



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:13 AM UTC

PDB ID : 7WNV / pdb_00007wnv
Title : Crystal structure of mutant estrogen receptor alpha Y537S in complex with CO9
Authors : Xiao, Y.; Lv, Y.
Deposited on : 2022-01-19
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

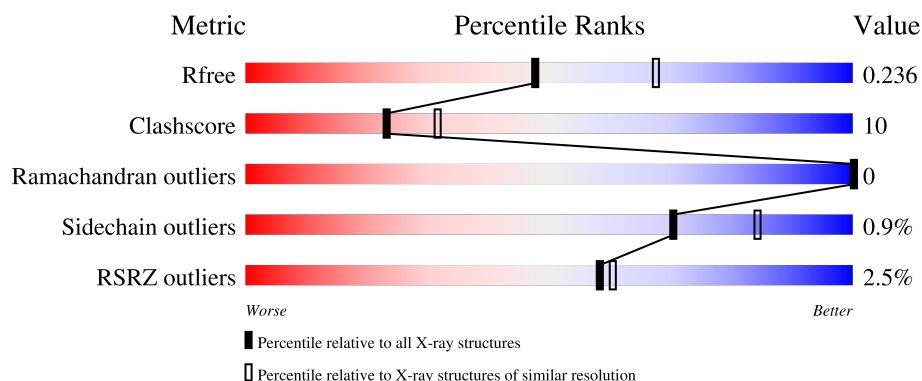
1 Overall quality at a glance

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	259	 2% 71% 15% 14%
1	B	259	 % 65% 18% 16%
1	C	259	 3% 66% 18% 15%
1	D	259	 2% 74% 13% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7148 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.

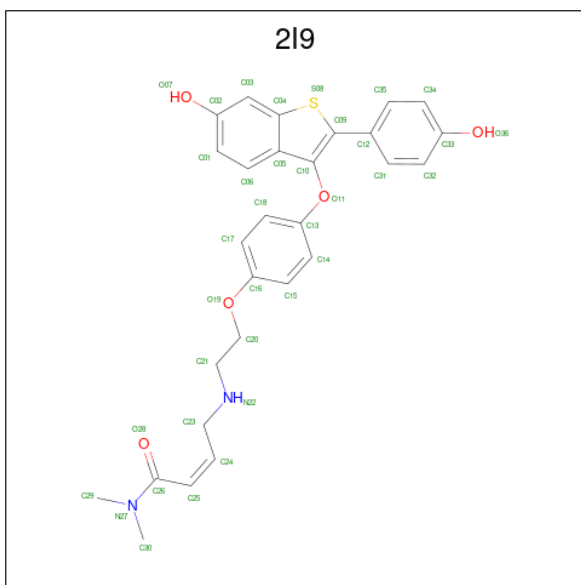
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1756	1122	301	315	18			
1	B	217	Total	C	N	O	S	0	0	0
			1697	1087	288	304	18			
1	C	219	Total	C	N	O	S	0	0	0
			1718	1099	294	307	18			
1	D	226	Total	C	N	O	S	0	0	0
			1748	1121	295	315	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	SER	-	expression tag	UNP P03372
A	417	SER	CYS	engineered mutation	UNP P03372
A	537	SER	TYR	engineered mutation	UNP P03372
B	296	SER	-	expression tag	UNP P03372
B	417	SER	CYS	engineered mutation	UNP P03372
B	537	SER	TYR	engineered mutation	UNP P03372
C	296	SER	-	expression tag	UNP P03372
C	417	SER	CYS	engineered mutation	UNP P03372
C	537	SER	TYR	engineered mutation	UNP P03372
D	296	SER	-	expression tag	UNP P03372
D	417	SER	CYS	engineered mutation	UNP P03372
D	537	SER	TYR	engineered mutation	UNP P03372

- Molecule 2 is ({Z})-4-[2-[4-[2-(4-hydroxyphenyl)-6-oxidanyl-1-benzothiophen-3-yl]oxy]phenoxy]ethylamino]- {N}, {N}-dimethyl-but-2-enamide (CCD ID: 2I9) (formula: C₂₈H₂₈N₂O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 36	C 28	N 2	O 5	S 1	0	0
2	B	1	Total 36	C 28	N 2	O 5	S 1	0	0
2	C	1	Total 36	C 28	N 2	O 5	S 1	0	0
2	D	1	Total 36	C 28	N 2	O 5	S 1	0	0

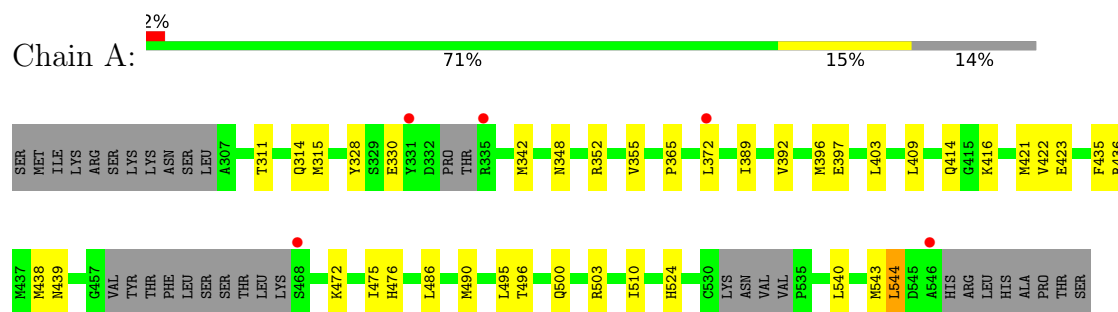
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	24	Total O 24 24	0	0
3	B	19	Total O 19 19	0	0
3	C	16	Total O 16 16	0	0
3	D	26	Total O 26 26	0	0

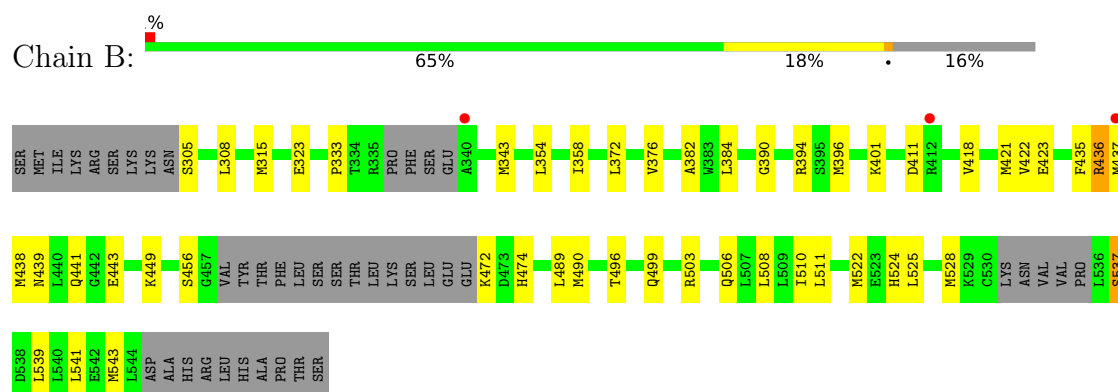
3 Residue-property plots [i](#)

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.

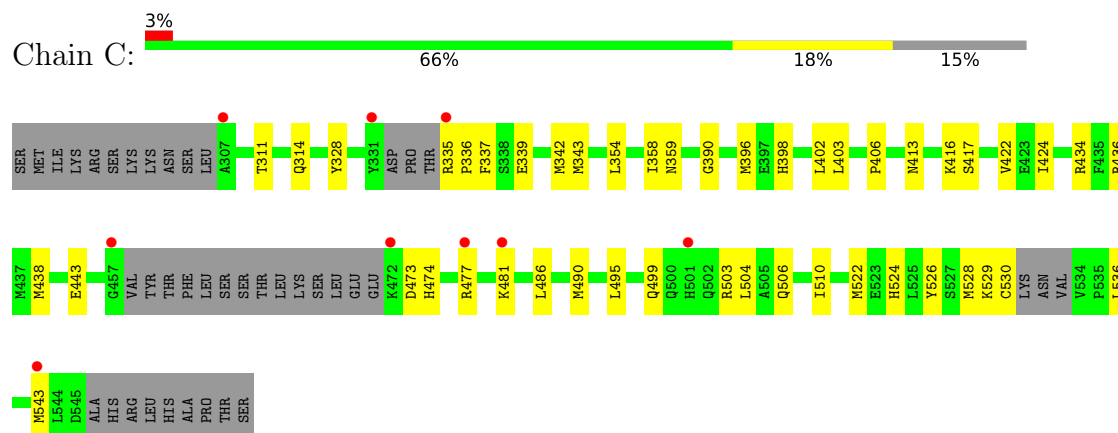
• Molecule 1: Estrogen receptor



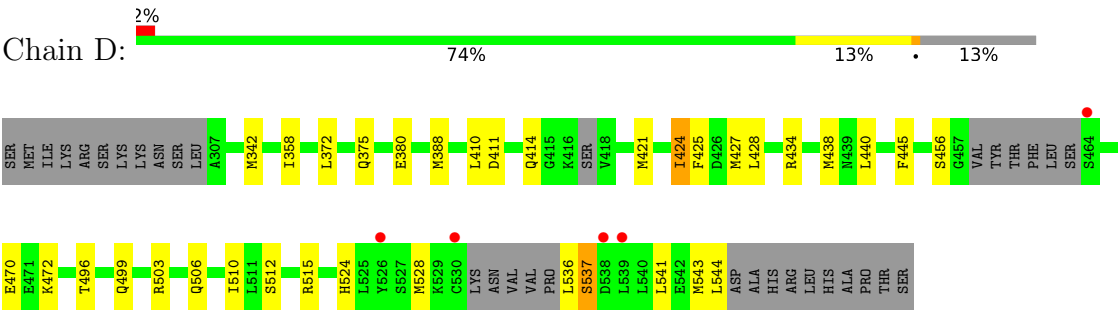
• Molecule 1: Estrogen receptor



• 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	53.93Å 58.83Å 93.06Å 90.31° 105.39° 117.15°	Depositor
Resolution (Å)	19.67 – 2.30 19.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.2 (19.67-2.30) 96.0 (19.67-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.30Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.203 , 0.235 0.204 , 0.236	Depositor DCC
R_{free} test set	1991 reflections (3.93%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.125 for h,-h-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7148	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 8.30% 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: 2I9

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	0.70	1/1784 (0.1%)	0.70	0/2405
1	B	0.59	1/1724 (0.1%)	0.72	2/2328 (0.1%)
1	C	0.71	0/1746	0.70	3/2357 (0.1%)
1	D	0.76	0/1777	0.69	0/2403
All	All	0.69	2/7031 (0.0%)	0.70	5/9493 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	333	PRO	N-CD	-6.28	1.39	1.47
1	A	475	ILE	C-O	-5.34	1.18	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	390	GLY	N-CA-C	-6.00	105.54	112.50
1	B	436	ARG	CA-C-N	-5.79	111.91	122.38
1	B	436	ARG	C-N-CA	-5.79	111.91	122.38
1	C	339	GLU	N-CA-C	-5.15	105.56	111.07
1	C	337	PHE	N-CA-C	5.12	118.55	109.96

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	1756	0	1791	36	0
1	B	1697	0	1727	42	0
1	C	1718	0	1748	37	0
1	D	1748	0	1758	28	0
2	A	36	0	0	1	0
2	B	36	0	0	3	0
2	C	36	0	0	1	0
2	D	36	0	0	4	0
3	A	24	0	0	0	0
3	B	19	0	0	0	0
3	C	16	0	0	0	0
3	D	26	0	0	0	0
All	All	7148	0	7024	145	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 10.

All (145) 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:B:401:LYS:NZ	1:B:411:ASP:HB3	1.43	1.30
1:D:421:MET:HE2	1:D:425:PHE:HD2	1.05	1.19
1:C:335:ARG:CB	1:C:336:PRO:HD2	1.77	1.15
1:D:524:HIS:ND1	2:D:601:2I9:O36	1.82	1.10
1:C:335:ARG:CB	1:C:336:PRO:CD	2.33	1.04
1:D:421:MET:HE2	1:D:425:PHE:CD2	1.93	1.03
1:B:401:LYS:HZ1	1:B:411:ASP:HB3	1.28	0.95
1:D:421:MET:CE	1:D:425:PHE:HD2	1.80	0.94
1:B:401:LYS:HZ3	1:B:411:ASP:HB3	1.11	0.93
1:B:401:LYS:NZ	1:B:411:ASP:CB	2.32	0.92
1:C:343:MET:HE2	1:C:528:MET:HE1	1.51	0.92
1:B:354:LEU:O	1:B:358:ILE:HD12	1.71	0.89
1:D:421:MET:CE	1:D:425:PHE:CD2	2.57	0.85
1:D:503:ARG:HA	1:D:506:GLN:OE1	1.84	0.76
1:D:358:ILE:HG21	1:D:543:MET:HG2	1.68	0.74
1:A:311:THR:HG23	1:A:314:GLN:H	1.51	0.73
1:B:401:LYS:HZ1	1:B:411:ASP:CB	1.96	0.73
1:B:490:MET:HE2	1:B:503:ARG:HG2	1.71	0.72
1:B:401:LYS:HZ3	1:B:411:ASP:CB	1.94	0.72
1:A:403:LEU:HD12	1:A:409:LEU:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:LEU:HD11	1:D:541:LEU:HD23	1.74	0.69
1:D:411:ASP:N	1:D:414:GLN:OE1	2.20	0.69
1:C:354:LEU:HD23	1:C:536:LEU:HD13	1.74	0.68
1:C:359:ASN:OD1	1:C:543:MET:HE1	1.95	0.66
1:A:396:MET:O	1:A:436:ARG:NH1	2.25	0.66
1:C:343:MET:HE2	1:C:528:MET:CE	2.25	0.65
1:B:372:LEU:O	1:B:376:VAL:HG23	1.97	0.65
1:C:473:ASP:OD1	1:C:477:ARG:NH1	2.29	0.64
1:D:424:ILE:HG21	2:D:601:2I9:C34	2.27	0.64
1:A:311:THR:HG22	1:A:314:GLN:OE1	1.98	0.64
1:D:380:GLU:OE2	1:D:537:SER:OG	2.16	0.63
1:D:410:LEU:HA	1:D:414:GLN:OE1	1.99	0.62
1:A:472:LYS:O	1:A:476:HIS:CD2	2.53	0.62
1:C:524:HIS:ND1	2:C:601:2I9:O36	2.21	0.61
1:A:328:TYR:O	1:A:352:ARG:NH2	2.27	0.60
1:A:439:ASN:ND2	1:D:470:GLU:OE2	2.22	0.60
1:D:421:MET:O	1:D:421:MET:HG2	2.01	0.60
1:B:472:LYS:HG3	1:B:474:HIS:H	1.67	0.59
1:A:416:LYS:HE2	1:A:422:VAL:HG21	1.84	0.59
1:A:421:MET:HB2	1:A:524:HIS:CE1	2.37	0.59
1:C:490:MET:HE2	1:C:503:ARG:HD3	1.85	0.59
1:C:311:THR:HG23	1:C:314:GLN:OE1	2.03	0.58
1:B:343:MET:HE2	1:B:528:MET:SD	2.44	0.58
1:A:490:MET:HB3	1:A:495:LEU:HD12	1.87	0.57
1:A:524:HIS:ND1	2:A:601:2I9:O36	2.33	0.57
1:C:434:ARG:O	1:C:438:MET:HG3	2.05	0.56
1:B:525:LEU:HB3	2:B:601:2I9:C30	2.36	0.56
1:B:382:ALA:HB2	1:B:456:SER:HB3	1.88	0.55
1:B:390:GLY:O	1:B:394:ARG:HG3	2.07	0.55
1:C:342:MET:HE2	1:C:417:SER:HB2	1.89	0.55
1:C:495:LEU:HG	1:C:499:GLN:HB3	1.88	0.54
1:D:434:ARG:HG3	1:D:438:MET:HE2	1.87	0.54
1:B:422:VAL:HG13	1:B:423:GLU:OE1	2.07	0.54
1:B:537:SER:O	1:B:541:LEU:CD2	2.56	0.54
1:A:490:MET:HE2	1:A:503:ARG:CD	2.38	0.54
1:A:486:LEU:O	1:A:490:MET:HG3	2.08	0.53
1:A:396:MET:HE3	1:A:435:PHE:C	2.34	0.53
1:B:537:SER:O	1:B:541:LEU:HD23	2.10	0.52
1:A:421:MET:HB2	1:A:524:HIS:HE1	1.74	0.52
1:A:490:MET:HE2	1:A:503:ARG:CG	2.40	0.52
1:B:438:MET:HE3	1:B:506:GLN:OE1	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:MET:HE2	1:B:503:ARG:CG	2.38	0.51
1:B:496:THR:HG23	1:B:499:GLN:OE1	2.10	0.51
1:A:490:MET:HE2	1:A:503:ARG:HG2	1.94	0.50
1:B:401:LYS:CE	1:B:411:ASP:HB3	2.38	0.50
1:D:421:MET:HB2	1:D:524:HIS:CE1	2.46	0.50
1:A:490:MET:HE2	1:A:503:ARG:HD3	1.94	0.50
1:C:490:MET:HE2	1:C:503:ARG:CG	2.42	0.50
1:D:438:MET:HE1	1:D:510:ILE:CD1	2.42	0.50
1:C:506:GLN:O	1:C:510:ILE:HG13	2.13	0.49
1:C:354:LEU:HD23	1:C:536:LEU:CD1	2.40	0.49
1:D:358:ILE:CG2	1:D:543:MET:HG2	2.38	0.49
1:D:456:SER:HA	1:D:515:ARG:NH2	2.27	0.48
1:B:418:VAL:HG11	1:B:421:MET:HE3	1.95	0.48
1:D:388:MET:HG2	1:D:428:LEU:HD21	1.96	0.48
1:A:342:MET:HE1	1:A:414:GLN:O	2.14	0.48
1:B:443:GLU:HG3	1:B:489:LEU:HD22	1.97	0.47
1:A:540:LEU:O	1:A:544:LEU:HB2	2.15	0.47
1:B:401:LYS:HZ1	1:B:411:ASP:CG	2.22	0.47
1:D:421:MET:HB2	1:D:524:HIS:HE1	1.79	0.47
1:A:372:LEU:HD11	1:A:544:LEU:HB3	1.97	0.47
2:D:601:2I9:O28	2:D:601:2I9:N22	2.47	0.47
1:B:396:MET:HE3	1:B:436:ARG:HA	1.97	0.47
1:C:354:LEU:CD2	1:C:536:LEU:HD13	2.41	0.47
1:D:424:ILE:HA	1:D:427:MET:HE3	1.97	0.47
1:B:423:GLU:OE1	1:B:423:GLU:N	2.47	0.46
1:A:423:GLU:H	1:A:423:GLU:CD	2.23	0.46
1:C:490:MET:HE2	1:C:503:ARG:CD	2.46	0.46
1:B:323:GLU:OE1	1:B:449:LYS:NZ	2.42	0.46
1:B:524:HIS:ND1	2:B:601:2I9:O36	2.41	0.46
1:D:375:GLN:OE1	1:D:544:LEU:HD22	2.16	0.46
1:B:418:VAL:CB	1:B:421:MET:HE3	2.46	0.45
1:C:403:LEU:HD21	1:C:406:PRO:HA	1.99	0.45
1:C:522:MET:HE3	1:C:526:TYR:CE2	2.51	0.45
1:A:355:VAL:HG13	1:A:543:MET:SD	2.56	0.45
1:C:443:GLU:H	1:C:443:GLU:CD	2.23	0.45
1:A:438:MET:HE1	1:A:510:ILE:HD13	1.99	0.45
1:B:539:LEU:O	1:B:543:MET:HG3	2.16	0.45
1:A:543:MET:HB3	1:A:543:MET:HE2	1.67	0.45
1:B:435:PHE:CE1	1:B:510:ILE:HG21	2.52	0.44
1:B:439:ASN:OD1	1:B:441:GLN:NE2	2.51	0.44
1:B:543:MET:HE2	1:B:543:MET:HB3	1.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:PHE:CE1	1:A:510:ILE:HG21	2.53	0.44
1:B:384:LEU:HB2	1:B:522:MET:HE2	1.99	0.44
1:A:438:MET:HE1	1:A:510:ILE:CD1	2.48	0.44
1:C:416:LYS:HA	1:C:422:VAL:CG2	2.48	0.43
1:C:398:HIS:NE2	1:C:403:LEU:HD12	2.33	0.43
1:D:440:LEU:HD21	1:D:445:PHE:HB2	2.00	0.43
1:C:358:ILE:HG21	1:C:543:MET:HB3	1.99	0.43
1:A:490:MET:CE	1:A:503:ARG:HG2	2.49	0.43
1:A:315:MET:SD	1:A:365:PRO:HG2	2.59	0.42
1:C:416:LYS:HG2	1:C:422:VAL:HG21	2.02	0.42
1:C:477:ARG:O	1:C:481:LYS:HG2	2.18	0.42
1:A:397:GLU:HA	1:A:397:GLU:OE1	2.19	0.42
1:A:403:LEU:HD12	1:A:409:LEU:CD1	2.47	0.42
1:B:508:LEU:O	1:B:511:LEU:HB2	2.19	0.42
1:C:413:ASN:HA	1:C:416:LYS:HG3	2.02	0.42
1:C:528:MET:HB2	1:C:528:MET:HE2	1.74	0.42
1:B:382:ALA:HB2	1:B:456:SER:CB	2.50	0.42
1:C:328:TYR:CE2	1:C:406:PRO:HB2	2.55	0.42
1:A:389:ILE:HA	1:A:392:VAL:HG22	2.01	0.42
1:B:537:SER:O	1:B:541:LEU:HD22	2.20	0.41
1:C:490:MET:HE1	1:C:504:LEU:N	2.35	0.41
1:A:496:THR:O	1:A:500:GLN:HG3	2.20	0.41
1:B:418:VAL:HB	1:B:421:MET:HE3	2.02	0.41
1:B:315:MET:HB2	1:B:315:MET:HE2	1.64	0.41
1:C:529:LYS:O	1:C:530:CYS:HB3	2.19	0.41
1:A:330:GLU:HG3	1:A:348:ASN:OD1	2.20	0.41
1:A:438:MET:HE3	1:A:438:MET:HB2	1.73	0.41
1:D:342:MET:HE3	1:D:342:MET:HB3	1.61	0.41
2:B:601:2I9:C26	2:B:601:2I9:N22	2.83	0.41
1:C:396:MET:HE3	1:C:436:ARG:HA	2.03	0.41
1:C:490:MET:HE2	1:C:503:ARG:HB3	2.03	0.41
1:A:416:LYS:NZ	1:A:422:VAL:HG11	2.36	0.41
1:C:342:MET:CE	1:C:417:SER:HB2	2.51	0.41
1:C:474:HIS:HA	1:C:477:ARG:NH2	2.36	0.41
1:D:496:THR:HG23	1:D:499:GLN:OE1	2.21	0.41
2:D:601:2I9:N22	2:D:601:2I9:C26	2.84	0.41
1:B:401:LYS:NZ	1:B:411:ASP:CG	2.78	0.40
1:C:486:LEU:O	1:C:490:MET:HG3	2.22	0.40
1:C:402:LEU:HD23	1:C:402:LEU:HA	1.91	0.40
1:D:524:HIS:NE2	1:D:528:MET:HE3	2.36	0.40
1:B:305:SER:N	1:B:308:LEU:HD12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:MET:HB3	1:B:437:MET:HE3	1.81	0.40
1:D:472:LYS:HB2	1:D:472:LYS:HE2	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	216/259 (83%)	214 (99%)	2 (1%)	0	100	100
1	B	209/259 (81%)	207 (99%)	2 (1%)	0	100	100
1	C	211/259 (82%)	209 (99%)	2 (1%)	0	100	100
1	D	218/259 (84%)	217 (100%)	1 (0%)	0	100	100
All	All	854/1036 (82%)	847 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/234 (83%)	194 (100%)	1 (0%)	81	90
1	B	188/234 (80%)	187 (100%)	1 (0%)	81	90
1	C	191/234 (82%)	190 (100%)	1 (0%)	81	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	191/234 (82%)	187 (98%)	4 (2%)	47	66
All	All	765/936 (82%)	758 (99%)	7 (1%)	70	84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	544	LEU
1	B	537	SER
1	C	424	ILE
1	D	424	ILE
1	D	512	SER
1	D	536	LEU
1	D	537	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	455	ASN
1	A	474	HIS
1	A	476	HIS
1	A	501	HIS
1	A	506	GLN
1	A	519	ASN
1	B	377	HIS
1	B	441	GLN
1	B	474	HIS
1	B	476	HIS
1	B	516	HIS
1	B	519	ASN
1	C	413	ASN
1	C	439	ASN
1	C	488	HIS
1	C	506	GLN
1	C	519	ASN
1	D	502	GLN
1	D	519	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2I9	B	601	1	37,39,39	6.28	24 (64%)	49,53,53	3.47	11 (22%)
2	2I9	D	601	1	37,39,39	6.13	24 (64%)	49,53,53	3.51	12 (24%)
2	2I9	A	601	1	37,39,39	6.22	24 (64%)	49,53,53	3.26	15 (30%)
2	2I9	C	601	1	37,39,39	6.27	25 (67%)	49,53,53	4.08	17 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2I9	B	601	1	-	5/22/22/22	0/4/4/4
2	2I9	D	601	1	-	7/22/22/22	0/4/4/4
2	2I9	A	601	1	-	4/22/22/22	0/4/4/4
2	2I9	C	601	1	-	3/22/22/22	0/4/4/4

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	2I9	C09-S08	-17.16	1.53	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	2I9	C09-S08	-14.55	1.56	1.74
2	B	601	2I9	C09-S08	-13.70	1.57	1.74
2	C	601	2I9	C09-S08	-13.46	1.58	1.74
2	D	601	2I9	C04-S08	-10.11	1.54	1.74
2	C	601	2I9	C06-C05	9.65	1.54	1.39
2	B	601	2I9	C15-C14	9.42	1.54	1.38
2	B	601	2I9	C03-C04	9.41	1.54	1.39
2	C	601	2I9	C15-C14	9.12	1.53	1.38
2	D	601	2I9	C18-C17	8.97	1.53	1.38
2	B	601	2I9	C06-C05	8.92	1.53	1.39
2	A	601	2I9	C06-C05	8.85	1.53	1.39
2	A	601	2I9	C03-C04	8.84	1.53	1.39
2	D	601	2I9	C03-C04	8.76	1.53	1.39
2	B	601	2I9	C35-C34	8.74	1.52	1.38
2	C	601	2I9	C35-C34	8.74	1.52	1.38
2	A	601	2I9	C32-C31	8.68	1.52	1.38
2	D	601	2I9	C06-C05	8.62	1.53	1.39
2	C	601	2I9	C10-C09	8.56	1.47	1.36
2	B	601	2I9	C32-C31	8.54	1.52	1.38
2	C	601	2I9	C03-C04	8.46	1.53	1.39
2	A	601	2I9	C31-C12	8.42	1.52	1.39
2	A	601	2I9	C35-C34	8.37	1.52	1.38
2	C	601	2I9	C35-C12	8.34	1.52	1.39
2	C	601	2I9	C32-C31	8.34	1.52	1.38
2	B	601	2I9	C03-C02	8.31	1.51	1.39
2	C	601	2I9	C31-C12	8.28	1.52	1.39
2	B	601	2I9	C35-C12	8.26	1.51	1.39
2	A	601	2I9	C18-C17	8.19	1.52	1.38
2	B	601	2I9	C31-C12	8.09	1.51	1.39
2	B	601	2I9	C15-C16	8.06	1.53	1.38
2	C	601	2I9	C18-C17	8.02	1.51	1.38
2	B	601	2I9	C18-C17	8.00	1.51	1.38
2	C	601	2I9	C14-C13	7.74	1.53	1.38
2	A	601	2I9	C03-C02	7.74	1.50	1.39
2	D	601	2I9	C32-C31	7.71	1.51	1.38
2	A	601	2I9	C10-C09	7.70	1.46	1.36
2	D	601	2I9	C15-C14	7.70	1.51	1.38
2	A	601	2I9	C15-C14	7.67	1.51	1.38
2	C	601	2I9	C15-C16	7.65	1.53	1.38
2	A	601	2I9	C17-C16	7.59	1.52	1.38
2	D	601	2I9	C35-C34	7.57	1.51	1.38
2	A	601	2I9	C35-C12	7.51	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	2I9	C04-S08	-7.47	1.59	1.74
2	B	601	2I9	C14-C13	7.44	1.52	1.38
2	C	601	2I9	C34-C33	7.40	1.52	1.39
2	B	601	2I9	C17-C16	7.38	1.52	1.38
2	A	601	2I9	C14-C13	7.34	1.52	1.38
2	A	601	2I9	C15-C16	7.32	1.52	1.38
2	A	601	2I9	C32-C33	7.30	1.52	1.39
2	C	601	2I9	C06-C01	7.29	1.50	1.38
2	D	601	2I9	C10-C09	7.21	1.45	1.36
2	A	601	2I9	C06-C01	7.20	1.50	1.38
2	C	601	2I9	C17-C16	7.17	1.52	1.38
2	B	601	2I9	C34-C33	7.15	1.52	1.39
2	B	601	2I9	C04-S08	-7.12	1.60	1.74
2	B	601	2I9	C10-C09	7.11	1.45	1.36
2	A	601	2I9	C04-S08	-7.11	1.60	1.74
2	A	601	2I9	C34-C33	7.06	1.52	1.39
2	A	601	2I9	C18-C13	7.05	1.51	1.38
2	B	601	2I9	C18-C13	7.04	1.51	1.38
2	D	601	2I9	C03-C02	7.01	1.49	1.39
2	D	601	2I9	C18-C13	7.00	1.51	1.38
2	C	601	2I9	C03-C02	6.95	1.49	1.39
2	B	601	2I9	C06-C01	6.93	1.50	1.38
2	D	601	2I9	C35-C12	6.93	1.49	1.39
2	B	601	2I9	C32-C33	6.79	1.51	1.39
2	D	601	2I9	C31-C12	6.74	1.49	1.39
2	C	601	2I9	C18-C13	6.67	1.51	1.38
2	D	601	2I9	C15-C16	6.65	1.51	1.38
2	D	601	2I9	C17-C16	6.61	1.51	1.38
2	D	601	2I9	C06-C01	6.52	1.49	1.38
2	C	601	2I9	C32-C33	6.47	1.51	1.39
2	A	601	2I9	C01-C02	6.27	1.50	1.39
2	D	601	2I9	C34-C33	6.26	1.50	1.39
2	B	601	2I9	C05-C10	6.18	1.60	1.45
2	B	601	2I9	C01-C02	5.93	1.50	1.39
2	D	601	2I9	C32-C33	5.72	1.49	1.39
2	C	601	2I9	C01-C02	5.70	1.49	1.39
2	C	601	2I9	C05-C10	5.69	1.58	1.45
2	D	601	2I9	C14-C13	5.64	1.49	1.38
2	D	601	2I9	C05-C10	5.43	1.58	1.45
2	D	601	2I9	C01-C02	5.15	1.48	1.39
2	C	601	2I9	C26-N27	4.98	1.47	1.34
2	C	601	2I9	C25-C26	4.88	1.55	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	2I9	C05-C10	4.73	1.56	1.45
2	A	601	2I9	C26-N27	4.72	1.46	1.34
2	A	601	2I9	C25-C26	4.69	1.55	1.48
2	B	601	2I9	C26-N27	4.52	1.46	1.34
2	D	601	2I9	C26-N27	4.08	1.44	1.34
2	D	601	2I9	C25-C26	3.90	1.54	1.48
2	B	601	2I9	C25-C26	2.99	1.52	1.48
2	A	601	2I9	C05-C04	2.91	1.45	1.41
2	C	601	2I9	C05-C04	2.83	1.45	1.41
2	B	601	2I9	C05-C04	2.80	1.45	1.41
2	D	601	2I9	O28-C26	-2.71	1.17	1.23
2	C	601	2I9	O28-C26	-2.05	1.19	1.23

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	2I9	C04-S08-C09	19.84	105.80	90.58
2	B	601	2I9	C04-S08-C09	18.34	104.64	90.58
2	C	601	2I9	C25-C26-N27	17.36	127.06	117.85
2	C	601	2I9	C04-S08-C09	16.99	103.61	90.58
2	A	601	2I9	C04-S08-C09	15.54	102.50	90.58
2	B	601	2I9	C25-C26-N27	7.45	121.80	117.85
2	A	601	2I9	C12-C09-S08	7.42	128.61	117.69
2	D	601	2I9	C12-C09-S08	6.91	127.85	117.69
2	A	601	2I9	C06-C05-C04	6.83	126.55	118.77
2	A	601	2I9	C03-C04-C05	-6.69	115.94	121.74
2	C	601	2I9	C12-C09-S08	6.50	127.25	117.69
2	B	601	2I9	C12-C09-S08	6.46	127.19	117.69
2	C	601	2I9	C03-C04-C05	-5.80	116.71	121.74
2	A	601	2I9	C12-C09-C10	-5.62	120.78	129.93
2	B	601	2I9	C03-C04-C05	-5.51	116.96	121.74
2	C	601	2I9	C06-C05-C04	5.28	124.78	118.77
2	D	601	2I9	C03-C04-C05	-4.93	117.46	121.74
2	D	601	2I9	C12-C09-C10	-4.62	122.41	129.93
2	D	601	2I9	C05-C10-C09	-4.56	106.79	114.49
2	B	601	2I9	C06-C05-C04	4.51	123.90	118.77
2	B	601	2I9	C12-C09-C10	-4.33	122.88	129.93
2	C	601	2I9	C12-C09-C10	-4.25	123.01	129.93
2	D	601	2I9	C06-C05-C04	4.05	123.38	118.77
2	B	601	2I9	C05-C10-C09	-3.87	107.94	114.49
2	D	601	2I9	C25-C26-N27	3.73	119.83	117.85
2	C	601	2I9	C05-C10-C09	-3.61	108.39	114.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	2I9	C05-C10-C09	-3.39	108.77	114.49
2	B	601	2I9	C03-C04-S08	3.34	134.40	126.07
2	A	601	2I9	C35-C12-C31	3.11	122.52	118.57
2	C	601	2I9	C24-C25-C26	3.11	130.84	122.94
2	B	601	2I9	C05-C04-S08	-3.06	108.64	112.24
2	A	601	2I9	C03-C04-S08	2.94	133.42	126.07
2	D	601	2I9	C03-C04-S08	2.87	133.24	126.07
2	C	601	2I9	C01-C02-C03	2.77	123.23	120.19
2	A	601	2I9	C06-C05-C10	-2.72	125.94	132.48
2	C	601	2I9	C03-C04-S08	2.70	132.82	126.07
2	D	601	2I9	C14-C15-C16	2.66	122.77	119.73
2	A	601	2I9	C34-C35-C12	-2.63	117.99	120.80
2	A	601	2I9	C01-C06-C05	-2.61	116.56	120.86
2	D	601	2I9	C05-C04-S08	-2.50	109.29	112.24
2	A	601	2I9	C31-C12-C09	-2.42	116.99	120.84
2	C	601	2I9	O28-C26-N27	-2.39	115.53	121.62
2	B	601	2I9	C35-C12-C31	2.38	121.60	118.57
2	D	601	2I9	C17-C18-C13	2.31	122.37	119.73
2	C	601	2I9	O11-C13-C14	2.29	125.53	119.09
2	C	601	2I9	O28-C26-C25	-2.29	117.41	122.02
2	A	601	2I9	C01-C02-C03	2.24	122.64	120.19
2	B	601	2I9	C06-C05-C10	-2.19	127.22	132.48
2	D	601	2I9	C01-C02-C03	2.15	122.55	120.19
2	C	601	2I9	C34-C35-C12	-2.11	118.54	120.80
2	C	601	2I9	C06-C05-C10	-2.10	127.44	132.48
2	A	601	2I9	C25-C26-N27	2.09	118.96	117.85
2	A	601	2I9	C04-C05-C10	-2.05	107.48	110.45
2	C	601	2I9	C01-C06-C05	-2.02	117.53	120.86
2	C	601	2I9	C20-O19-C16	2.01	123.14	117.93

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	2I9	C24-C25-C26-N27
2	C	601	2I9	C24-C25-C26-O28
2	D	601	2I9	C20-C21-N22-C23
2	D	601	2I9	O19-C20-C21-N22
2	B	601	2I9	C24-C25-C26-O28
2	B	601	2I9	C24-C25-C26-N27
2	A	601	2I9	C20-C21-N22-C23
2	C	601	2I9	O19-C20-C21-N22

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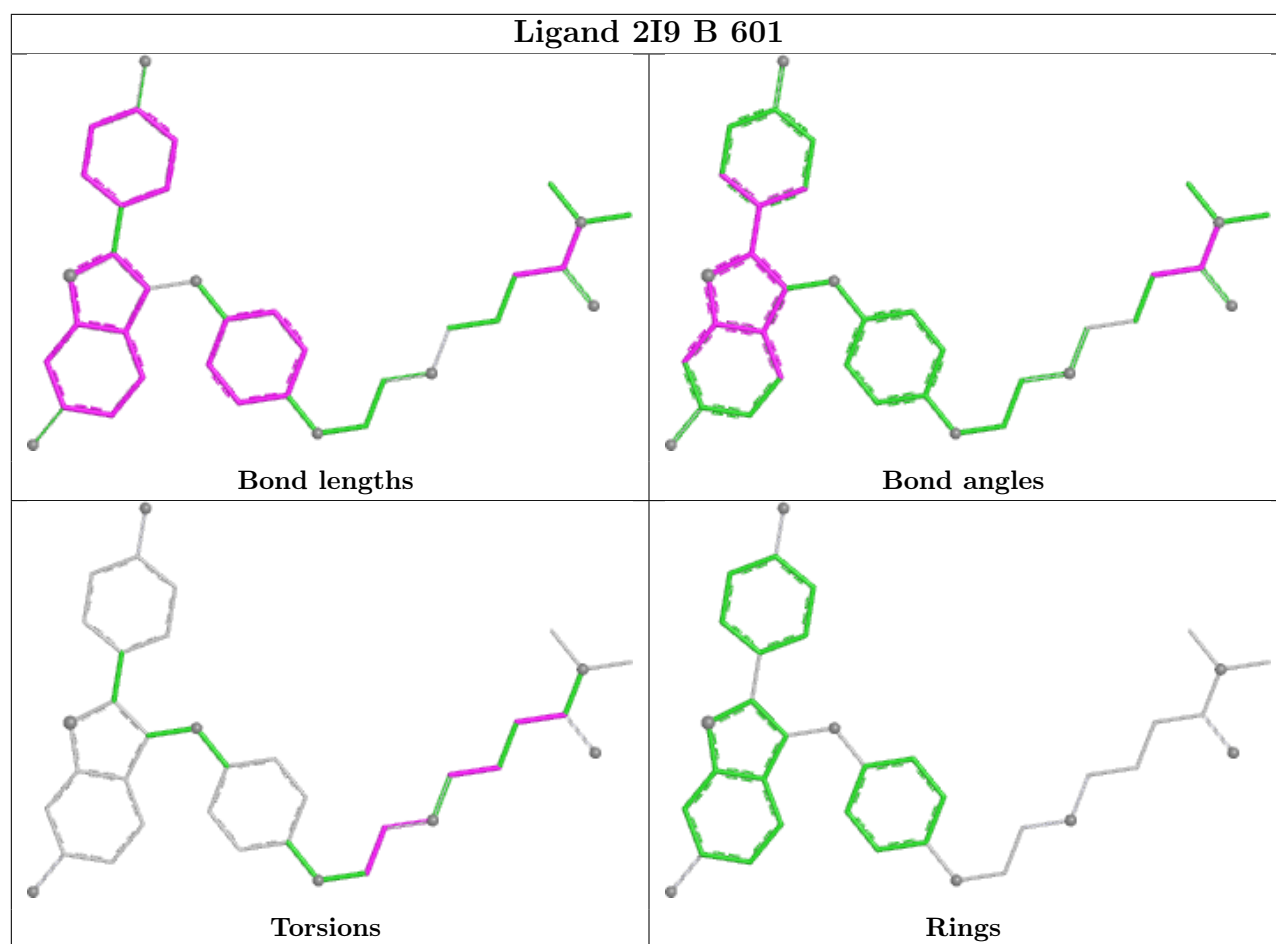
Mol	Chain	Res	Type	Atoms
2	D	601	2I9	C24-C23-N22-C21
2	B	601	2I9	C20-C21-N22-C23
2	D	601	2I9	C21-C20-O19-C16
2	B	601	2I9	O19-C20-C21-N22
2	D	601	2I9	N22-C23-C24-C25
2	D	601	2I9	C17-C16-O19-C20
2	D	601	2I9	C15-C16-O19-C20
2	B	601	2I9	N22-C23-C24-C25
2	A	601	2I9	C10-C09-C12-C31
2	A	601	2I9	C24-C23-N22-C21
2	A	601	2I9	C10-C09-C12-C35

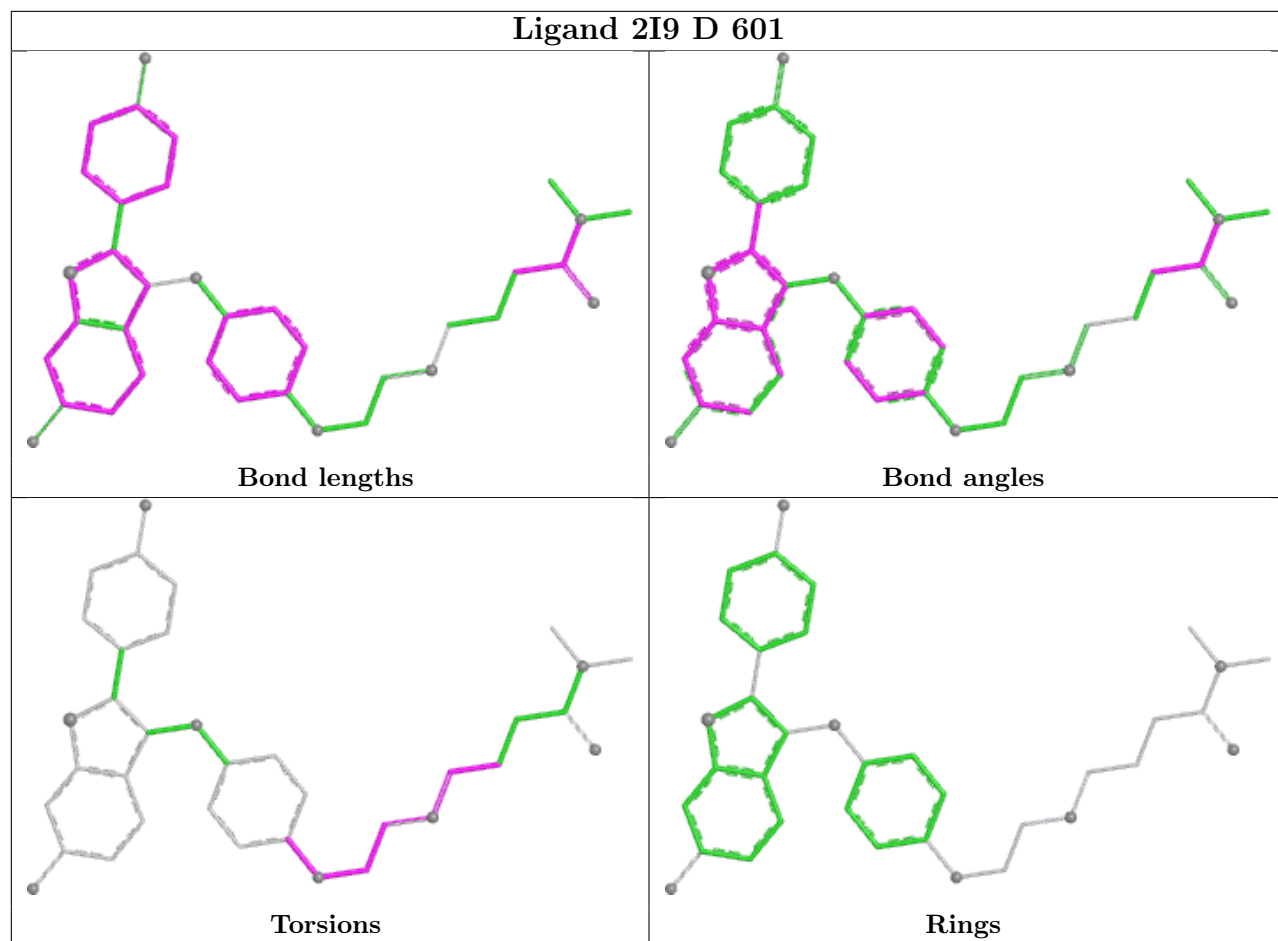
There are no ring outliers.

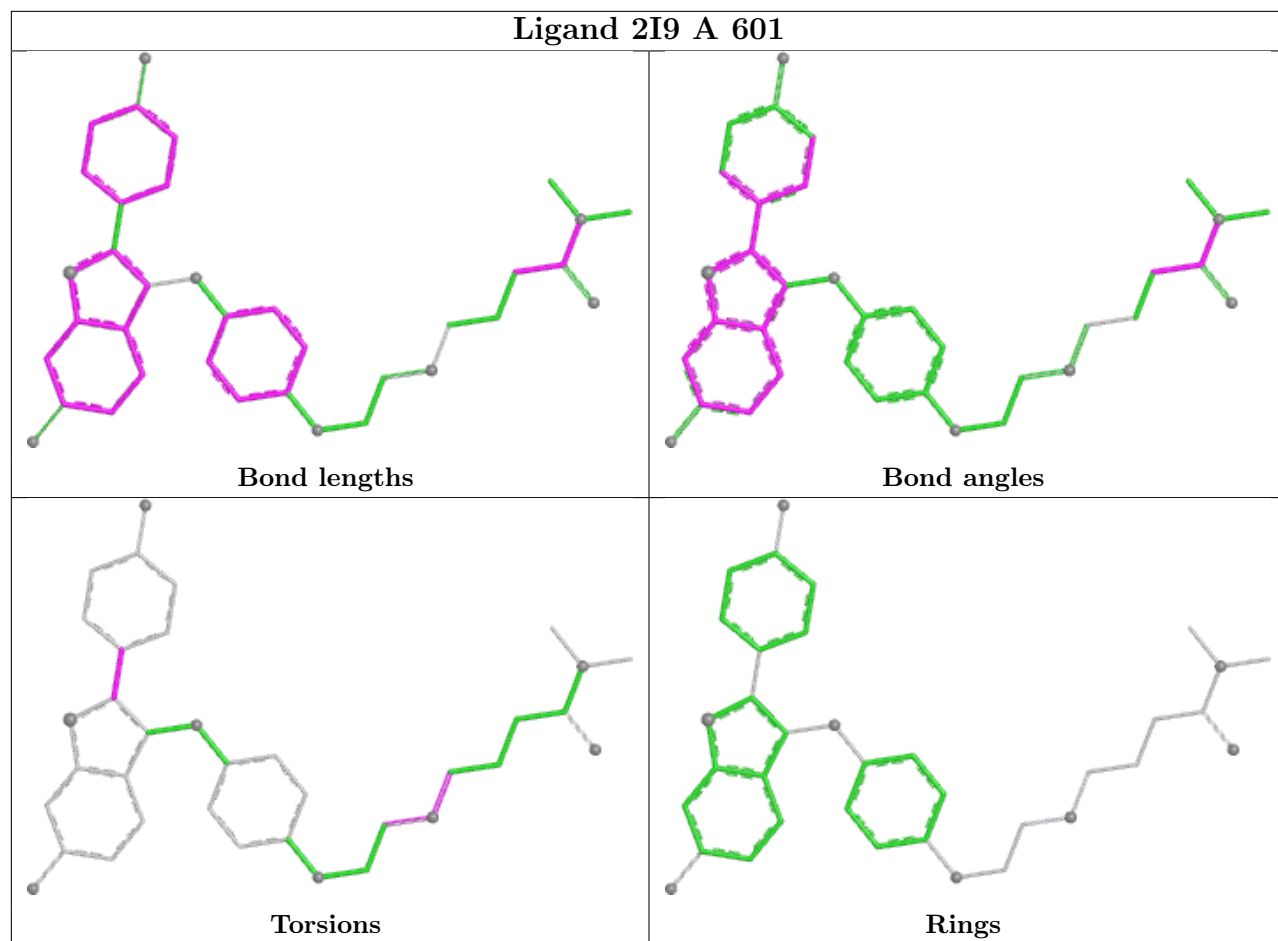
4 monomers are involved in 9 short contacts:

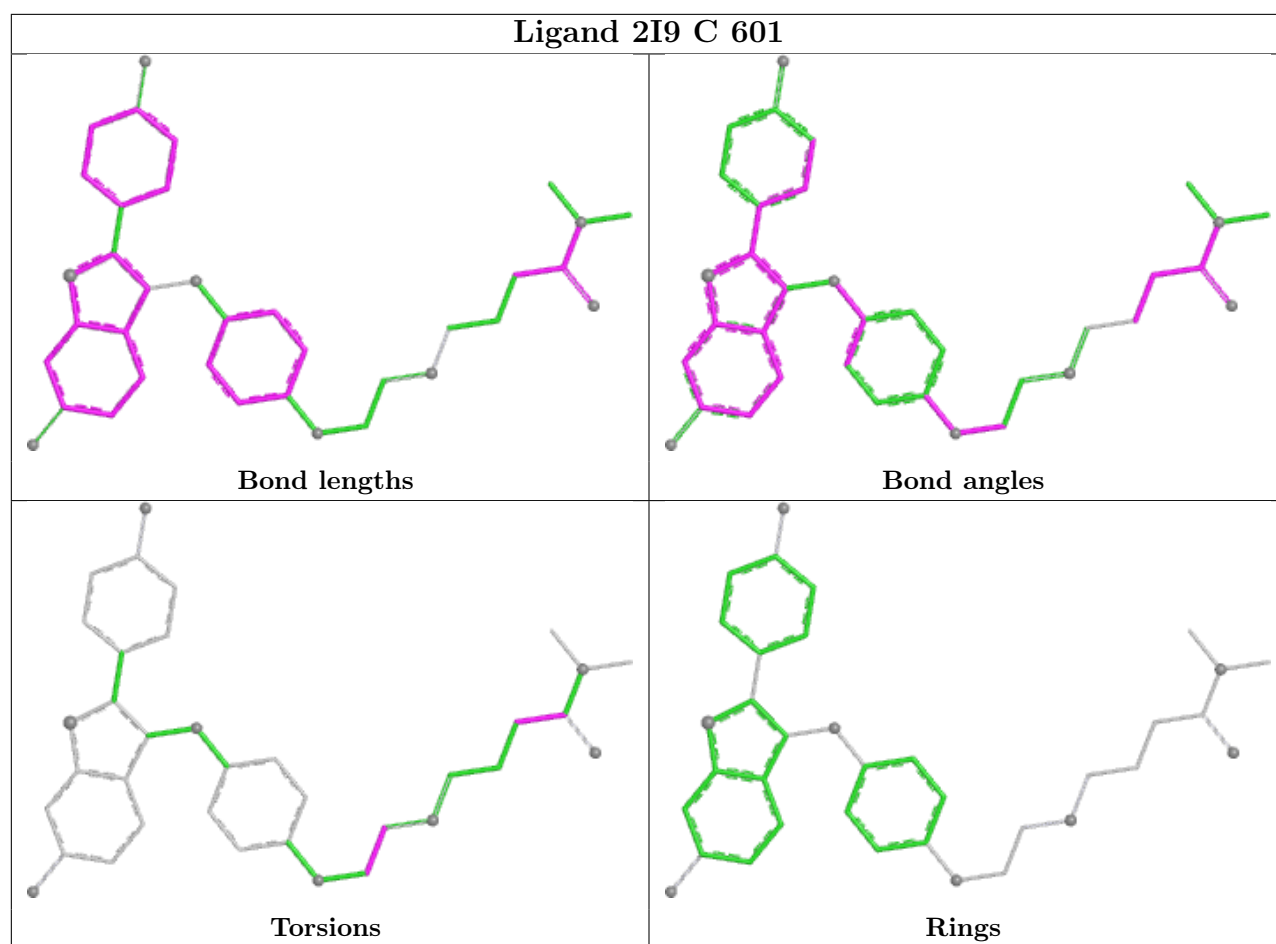
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	2I9	3	0
2	D	601	2I9	4	0
2	A	601	2I9	1	0
2	C	601	2I9	1	0

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	224/259 (86%)	0.02	5 (2%) 62 64	24, 37, 63, 85	0
1	B	217/259 (83%)	0.08	3 (1%) 73 75	23, 38, 71, 85	0
1	C	219/259 (84%)	0.18	9 (4%) 41 43	26, 41, 68, 95	0
1	D	226/259 (87%)	0.12	5 (2%) 62 64	22, 39, 72, 87	0
All	All	886/1036 (85%)	0.10	22 (2%) 58 60	22, 39, 70, 95	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	ARG	3.9
1	B	437	MET	3.7
1	C	331	TYR	3.7
1	B	340	ALA	3.6
1	C	472	LYS	3.1
1	A	468	SER	3.1
1	C	307	ALA	3.0
1	C	457	GLY	2.8
1	D	539	LEU	2.7
1	D	464	SER	2.6
1	A	546	ALA	2.6
1	D	526	TYR	2.5
1	C	481	LYS	2.5
1	D	530	CYS	2.4
1	C	543	MET	2.4
1	A	331	TYR	2.3
1	D	538	ASP	2.3
1	A	372	LEU	2.3
1	C	501	HIS	2.2
1	C	477	ARG	2.2
1	C	335	ARG	2.1
1	B	412	ARG	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](#)

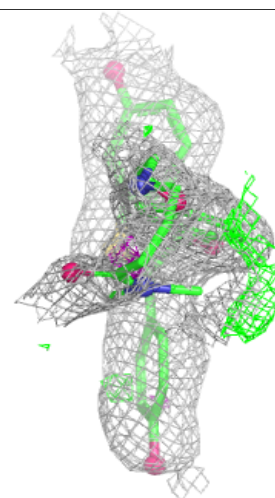
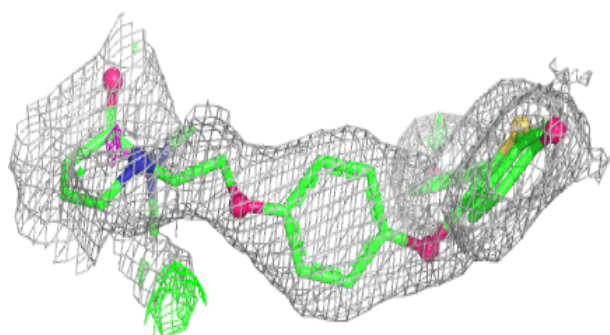
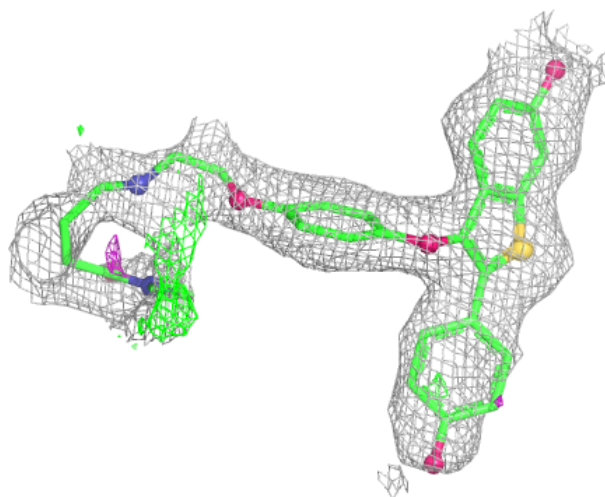
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	2I9	B	601	36/36	0.89	0.12	37,46,69,70	0
2	2I9	D	601	36/36	0.90	0.11	35,44,59,63	0
2	2I9	A	601	36/36	0.91	0.11	31,38,52,55	0
2	2I9	C	601	36/36	0.92	0.10	33,41,60,61	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.

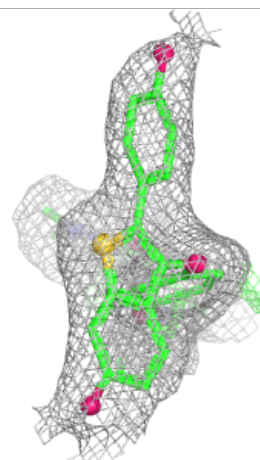
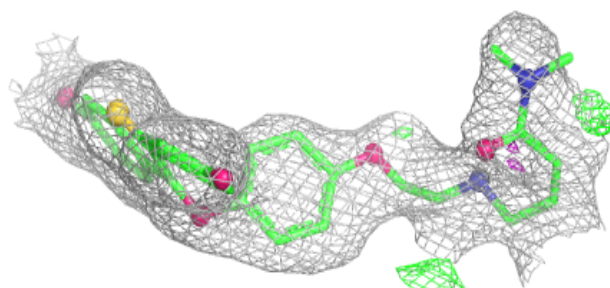
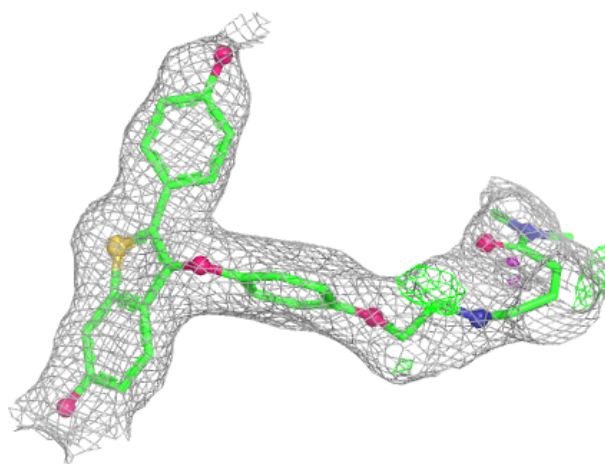
Electron density around 2I9 B 601:

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



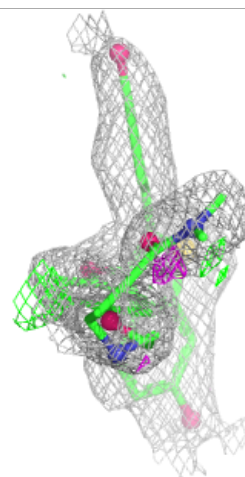
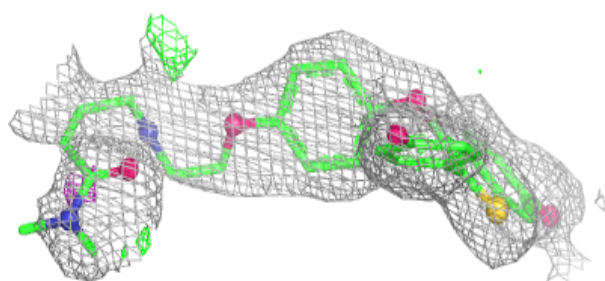
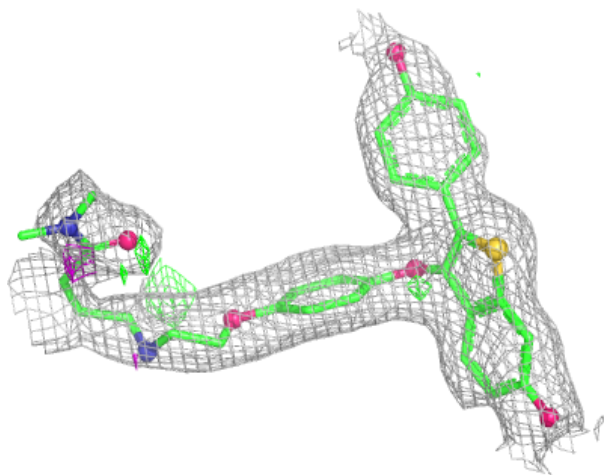
Electron density around 2I9 D 601:

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



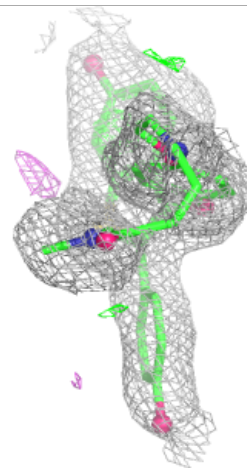
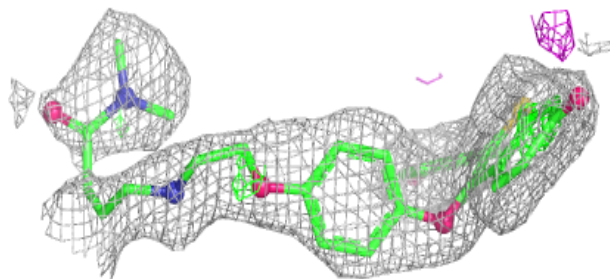
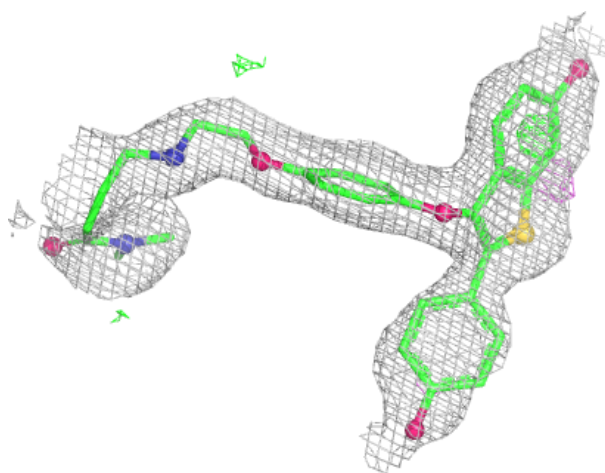
Electron density around 2I9 A 601:

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



Electron density around 2I9 C 601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.