



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:44 PM UTC

PDB ID : 4DMA / pdb_00004dma
Title : Crystal structure of ERa LBD in complex with RU100132
Authors : Osz, J.; Breliet, Y.; Peluso-Iltis, C.; Cura, V.; Eiler, S.; Ruff, M.; Bourguet, W.; Rochel, N.; Moras, D.
Deposited on : 2012-02-07
Resolution : 2.30 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

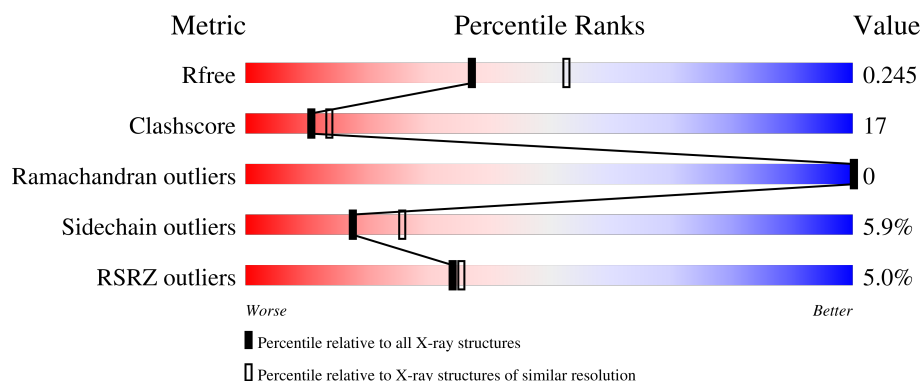
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	247	4% 68% 26% • •
1	B	247	4% 65% 26% • 5%
2	E	15	20% 53% 20% 27%
2	F	15	13% 60% 20% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4140 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	238	Total	C	N	O	S	0	0	0
			1906	1223	325	340	18			
1	B	235	Total	C	N	O	S	0	0	0
			1879	1205	323	333	18			

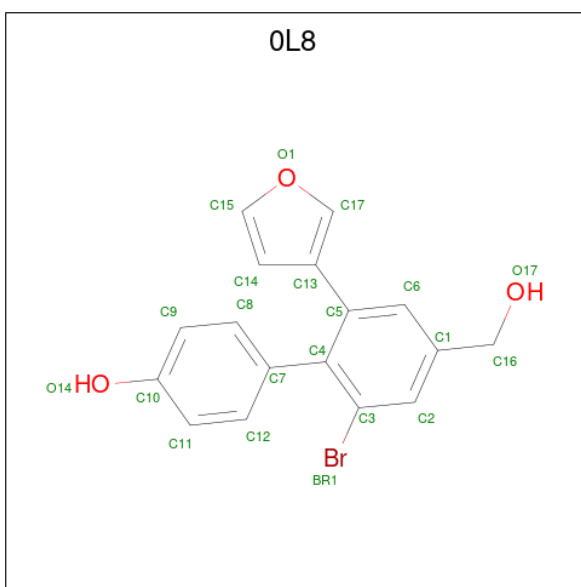
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	530	ALA	CYS	engineered mutation	UNP P03372
B	1530	ALA	CYS	engineered mutation	UNP P03372

- Molecule 2 is a protein called Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	0	0	0
			94	60	20	14			
2	F	12	Total	C	N	O	0	0	0
			99	63	21	15			

- Molecule 3 is 2'-bromo-6'-(furan-3-yl)-4'-(hydroxymethyl)biphenyl-4-ol (CCD ID: 0L8) (formula: C₁₇H₁₃BrO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	Br	C	O	0	0
			21	1	17	3		
3	B	1	Total	Br	C	O	0	0
			21	1	17	3		

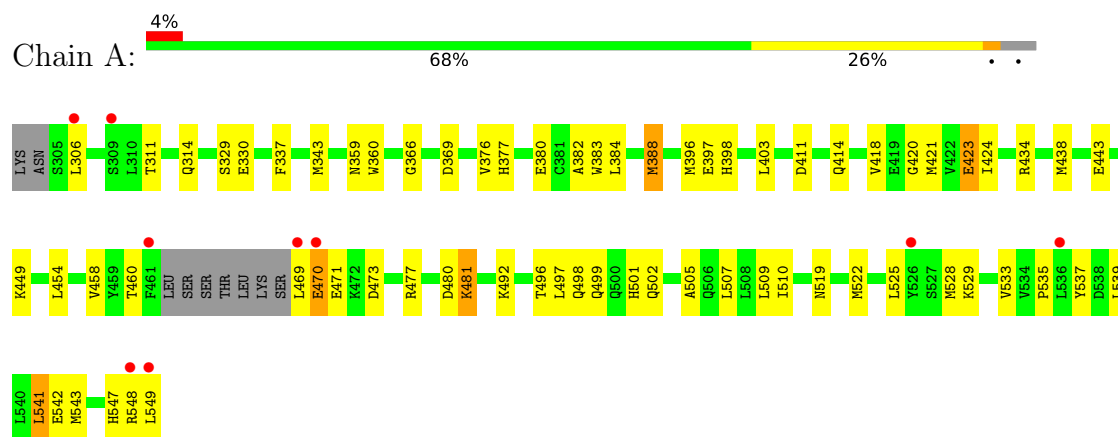
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	61	Total	O	0	0
			61	61		
4	E	6	Total	O	0	0
			6	6		
4	F	2	Total	O	0	0
			2	2		

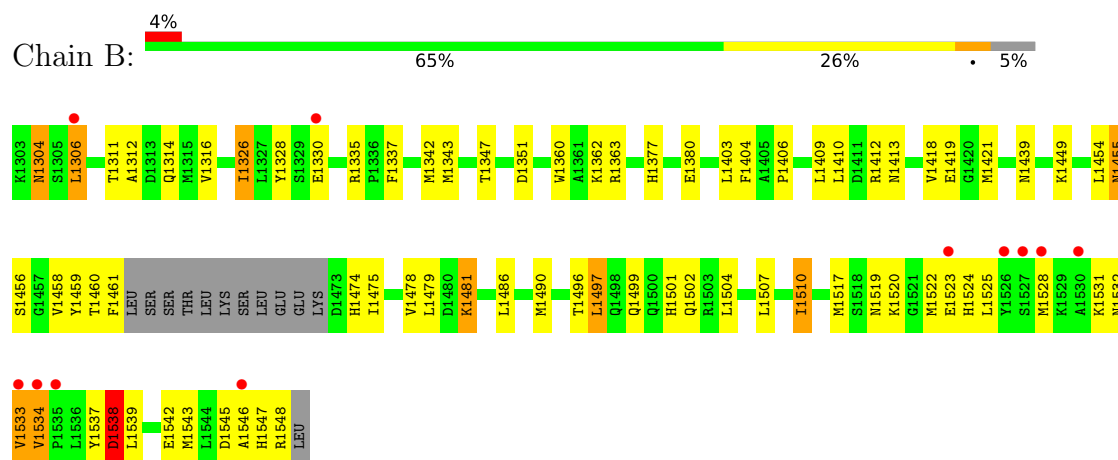
3 Residue-property plots

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 1



• Molecule 2: Nuclear receptor coactivator 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.28Å 81.79Å 58.30Å 90.00° 111.17° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.30) 95.1 (30.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.58 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.251 0.201 , 0.245	Depositor DCC
R_{free} test set	2097 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.754	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4140	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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: 0L8

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	0.39	0/1942	0.85	4/2623 (0.2%)
1	B	0.43	0/1915	0.91	5/2588 (0.2%)
2	E	0.33	0/95	0.74	0/125
2	F	0.32	0/100	0.73	0/132
All	All	0.41	0/4052	0.88	9/5468 (0.2%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1538	ASP	N-CA-C	10.70	124.08	111.02
1	B	1456	SER	N-CA-C	6.24	118.88	111.33
1	B	1304	ASN	N-CA-C	-6.05	102.73	110.53
1	A	382	ALA	N-CA-C	5.79	120.50	113.38
1	A	383	TRP	N-CA-C	5.75	118.00	111.11
1	B	1455	ASN	N-CA-C	5.57	120.19	112.45
1	B	1538	ASP	CB-CA-C	-5.35	102.42	110.92
1	A	388	MET	N-CA-C	5.17	116.60	111.07
1	A	424	ILE	N-CA-C	-5.05	105.50	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1906	0	1954	65	0
1	B	1879	0	1926	71	0
2	E	94	0	100	2	0
2	F	99	0	102	4	0
3	A	21	0	13	3	0
3	B	21	0	12	1	0
4	A	51	0	0	1	0
4	B	61	0	0	4	0
4	E	6	0	0	1	0
4	F	2	0	0	0	0
All	All	4140	0	4107	135	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 17.

All (135) 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:549:LEU:HD12	1:A:549:LEU:OXT	1.48	1.12
1:B:1326:ILE:HD13	1:B:1326:ILE:H	1.27	0.97
1:B:1533:VAL:HG13	1:B:1534:VAL:H	1.29	0.97
1:A:528:MET:HE3	1:A:533:VAL:HG21	1.48	0.94
1:B:1520:LYS:O	1:B:1523:GLU:HG2	1.73	0.87
1:B:1343:MET:HB3	1:B:1534:VAL:HG22	1.60	0.82
1:B:1343:MET:HB3	1:B:1534:VAL:CG2	2.11	0.81
1:A:549:LEU:OXT	1:A:549:LEU:CD1	2.29	0.80
1:A:434:ARG:NE	1:A:438:MET:HE2	2.00	0.76
1:B:1533:VAL:HG13	1:B:1534:VAL:HG23	1.66	0.76
1:B:1343:MET:HE1	1:B:1421:MET:HE2	1.68	0.75
1:B:1347:THR:HG21	1:B:1534:VAL:HG11	1.70	0.73
1:B:1475:ILE:O	1:B:1479:LEU:HD23	1.90	0.71
1:A:498:GLN:O	1:A:502:GLN:HG3	1.91	0.70
1:B:1347:THR:CG2	1:B:1534:VAL:HG11	2.20	0.70
1:B:1377:HIS:NE2	1:B:1460:THR:HB	2.05	0.70
1:B:1548:ARG:CD	1:B:1548:ARG:H	2.05	0.69
1:B:1343:MET:HE1	1:B:1421:MET:CE	2.22	0.69
1:A:477:ARG:O	1:A:481:LYS:HG2	1.94	0.68
1:B:1525:LEU:HD13	3:B:1701:OL8:H2	1.74	0.68
1:B:1496:THR:OG1	1:B:1499:GLN:HG3	1.93	0.68
1:A:542:GLU:OE2	2:E:688:LYS:HB3	1.95	0.66
1:B:1538:ASP:O	1:B:1542:GLU:HG3	1.96	0.65
1:B:1343:MET:CB	1:B:1534:VAL:HG22	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:GLU:H	1:A:443:GLU:CD	2.05	0.65
1:A:470:GLU:HA	1:A:473:ASP:OD2	1.98	0.64
1:B:1326:ILE:H	1:B:1326:ILE:CD1	2.05	0.63
1:B:1343:MET:HE3	1:B:1418:VAL:HG11	1.79	0.63
1:A:481:LYS:HZ2	1:A:481:LYS:HB3	1.63	0.63
1:B:1533:VAL:HG22	1:B:1534:VAL:N	2.14	0.63
1:B:1362:LYS:HZ1	2:F:697:GLY:HA3	1.64	0.63
1:A:376:VAL:O	1:A:380:GLU:HG3	1.99	0.62
1:A:519:ASN:ND2	1:B:1519:ASN:OD1	2.29	0.61
1:B:1306:LEU:HD13	1:B:1306:LEU:O	2.01	0.60
1:B:1548:ARG:H	1:B:1548:ARG:HD2	1.67	0.60
1:A:366:GLY:HA2	1:A:369:ASP:OD2	2.01	0.59
1:A:548:ARG:HB3	1:A:548:ARG:NH1	2.17	0.59
1:B:1528:MET:O	1:B:1533:VAL:HG12	2.02	0.59
1:B:1326:ILE:HD13	1:B:1326:ILE:N	2.08	0.59
1:B:1533:VAL:HG13	1:B:1534:VAL:N	2.09	0.58
1:A:384:LEU:HD13	3:A:701:OL8:H11	1.86	0.58
1:B:1363:ARG:HD3	4:B:1823:HOH:O	2.05	0.56
1:B:1486:LEU:HG	1:B:1490:MET:HE3	1.89	0.55
1:A:496:THR:OG1	1:A:499:GLN:HG3	2.07	0.54
1:A:470:GLU:OE1	1:A:471:GLU:N	2.39	0.54
1:A:397:GLU:HG3	1:A:398:HIS:CE1	2.43	0.54
1:B:1343:MET:HE3	1:B:1418:VAL:HG21	1.89	0.54
1:A:529:LYS:HD2	1:A:541:LEU:HD11	1.90	0.53
1:B:1419:GLU:OE1	1:B:1531:LYS:NZ	2.41	0.53
1:B:1404:PHE:CE2	1:B:1410:LEU:HD12	2.44	0.53
2:E:692:ARG:NE	4:E:801:HOH:O	2.38	0.53
1:B:1362:LYS:NZ	2:F:697:GLY:HA3	2.24	0.52
1:A:529:LYS:CE	1:A:541:LEU:HD11	2.39	0.52
1:A:423:GLU:H	1:A:423:GLU:CD	2.15	0.52
1:A:306:LEU:N	1:A:306:LEU:HD12	2.26	0.51
2:F:696:GLU:OE2	2:F:696:GLU:HA	2.08	0.51
1:B:1454:LEU:HB3	1:B:1479:LEU:HD21	1.92	0.50
1:B:1548:ARG:CD	1:B:1548:ARG:N	2.75	0.50
1:B:1328:TYR:CE1	1:B:1406:PRO:HB2	2.47	0.50
1:A:411:ASP:OD1	1:A:414:GLN:HG3	2.12	0.50
1:A:434:ARG:HG2	1:B:1459:TYR:CZ	2.47	0.50
1:A:458:VAL:HG22	1:A:458:VAL:O	2.12	0.49
1:A:535:PRO:HB2	1:A:537:TYR:CE2	2.47	0.49
1:B:1538:ASP:HB2	2:F:689:ILE:CD1	2.43	0.49
1:A:343:MET:HE2	1:A:528:MET:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1343:MET:HB3	1:B:1534:VAL:HG21	1.90	0.49
1:B:1461:PHE:HB2	4:B:1861:HOH:O	2.12	0.49
1:B:1523:GLU:CG	1:B:1524:HIS:N	2.76	0.49
1:B:1481:LYS:HE3	1:B:1481:LYS:HA	1.93	0.49
1:B:1548:ARG:HD2	1:B:1548:ARG:N	2.28	0.48
1:A:496:THR:HG23	1:A:499:GLN:OE1	2.13	0.48
1:B:1306:LEU:O	1:B:1306:LEU:HD22	2.13	0.48
1:A:420:GLY:HA2	1:A:423:GLU:OE2	2.13	0.48
1:A:434:ARG:CZ	1:A:438:MET:HE2	2.44	0.48
1:A:384:LEU:CD1	3:A:701:OL8:H11	2.44	0.47
1:A:501:HIS:HB3	4:B:1849:HOH:O	2.13	0.47
1:B:1510:ILE:CD1	4:B:1812:HOH:O	2.61	0.47
1:A:505:ALA:O	1:A:509:LEU:HG	2.15	0.47
1:A:403:LEU:O	1:A:403:LEU:HD23	2.15	0.47
1:A:525:LEU:HD13	3:A:701:OL8:H2	1.97	0.47
1:B:1533:VAL:CG1	1:B:1534:VAL:H	2.06	0.47
1:B:1403:LEU:HD12	1:B:1409:LEU:HD13	1.96	0.46
1:B:1507:LEU:O	1:B:1510:ILE:HB	2.15	0.46
1:A:470:GLU:CD	1:A:471:GLU:N	2.74	0.46
1:A:434:ARG:HG3	1:A:438:MET:HE3	1.98	0.46
1:B:1306:LEU:HD13	1:B:1306:LEU:C	2.41	0.46
1:A:329:SER:HB2	4:A:808:HOH:O	2.14	0.45
1:A:481:LYS:HB3	1:A:481:LYS:NZ	2.29	0.45
1:B:1360:TRP:CZ2	1:B:1449:LYS:HG2	2.50	0.45
1:B:1497:LEU:HD12	1:B:1501:HIS:CE1	2.51	0.45
1:B:1335:ARG:CZ	1:B:1337:PHE:CZ	2.99	0.45
1:A:528:MET:HE3	1:A:533:VAL:CG2	2.35	0.45
1:B:1311:THR:H	1:B:1314:GLN:HE21	1.64	0.44
1:A:480:ASP:OD1	1:B:1502:GLN:HG2	2.18	0.44
1:B:1474:HIS:O	1:B:1478:VAL:HG23	2.17	0.44
1:A:384:LEU:O	1:A:388:MET:HG3	2.17	0.44
1:A:528:MET:O	1:A:533:VAL:HG22	2.18	0.44
1:B:1380:GLU:HB3	1:B:1546:ALA:HB1	1.99	0.44
1:A:330:GLU:HA	1:A:330:GLU:OE2	2.18	0.43
1:A:492:LYS:HE2	1:A:492:LYS:HB3	1.80	0.43
1:A:539:LEU:O	1:A:543:MET:HG2	2.18	0.43
1:B:1312:ALA:O	1:B:1316:VAL:HG23	2.19	0.43
1:B:1458:VAL:HG13	1:B:1459:TYR:HD1	1.84	0.43
1:A:377:HIS:HE1	1:A:460:THR:OG1	2.01	0.43
1:A:522:MET:HE3	1:A:547:HIS:CD2	2.53	0.42
1:B:1460:THR:HG22	1:B:1460:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:MET:HG3	1:A:528:MET:HE2	2.01	0.42
1:A:548:ARG:HB3	1:A:548:ARG:HH11	1.85	0.42
1:B:1522:MET:HE3	1:B:1547:HIS:CE1	2.54	0.42
1:B:1548:ARG:H	1:B:1548:ARG:HD3	1.84	0.42
1:A:360:TRP:CZ2	1:A:449:LYS:HD2	2.55	0.42
1:A:411:ASP:H	1:A:414:GLN:NE2	2.17	0.42
1:B:1455:ASN:O	1:B:1458:VAL:HG12	2.19	0.42
1:B:1326:ILE:CD1	1:B:1326:ILE:N	2.76	0.42
1:B:1539:LEU:O	1:B:1543:MET:HG2	2.19	0.42
1:A:469:LEU:HD22	1:A:469:LEU:N	2.35	0.41
1:A:548:ARG:O	1:A:549:LEU:C	2.63	0.41
1:A:507:LEU:O	1:A:510:ILE:HB	2.19	0.41
1:A:311:THR:OG1	1:A:314:GLN:HG3	2.20	0.41
1:A:529:LYS:HE3	1:A:541:LEU:HD11	2.02	0.41
1:B:1380:GLU:O	1:B:1547:HIS:HE1	2.04	0.41
1:A:377:HIS:CE1	1:A:460:THR:OG1	2.74	0.41
1:B:1351:ASP:CG	1:B:1537:TYR:HB2	2.46	0.41
1:A:411:ASP:H	1:A:414:GLN:HE21	1.68	0.41
1:B:1326:ILE:HG12	1:B:1326:ILE:O	2.20	0.41
1:B:1523:GLU:HG3	1:B:1524:HIS:N	2.36	0.41
1:A:418:VAL:HB	1:A:421:MET:HB2	2.03	0.40
1:A:509:LEU:HD23	1:A:509:LEU:HA	1.87	0.40
1:B:1486:LEU:HD23	1:B:1504:LEU:HD12	2.03	0.40
1:A:403:LEU:HD23	1:A:403:LEU:C	2.46	0.40
1:A:529:LYS:HE3	1:A:541:LEU:CD1	2.51	0.40
1:A:529:LYS:CD	1:A:541:LEU:HD11	2.51	0.40
1:B:1454:LEU:CB	1:B:1479:LEU:HD21	2.52	0.40
1:A:366:GLY:O	1:A:369:ASP:HB2	2.21	0.40
1:B:1342:MET:HG2	1:B:1418:VAL:HG23	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	234/247 (95%)	225 (96%)	9 (4%)	0	100	100
1	B	231/247 (94%)	223 (96%)	8 (4%)	0	100	100
2	E	9/15 (60%)	9 (100%)	0	0	100	100
2	F	10/15 (67%)	9 (90%)	1 (10%)	0	100	100
All	All	484/524 (92%)	466 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	213/222 (96%)	204 (96%)	9 (4%)	26	40
1	B	210/222 (95%)	194 (92%)	16 (8%)	12	16
2	E	10/14 (71%)	9 (90%)	1 (10%)	7	9
2	F	10/14 (71%)	10 (100%)	0	100	100
All	All	443/472 (94%)	417 (94%)	26 (6%)	18	26

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	PHE
1	A	359	ASN
1	A	396	MET
1	A	423	GLU
1	A	454	LEU
1	A	470	GLU
1	A	481	LYS
1	A	497	LEU
1	A	541	LEU
1	B	1304	ASN
1	B	1306	LEU
1	B	1326	ILE
1	B	1330	GLU

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Mol	Chain	Res	Type
1	B	1412	ARG
1	B	1413	ASN
1	B	1439	ASN
1	B	1481	LYS
1	B	1497	LEU
1	B	1510	ILE
1	B	1517	MET
1	B	1532	ASN
1	B	1533	VAL
1	B	1534	VAL
1	B	1538	ASP
1	B	1545	ASP
2	E	695	GLN

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	377	HIS
1	A	414	GLN
1	A	439	ASN
1	A	488	HIS
1	A	519	ASN
1	A	532	ASN
1	B	1314	GLN
1	B	1474	HIS
1	B	1501	HIS
1	B	1506	GLN
1	B	1516	HIS
1	B	1519	ASN
1	B	1547	HIS
2	E	695	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0L8	A	701	-	22,23,23	2.78	11 (50%)	30,32,32	1.63	5 (16%)
3	0L8	B	1701	-	22,23,23	2.87	12 (54%)	30,32,32	1.50	5 (16%)

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	0L8	A	701	-	-	4/10/10/10	0/3/3/3
3	0L8	B	1701	-	-	4/10/10/10	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	0L8	C4-C3	7.01	1.49	1.39
3	A	701	0L8	C5-C4	6.00	1.48	1.40
3	B	1701	0L8	C4-C3	5.73	1.47	1.39
3	B	1701	0L8	C5-C4	5.11	1.47	1.40
3	B	1701	0L8	C4-C7	4.50	1.58	1.50
3	B	1701	0L8	C8-C7	3.76	1.46	1.39
3	A	701	0L8	C9-C8	3.72	1.44	1.38
3	A	701	0L8	C4-C7	3.70	1.56	1.50
3	B	1701	0L8	C11-C10	3.68	1.45	1.39
3	B	1701	0L8	C6-C5	3.44	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1701	OL8	C12-C11	3.32	1.44	1.38
3	B	1701	OL8	C9-C8	3.31	1.44	1.38
3	B	1701	OL8	C2-C3	3.21	1.44	1.38
3	B	1701	OL8	C12-C7	3.19	1.45	1.39
3	A	701	OL8	C12-C11	3.00	1.43	1.38
3	A	701	OL8	C9-C10	2.90	1.44	1.39
3	A	701	OL8	C12-C7	2.87	1.45	1.39
3	A	701	OL8	C6-C5	2.64	1.44	1.39
3	A	701	OL8	C11-C10	2.52	1.43	1.39
3	B	1701	OL8	C9-C10	2.49	1.43	1.39
3	A	701	OL8	C2-C3	2.45	1.43	1.38
3	A	701	OL8	C8-C7	2.32	1.44	1.39
3	B	1701	OL8	O1-C17	-2.03	1.32	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	OL8	C6-C5-C13	-4.31	112.42	119.12
3	A	701	OL8	BR1-C3-C2	-4.17	110.67	118.28
3	B	1701	OL8	C5-C4-C3	-3.86	114.39	116.97
3	A	701	OL8	C5-C4-C3	-3.68	114.51	116.97
3	B	1701	OL8	C6-C5-C13	-3.67	113.41	119.12
3	A	701	OL8	BR1-C3-C4	3.65	127.51	120.86
3	B	1701	OL8	BR1-C3-C2	-3.28	112.30	118.28
3	B	1701	OL8	BR1-C3-C4	2.55	125.51	120.86
3	B	1701	OL8	C15-C14-C13	-2.27	103.37	107.92
3	A	701	OL8	C7-C4-C3	2.18	124.30	122.00

There are no chirality outliers.

All (8) torsion outliers are listed below:

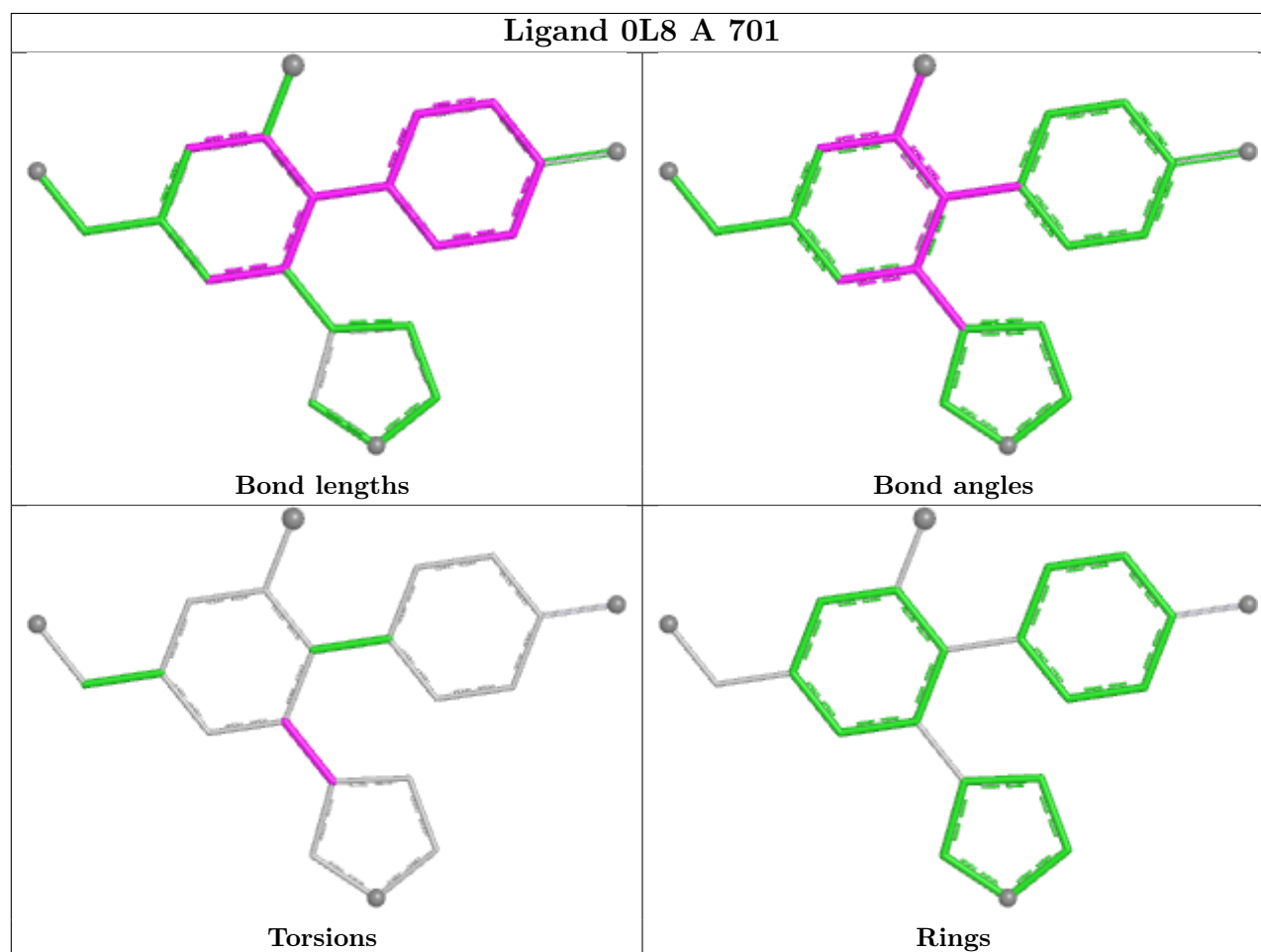
Mol	Chain	Res	Type	Atoms
3	A	701	OL8	C14-C13-C5-C4
3	B	1701	OL8	C17-C13-C5-C4
3	B	1701	OL8	C14-C13-C5-C6
3	A	701	OL8	C17-C13-C5-C6
3	B	1701	OL8	C17-C13-C5-C6
3	A	701	OL8	C14-C13-C5-C6
3	A	701	OL8	C17-C13-C5-C4
3	B	1701	OL8	C14-C13-C5-C4

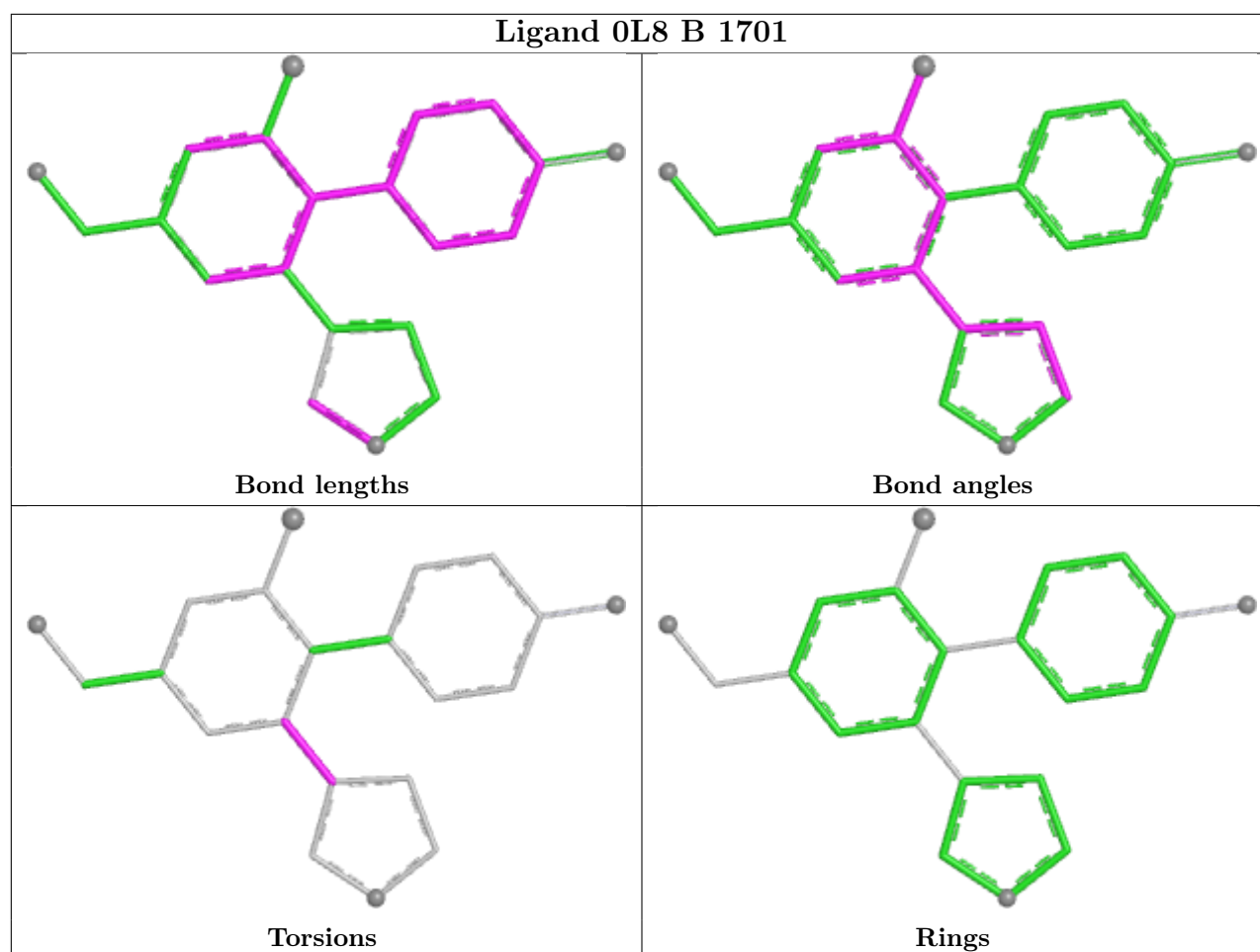
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	0L8	3	0
3	B	1701	0L8	1	0

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





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	238/247 (96%)	0.32	9 (3%) 44 46	12, 29, 54, 71	0
1	B	235/247 (95%)	0.29	11 (4%) 36 38	13, 26, 49, 63	0
2	E	11/15 (73%)	1.20	3 (27%) 1 1	28, 38, 54, 57	0
2	F	12/15 (80%)	0.37	2 (16%) 4 5	23, 32, 52, 52	0
All	All	496/524 (94%)	0.33	25 (5%) 34 35	12, 28, 53, 71	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	549	LEU	4.7
1	B	1527	SER	3.6
1	A	470	GLU	3.3
1	B	1530	ALA	3.0
1	A	469	LEU	2.8
1	B	1533	VAL	2.8
1	A	306	LEU	2.7
1	B	1546	ALA	2.7
1	B	1330	GLU	2.7
1	A	548	ARG	2.7
1	B	1534	VAL	2.6
2	E	697	GLY	2.6
1	B	1528	MET	2.6
2	F	697	GLY	2.6
2	E	687	HIS	2.5
1	B	1535	PRO	2.5
1	A	461	PHE	2.5
1	A	309	SER	2.4
1	A	536	LEU	2.4
1	B	1526	TYR	2.3
2	F	696	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	695	GLN	2.2
1	B	1306	LEU	2.1
1	B	1523	GLU	2.0
1	A	526	TYR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

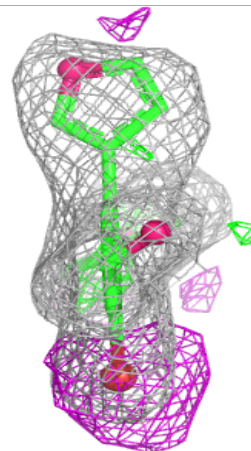
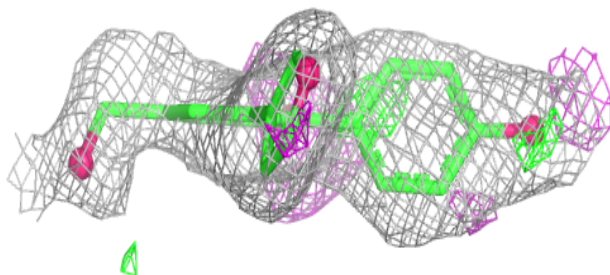
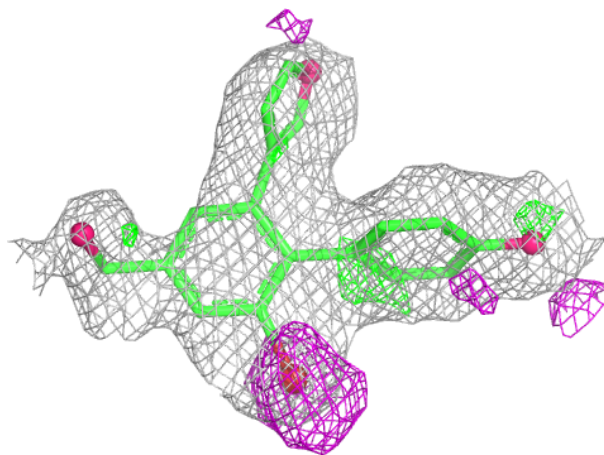
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	0L8	B	1701	21/21	0.68	0.20	42,49,58,74	0
3	0L8	A	701	21/21	0.73	0.20	32,52,57,75	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.

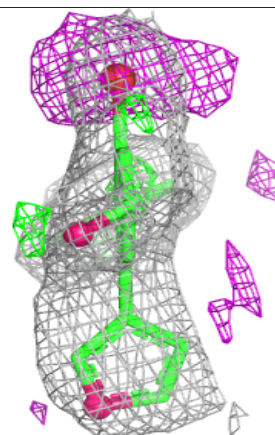
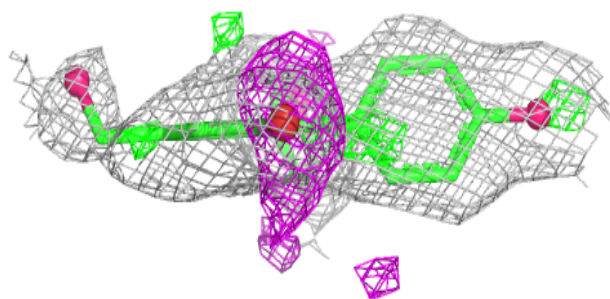
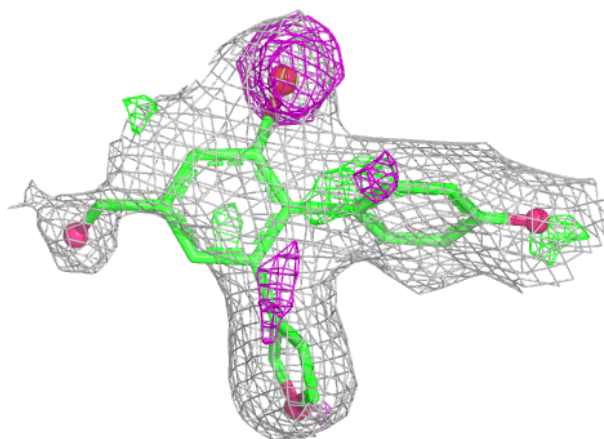
Electron density around 0L8 B 1701:

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



Electron density around 0L8 A 701:

$2mF_o-DF_c$ (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.