



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 01:49 PM EDT

PDB ID : 2G44
Title : Human Estrogen Receptor Alpha Ligand-Binding Domain In Complex With
OBCP-1M-G and A Glucocorticoid Receptor Interacting Protein 1 NR Box II
Peptide
Authors : Rajan, S.S.; Hsieh, R.W.; Sharma, S.K.; Greene, G.L.
Deposited on : 2006-02-21
Resolution : 2.65 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 : 2.23.2
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) : 2.23.2

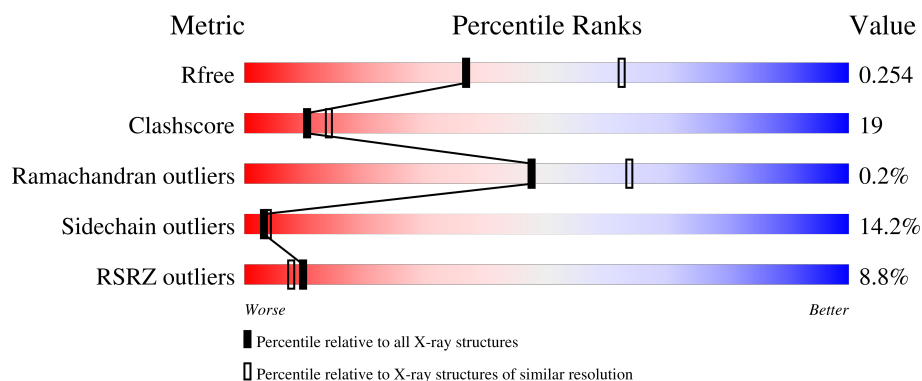
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	
1	B	257	
2	C	13	
2	D	13	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4040 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	237	Total	C	N	O	S	0	3	0
			1922	1228	328	342	24			
1	B	237	Total	C	N	O	S	0	3	0
			1920	1229	330	337	24			

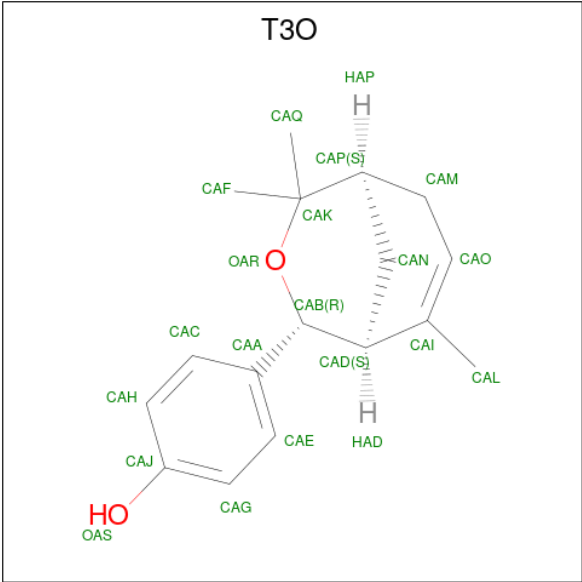
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	CME	CYS	modified residue	UNP P03372
A	417	CME	CYS	modified residue	UNP P03372
A	530	CME	CYS	modified residue	UNP P03372
A	537	SER	TYR	engineered mutation	UNP P03372
B	381	CME	CYS	modified residue	UNP P03372
B	417	CME	CYS	modified residue	UNP P03372
B	530	CME	CYS	modified residue	UNP P03372
B	537	SER	TYR	engineered mutation	UNP P03372

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			79	51	16	12			
2	D	9	Total	C	N	O	0	0	0
			75	49	15	11			

- Molecule 3 is 4-[(1S,2R,5S)-4,4,8-TRIMETHYL-3-OXABICYCLO[3.3.1]NON-7-EN-2-YL]PHENOL (three-letter code: T3O) (formula: C₁₇H₂₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			19	17	2		
3	B	1	Total	C	O	0	0
			19	17	2		

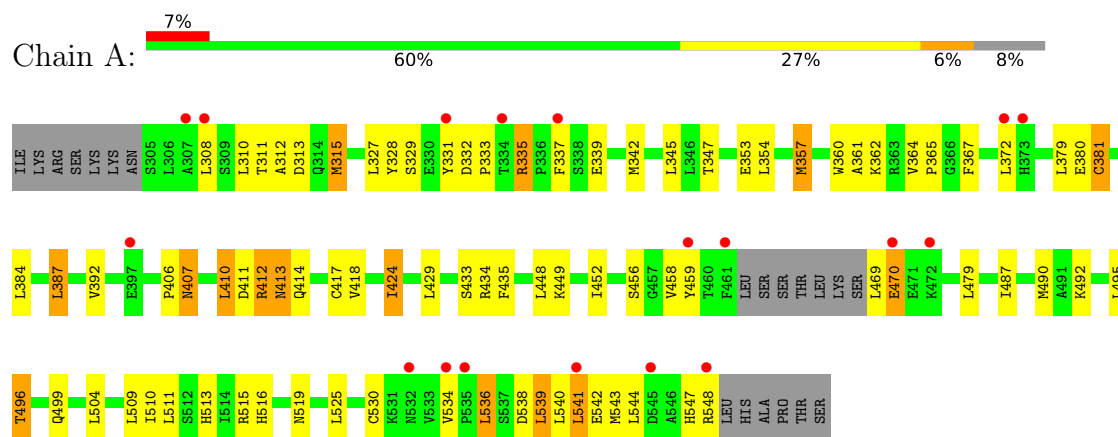
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	2	Total	O	0	0
			2	2		

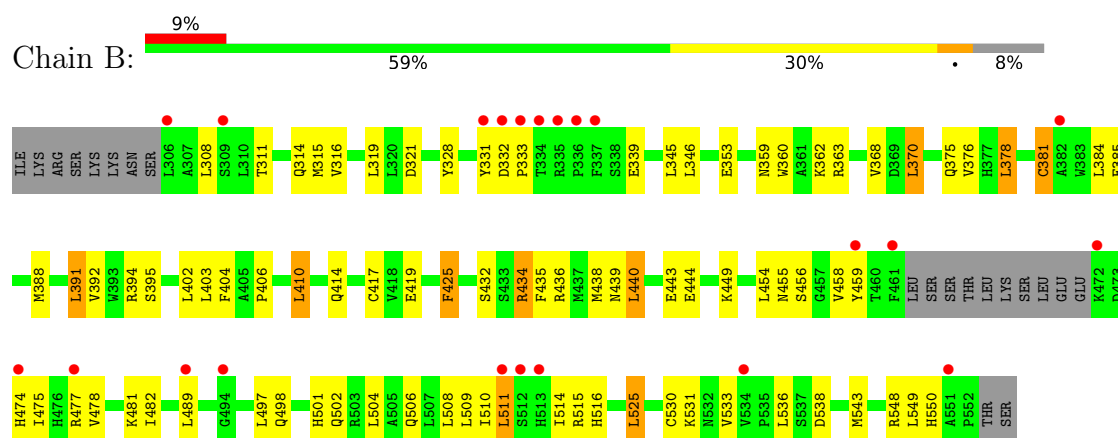
3 Residue-property plots [i](#)

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.

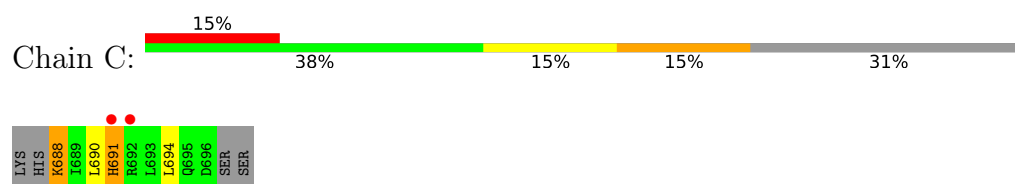
• Molecule 1: Estrogen receptor



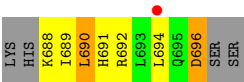
• Molecule 1: Estrogen receptor



• Molecule 2: Nuclear receptor coactivator 2



• Molecule 2: Nuclear receptor coactivator 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.25Å 81.91Å 58.34Å 90.00° 111.23° 90.00°	Depositor
Resolution (Å)	19.70 – 2.65 27.19 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.1 (19.70-2.65) 96.9 (27.19-2.61)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.256 0.220 , 0.254	Depositor DCC
R_{free} test set	703 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4040	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% 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: CME, T3O

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	0.35	0/1928	0.51	0/2600
1	B	0.42	1/1928 (0.1%)	0.60	0/2602
2	C	0.67	0/79	0.64	0/104
2	D	0.53	0/75	0.67	0/99
All	All	0.40	1/4010 (0.0%)	0.56	0/5405

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	359	ASN	CG-ND2	-5.94	1.18	1.32

There are no bond angle outliers.

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	1922	0	1966	91	0
1	B	1920	0	1968	73	0
2	C	79	0	88	5	0
2	D	75	0	82	7	0
3	A	19	0	22	5	0
3	B	19	0	22	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	0	0	0
4	B	2	0	0	0	0
All	All	4040	0	4148	153	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 19.

All (153) 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:458:VAL:HG13	1:A:459:TYR:CD1	1.94	1.02
1:A:458:VAL:HG13	1:A:459:TYR:HD1	1.34	0.91
1:A:407:ASN:H	1:A:407:ASN:HD22	1.26	0.82
1:A:513[A]:HIS:CE1	1:B:459:TYR:CD1	2.70	0.79
1:A:496:THR:H	1:A:499:GLN:HE21	1.30	0.79
1:A:434:ARG:HD3	1:B:459:TYR:HE2	1.47	0.78
1:A:434:ARG:HD3	1:B:459:TYR:CE2	2.17	0.78
1:A:456:SER:HA	1:A:515:ARG:NH2	1.99	0.78
1:B:311:THR:HG23	1:B:314:GLN:H	1.48	0.78
1:A:315:MET:CE	1:A:365:PRO:HG2	2.14	0.78
1:A:459:TYR:HE2	1:B:510:ILE:HG12	1.50	0.76
1:A:315:MET:HE3	1:A:365:PRO:HG2	1.69	0.75
1:A:496:THR:H	1:A:499:GLN:NE2	1.85	0.74
1:A:331:TYR:CZ	1:A:333:PRO:HA	2.22	0.74
1:A:547:HIS:O	1:A:548:ARG:HB3	1.88	0.74
1:A:384:LEU:HD11	3:A:700:T3O:HAN1	1.68	0.74
1:A:411:ASP:H	1:A:414:GLN:NE2	1.88	0.72
1:B:394:ARG:HG2	1:B:403:LEU:HD22	1.70	0.71
1:A:357:MET:CE	1:A:387:LEU:HD13	2.20	0.71
1:A:459:TYR:CE2	1:B:434:ARG:HG3	2.26	0.71
1:A:459:TYR:CE2	1:B:510:ILE:HG12	2.25	0.71
1:A:361:ALA:O	1:A:364:VAL:HG12	1.91	0.71
1:A:513[A]:HIS:CE1	1:B:459:TYR:HD1	2.08	0.71
1:B:331:TYR:CZ	1:B:333:PRO:HA	2.27	0.70
1:A:411:ASP:H	1:A:414:GLN:HE21	1.38	0.69
1:A:412:ARG:HB3	1:A:429:LEU:HD11	1.75	0.68
1:B:311:THR:HG22	1:B:314:GLN:NE2	2.10	0.67
1:A:332:ASP:O	1:A:335:ARG:HD2	1.95	0.66
1:A:424:ILE:CD1	1:A:424:ILE:N	2.57	0.66
1:A:332:ASP:HB3	1:A:335:ARG:HE	1.59	0.65
1:B:525:LEU:CD1	1:B:536:LEU:HD11	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:THR:HG22	1:A:499:GLN:H	1.62	0.64
1:A:458:VAL:HG13	1:A:459:TYR:CE1	2.33	0.64
1:B:360:TRP:CZ2	1:B:449:LYS:HD3	2.32	0.64
1:A:332:ASP:HB3	1:A:335:ARG:NE	2.13	0.64
1:A:311:THR:CG2	1:A:312:ALA:N	2.61	0.63
1:A:329:SER:H	1:A:407:ASN:HD21	1.45	0.63
1:B:311:THR:H	1:B:314:GLN:HE21	1.45	0.63
1:A:547:HIS:O	1:A:548:ARG:CB	2.48	0.62
1:A:513[A]:HIS:CD2	1:B:459:TYR:HD1	2.18	0.61
1:A:424:ILE:H	1:A:424:ILE:HD13	1.65	0.61
1:A:424:ILE:N	1:A:424:ILE:HD13	2.14	0.60
1:A:516:HIS:CD2	1:B:381[A]:CME:HH	2.21	0.59
1:B:443:GLU:HB3	1:B:489:LEU:HD11	1.83	0.59
1:A:331:TYR:O	1:A:333:PRO:HD3	2.03	0.59
1:A:315:MET:HE1	1:A:365:PRO:HG2	1.86	0.58
1:A:513[A]:HIS:CE1	1:B:459:TYR:CE1	2.91	0.58
1:B:392:VAL:HG13	1:B:432:SER:CA	2.34	0.58
2:C:688:LYS:HE2	2:C:691:HIS:HB2	1.87	0.57
1:B:531:LYS:HG3	1:B:533:VAL:HG13	1.85	0.57
1:A:519:ASN:HD21	1:B:516:HIS:CD2	2.23	0.57
1:B:384:LEU:HD11	3:B:701:T3O:HAN1	1.87	0.56
1:A:513[A]:HIS:CG	1:B:459:TYR:HD1	2.24	0.56
1:B:455:ASN:O	1:B:458:VAL:HG12	2.05	0.56
1:A:339:GLU:HG3	1:A:418:VAL:HA	1.87	0.56
1:B:331:TYR:HB2	1:B:345:LEU:HD13	1.87	0.56
1:B:331:TYR:CE1	1:B:333:PRO:HA	2.42	0.55
1:A:513[A]:HIS:HE1	1:B:455:ASN:OD1	1.89	0.55
1:B:311:THR:CG2	1:B:314:GLN:HG3	2.36	0.55
1:A:327:LEU:HD12	1:A:353:GLU:HG2	1.87	0.55
1:B:311:THR:HG22	1:B:314:GLN:CG	2.37	0.54
1:A:311:THR:HG22	1:A:312:ALA:N	2.22	0.54
1:B:376:VAL:HG21	2:D:691:HIS:CD2	2.42	0.54
1:B:385:GLU:HG2	1:B:514:ILE:HG22	1.87	0.54
2:D:692:ARG:O	2:D:696:ASP:HB3	2.08	0.54
1:A:381[B]:CME:HZ2	1:A:547:HIS:CD2	2.43	0.54
1:A:456:SER:HA	1:A:515:ARG:HH22	1.71	0.54
1:B:315:MET:CE	1:B:482:ILE:HG12	2.38	0.54
1:A:360:TRP:CZ2	1:A:449:LYS:HE2	2.43	0.53
1:B:456:SER:HA	1:B:515:ARG:NH2	2.24	0.53
1:A:380:GLU:O	1:A:547:HIS:HE1	1.92	0.53
1:A:380:GLU:O	1:A:547:HIS:CE1	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:GLU:HG2	1:A:470:GLU:O	2.08	0.52
1:A:328:TYR:CE1	1:A:406:PRO:HB2	2.45	0.52
1:A:459:TYR:HD1	1:A:459:TYR:N	2.08	0.51
1:A:513[A]:HIS:NE2	1:B:459:TYR:HD1	2.07	0.51
1:B:311:THR:HG22	1:B:314:GLN:HE21	1.76	0.51
1:A:347:THR:HG21	1:A:536:LEU:HD12	1.92	0.51
1:A:424:ILE:HG21	3:A:700:T3O:CAQ	2.41	0.51
1:A:362:LYS:HE2	2:C:694:LEU:O	2.11	0.51
1:A:538:ASP:HA	1:A:541:LEU:HD23	1.92	0.51
1:A:452:ILE:HD11	1:A:511:LEU:HD22	1.93	0.50
1:B:435:PHE:HE2	1:B:510:ILE:HG21	1.76	0.50
1:A:459:TYR:CD1	1:A:459:TYR:N	2.80	0.49
1:A:542:GLU:OE1	2:C:688:LYS:HA	2.12	0.49
1:B:392:VAL:HG13	1:B:432:SER:HA	1.93	0.49
1:A:412:ARG:HB3	1:A:429:LEU:CD1	2.42	0.49
1:A:513[A]:HIS:NE2	1:B:459:TYR:CD1	2.80	0.49
1:A:519:ASN:HD21	1:B:516:HIS:HD2	1.61	0.49
3:B:701:T3O:CAO	3:B:701:T3O:HAF3	2.42	0.49
1:A:543:MET:CE	2:C:690:LEU:HD13	2.42	0.48
1:B:508:LEU:HA	1:B:511:LEU:HD22	1.96	0.47
1:A:392:VAL:HG12	1:A:435:PHE:CD1	2.49	0.47
1:B:402:LEU:HD12	1:B:425:PHE:CE2	2.50	0.47
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.97	0.47
1:B:509:LEU:HD23	1:B:509:LEU:HA	1.80	0.47
1:B:525:LEU:HD11	1:B:536:LEU:HD11	1.95	0.47
1:A:487:ILE:HA	1:A:490:MET:CE	2.45	0.46
1:B:368:VAL:HA	1:B:375:GLN:NE2	2.30	0.46
3:A:700:T3O:HAF3	3:A:700:T3O:CAO	2.45	0.46
1:B:438:MET:HE1	1:B:510:ILE:HD12	1.97	0.46
1:B:531:LYS:HE2	1:B:533:VAL:HG11	1.97	0.46
1:B:378:LEU:HD12	1:B:378:LEU:HA	1.66	0.46
1:B:440:LEU:CD2	1:B:444:GLU:HB2	2.45	0.45
1:A:357:MET:HE1	1:A:387:LEU:HD13	1.98	0.45
1:A:407:ASN:HD22	1:A:407:ASN:N	1.96	0.45
1:B:370:LEU:HD21	1:B:475:ILE:HG12	1.99	0.45
1:A:407:ASN:H	1:A:407:ASN:ND2	2.04	0.45
1:B:498:GLN:HA	1:B:501:HIS:CE1	2.51	0.45
1:B:311:THR:HG22	1:B:314:GLN:HG3	1.97	0.44
1:B:531:LYS:HE2	1:B:533:VAL:CG1	2.46	0.44
2:D:692:ARG:HH11	2:D:692:ARG:HG3	1.81	0.44
1:A:540:LEU:HD23	1:A:540:LEU:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:MET:CE	1:A:387:LEU:CD1	2.94	0.44
1:B:360:TRP:CE2	1:B:449:LYS:HD3	2.52	0.44
1:B:376:VAL:HG21	2:D:691:HIS:NE2	2.33	0.44
1:B:502:GLN:O	1:B:506:GLN:HG3	2.18	0.44
1:B:538:ASP:HB3	2:D:689:ILE:HD11	1.98	0.44
1:A:411:ASP:OD1	1:A:413:ASN:HB2	2.18	0.44
1:A:496:THR:CG2	1:A:499:GLN:H	2.29	0.44
1:A:487:ILE:HA	1:A:490:MET:HE2	1.99	0.43
1:B:404:PHE:CD2	1:B:410:LEU:HD23	2.52	0.43
1:B:315:MET:HE2	1:B:482:ILE:HG12	2.00	0.43
2:D:688:LYS:HE3	2:D:688:LYS:HB2	1.56	0.43
1:A:424:ILE:HG21	3:A:700:T3O:HAQ3	2.01	0.43
1:A:410:LEU:HD12	1:A:410:LEU:HA	1.85	0.43
1:A:543:MET:HE2	2:C:690:LEU:HD13	2.01	0.43
1:B:328:TYR:CE2	1:B:406:PRO:HB2	2.54	0.43
1:A:360:TRP:CE2	1:A:449:LYS:HE2	2.54	0.42
1:A:509:LEU:HD23	1:A:509:LEU:HA	1.89	0.42
1:B:311:THR:H	1:B:314:GLN:NE2	2.12	0.42
1:A:364:VAL:HG13	1:A:367:PHE:HB2	2.02	0.42
1:B:332:ASP:HA	1:B:333:PRO:HD2	1.46	0.42
1:B:311:THR:HG22	1:B:314:GLN:CD	2.40	0.42
1:B:497:LEU:HD12	1:B:497:LEU:HA	1.85	0.41
1:A:434:ARG:HD2	1:A:434:ARG:HA	1.86	0.41
3:A:700:T3O:HAF2	3:A:700:T3O:HAM2	1.92	0.41
1:B:391:LEU:HD13	1:B:402:LEU:HD22	2.02	0.41
1:B:435:PHE:CD1	1:B:440:LEU:HD12	2.56	0.41
1:A:311:THR:HG22	1:A:313:ASP:H	1.84	0.41
1:A:434:ARG:CD	1:B:459:TYR:CE2	2.99	0.41
1:A:413:ASN:HD22	1:A:413:ASN:HA	1.53	0.41
1:A:513[A]:HIS:ND1	1:B:459:TYR:HD1	2.17	0.41
1:A:448:LEU:HD23	1:A:448:LEU:HA	1.86	0.41
1:A:539:LEU:HD23	1:A:539:LEU:HA	1.89	0.41
1:B:331:TYR:OH	1:B:333:PRO:HA	2.20	0.41
1:B:388:MET:HE2	3:B:701:T3O:HAQ2	2.03	0.41
1:B:410:LEU:HD12	1:B:414:GLN:NE2	2.35	0.41
1:A:337:PHE:HE2	1:A:345:LEU:HD12	1.85	0.41
1:A:411:ASP:HB3	1:A:414:GLN:HE21	1.86	0.40
1:B:474:HIS:O	1:B:478:VAL:HG23	2.21	0.40
1:A:513[A]:HIS:ND1	1:B:459:TYR:CD1	2.90	0.40
2:D:690:LEU:HD22	2:D:694:LEU:HD12	2.04	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	232/257 (90%)	226 (97%)	5 (2%)	1 (0%)	34	48
1	B	232/257 (90%)	227 (98%)	5 (2%)	0	100	100
2	C	7/13 (54%)	7 (100%)	0	0	100	100
2	D	7/13 (54%)	7 (100%)	0	0	100	100
All	All	478/540 (88%)	467 (98%)	10 (2%)	1 (0%)	47	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	MET

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	212/229 (93%)	183 (86%)	29 (14%)	3	4
1	B	211/229 (92%)	182 (86%)	29 (14%)	3	4
2	C	9/13 (69%)	7 (78%)	2 (22%)	1	0
2	D	8/13 (62%)	6 (75%)	2 (25%)	0	0
All	All	440/484 (91%)	378 (86%)	62 (14%)	3	4

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	308	LEU
1	A	310	LEU
1	A	315	MET
1	A	335	ARG
1	A	354	LEU
1	A	357	MET
1	A	372	LEU
1	A	379	LEU
1	A	387	LEU
1	A	407	ASN
1	A	410	LEU
1	A	412	ARG
1	A	413	ASN
1	A	424	ILE
1	A	433	SER
1	A	469	LEU
1	A	470	GLU
1	A	479	LEU
1	A	492	LYS
1	A	495	LEU
1	A	496	THR
1	A	504	LEU
1	A	510	ILE
1	A	525	LEU
1	A	534	VAL
1	A	536	LEU
1	A	539	LEU
1	A	541	LEU
1	A	544	LEU
1	B	308	LEU
1	B	319	LEU
1	B	321	ASP
1	B	339	GLU
1	B	346	LEU
1	B	353	GLU
1	B	362	LYS
1	B	363	ARG
1	B	370	LEU
1	B	378	LEU
1	B	391	LEU
1	B	395	SER
1	B	410	LEU
1	B	419	GLU

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Mol	Chain	Res	Type
1	B	425	PHE
1	B	434	ARG
1	B	436	ARG
1	B	439	ASN
1	B	440	LEU
1	B	454	LEU
1	B	477	ARG
1	B	481	LYS
1	B	504	LEU
1	B	511	LEU
1	B	525	LEU
1	B	543	MET
1	B	548	ARG
1	B	549	LEU
1	B	550	HIS
2	C	688	LYS
2	C	691	HIS
2	D	690	LEU
2	D	696	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	ASN
1	A	413	ASN
1	A	414	GLN
1	A	499	GLN
1	A	500	GLN
1	A	524	HIS
1	A	547	HIS
1	B	314	GLN
1	B	348	ASN
1	B	356	HIS
1	B	498	GLN
1	B	502	GLN
1	B	506	GLN
1	B	516	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	CME	B	417	1	8,9,10	0.82	0	5,9,11	1.56	1 (20%)
1	CME	B	530	1	8,9,10	0.85	0	5,9,11	1.21	1 (20%)
1	CME	A	381[B]	-	8,9,10	0.80	0	5,9,11	1.37	1 (20%)
1	CME	B	381[B]	-	8,9,10	0.86	0	5,9,11	1.35	1 (20%)
1	CME	A	417	1	8,9,10	0.80	0	5,9,11	1.37	1 (20%)
1	CME	A	530	1	8,9,10	0.84	0	5,9,11	1.44	1 (20%)
1	CME	A	381[A]	-	8,9,10	0.81	0	5,9,11	1.39	1 (20%)
1	CME	B	381[A]	-	8,9,10	0.75	0	5,9,11	1.21	1 (20%)

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	CME	B	417	1	-	3/5/8/10	-
1	CME	B	530	1	-	1/5/8/10	-
1	CME	A	381[B]	-	-	3/5/8/10	-
1	CME	B	381[B]	-	-	2/5/8/10	-
1	CME	A	417	1	-	3/5/8/10	-
1	CME	A	530	1	-	3/5/8/10	-
1	CME	A	381[A]	-	-	3/5/8/10	-
1	CME	B	381[A]	-	-	1/5/8/10	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	417	CME	CE-SD-SG	2.68	115.79	103.45
1	A	417	CME	CE-SD-SG	2.62	115.50	103.45
1	A	381[B]	CME	CE-SD-SG	2.61	115.48	103.45
1	A	530	CME	CE-SD-SG	2.59	115.40	103.45
1	A	381[A]	CME	CE-SD-SG	2.45	114.72	103.45
1	B	381[B]	CME	CE-SD-SG	2.39	114.45	103.45
1	B	530	CME	CE-SD-SG	2.21	113.62	103.45
1	B	381[A]	CME	CE-SD-SG	2.18	113.51	103.45

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	381[A]	CME	SD-CE-CZ-OH
1	A	381[B]	CME	CE-SD-SG-CB
1	A	530	CME	SD-CE-CZ-OH
1	B	381[B]	CME	CE-SD-SG-CB
1	B	417	CME	CE-SD-SG-CB
1	B	417	CME	SD-CE-CZ-OH
1	A	381[A]	CME	CE-SD-SG-CB
1	B	381[A]	CME	CE-SD-SG-CB
1	A	530	CME	CE-SD-SG-CB
1	B	530	CME	CE-SD-SG-CB
1	A	381[B]	CME	CA-CB-SG-SD
1	A	530	CME	CA-CB-SG-SD
1	A	417	CME	CE-SD-SG-CB
1	B	381[B]	CME	SD-CE-CZ-OH
1	B	417	CME	CZ-CE-SD-SG
1	A	417	CME	CA-CB-SG-SD
1	A	381[A]	CME	CZ-CE-SD-SG
1	A	381[B]	CME	CZ-CE-SD-SG
1	A	417	CME	CZ-CE-SD-SG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	381[B]	CME	1	0
1	B	381[A]	CME	1	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

2 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	T3O	B	701	-	21,21,21	0.69	0	28,32,32	0.98	2 (7%)
3	T3O	A	700	-	21,21,21	0.74	0	28,32,32	1.25	4 (14%)

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	T3O	B	701	-	-	0/4/32/32	1/3/3/3
3	T3O	A	700	-	-	0/4/32/32	1/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	700	T3O	CAM-CAP-CAK	-3.53	112.38	117.30
3	A	700	T3O	CAQ-CAK-CAP	-2.73	107.56	112.60
3	B	701	T3O	CAQ-CAK-CAP	-2.47	108.03	112.60
3	B	701	T3O	CAM-CAP-CAK	-2.44	113.90	117.30
3	A	700	T3O	CAN-CAD-CAB	2.43	111.26	106.62
3	A	700	T3O	CAD-CAN-CAP	-2.29	107.87	112.66

There are no chirality outliers.

There are no torsion outliers.

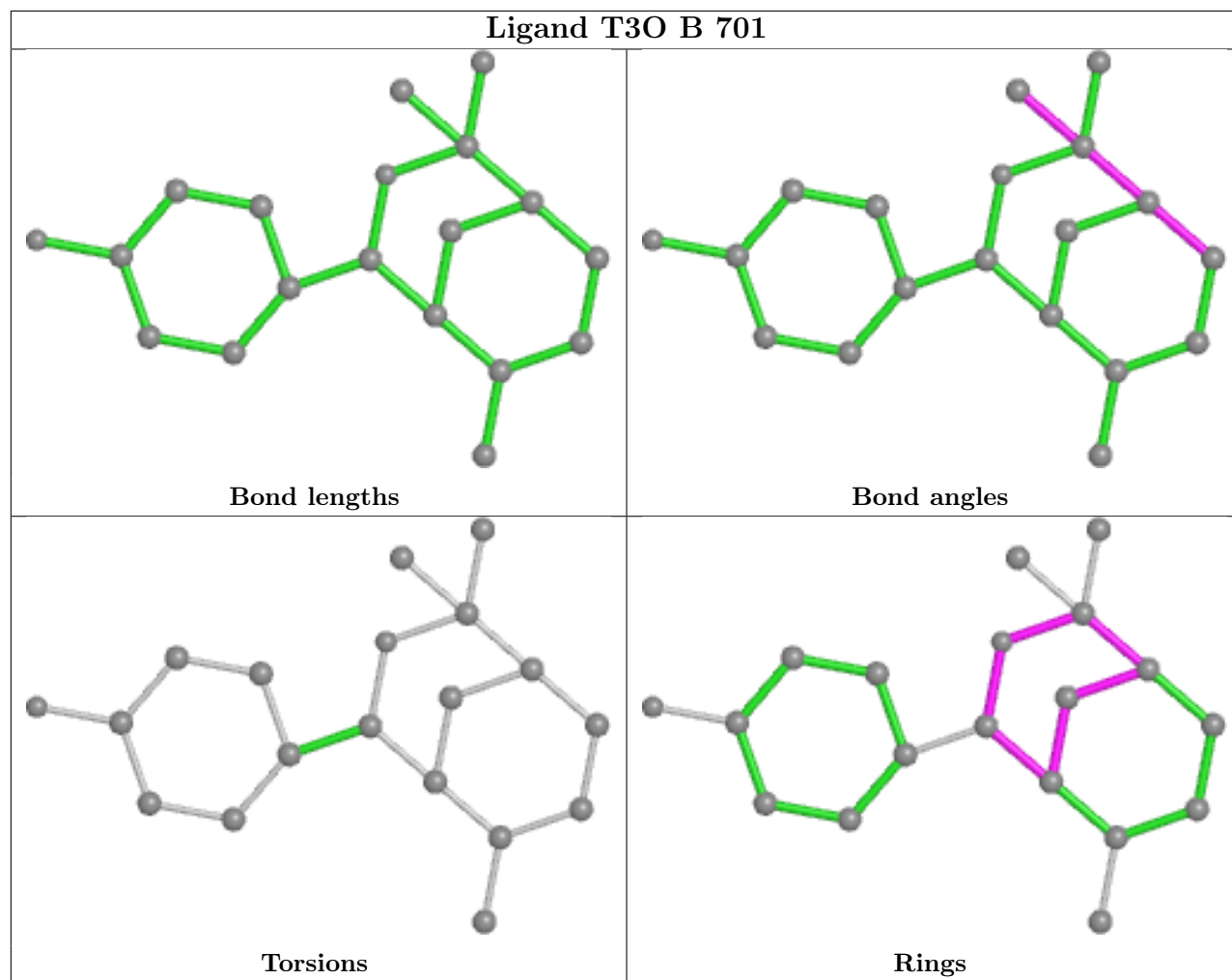
All (2) ring outliers are listed below:

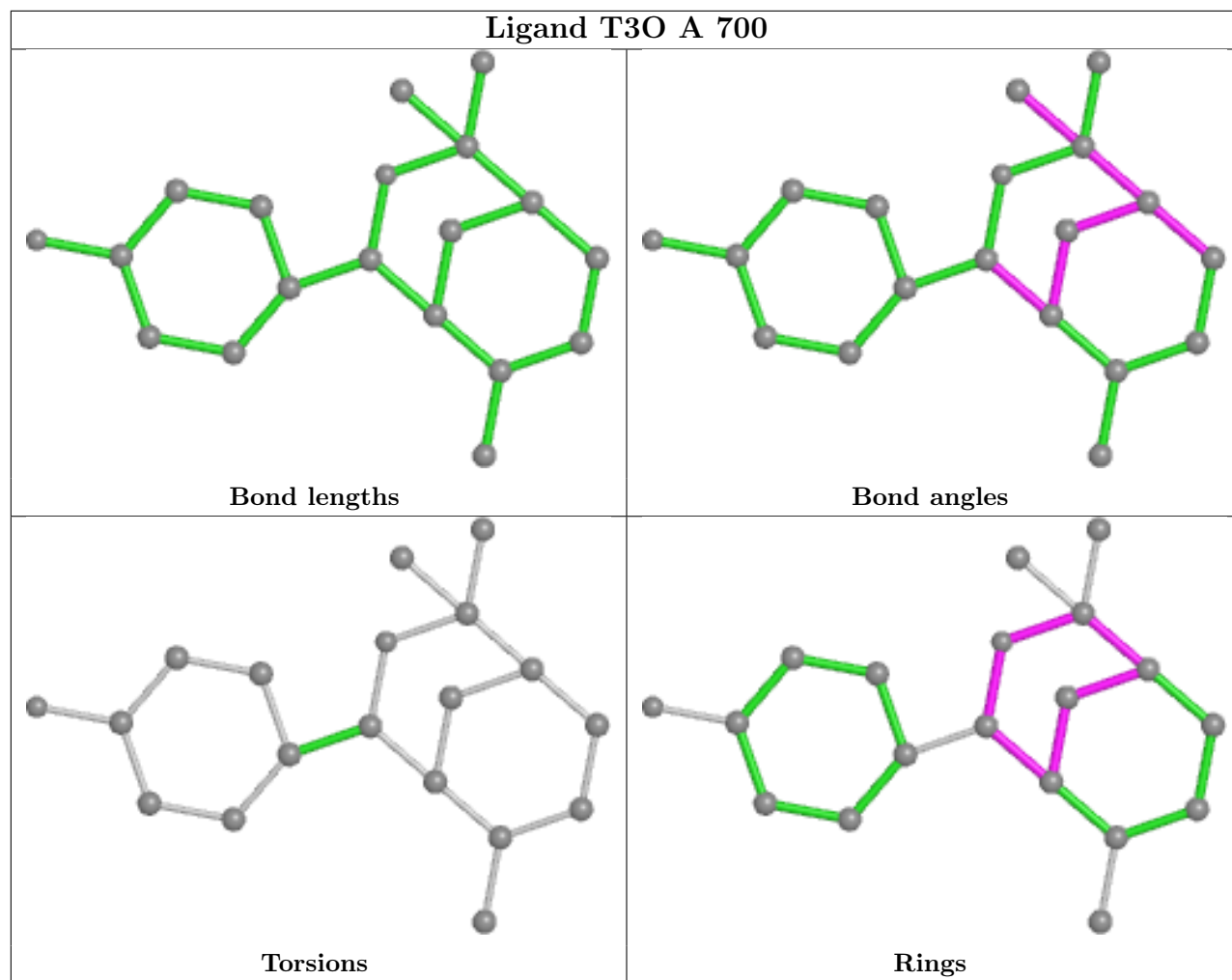
Mol	Chain	Res	Type	Atoms
3	A	700	T3O	CAB-CAD-CAK-CAN-CAP-OAR
3	B	701	T3O	CAB-CAD-CAK-CAN-CAP-OAR

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	T3O	3	0
3	A	700	T3O	5	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	234/257 (91%)	0.47	18 (7%) 13 10	34, 55, 81, 101	0
1	B	234/257 (91%)	0.56	22 (9%) 8 6	33, 55, 80, 98	0
2	C	9/13 (69%)	1.17	2 (22%) 0 0	56, 59, 84, 86	0
2	D	9/13 (69%)	0.60	1 (11%) 5 3	57, 59, 85, 86	0
All	All	486/540 (90%)	0.53	43 (8%) 10 8	33, 56, 82, 101	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	PRO	14.5
1	B	334	THR	7.3
1	A	459	TYR	7.0
1	B	331	TYR	4.6
1	B	477	ARG	4.4
1	B	551	ALA	4.1
1	B	335	ARG	3.9
1	A	461	PHE	3.9
1	B	534	VAL	3.9
1	A	535	PRO	3.9
1	A	472	LYS	3.8
1	B	459	TYR	3.7
1	B	333	PRO	3.7
1	B	337	PHE	3.7
1	B	494	GLY	3.7
1	A	372	LEU	3.6
1	A	331	TYR	3.4
1	A	541	LEU	3.4
1	A	337	PHE	3.3
1	A	334	THR	3.3
1	B	382	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	513[A]	HIS	3.0
1	B	306	LEU	3.0
1	A	532	ASN	2.9
1	B	461	PHE	2.9
2	C	691	HIS	2.8
1	B	511	LEU	2.7
1	A	545	ASP	2.7
1	A	397	GLU	2.6
1	A	373[A]	HIS	2.5
1	B	472	LYS	2.5
1	A	470	GLU	2.4
1	A	307	ALA	2.4
1	B	309	SER	2.4
1	B	474	HIS	2.4
2	C	692	ARG	2.4
2	D	694	LEU	2.3
1	B	489	LEU	2.3
1	B	332	ASP	2.2
1	A	534	VAL	2.2
1	B	512	SER	2.1
1	A	548	ARG	2.1
1	A	308	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	CME	B	530	10/11	0.81	0.22	58,58,59,59	5
1	CME	A	381[B]	10/11	0.82	0.26	54,55,56,56	6
1	CME	A	417	10/11	0.82	0.23	56,59,62,62	5
1	CME	A	381[A]	10/11	0.82	0.26	54,57,62,63	6
1	CME	A	530	10/11	0.88	0.33	59,59,59,60	5
1	CME	B	381[B]	10/11	0.89	0.26	54,55,58,59	6
1	CME	B	381[A]	10/11	0.89	0.26	54,57,63,64	6
1	CME	B	417	10/11	0.91	0.20	57,59,63,63	5

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

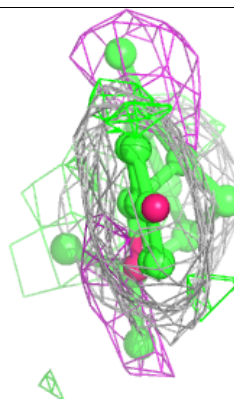
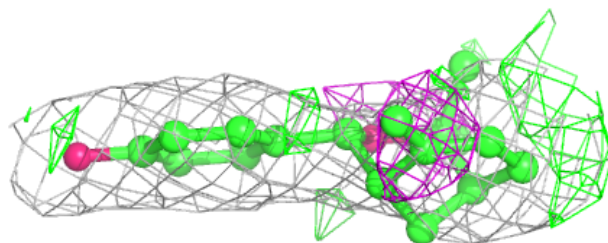
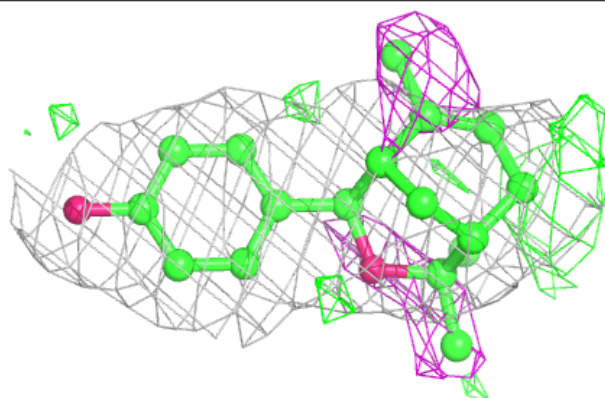
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	T3O	B	701	19/19	0.74	0.31	47,51,52,52	0
3	T3O	A	700	19/19	0.79	0.31	47,50,52,52	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.

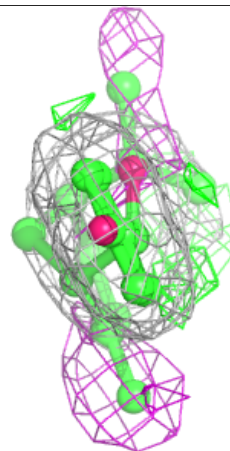
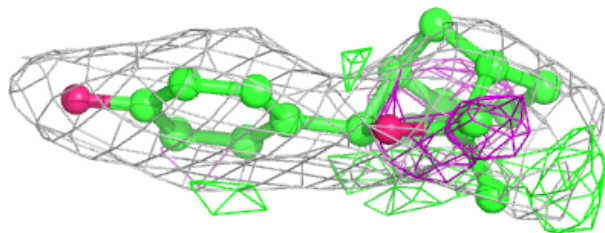
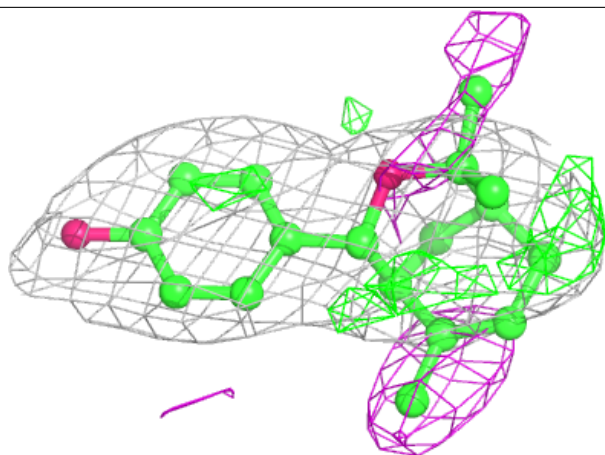
Electron density around T3O B 701:

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 T3O A 700:

$2mF_o-DF_c$ (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.