



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2021 – 10:03 PM EDT

PDB ID : 7RS3
Title : Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with DMERI-29
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 : 1.84 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
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) : 2.23.1

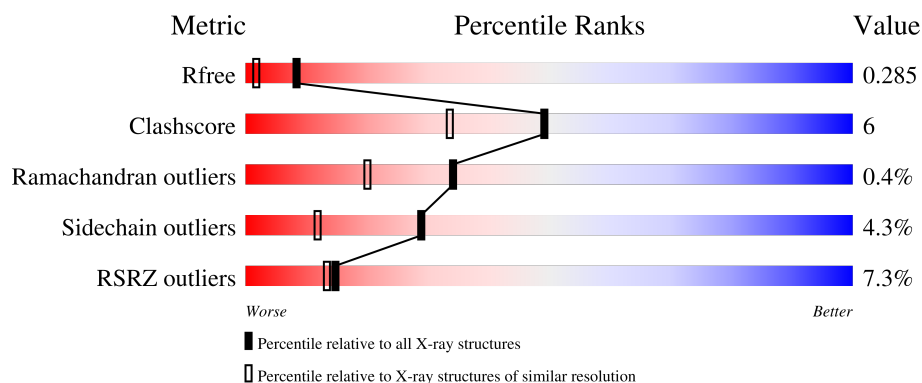
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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> <div>8%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	257	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>9%</div> <div>•</div> <div>18%</div> </div> </div>
1	C	257	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>5%</div> <div></div> <div>23%</div> </div> </div>
1	D	257	<div> <div>9%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>••</div> <div>8%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7212 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.

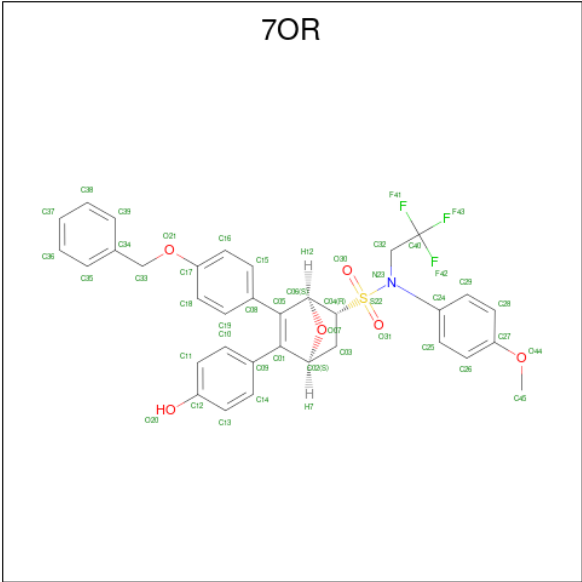
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	1	0
			1779	1138	302	321	18			
1	B	212	Total	C	N	O	S	0	0	0
			1681	1074	292	299	16			
1	C	198	Total	C	N	O	S	0	1	0
			1591	1017	276	284	14			
1	D	237	Total	C	N	O	S	0	0	0
			1890	1208	321	343	18			

There are 8 discrepancies between the modelled and reference sequences:

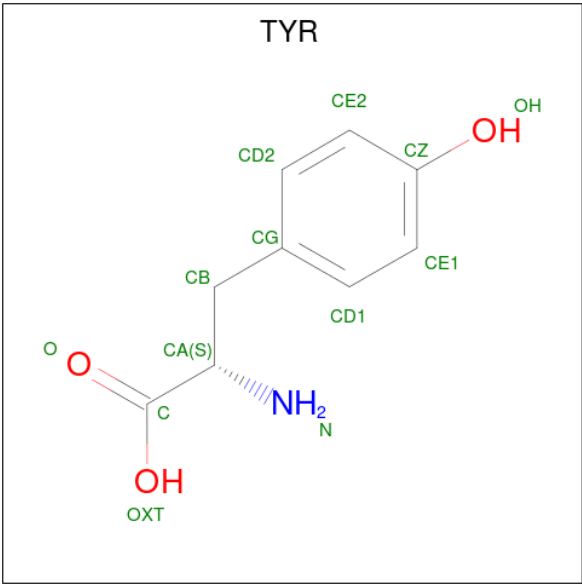
Chain	Residue	Modelled	Actual	Comment	Reference
A	372	SER	LEU	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	UNP P03372
B	372	SER	LEU	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372
C	372	SER	LEU	engineered mutation	UNP P03372
C	536	SER	LEU	engineered mutation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

- Molecule 2 is (1S,2R,4S)-6-[4-(benzyloxy)phenyl]-5-(4-hydroxyphenyl)-N-(4-methoxyphenyl)-N-(2,2,2-trifluoroethyl)-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonamide (three-letter code: 7OR) (formula: C₃₄H₃₀F₃NO₆S) (labeled as "Ligand of Interest" by depositor).



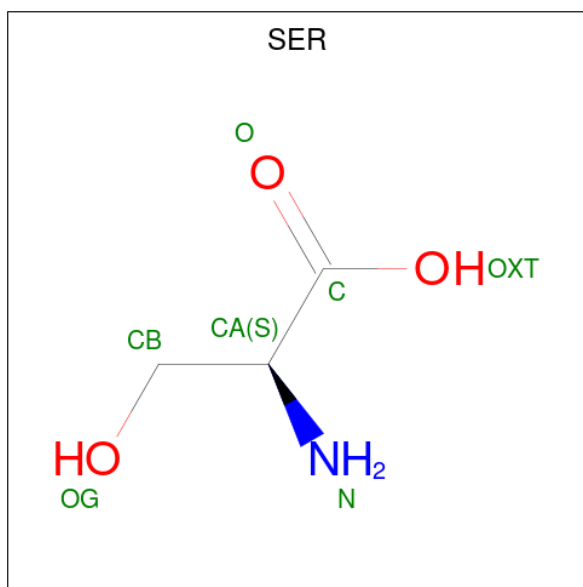
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			45	34	3	1	6	1		
2	B	1	Total	C	F	N	O	S	0	0
			45	34	3	1	6	1		
2	C	1	Total	C	F	N	O	S	0	0
			45	34	3	1	6	1		
2	D	1	Total	C	F	N	O	S	0	0
			45	34	3	1	6	1		

- Molecule 3 is TYROSINE (three-letter code: TYR) (formula: C₉H₁₁NO₃).



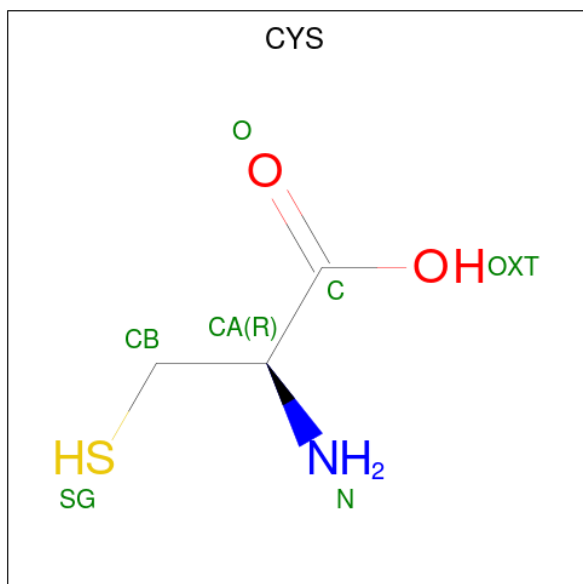
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 4 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 5 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			5	3	1	1		

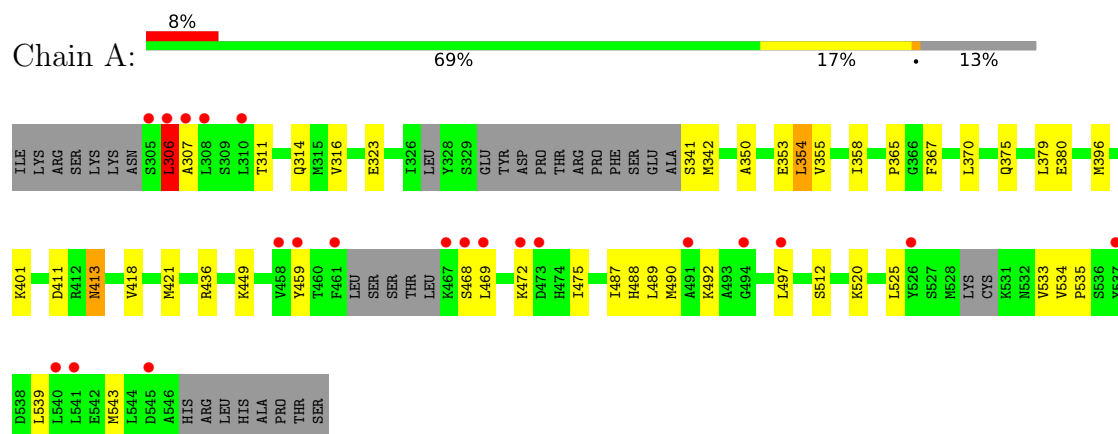
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	29	Total	O	0	0
			29	29		
6	C	17	Total	O	0	0
			17	17		
6	D	12	Total	O	0	0
			12	12		

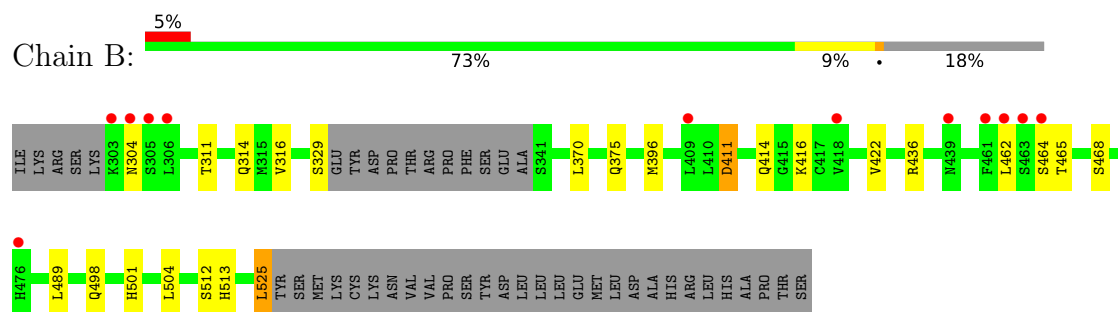
3 Residue-property plots [i](#)

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.

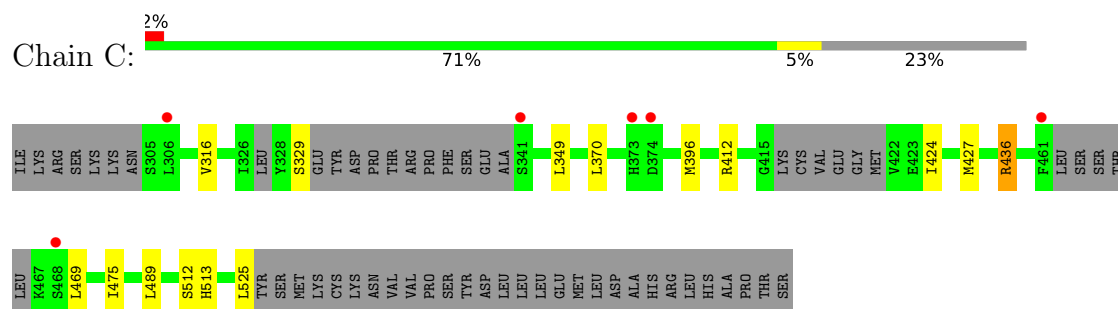
• Molecule 1: Estrogen receptor



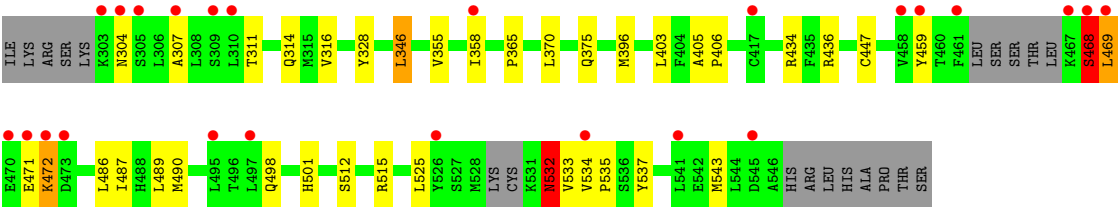
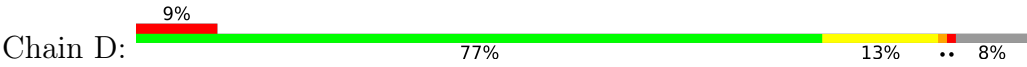
• Molecule 1: Estrogen receptor



• 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	52.56Å 58.98Å 91.67Å 89.03° 74.59° 63.60°	Depositor
Resolution (Å)	87.76 – 1.84 87.76 – 1.84	Depositor EDS
% Data completeness (in resolution range)	51.0 (87.76-1.84) 51.0 (87.76-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.236 , 0.283 0.243 , 0.285	Depositor DCC
R_{free} test set	2072 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.209 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7212	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.07% 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: 7OR, 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	0.54	0/1796	0.74	1/2419 (0.0%)
1	B	0.52	0/1698	0.73	0/2289
1	C	0.52	0/1605	0.74	2/2160 (0.1%)
1	D	0.53	0/1913	0.73	0/2582
All	All	0.53	0/7012	0.73	3/9450 (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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	436	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	A	306	LEU	CA-CB-CG	6.03	129.16	115.30
1	C	349	LEU	CB-CG-CD2	-5.63	101.42	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	462	LEU	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	1779	0	1812	33	0
1	B	1681	0	1737	20	0
1	C	1591	0	1629	7	0
1	D	1890	0	1921	28	0
2	A	45	0	0	2	0
2	B	45	0	0	0	0
2	C	45	0	0	0	0
2	D	45	0	0	3	0
3	B	5	0	1	0	0
3	C	5	0	1	0	0
4	B	5	0	2	0	0
5	B	5	0	2	0	0
6	A	13	0	0	0	0
6	B	29	0	0	1	0
6	C	17	0	0	0	0
6	D	12	0	0	0	0
All	All	7212	0	7105	84	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (84) 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:447:CYS:HB3	1:D:486:LEU:HD21	1.58	0.84
1:B:311:THR:H	1:B:314:GLN:HE21	1.26	0.82
1:A:534:VAL:HG22	1:A:535:PRO:HD2	1.64	0.80
1:A:367:PHE:HZ	1:A:379:LEU:CD2	1.99	0.75
1:D:469:LEU:O	1:D:472:LYS:HG3	1.87	0.75
1:A:367:PHE:CZ	1:A:379:LEU:CD2	2.70	0.74
1:B:311:THR:H	1:B:314:GLN:NE2	1.85	0.74
1:D:447:CYS:HB3	1:D:486:LEU:CD2	2.17	0.73
1:A:358:ILE:HD13	1:A:543:MET:HE2	1.69	0.73
1:D:358:ILE:HD13	1:D:543:MET:HE2	1.71	0.71
1:A:367:PHE:CZ	1:A:379:LEU:HD21	2.26	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:487:ILE:HD13	1:D:490:MET:CE	2.24	0.67
1:A:487:ILE:HD13	1:A:490:MET:CE	2.25	0.67
1:B:504:LEU:C	1:B:504:LEU:HD13	2.14	0.66
1:A:342:MET:HE3	1:A:418:VAL:HG23	1.79	0.63
1:B:465:THR:HG23	1:B:468:SER:HB2	1.81	0.63
1:A:534:VAL:CG2	1:A:535:PRO:HD2	2.28	0.63
1:A:342:MET:CE	1:A:418:VAL:HG23	2.31	0.61
1:D:447:CYS:CB	1:D:486:LEU:HD21	2.31	0.60
1:A:367:PHE:HZ	1:A:379:LEU:HD23	1.67	0.58
1:A:306:LEU:H	1:A:306:LEU:HD22	1.70	0.57
1:A:375:GLN:O	1:A:379:LEU:HD23	2.05	0.56
1:B:416:LYS:HA	1:B:422:VAL:HG22	1.86	0.56
1:C:424:ILE:HD13	1:C:427:MET:CE	2.36	0.55
1:A:396:MET:O	1:A:436:ARG:HD3	2.06	0.55
1:A:468:SER:O	1:A:472:LYS:HD3	2.06	0.55
1:D:525:LEU:HD21	1:D:534:VAL:CG2	2.36	0.55
1:D:534:VAL:HG13	1:D:535:PRO:HD2	1.88	0.54
1:A:487:ILE:HD13	1:A:490:MET:HE3	1.90	0.54
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.90	0.54
1:B:436:ARG:NH1	6:B:703:HOH:O	2.37	0.54
1:D:487:ILE:HD13	1:D:490:MET:HE3	1.90	0.53
1:C:396:MET:O	1:C:436:ARG:HD3	2.10	0.52
1:D:447:CYS:CB	1:D:486:LEU:CD2	2.87	0.52
1:D:346:LEU:HB3	2:D:601:7OR:C15	2.40	0.52
1:B:465:THR:CG2	1:B:468:SER:HB2	2.40	0.51
1:B:525:LEU:HD22	1:B:525:LEU:O	2.10	0.51
1:C:316:VAL:HG21	1:C:489:LEU:HD21	1.93	0.51
1:B:311:THR:N	1:B:314:GLN:HE21	2.02	0.51
1:A:413:ASN:HD22	1:A:413:ASN:N	2.08	0.51
1:A:459:TYR:CD2	1:B:513:HIS:HB2	2.45	0.51
1:D:316:VAL:HG21	1:D:489:LEU:HD21	1.93	0.51
1:A:323:GLU:OE1	1:A:449:LYS:NZ	2.30	0.50
1:D:525:LEU:HD22	2:D:601:7OR:C27	2.42	0.50
1:B:525:LEU:HD22	1:B:525:LEU:C	2.33	0.49
1:A:534:VAL:HG22	1:A:535:PRO:CD	2.40	0.49
1:A:316:VAL:HG21	1:A:489:LEU:HD21	1.95	0.49
1:D:307:ALA:HB1	1:D:365:PRO:HB3	1.95	0.49
1:B:411:ASP:H	1:B:414:GLN:NE2	2.11	0.48
1:A:307:ALA:HB1	1:A:365:PRO:HB3	1.95	0.48
1:A:311:THR:HG23	1:A:314:GLN:H	1.79	0.48
1:A:468:SER:O	1:A:472:LYS:CD	2.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:HIS:NE2	1:A:492:LYS:HD2	2.30	0.47
1:C:513:HIS:HB2	1:D:459:TYR:CD2	2.49	0.47
1:B:498:GLN:HA	1:B:501:HIS:CE1	2.50	0.47
1:D:311:THR:HG23	1:D:314:GLN:H	1.80	0.47
1:D:355:VAL:HG22	1:D:543:MET:HE3	1.97	0.47
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.50	0.46
1:A:355:VAL:HG22	1:A:543:MET:HE3	1.98	0.46
1:A:401:LYS:CD	1:A:411:ASP:HB3	2.46	0.45
1:D:403:LEU:HD12	1:D:405:ALA:O	2.16	0.45
1:B:525:LEU:C	1:B:525:LEU:CD2	2.85	0.45
1:D:328:TYR:CE1	1:D:406:PRO:HB2	2.51	0.45
1:B:411:ASP:H	1:B:414:GLN:HE21	1.64	0.45
1:C:370:LEU:HD11	1:C:475:ILE:HD11	1.99	0.44
1:D:525:LEU:HD13	2:D:601:7OR:C28	2.47	0.44
1:B:396:MET:O	1:B:436:ARG:NE	2.47	0.44
1:A:413:ASN:HD22	1:A:413:ASN:H	1.65	0.44
1:A:525:LEU:HG	2:A:601:7OR:C27	2.47	0.44
1:D:532:ASN:HD22	1:D:532:ASN:HA	1.63	0.44
1:A:350:ALA:O	1:A:354:LEU:HD13	2.18	0.43
1:C:513:HIS:HB2	1:D:459:TYR:CE2	2.53	0.43
1:D:370:LEU:O	1:D:375:GLN:NE2	2.51	0.43
1:A:370:LEU:O	1:A:375:GLN:NE2	2.51	0.42
1:B:465:THR:HG23	1:B:468:SER:H	1.85	0.42
1:D:468:SER:HA	1:D:471:GLU:HG3	2.02	0.42
1:A:353:GLU:OE2	2:A:601:7OR:O20	2.38	0.42
1:A:401:LYS:HE3	1:A:411:ASP:HB3	2.01	0.41
1:D:311:THR:HG22	1:D:314:GLN:CD	2.41	0.41
1:C:513:HIS:CD2	1:D:459:TYR:HB2	2.54	0.41
1:A:370:LEU:HD11	1:A:475:ILE:HD11	2.02	0.41
1:D:396:MET:O	1:D:436:ARG:NE	2.48	0.41
1:B:504:LEU:C	1:B:504:LEU:CD1	2.86	0.40
1:B:370:LEU:O	1:B:375:GLN:NE2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/257 (83%)	211 (99%)	2 (1%)	0	100	100
1	B	207/257 (80%)	204 (99%)	3 (1%)	0	100	100
1	C	188/257 (73%)	187 (100%)	1 (0%)	0	100	100
1	D	230/257 (90%)	224 (97%)	3 (1%)	3 (1%)	12	3
All	All	838/1028 (82%)	826 (99%)	9 (1%)	3 (0%)	34	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	304	ASN
1	D	468	SER
1	D	532	ASN

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	198/231 (86%)	186 (94%)	12 (6%)	18	5
1	B	188/231 (81%)	182 (97%)	6 (3%)	39	21
1	C	177/231 (77%)	172 (97%)	5 (3%)	43	26
1	D	211/231 (91%)	201 (95%)	10 (5%)	26	10
All	All	774/924 (84%)	741 (96%)	33 (4%)	29	12

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	LEU
1	A	341	SER
1	A	354	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	380	GLU
1	A	413	ASN
1	A	421	MET
1	A	469	LEU
1	A	497	LEU
1	A	512	SER
1	A	520	LYS
1	A	533	VAL
1	A	539	LEU
1	B	304	ASN
1	B	329	SER
1	B	411	ASP
1	B	464	SER
1	B	512	SER
1	B	525	LEU
1	C	329	SER
1	C	412	ARG
1	C	469	LEU
1	C	512	SER
1	C	525	LEU
1	D	346	LEU
1	D	434	ARG
1	D	468	SER
1	D	469	LEU
1	D	472	LYS
1	D	512	SER
1	D	515	ARG
1	D	532	ASN
1	D	533	VAL
1	D	537	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	HIS
1	A	413	ASN
1	A	519	ASN
1	B	314	GLN
1	B	414	GLN
1	B	488	HIS
1	B	519	ASN
1	C	398	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	488	HIS
1	C	519	ASN
1	D	519	ASN
1	D	532	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	381	1	7,9,10	0.49	0	4,10,12	0.60	0
1	YCM	B	381	1	7,9,10	0.48	0	4,10,12	0.51	0
1	YCM	C	381	1	7,9,10	0.57	0	4,10,12	0.56	0
1	YCM	D	381	1	7,9,10	0.50	0	4,10,12	0.41	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	381	1	-	2/6/8/10	-
1	YCM	B	381	1	-	2/6/8/10	-
1	YCM	C	381	1	-	3/6/8/10	-
1	YCM	D	381	1	-	2/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) 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-OZ1
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	A	381	YCM	SG-CD-CE-OZ1
1	C	381	YCM	SG-CD-CE-OZ1
1	D	381	YCM	SG-CD-CE-OZ1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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$
5	CYS	B	603	-	3,4,6	0.58	0	2,4,7	0.83	0
2	7OR	C	602	-	47,50,50	3.00	11 (23%)	61,74,74	2.01	15 (24%)
2	7OR	A	601	-	47,50,50	3.22	10 (21%)	61,74,74	2.09	17 (27%)
3	TYR	C	601	-	3,4,13	0.84	0	2,4,17	0.43	0
3	TYR	B	601	-	3,4,13	0.54	0	2,4,17	0.76	0
4	SER	B	602	-	3,4,6	0.67	0	2,4,7	1.00	0
2	7OR	D	601	-	47,50,50	2.92	7 (14%)	61,74,74	1.93	17 (27%)
2	7OR	B	604	-	47,50,50	2.98	11 (23%)	61,74,74	2.03	20 (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
5	CYS	B	603	-	-	0/0/2/6	-
2	7OR	C	602	-	-	16/34/60/60	0/7/6/6
2	7OR	A	601	-	-	13/34/60/60	0/7/6/6
3	TYR	C	601	-	-	0/0/2/8	-
3	TYR	B	601	-	-	0/0/2/8	-
4	SER	B	602	-	-	0/0/2/6	-
2	7OR	D	601	-	-	13/34/60/60	0/7/6/6
2	7OR	B	604	-	-	13/34/60/60	0/7/6/6

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	7OR	C05-C01	13.13	1.60	1.34
2	D	601	7OR	C05-C01	12.64	1.59	1.34
2	C	602	7OR	C05-C01	11.89	1.58	1.34
2	B	604	7OR	C05-C01	11.10	1.56	1.34
2	C	602	7OR	C03-C04	9.57	1.66	1.54
2	A	601	7OR	C03-C04	8.96	1.65	1.54
2	B	604	7OR	C03-C04	8.88	1.65	1.54
2	D	601	7OR	C03-C04	8.52	1.64	1.54
2	A	601	7OR	C32-C40	7.71	1.60	1.50
2	A	601	7OR	C02-C01	-7.61	1.40	1.51
2	B	604	7OR	C32-C40	6.57	1.59	1.50
2	B	604	7OR	C02-C01	-6.53	1.42	1.51
2	D	601	7OR	C02-C01	-6.47	1.42	1.51
2	C	602	7OR	C02-C01	-6.45	1.42	1.51
2	C	602	7OR	C06-C05	-6.43	1.43	1.50
2	D	601	7OR	C32-C40	6.21	1.58	1.50
2	A	601	7OR	C06-C05	-5.95	1.44	1.50
2	B	604	7OR	C06-C05	-5.92	1.44	1.50
2	D	601	7OR	C06-C05	-5.33	1.44	1.50
2	C	602	7OR	C32-C40	4.70	1.56	1.50
2	B	604	7OR	S22-N23	4.35	1.76	1.67
2	C	602	7OR	C03-C02	-3.34	1.46	1.53
2	A	601	7OR	C33-C34	3.33	1.58	1.50
2	C	602	7OR	O31-S22	-3.23	1.40	1.43
2	A	601	7OR	S22-N23	3.17	1.73	1.67
2	C	602	7OR	S22-N23	3.15	1.73	1.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	7OR	C03-C02	-3.12	1.46	1.53
2	B	604	7OR	C03-C02	-2.99	1.46	1.53
2	D	601	7OR	O30-S22	-2.94	1.41	1.43
2	B	604	7OR	O31-S22	-2.57	1.41	1.43
2	C	602	7OR	C24-N23	2.47	1.48	1.44
2	A	601	7OR	C03-C02	-2.46	1.48	1.53
2	A	601	7OR	C15-C08	2.44	1.43	1.39
2	B	604	7OR	C08-C05	-2.33	1.44	1.48
2	C	602	7OR	C18-C17	2.19	1.43	1.38
2	B	604	7OR	C33-C34	2.06	1.55	1.50
2	A	601	7OR	O30-S22	-2.02	1.41	1.43
2	C	602	7OR	C29-C24	2.02	1.43	1.39
2	B	604	7OR	C09-C01	-2.01	1.44	1.48

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	7OR	C09-C01-C02	7.77	134.11	121.44
2	D	601	7OR	C09-C01-C02	7.21	133.19	121.44
2	C	602	7OR	C09-C01-C02	7.07	132.97	121.44
2	B	604	7OR	C09-C01-C02	7.06	132.96	121.44
2	A	601	7OR	C40-C32-N23	5.44	117.42	112.14
2	C	602	7OR	O31-S22-O30	-5.34	115.79	119.22
2	B	604	7OR	O07-C02-C03	-4.72	95.35	104.64
2	C	602	7OR	O07-C02-C03	-4.61	95.58	104.64
2	A	601	7OR	O07-C02-C03	-4.58	95.62	104.64
2	A	601	7OR	O31-S22-O30	-4.53	116.31	119.22
2	C	602	7OR	C02-C03-C04	-4.45	96.68	100.61
2	B	604	7OR	C02-C03-C04	-4.22	96.89	100.61
2	D	601	7OR	O07-C02-C03	-4.09	96.59	104.64
2	C	602	7OR	C02-C01-C05	-3.74	99.12	106.97
2	B	604	7OR	O31-S22-O30	-3.71	116.83	119.22
2	B	604	7OR	C02-C01-C05	-3.71	99.18	106.97
2	D	601	7OR	C02-C01-C05	-3.71	99.19	106.97
2	A	601	7OR	C25-C24-N23	3.68	125.65	120.16
2	A	601	7OR	C02-C01-C05	-3.54	99.53	106.97
2	D	601	7OR	C02-C03-C04	-3.44	97.57	100.61
2	D	601	7OR	C40-C32-N23	3.33	115.37	112.14
2	A	601	7OR	C19-C08-C05	3.19	125.03	120.91
2	B	604	7OR	C40-C32-N23	3.14	115.19	112.14
2	D	601	7OR	C08-C05-C06	-3.08	116.20	121.27
2	C	602	7OR	O21-C33-C34	3.01	118.18	109.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	7OR	C25-C24-N23	2.98	124.61	120.16
2	C	602	7OR	C18-C17-C16	-2.91	115.69	120.18
2	A	601	7OR	O21-C33-C34	2.91	117.90	109.16
2	B	604	7OR	C25-C24-N23	2.91	124.51	120.16
2	B	604	7OR	C28-C27-C26	-2.89	115.72	120.18
2	D	601	7OR	C28-C27-C26	-2.86	115.77	120.18
2	A	601	7OR	C02-C03-C04	-2.85	98.09	100.61
2	C	602	7OR	C25-C24-N23	2.82	124.38	120.16
2	B	604	7OR	C15-C08-C05	-2.76	117.34	120.91
2	D	601	7OR	C18-C17-C16	-2.76	115.93	120.18
2	D	601	7OR	C29-C24-C25	-2.74	113.58	119.16
2	B	604	7OR	C19-C08-C05	2.72	124.43	120.91
2	A	601	7OR	C28-C27-C26	-2.67	116.06	120.18
2	B	604	7OR	C29-C24-C25	-2.56	113.95	119.16
2	A	601	7OR	C18-C17-C16	-2.56	116.24	120.18
2	B	604	7OR	C18-C17-C16	-2.50	116.33	120.18
2	C	602	7OR	C28-C27-C26	-2.49	116.35	120.18
2	C	602	7OR	C29-C24-C25	-2.48	114.12	119.16
2	C	602	7OR	C14-C09-C01	2.47	124.10	120.91
2	D	601	7OR	C28-C29-C24	2.46	123.56	120.32
2	A	601	7OR	C28-C29-C24	2.44	123.54	120.32
2	A	601	7OR	C08-C05-C06	-2.44	117.26	121.27
2	D	601	7OR	C26-C25-C24	2.42	123.51	120.32
2	B	604	7OR	C28-C29-C24	2.41	123.50	120.32
2	D	601	7OR	O21-C33-C34	2.38	116.30	109.16
2	D	601	7OR	C14-C09-C01	2.35	123.95	120.91
2	D	601	7OR	O31-S22-O30	-2.32	117.72	119.22
2	B	604	7OR	C08-C05-C06	-2.30	117.50	121.27
2	B	604	7OR	C25-C26-C27	2.28	122.53	119.73
2	C	602	7OR	C19-C18-C17	2.25	122.48	119.73
2	A	601	7OR	C39-C34-C35	-2.23	114.66	118.17
2	B	604	7OR	O31-S22-N23	2.23	110.28	107.56
2	A	601	7OR	C29-C24-C25	-2.22	114.64	119.16
2	C	602	7OR	C28-C29-C24	2.22	123.24	120.32
2	B	604	7OR	C14-C09-C01	2.21	123.77	120.91
2	B	604	7OR	C33-O21-C17	2.20	123.09	117.65
2	A	601	7OR	C15-C08-C05	-2.19	118.07	120.91
2	A	601	7OR	C19-C18-C17	2.12	122.32	119.73
2	B	604	7OR	C26-C25-C24	2.11	123.10	120.32
2	B	604	7OR	O21-C33-C34	2.09	115.43	109.16
2	C	602	7OR	C26-C25-C24	2.08	123.06	120.32
2	D	601	7OR	C19-C08-C05	2.08	123.59	120.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	7OR	C19-C18-C17	2.07	122.27	119.73
2	C	602	7OR	C19-C08-C05	2.03	123.53	120.91

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	7OR	C24-N23-S22-O30
2	A	601	7OR	C32-N23-S22-O30
2	A	601	7OR	C32-N23-S22-O31
2	A	601	7OR	N23-C32-C40-F41
2	A	601	7OR	N23-C32-C40-F42
2	A	601	7OR	N23-C32-C40-F43
2	B	604	7OR	C03-C04-S22-O30
2	B	604	7OR	C06-C04-S22-O30
2	B	604	7OR	C32-N23-S22-O30
2	B	604	7OR	C32-N23-S22-O31
2	B	604	7OR	N23-C32-C40-F41
2	C	602	7OR	C03-C04-S22-O30
2	C	602	7OR	C06-C04-S22-O30
2	C	602	7OR	C24-N23-S22-O30
2	C	602	7OR	C32-N23-S22-O30
2	C	602	7OR	C32-N23-S22-O31
2	C	602	7OR	N23-C32-C40-F41
2	C	602	7OR	N23-C32-C40-F42
2	C	602	7OR	N23-C32-C40-F43
2	D	601	7OR	C24-N23-S22-O30
2	D	601	7OR	C32-N23-S22-O30
2	D	601	7OR	C32-N23-S22-O31
2	D	601	7OR	N23-C32-C40-F41
2	D	601	7OR	N23-C32-C40-F42
2	D	601	7OR	N23-C32-C40-F43
2	C	602	7OR	C28-C27-O44-C45
2	C	602	7OR	C26-C27-O44-C45
2	A	601	7OR	C25-C24-N23-S22
2	B	604	7OR	C25-C24-N23-S22
2	C	602	7OR	C25-C24-N23-S22
2	D	601	7OR	C25-C24-N23-S22
2	D	601	7OR	C29-C24-N23-S22
2	A	601	7OR	C03-C04-S22-O30
2	D	601	7OR	C03-C04-S22-O30
2	A	601	7OR	C32-N23-S22-C04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	604	7OR	C32-N23-S22-C04
2	C	602	7OR	C32-N23-S22-C04
2	A	601	7OR	C06-C05-C08-C15
2	A	601	7OR	C06-C05-C08-C19
2	B	604	7OR	C29-C24-N23-S22
2	B	604	7OR	C03-C04-S22-O31
2	C	602	7OR	C03-C04-S22-O31
2	B	604	7OR	N23-C32-C40-F42
2	A	601	7OR	C29-C24-N23-S22
2	C	602	7OR	C29-C24-N23-S22
2	D	601	7OR	C32-N23-S22-C04
2	B	604	7OR	C06-C05-C08-C15
2	B	604	7OR	C06-C05-C08-C19
2	C	602	7OR	C06-C05-C08-C15
2	C	602	7OR	C06-C05-C08-C19
2	D	601	7OR	C06-C05-C08-C15
2	D	601	7OR	C06-C05-C08-C19
2	B	604	7OR	N23-C32-C40-F43
2	A	601	7OR	C06-C04-S22-O30
2	D	601	7OR	C06-C04-S22-O30

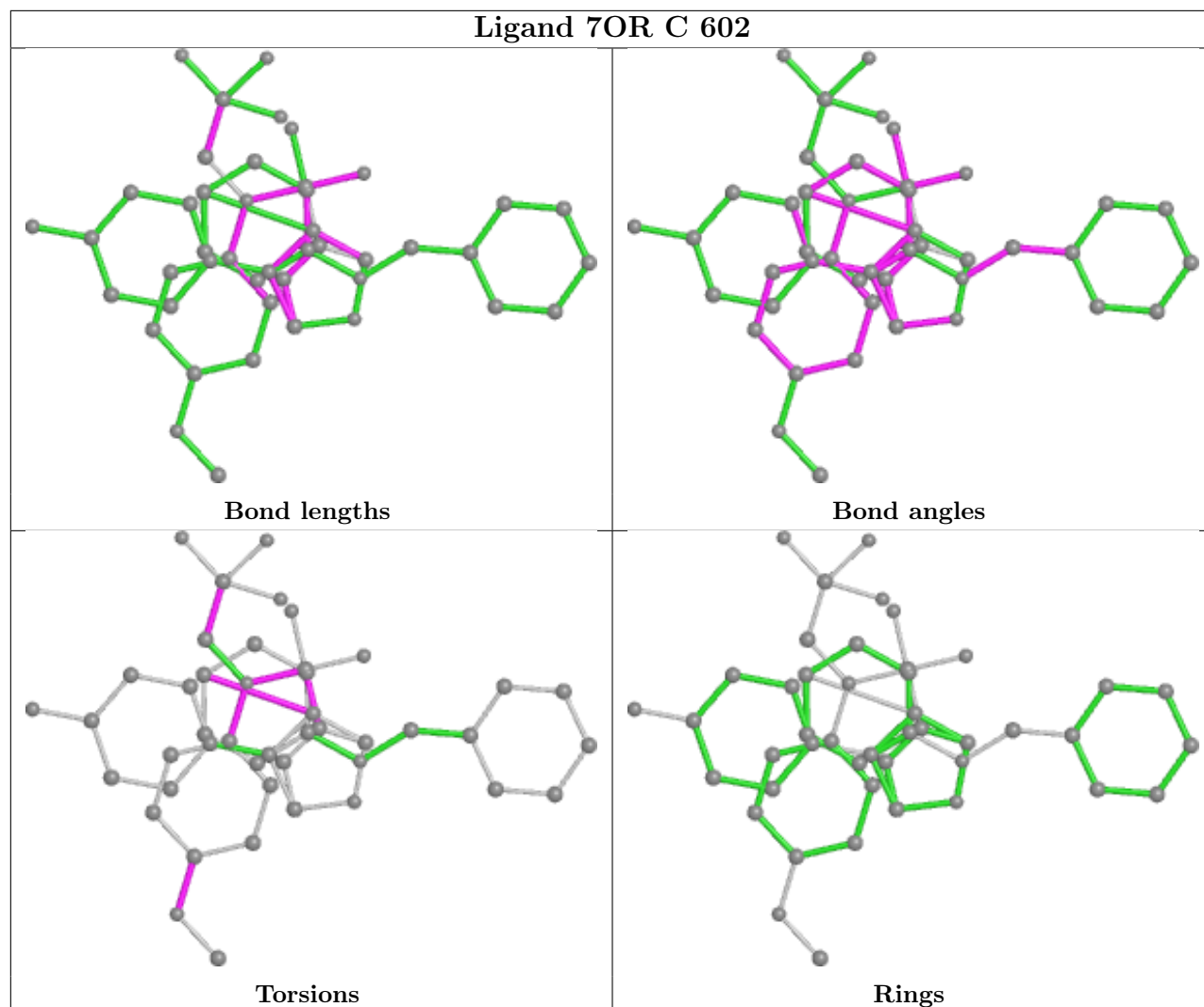
There are no ring outliers.

2 monomers are involved in 5 short contacts:

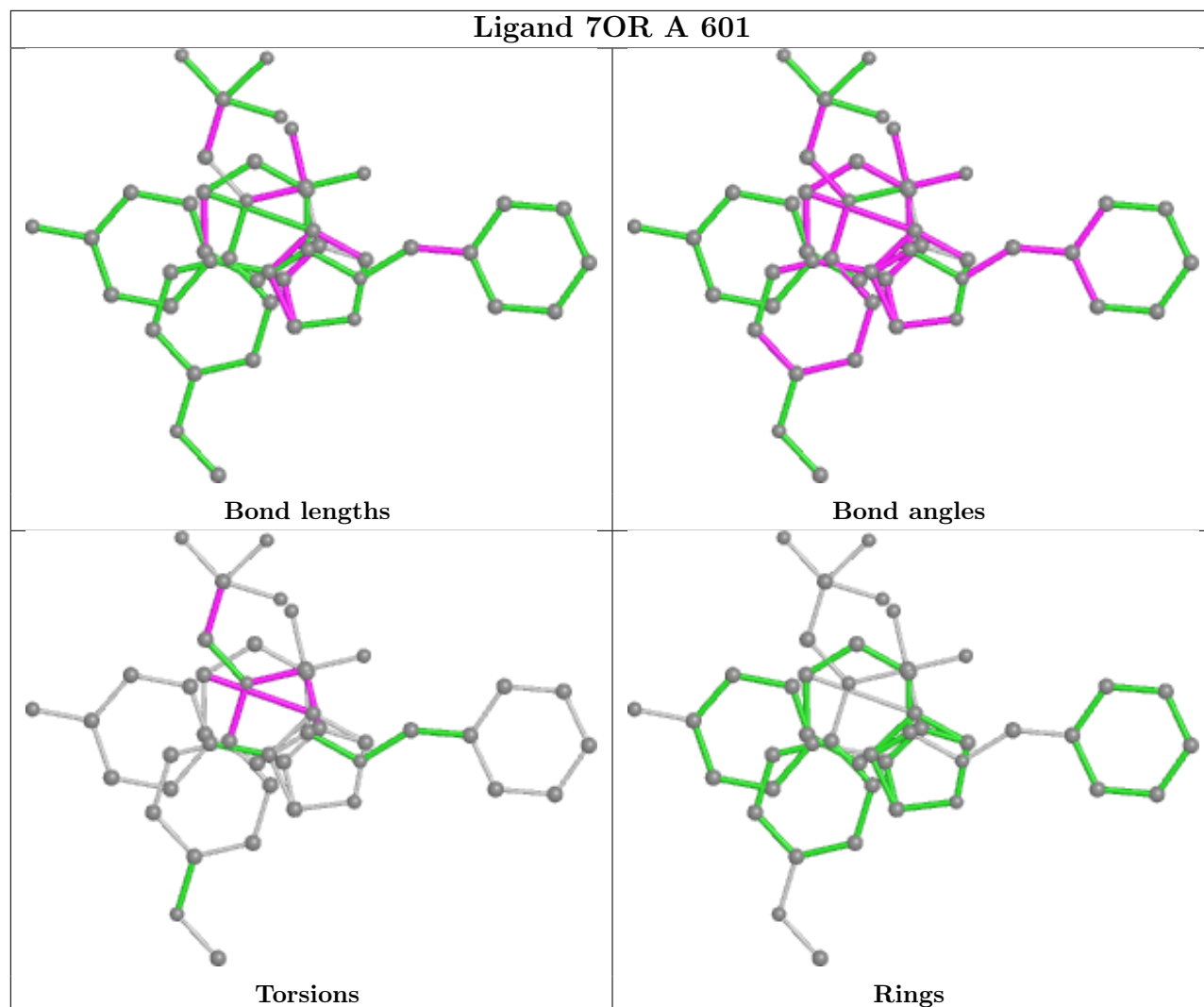
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	7OR	2	0
2	D	601	7OR	3	0

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.

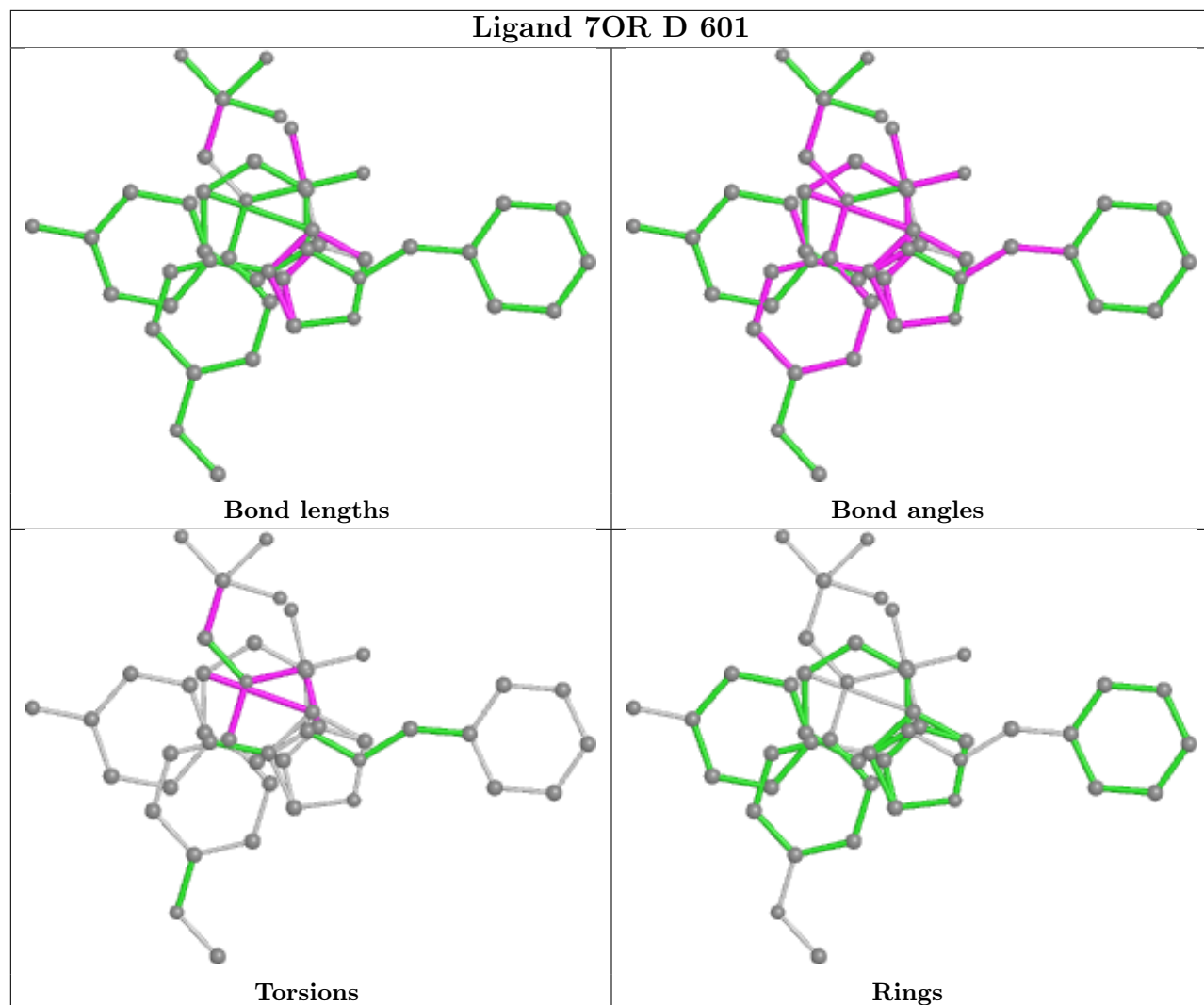
Ligand 7OR C 602

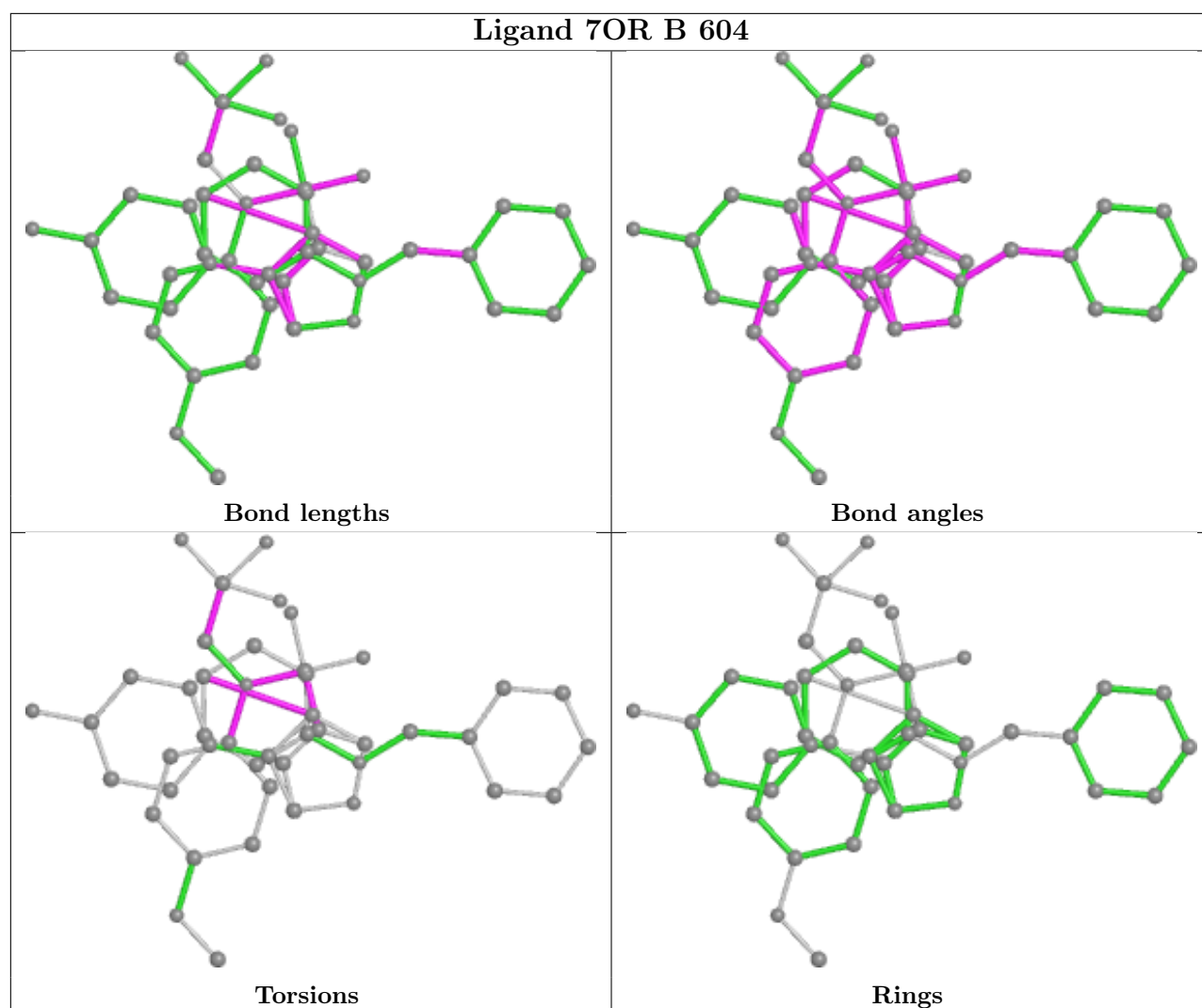


Ligand 7OR A 601



Ligand 7OR 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	222/257 (86%)	0.68	21 (9%) 8 7	19, 40, 88, 124	0
1	B	211/257 (82%)	0.44	12 (5%) 23 21	17, 36, 77, 102	0
1	C	197/257 (76%)	0.34	6 (3%) 50 47	17, 36, 74, 90	0
1	D	236/257 (91%)	0.77	24 (10%) 6 5	18, 41, 94, 135	0
All	All	866/1028 (84%)	0.57	63 (7%) 15 13	17, 38, 83, 135	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	459	TYR	13.2
1	A	459	TYR	12.2
1	D	305	SER	8.5
1	D	469	LEU	7.5
1	D	304	ASN	6.8
1	D	472	LYS	6.7
1	A	467	LYS	5.9
1	D	307	ALA	5.7
1	B	304	ASN	5.6
1	D	470	GLU	5.5
1	A	472	LYS	5.3
1	D	526	TYR	4.9
1	A	310	LEU	4.8
1	A	491	ALA	4.4
1	D	468	SER	4.4
1	A	308	LEU	4.3
1	B	305	SER	4.0
1	B	462	LEU	4.0
1	B	463	SER	3.9
1	A	458	VAL	3.9
1	D	458	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	467	LYS	3.8
1	C	373	HIS	3.8
1	D	473	ASP	3.7
1	D	497	LEU	3.7
1	A	306	LEU	3.5
1	D	310	LEU	3.5
1	C	461	PHE	3.5
1	A	305	SER	3.5
1	D	534	VAL	3.4
1	B	461	PHE	3.4
1	B	303	LYS	3.4
1	A	307	ALA	3.3
1	C	306	LEU	3.3
1	B	418	VAL	3.3
1	A	461	PHE	3.2
1	A	497	LEU	3.2
1	D	545	ASP	3.2
1	A	526	TYR	3.1
1	D	303	LYS	3.1
1	D	417	CYS	2.8
1	C	468	SER	2.7
1	A	473	ASP	2.6
1	A	545	ASP	2.6
1	D	358	ILE	2.6
1	C	341	SER	2.6
1	A	469	LEU	2.5
1	C	374	ASP	2.5
1	D	309	SER	2.4
1	A	494	GLY	2.4
1	B	306	LEU	2.3
1	D	471	GLU	2.3
1	A	537	TYR	2.3
1	A	541	LEU	2.3
1	A	468	SER	2.2
1	D	541	LEU	2.2
1	B	476	HIS	2.2
1	B	409	LEU	2.2
1	D	461	PHE	2.2
1	D	495	LEU	2.1
1	B	439	ASN	2.1
1	A	540	LEU	2.0
1	B	464	SER	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	381	10/11	0.93	0.13	23,25,39,40	0
1	YCM	D	381	10/11	0.93	0.16	27,32,61,76	0
1	YCM	C	381	10/11	0.94	0.11	28,32,48,53	0
1	YCM	A	381	10/11	0.94	0.13	26,33,55,70	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

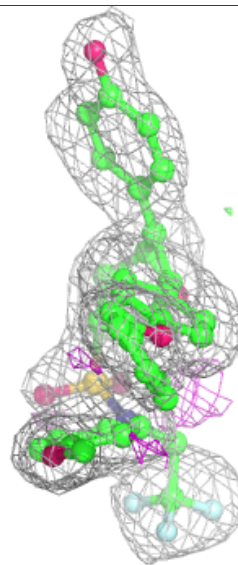
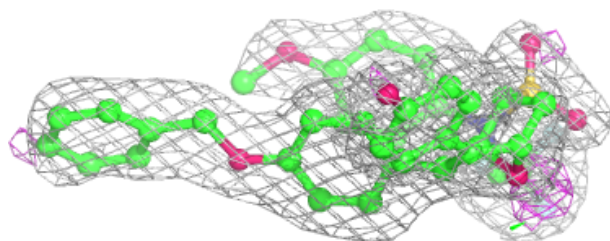
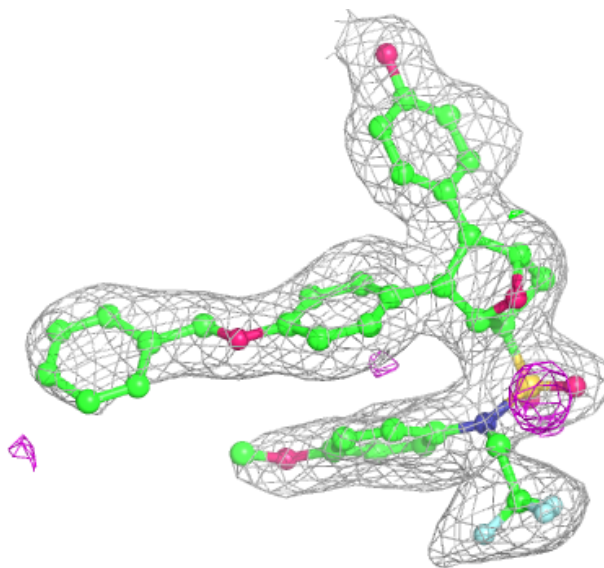
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TYR	B	601	5/13	0.74	0.19	30,30,30,30	0
3	TYR	C	601	5/13	0.78	0.22	30,30,30,30	0
4	SER	B	602	5/7	0.87	0.21	30,30,30,30	0
5	CYS	B	603	5/7	0.88	0.15	30,30,30,30	0
2	7OR	B	604	45/45	0.92	0.12	24,33,62,67	0
2	7OR	C	602	45/45	0.94	0.12	16,32,77,83	0
2	7OR	D	601	45/45	0.94	0.10	20,26,46,50	0
2	7OR	A	601	45/45	0.95	0.11	19,30,51,59	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.

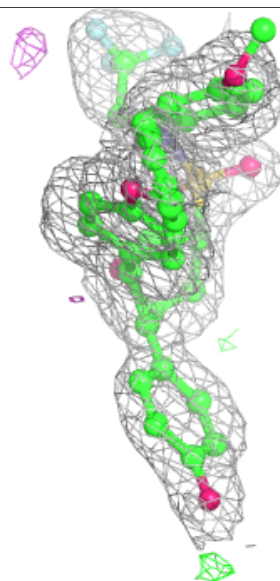
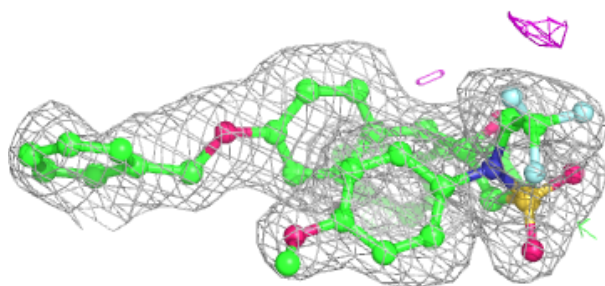
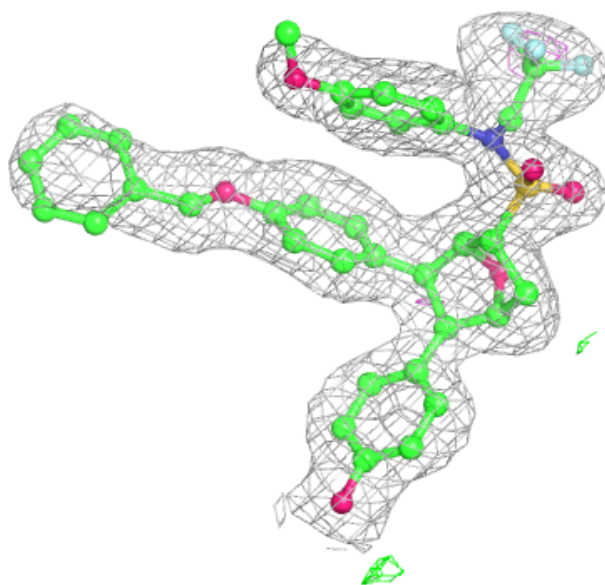
Electron density around 7OR B 604:

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



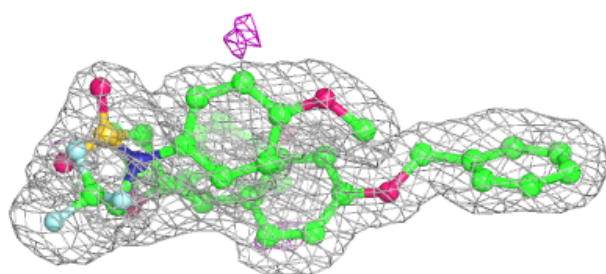
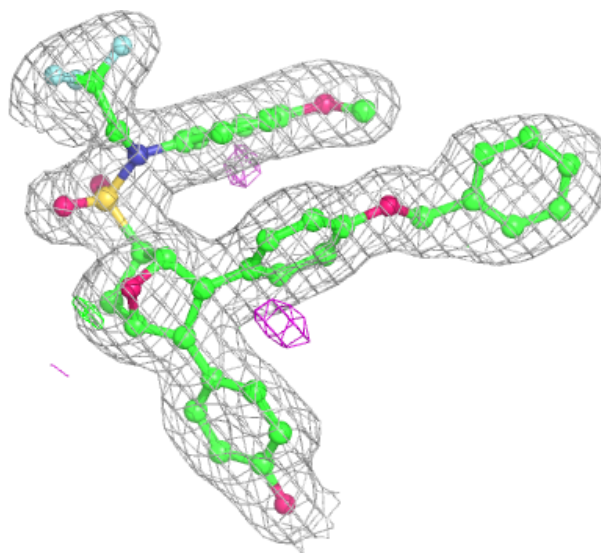
Electron density around 7OR C 602:

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



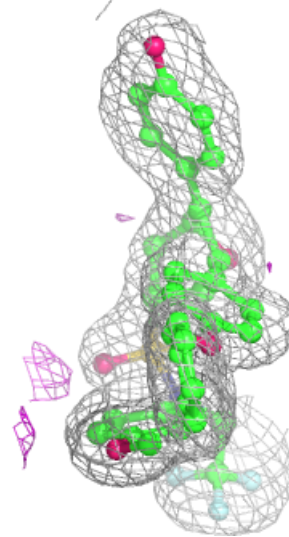
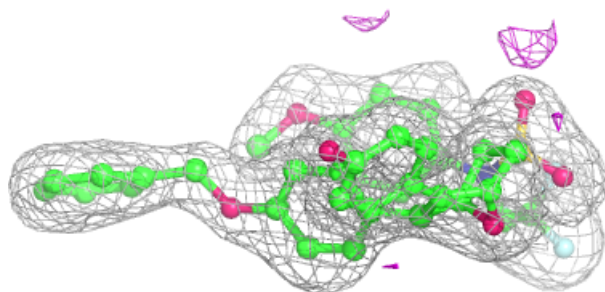
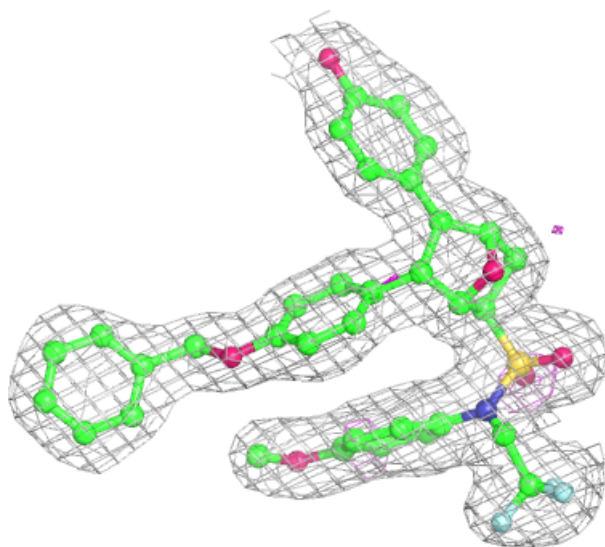
Electron density around 7OR D 601:

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



Electron density around 7OR 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.