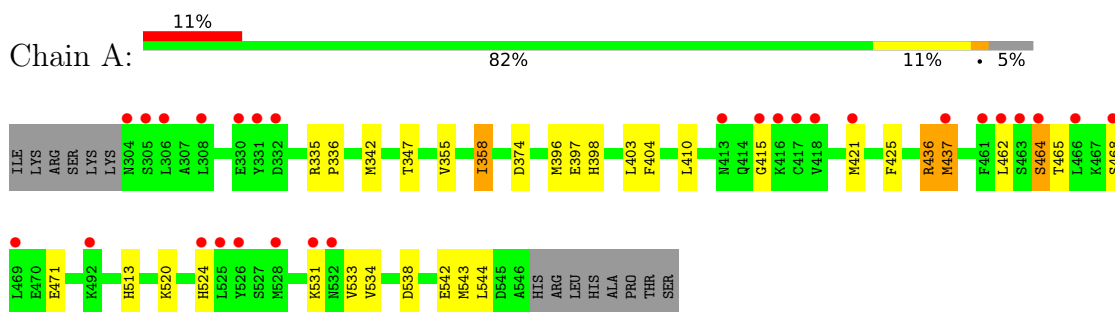
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	60	Total	O	0	0
			60	60		
3	B	48	Total	O	0	0
			48	48		
3	C	71	Total	O	0	0
			71	71		
3	D	56	Total	O	0	0
			56	56		

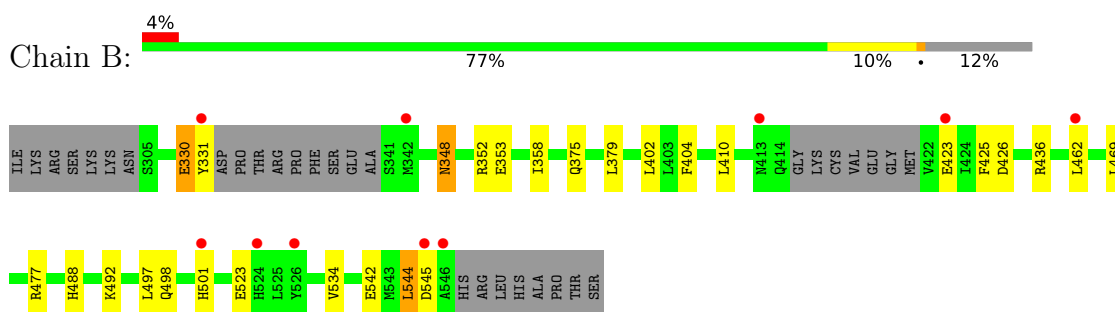
3 Residue-property plots [i](#)

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.

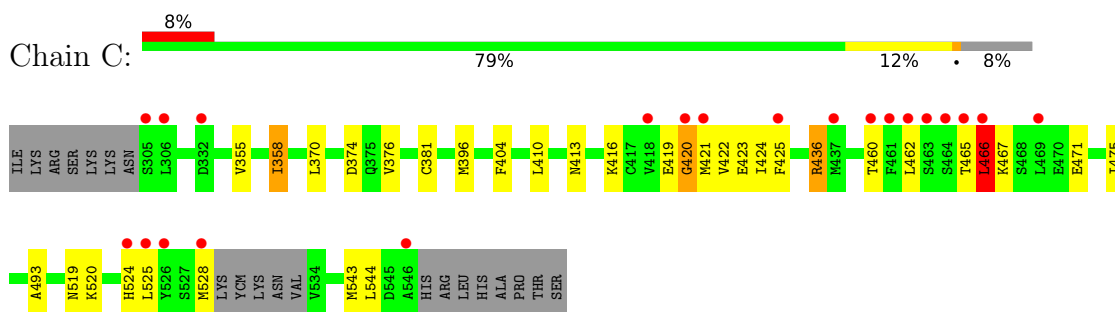
- Molecule 1: Estrogen receptor



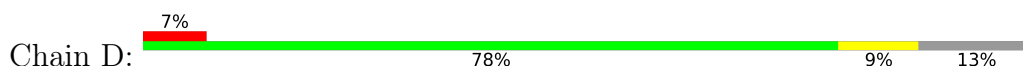
- Molecule 1: Estrogen receptor

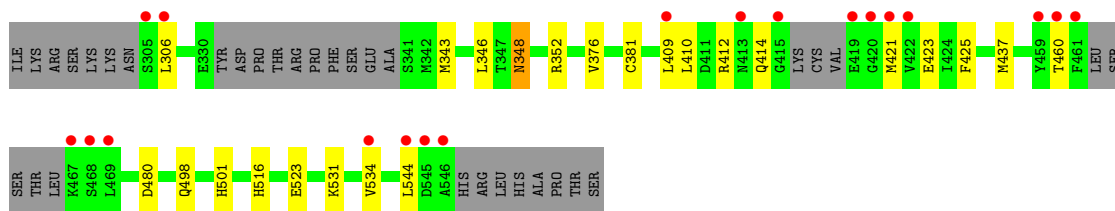


- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.57Å 58.81Å 92.86Å 86.70° 75.09° 62.91°	Depositor
Resolution (Å)	89.52 – 1.70 89.51 – 1.70	Depositor EDS
% Data completeness (in resolution range)	58.9 (89.52-1.70) 58.9 (89.51-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.214 , 0.252 0.225 , 0.256	Depositor DCC
R_{free} test set	3121 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtrriage
Anisotropy	0.027	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.115 for h,h-k,h-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7809	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% 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, 7OI

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	0.55	0/1957	0.73	1/2642 (0.0%)
1	B	0.55	0/1822	0.75	1/2457 (0.0%)
1	C	0.57	0/1921	0.75	1/2595 (0.0%)
1	D	0.56	0/1795	0.74	1/2416 (0.0%)
All	All	0.56	0/7495	0.74	4/10110 (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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	C	436	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	B	436	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	480	ASP	CB-CG-OD2	-5.09	113.72	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	335	ARG	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	1939	0	1976	16	1
1	B	1809	0	1857	16	0
1	C	1897	0	1930	29	1
1	D	1788	0	1829	13	0
2	A	36	0	0	2	0
2	B	37	0	0	1	0
2	C	31	0	0	0	0
2	D	37	0	0	4	0
3	A	60	0	0	1	0
3	B	48	0	0	1	0
3	C	71	0	0	1	0
3	D	56	0	0	1	0
All	All	7809	0	7592	72	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 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:C:421:MET:SD	1:C:423:GLU:HB2	1.92	1.10
1:D:348:ASN:ND2	3:D:701:HOH:O	1.98	0.94
1:C:370:LEU:HD11	1:C:475:ILE:HD11	1.56	0.87
1:A:397[B]:GLU:HA	1:A:397[B]:GLU:OE1	1.76	0.86
1:C:416:LYS:HG2	1:C:422:VAL:HG21	1.60	0.84
1:A:513:HIS:ND1	3:A:701:HOH:O	2.17	0.77
1:A:355:VAL:HG22	1:A:543:MET:CE	2.17	0.75
1:A:355:VAL:HG22	1:A:543:MET:HE1	1.69	0.73
1:C:413:ASN:OD1	3:C:701:HOH:O	2.09	0.71
1:C:421:MET:SD	1:C:423:GLU:CB	2.78	0.67
1:A:464:SER:O	1:A:468:SER:HB2	1.97	0.65
1:C:355:VAL:HG22	1:C:543:MET:CE	2.28	0.64
1:A:404:PHE:CE2	1:A:410:LEU:HD12	2.39	0.58
1:C:421:MET:CE	1:C:524:HIS:CE1	2.88	0.57
1:B:469:LEU:HD13	1:C:493:ALA:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:PHE:CE2	1:B:410:LEU:HD12	2.41	0.56
1:C:404:PHE:CE2	1:C:410:LEU:HD12	2.41	0.56
1:D:343:MET:HE1	2:D:601:7OI:C18	2.37	0.55
1:A:347:THR:HG23	1:A:533:VAL:HG22	1.88	0.55
1:B:542:GLU:HA	1:B:545:ASP:OD1	2.07	0.55
1:D:346:LEU:CD1	2:D:601:7OI:C16	2.86	0.53
1:B:488:HIS:NE2	1:B:492:LYS:HD2	2.24	0.52
1:D:343:MET:CE	2:D:601:7OI:C18	2.88	0.51
1:C:419:GLU:O	1:C:420:GLY:C	2.49	0.50
1:C:419:GLU:O	1:C:420:GLY:O	2.30	0.49
1:B:358:ILE:HG23	1:B:544:LEU:HD13	1.95	0.49
1:C:466:LEU:HG	1:C:467:LYS:N	2.27	0.49
1:C:462:LEU:HG	1:C:462:LEU:O	2.13	0.49
1:B:477:ARG:NH2	3:B:701:HOH:O	2.33	0.48
2:A:601:7OI:O01	2:A:601:7OI:C12	2.62	0.48
1:B:488:HIS:CD2	1:B:492:LYS:HD2	2.49	0.48
1:A:358:ILE:HG23	1:A:544:LEU:HD23	1.97	0.47
1:C:355:VAL:HG22	1:C:543:MET:HE3	1.97	0.47
1:C:465:THR:O	1:C:467:LYS:N	2.47	0.47
1:C:421:MET:HE2	1:C:524:HIS:CE1	2.51	0.46
1:A:462:LEU:HG	1:B:426:ASP:HB3	1.98	0.46
1:C:355:VAL:HA	1:C:543:MET:CE	2.46	0.46
1:A:415:GLY:O	1:A:421:MET:HB3	2.15	0.46
1:C:520:LYS:O	1:C:524:HIS:CD2	2.69	0.46
1:D:346:LEU:HD12	2:D:601:7OI:C16	2.46	0.46
1:C:396:MET:O	1:C:436:ARG:HD3	2.15	0.45
1:C:519:ASN:HD21	1:D:516:HIS:HA	1.81	0.45
1:A:520:LYS:O	1:A:524:HIS:CD2	2.70	0.45
1:C:358:ILE:HG23	1:C:544:LEU:HD23	1.99	0.45
1:B:375:GLN:HB3	1:B:544:LEU:HD21	1.98	0.45
1:B:330:GLU:HA	1:B:330:GLU:OE1	2.18	0.44
1:B:353:GLU:OE2	2:B:601:7OI:O03	2.35	0.44
1:D:348:ASN:HD21	1:D:352:ARG:HH21	1.63	0.44
1:A:396:MET:O	1:A:436:ARG:HD3	2.18	0.43
1:B:542:GLU:O	1:B:545:ASP:OD1	2.36	0.43
1:B:498:GLN:HA	1:B:501:HIS:CE1	2.53	0.43
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.53	0.43
1:C:525:LEU:O	1:C:528:MET:HG3	2.18	0.43
1:D:412:ARG:HA	1:D:425:PHE:CE1	2.54	0.42
1:C:421:MET:HB3	1:C:424:ILE:H	1.84	0.42
1:C:421:MET:HE1	1:C:524:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:LEU:HD12	1:B:425:PHE:CE2	2.55	0.42
1:C:374:ASP:OD2	1:C:471:GLU:OE2	2.37	0.42
1:D:409:LEU:C	1:D:410:LEU:HD12	2.40	0.42
1:A:437:MET:HE3	1:A:437:MET:O	2.20	0.42
1:B:348:ASN:HD21	1:B:352:ARG:HH21	1.66	0.42
1:D:376:VAL:CG2	1:D:544:LEU:HD12	2.50	0.41
1:C:355:VAL:HA	1:C:543:MET:HE2	2.03	0.41
1:A:398:HIS:CE1	1:A:403:LEU:HD12	2.55	0.41
1:C:466:LEU:HG	1:C:467:LYS:H	1.84	0.41
1:D:348:ASN:ND2	1:D:352:ARG:HH21	2.19	0.41
1:A:533:VAL:HG13	2:A:601:7OI:O06	2.21	0.41
1:A:374:ASP:OD2	1:A:471:GLU:OE1	2.39	0.40
1:C:376:VAL:CG2	1:C:544:LEU:HD12	2.52	0.40
1:D:381:YCM:NZ2	1:D:460:THR:HG21	2.37	0.40
1:C:381:YCM:NZ2	1:C:460:THR:HG21	2.36	0.40
1:B:358:ILE:CD1	1:B:379:LEU:HD13	2.52	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)
1:A:542:GLU:OE2	1:C:465:THR:OG1[1_556]	2.16	0.04

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	240/257 (93%)	233 (97%)	4 (2%)	3 (1%)	12 2
1	B	218/257 (85%)	216 (99%)	2 (1%)	0	100 100
1	C	233/257 (91%)	226 (97%)	5 (2%)	2 (1%)	17 5
1	D	214/257 (83%)	210 (98%)	3 (1%)	1 (0%)	29 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	905/1028 (88%)	885 (98%)	14 (2%)	6 (1%)	22	8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	PRO
1	C	466	LEU
1	D	421	MET
1	A	465	THR
1	C	420	GLY
1	A	464	SER

5.3.2 Protein sidechains [i](#)

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	217/230 (94%)	210 (97%)	7 (3%)	39	20
1	B	203/230 (88%)	194 (96%)	9 (4%)	28	11
1	C	213/230 (93%)	210 (99%)	3 (1%)	67	53
1	D	198/230 (86%)	190 (96%)	8 (4%)	31	13
All	All	831/920 (90%)	804 (97%)	27 (3%)	38	20

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	MET
1	A	358	ILE
1	A	425	PHE
1	A	437	MET
1	A	531	LYS
1	A	534	VAL
1	A	538	ASP
1	B	330	GLU
1	B	331	TYR

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Mol	Chain	Res	Type
1	B	348	ASN
1	B	423	GLU
1	B	462	LEU
1	B	497	LEU
1	B	523	GLU
1	B	534	VAL
1	B	544	LEU
1	C	358	ILE
1	C	425	PHE
1	C	466	LEU
1	D	306	LEU
1	D	348	ASN
1	D	414	GLN
1	D	423	GLU
1	D	437	MET
1	D	523	GLU
1	D	531	LYS
1	D	534	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	HIS
1	A	519	ASN
1	A	524	HIS
1	B	373	HIS
1	B	519	ASN
1	C	398	HIS
1	C	488	HIS
1	C	519	ASN
1	C	524	HIS
1	D	519	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	530	1	4,5,10	0.69	0	1,5,12	0.16	0
1	YCM	C	381	1	7,9,10	0.45	0	4,10,12	0.32	0
1	YCM	B	530	1	4,5,10	0.80	0	1,5,12	0.28	0
1	YCM	D	381	1	7,9,10	0.65	0	4,10,12	0.22	0
1	YCM	D	530	1	7,9,10	0.44	0	4,10,12	0.48	0
1	YCM	B	381	1	7,9,10	0.67	0	4,10,12	0.31	0
1	YCM	A	381	1	7,9,10	0.44	0	4,10,12	0.20	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	530	1	-	0/1/4/10	-
1	YCM	C	381	1	-	1/6/8/10	-
1	YCM	B	530	1	-	0/1/4/10	-
1	YCM	D	381	1	-	1/6/8/10	-
1	YCM	D	530	1	-	0/6/8/10	-
1	YCM	B	381	1	-	1/6/8/10	-
1	YCM	A	381	1	-	1/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	7OI	A	601	-	37,40,49	3.00	15 (40%)	48,61,73	2.69	13 (27%)
2	7OI	B	601	-	38,41,49	2.91	10 (26%)	50,63,73	2.53	15 (30%)
2	7OI	C	601	-	31,34,49	2.77	11 (35%)	40,53,73	2.44	6 (15%)
2	7OI	D	601	-	38,41,49	3.57	24 (63%)	50,63,73	2.84	22 (44%)

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	7OI	A	601	-	-	10/27/53/58	0/6/5/6
2	7OI	B	601	-	-	11/27/53/58	0/6/5/6
2	7OI	C	601	-	-	8/21/49/58	0/5/4/6
2	7OI	D	601	-	-	9/27/53/58	0/6/5/6

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	7OI	C14-N01	-14.22	1.24	1.44
2	A	601	7OI	C14-N01	-11.35	1.28	1.44
2	B	601	7OI	C14-N01	-10.89	1.29	1.44
2	C	601	7OI	C14-N01	-7.88	1.29	1.47
2	A	601	7OI	C22-C11	-7.11	1.35	1.48
2	C	601	7OI	C01-C20	-6.87	1.35	1.48
2	A	601	7OI	C01-C20	-6.71	1.35	1.48
2	C	601	7OI	C22-C11	-6.59	1.36	1.48
2	B	601	7OI	C01-C20	-6.37	1.36	1.48
2	B	601	7OI	C22-C11	-5.98	1.37	1.48
2	D	601	7OI	C01-C20	-5.81	1.37	1.48
2	D	601	7OI	C22-C11	-5.69	1.37	1.48
2	D	601	7OI	O05-S01	-5.30	1.39	1.43
2	D	601	7OI	C03-C11	5.21	1.56	1.50
2	B	601	7OI	O04-S01	4.90	1.47	1.43
2	D	601	7OI	O04-S01	-4.26	1.40	1.43
2	A	601	7OI	O04-S01	3.78	1.46	1.43
2	B	601	7OI	C03-C11	3.41	1.54	1.50
2	C	601	7OI	O04-S01	3.30	1.46	1.43
2	B	601	7OI	O05-S01	3.29	1.46	1.43
2	A	601	7OI	O05-S01	3.01	1.46	1.43
2	C	601	7OI	C03-C11	3.00	1.53	1.50
2	C	601	7OI	C12-N01	2.90	1.52	1.47
2	D	601	7OI	C16-C17	-2.89	1.33	1.38
2	D	601	7OI	C06-C07	-2.86	1.33	1.38
2	D	601	7OI	C19-C14	-2.81	1.33	1.39
2	D	601	7OI	C23-C24	-2.81	1.33	1.38
2	D	601	7OI	O01-C03	-2.75	1.40	1.43
2	A	601	7OI	C09-C06	-2.70	1.33	1.38
2	D	601	7OI	C08-C07	-2.68	1.33	1.38
2	D	601	7OI	O01-C02	-2.67	1.38	1.44
2	D	601	7OI	C24-C25	-2.67	1.33	1.38
2	D	601	7OI	C27-C22	-2.66	1.34	1.39
2	D	601	7OI	C15-C14	-2.65	1.34	1.39
2	D	601	7OI	C27-C26	-2.61	1.34	1.38
2	C	601	7OI	O05-S01	2.59	1.45	1.43
2	D	601	7OI	C26-C25	-2.48	1.34	1.38
2	B	601	7OI	C08-C10	-2.43	1.34	1.38
2	A	601	7OI	O01-C03	-2.38	1.40	1.43
2	B	601	7OI	C18-C17	-2.36	1.34	1.38
2	D	601	7OI	C18-C17	-2.28	1.34	1.38
2	D	601	7OI	C19-C18	-2.25	1.34	1.38
2	A	601	7OI	C27-C26	-2.22	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	7OI	C03-C11	2.19	1.53	1.50
2	D	601	7OI	C16-C15	-2.16	1.34	1.38
2	A	601	7OI	C26-C25	-2.12	1.34	1.38
2	C	601	7OI	C08-C10	-2.11	1.34	1.38
2	B	601	7OI	C06-C07	-2.11	1.34	1.38
2	A	601	7OI	C23-C24	-2.10	1.34	1.38
2	A	601	7OI	C18-C19	-2.08	1.34	1.38
2	D	601	7OI	C23-C22	-2.07	1.35	1.39
2	C	601	7OI	C27-C26	-2.06	1.35	1.38
2	C	601	7OI	C27-C22	-2.03	1.35	1.39
2	A	601	7OI	C06-C07	-2.03	1.35	1.38
2	D	601	7OI	C09-C06	-2.02	1.35	1.38
2	C	601	7OI	C08-C07	-2.02	1.35	1.38
2	D	601	7OI	C09-C01	-2.02	1.35	1.39
2	A	601	7OI	C10-C01	-2.02	1.35	1.39
2	A	601	7OI	C23-C22	-2.02	1.35	1.39
2	B	601	7OI	C26-C25	-2.00	1.35	1.38

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	7OI	O05-S01-N01	11.73	119.45	107.49
2	B	601	7OI	O05-S01-N01	9.99	119.79	107.56
2	A	601	7OI	O05-S01-N01	9.94	119.74	107.56
2	D	601	7OI	C13-C12-N01	9.65	121.51	112.14
2	A	601	7OI	C13-C12-N01	9.62	121.49	112.14
2	B	601	7OI	C13-C12-N01	7.93	119.84	112.14
2	D	601	7OI	O05-S01-N01	7.80	117.11	107.56
2	D	601	7OI	O04-S01-O05	6.66	123.50	119.22
2	C	601	7OI	O04-S01-N01	6.42	114.04	107.49
2	A	601	7OI	O04-S01-N01	5.65	114.48	107.56
2	B	601	7OI	C19-C14-N01	5.13	127.82	120.16
2	D	601	7OI	C22-C11-C03	5.07	129.60	121.27
2	D	601	7OI	C23-C22-C11	4.27	126.44	120.91
2	A	601	7OI	C12-N01-C14	4.03	122.97	117.59
2	A	601	7OI	C19-C14-N01	3.88	125.95	120.16
2	B	601	7OI	O04-S01-N01	3.61	111.98	107.56
2	D	601	7OI	F02-C13-C12	3.60	118.04	112.13
2	D	601	7OI	C09-C01-C10	-3.57	113.50	118.59
2	D	601	7OI	C27-C22-C23	-3.33	113.85	118.59
2	D	601	7OI	C02-C20-C11	-3.15	100.36	106.97
2	A	601	7OI	O04-S01-O05	3.14	121.24	119.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	7OI	O01-C02-C04	-3.12	98.51	104.64
2	D	601	7OI	O04-S01-N01	3.11	111.36	107.56
2	B	601	7OI	C27-C22-C23	-3.01	114.30	118.59
2	A	601	7OI	C01-C20-C11	2.82	136.12	128.81
2	D	601	7OI	C12-N01-C14	-2.82	113.83	117.59
2	B	601	7OI	C19-C18-C17	2.80	122.95	119.88
2	A	601	7OI	C22-C11-C20	2.76	135.96	128.81
2	B	601	7OI	C23-C22-C11	2.74	124.45	120.91
2	B	601	7OI	O01-C02-C20	-2.72	98.20	101.99
2	D	601	7OI	O01-C02-C20	-2.71	98.23	101.99
2	B	601	7OI	C19-C14-C15	-2.62	113.83	119.16
2	B	601	7OI	C16-C15-C14	2.57	123.70	120.32
2	B	601	7OI	C18-C17-C16	-2.54	115.49	119.77
2	A	601	7OI	C18-C19-C14	2.52	122.98	119.68
2	B	601	7OI	C02-C20-C11	-2.47	101.78	106.97
2	C	601	7OI	C02-C20-C11	-2.41	101.91	106.97
2	C	601	7OI	C01-C20-C11	2.36	134.92	128.81
2	D	601	7OI	C26-C27-C22	2.35	123.51	120.78
2	D	601	7OI	C18-C17-C16	-2.33	115.84	119.77
2	A	601	7OI	C16-C15-C14	2.33	122.73	119.68
2	C	601	7OI	O01-C02-C20	-2.32	98.77	101.99
2	B	601	7OI	C26-C25-C24	-2.27	115.94	119.77
2	D	601	7OI	C10-C01-C20	2.26	123.83	120.91
2	A	601	7OI	C19-C14-C15	-2.25	114.58	119.16
2	A	601	7OI	C10-C01-C20	2.25	123.82	120.91
2	D	601	7OI	C19-C14-N01	2.24	123.50	120.16
2	B	601	7OI	C22-C11-C03	2.22	124.92	121.27
2	D	601	7OI	C06-C09-C01	2.12	123.25	120.78
2	D	601	7OI	C24-C23-C22	2.09	123.20	120.78
2	C	601	7OI	C27-C22-C23	-2.08	115.63	118.59
2	D	601	7OI	C08-C07-C06	-2.07	116.28	119.77
2	D	601	7OI	C08-C10-C01	2.04	123.15	120.78
2	D	601	7OI	C19-C18-C17	2.02	122.09	119.88
2	A	601	7OI	C02-C20-C11	-2.01	102.75	106.97
2	B	601	7OI	C26-C27-C22	2.01	123.11	120.78

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	7OI	N01-C12-C13-F01
2	A	601	7OI	N01-C12-C13-F02

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Mol	Chain	Res	Type	Atoms
2	A	601	7OI	N01-C12-C13-F03
2	A	601	7OI	C13-C12-N01-S01
2	A	601	7OI	C13-C12-N01-C14
2	A	601	7OI	C03-C05-S01-O05
2	B	601	7OI	C12-N01-S01-O05
2	B	601	7OI	C13-C12-N01-S01
2	B	601	7OI	C13-C12-N01-C14
2	B	601	7OI	C03-C05-S01-O05
2	C	601	7OI	N01-C12-C13-F01
2	C	601	7OI	N01-C12-C13-F03
2	C	601	7OI	C03-C05-S01-O05
2	C	601	7OI	C04-C05-S01-O05
2	D	601	7OI	C12-N01-S01-O04
2	D	601	7OI	C03-C05-S01-O05
2	D	601	7OI	C04-C05-S01-O05
2	D	601	7OI	C03-C05-S01-O04
2	D	601	7OI	C04-C05-S01-O04
2	C	601	7OI	N01-C12-C13-F02
2	B	601	7OI	C03-C05-S01-O04
2	C	601	7OI	C03-C05-S01-O04
2	A	601	7OI	C04-C05-S01-O04
2	B	601	7OI	C04-C05-S01-O05
2	B	601	7OI	C04-C05-S01-O04
2	C	601	7OI	C04-C05-S01-O04
2	B	601	7OI	C12-N01-S01-C05
2	D	601	7OI	C12-N01-S01-C05
2	C	601	7OI	C14-N01-S01-O05
2	B	601	7OI	C12-N01-S01-O04
2	D	601	7OI	C12-N01-S01-O05
2	A	601	7OI	C03-C05-S01-O04
2	A	601	7OI	C19-C14-N01-S01
2	B	601	7OI	C09-C01-C20-C11
2	D	601	7OI	C10-C01-C20-C11
2	A	601	7OI	C14-N01-S01-C05
2	B	601	7OI	C10-C01-C20-C11
2	D	601	7OI	C09-C01-C20-C11

There are no ring outliers.

3 monomers are involved in 7 short contacts:

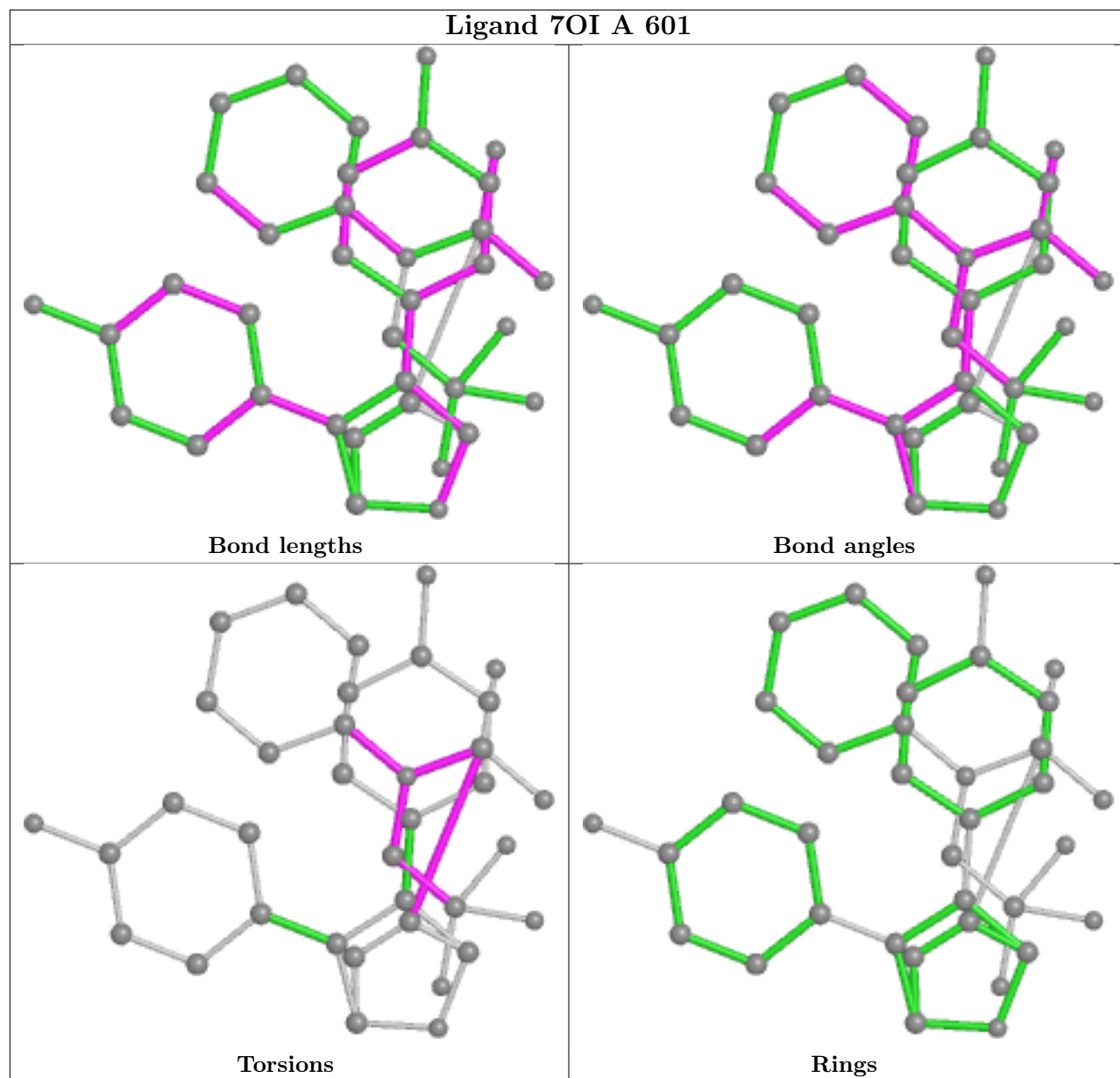
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	7OI	2	0

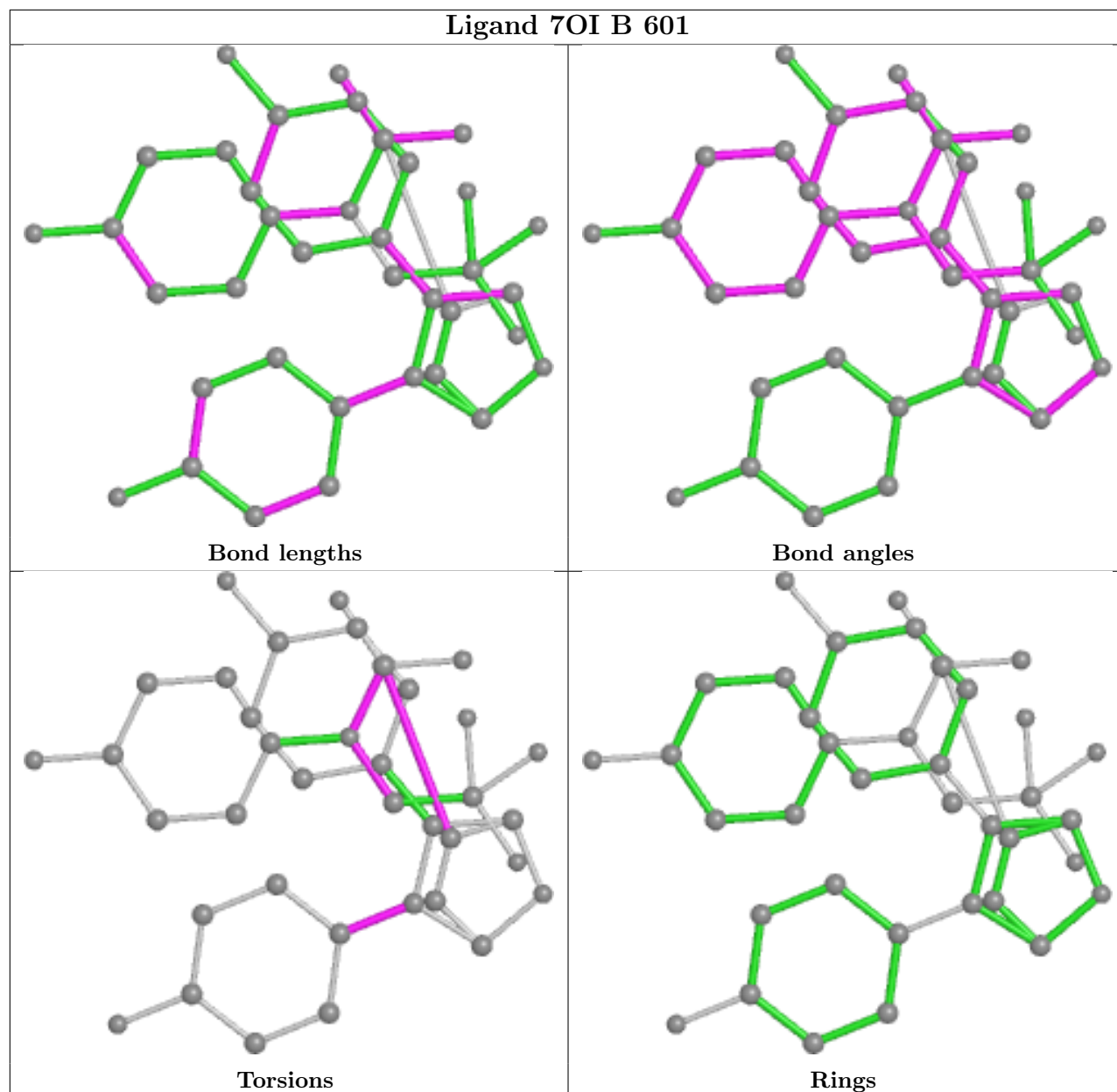
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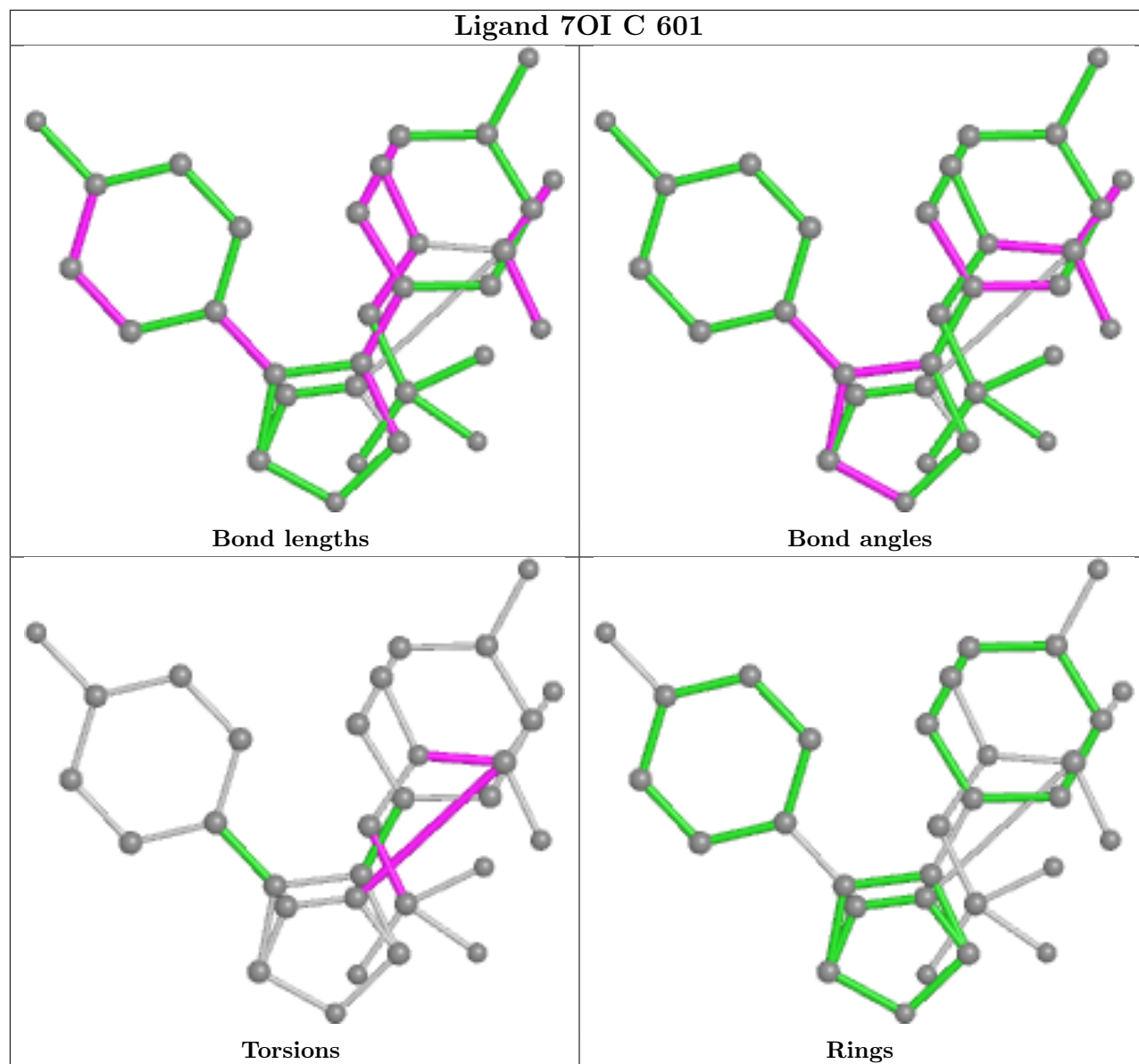
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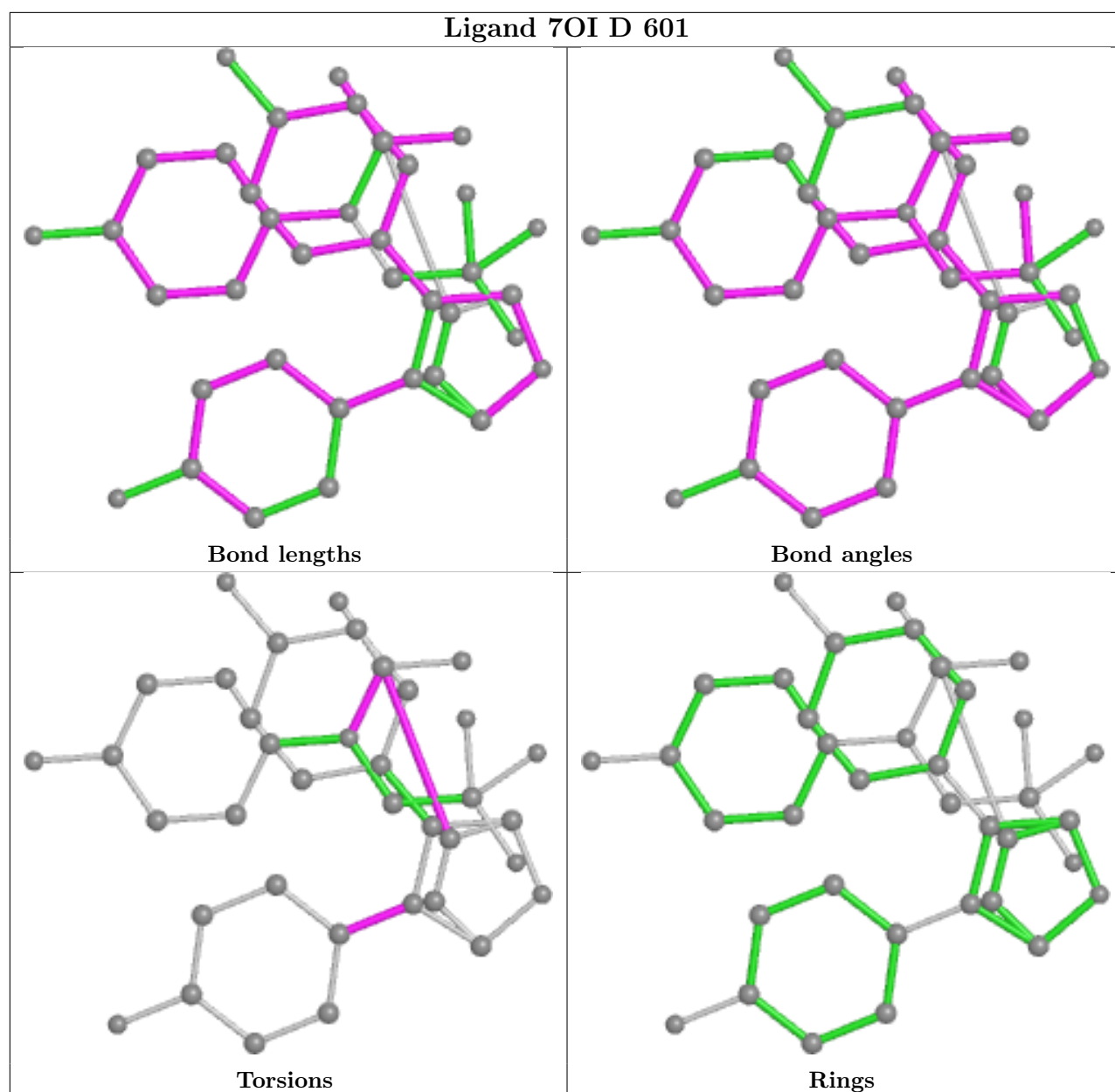
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	7OI	1	0
2	D	601	7OI	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	241/257 (93%)	0.66	28 (11%) 4 5	17, 36, 78, 101	0
1	B	224/257 (87%)	0.43	10 (4%) 33 37	18, 34, 68, 92	0
1	C	236/257 (91%)	0.58	21 (8%) 9 11	18, 33, 79, 126	0
1	D	222/257 (86%)	0.50	19 (8%) 10 12	19, 33, 74, 96	0
All	All	923/1028 (89%)	0.54	78 (8%) 10 12	17, 34, 76, 126	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	526	TYR	8.6
1	C	464	SER	8.2
1	C	462	LEU	7.5
1	A	462	LEU	7.3
1	C	420	GLY	6.6
1	A	464	SER	6.3
1	B	546	ALA	6.0
1	D	420	GLY	5.8
1	A	463	SER	5.3
1	D	461	PHE	5.2
1	A	305	SER	4.6
1	D	545	ASP	4.5
1	A	466	LEU	4.4
1	D	546	ALA	4.1
1	C	463	SER	3.9
1	B	331	TYR	3.9
1	D	305	SER	3.8
1	C	421	MET	3.8
1	A	418	VAL	3.7
1	B	413	ASN	3.6
1	A	304	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	467	LYS	3.5
1	A	332	ASP	3.5
1	A	437	MET	3.5
1	C	305	SER	3.5
1	A	528	MET	3.4
1	C	461	PHE	3.4
1	A	526	TYR	3.3
1	A	306	LEU	3.3
1	B	526	TYR	3.2
1	A	417	CYS	3.2
1	D	422	VAL	3.2
1	A	421	MET	3.2
1	D	534	VAL	3.1
1	B	462	LEU	3.1
1	C	528	MET	3.0
1	C	524	HIS	3.0
1	D	468	SER	3.0
1	D	415	GLY	3.0
1	B	545	ASP	2.9
1	A	461	PHE	2.9
1	D	421	MET	2.8
1	A	330	GLU	2.8
1	D	413	ASN	2.8
1	A	413	ASN	2.8
1	A	415	GLY	2.7
1	A	524	HIS	2.7
1	C	465	THR	2.7
1	D	459	TYR	2.7
1	B	524	HIS	2.6
1	A	492	LYS	2.6
1	C	460	THR	2.6
1	C	469	LEU	2.6
1	A	532	ASN	2.6
1	A	416	LYS	2.5
1	D	544	LEU	2.5
1	C	425	PHE	2.5
1	A	308	LEU	2.4
1	C	437	MET	2.4
1	A	531	LYS	2.4
1	C	332	ASP	2.4
1	D	460	THR	2.3
1	A	469	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	546	ALA	2.3
1	A	331	TYR	2.3
1	C	466	LEU	2.2
1	D	419	GLU	2.2
1	C	306	LEU	2.1
1	A	468	SER	2.1
1	B	342	MET	2.1
1	A	525	LEU	2.1
1	D	306	LEU	2.1
1	D	409	LEU	2.1
1	B	423	GLU	2.1
1	B	501	HIS	2.1
1	C	418	VAL	2.1
1	C	525	LEU	2.0
1	D	469	LEU	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	D	530	10/11	0.88	0.15	42,52,70,82	0
1	YCM	B	530	6/11	0.89	0.20	49,57,59,61	0
1	YCM	A	530	6/11	0.90	0.32	95,107,118,152	0
1	YCM	C	381	10/11	0.92	0.15	21,28,59,67	0
1	YCM	A	381	10/11	0.92	0.13	23,29,48,54	0
1	YCM	D	381	10/11	0.95	0.12	25,28,59,62	0
1	YCM	B	381	10/11	0.97	0.10	23,29,64,71	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

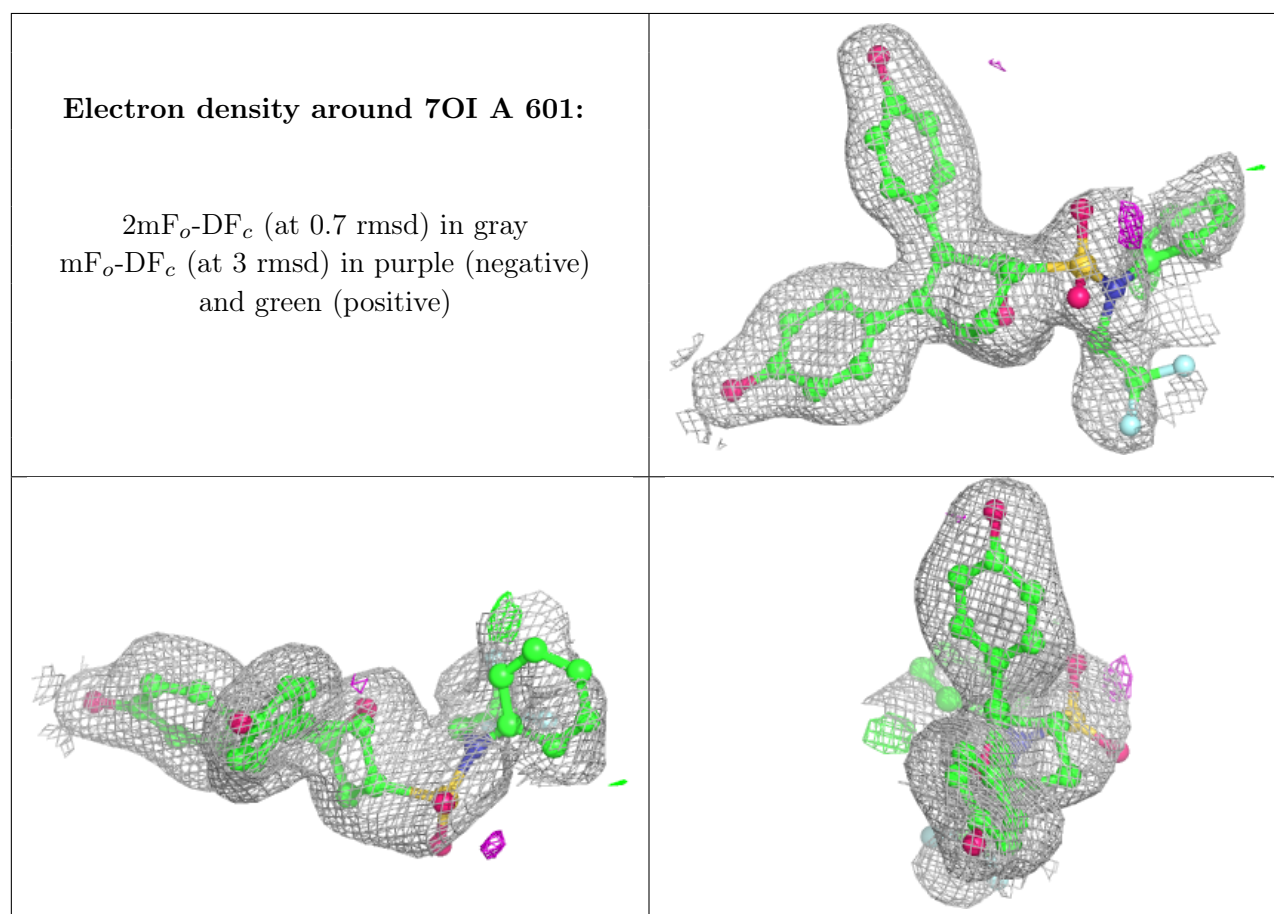
6.4 Ligands [i](#)

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.

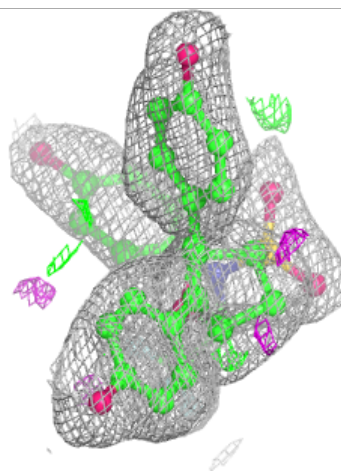
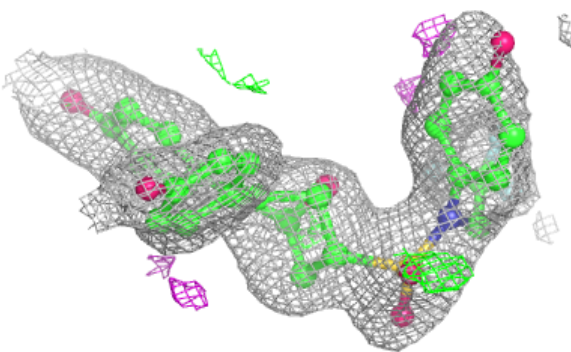
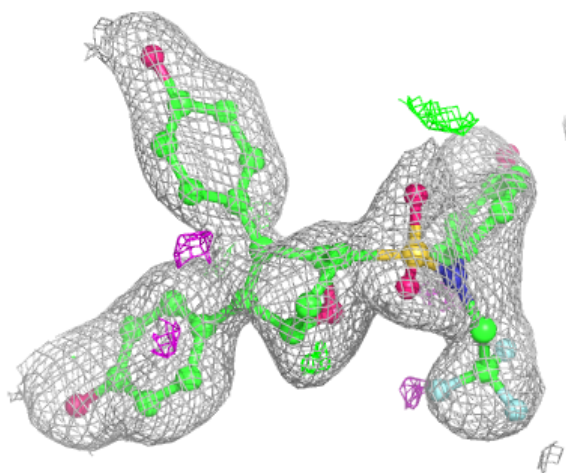
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	7OI	A	601	36/44	0.89	0.16	30,58,129,171	0
2	7OI	B	601	37/44	0.89	0.14	27,53,78,83	0
2	7OI	C	601	31/44	0.89	0.11	27,45,125,136	0
2	7OI	D	601	37/44	0.91	0.12	22,44,71,77	0

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.



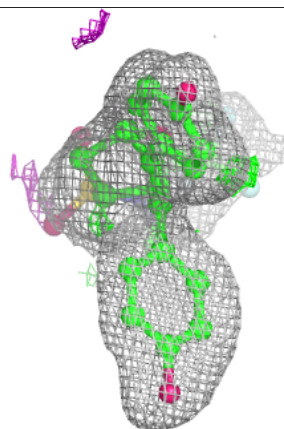
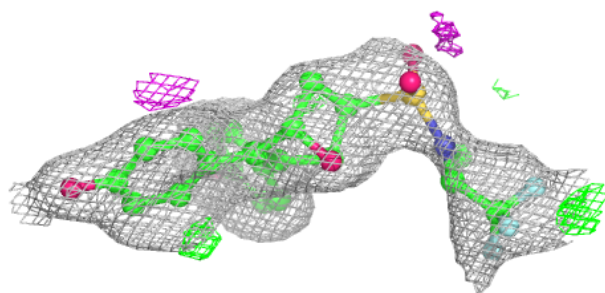
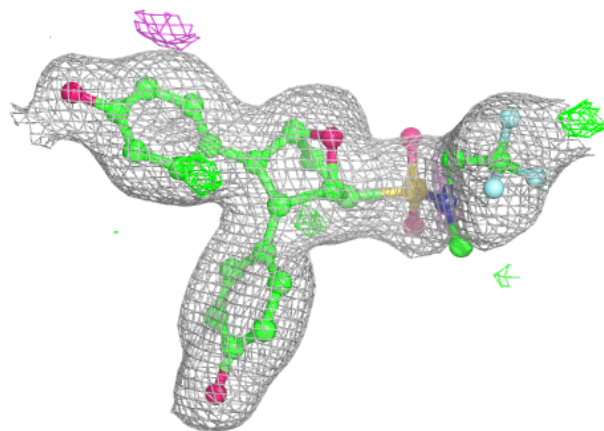
Electron density around 7OI B 601:

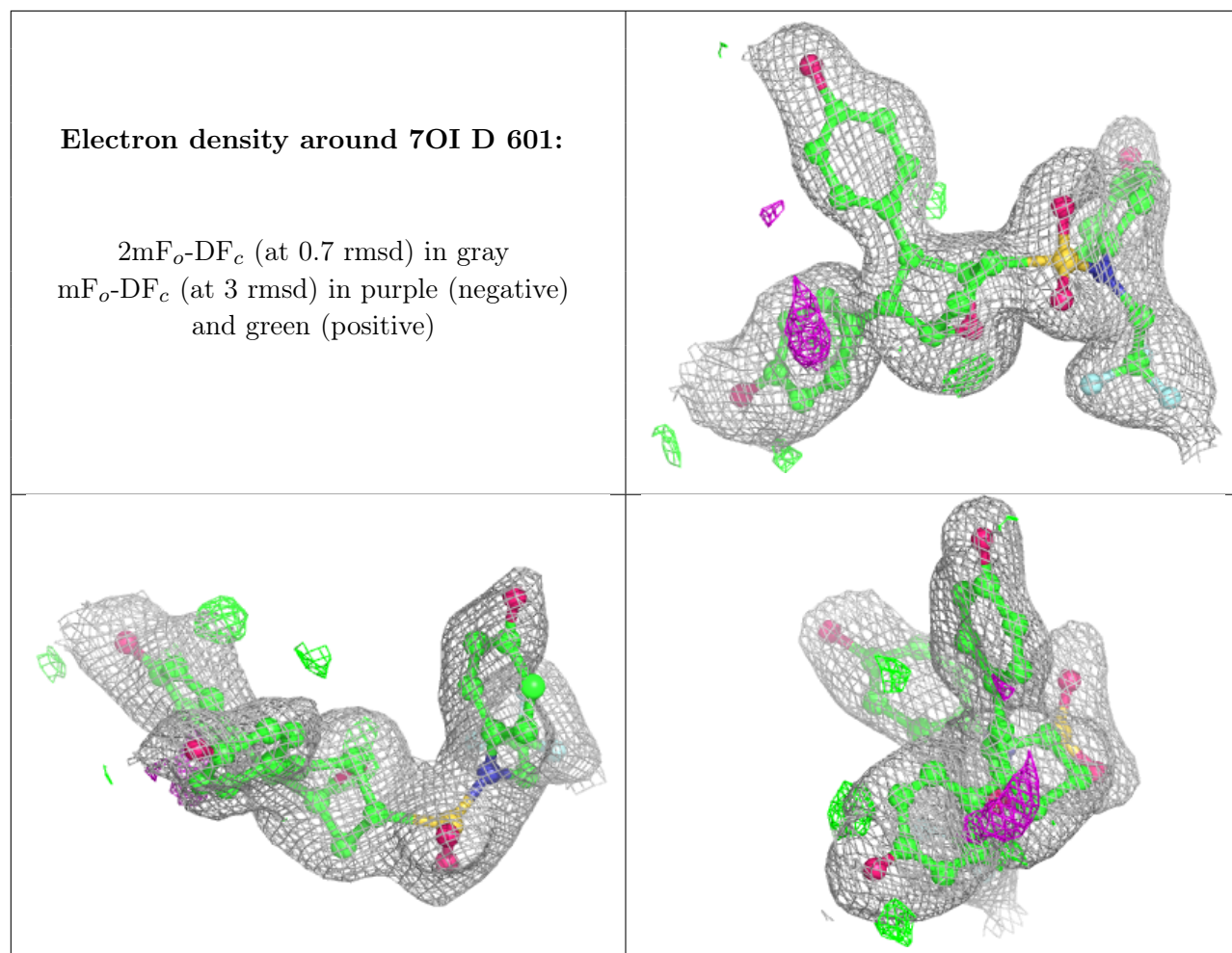
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 7OI 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.