



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:36 PM UTC

PDB ID : 4XI3 / pdb_00004xi3
Title : Estrogen Receptor Alpha Ligand Binding Domain in Complex with Bazedoxifene
Authors : Fanning, S.W.; Mayne, C.G.; Toy, W.; Carlson, K.; Greene, B.; Nowak, J.; Walter, R.; Panchamukhi, S.; Tajhorshid, E.; Nettles, K.W.; Chandarlapaty, S.; Katzenellenbogen, J.; Greene, G.L.
Deposited on : 2015-01-06
Resolution : 2.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 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

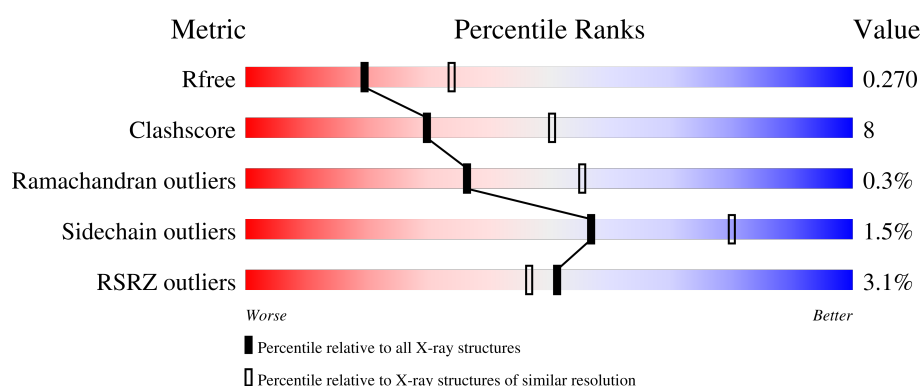
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	243	3% 78% 16% • 5%
1	B	243	2% 83% 12% • •
1	C	243	2% 77% 19% • •
1	D	243	5% 74% 16% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	29S	D	601	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7207 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.

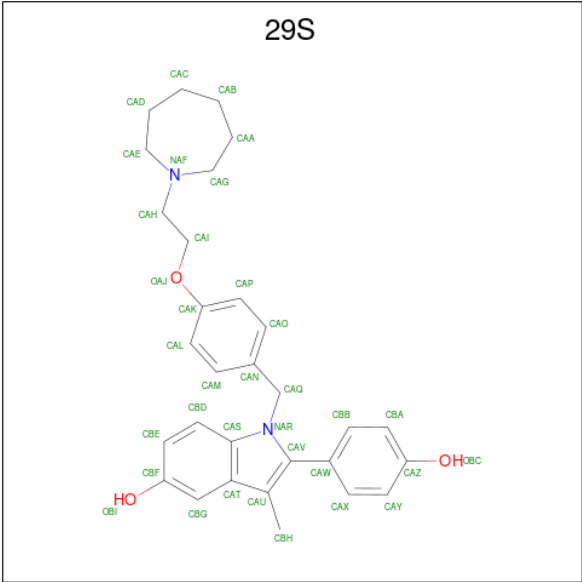
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	3	0
			1771	1138	304	312	17			
1	B	233	Total	C	N	O	S	0	1	0
			1804	1155	308	323	18			
1	C	236	Total	C	N	O	S	0	0	0
			1794	1148	306	322	18			
1	D	219	Total	C	N	O	S	0	2	0
			1659	1060	289	294	16			

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is Bazedoxifene (CCD ID: 29S) (formula: $C_{30}H_{34}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	30	2	3		
2	B	1	Total	C	N	O	0	0
			35	30	2	3		
2	C	1	Total	C	N	O	0	0
			35	30	2	3		
2	D	1	Total	C	N	O	0	0
			35	30	2	3		

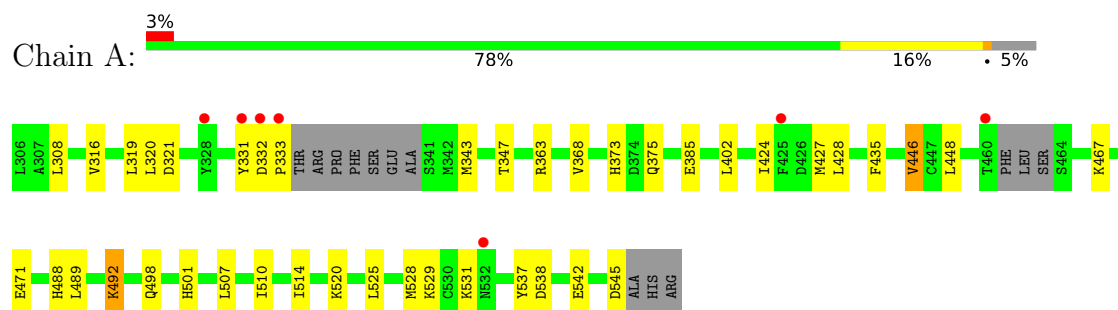
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	6	Total	O	0	0
			6	6		
3	C	7	Total	O	0	0
			7	7		
3	D	10	Total	O	0	0
			10	10		

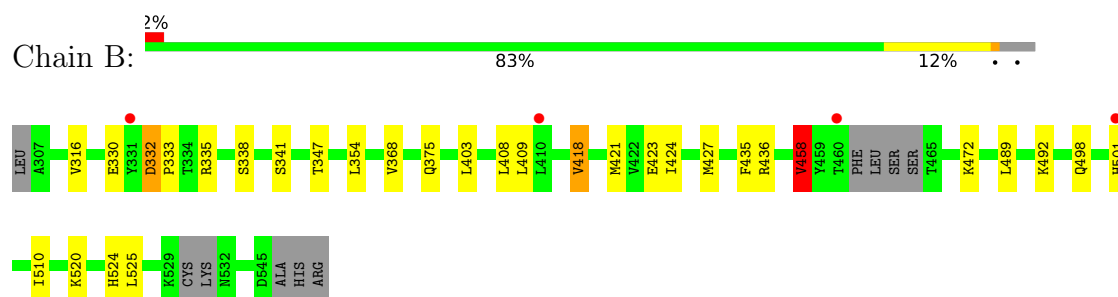
3 Residue-property plots [i](#)

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.

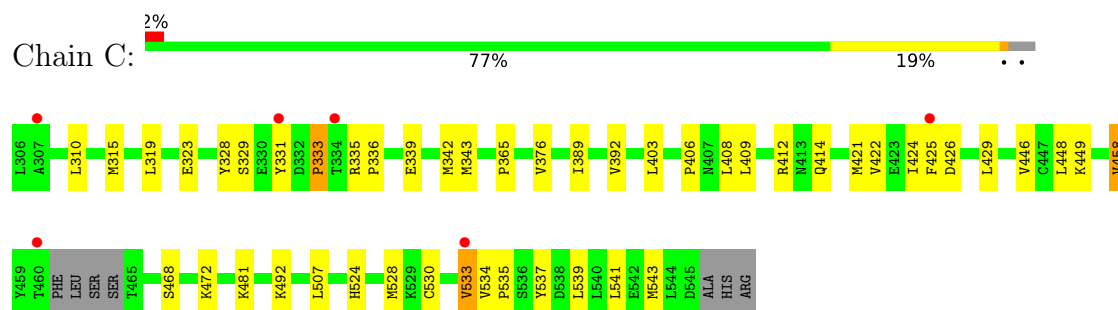
• Molecule 1: Estrogen receptor



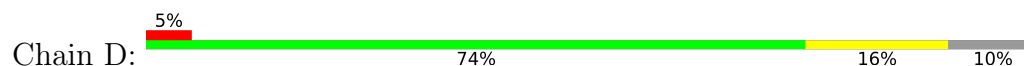
• Molecule 1: Estrogen receptor

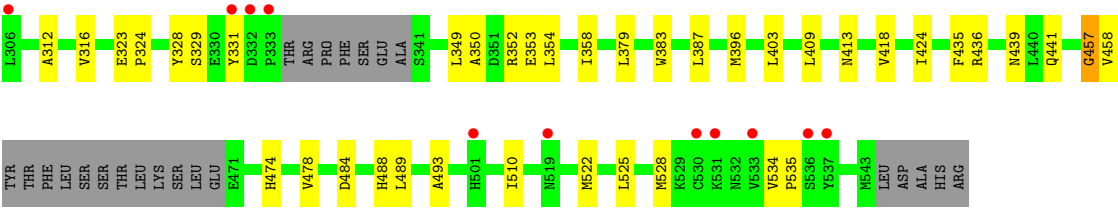


• Molecule 1: Estrogen receptor



• 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	53.58Å 59.16Å 94.14Å 86.76° 75.36° 63.03°	Depositor
Resolution (Å)	46.20 – 2.49 46.20 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.4 (46.20-2.49) 90.0 (46.20-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.215 , 0.268 0.219 , 0.270	Depositor DCC
R_{free} test set	1706 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.119 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7207	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.03% 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: 29S

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	0.38	1/1809 (0.1%)	0.86	4/2453 (0.2%)
1	B	0.35	0/1837	0.82	2/2489 (0.1%)
1	C	0.34	0/1826	0.86	2/2479 (0.1%)
1	D	0.41	0/1691	0.85	1/2295 (0.0%)
All	All	0.37	1/7163 (0.0%)	0.85	9/9716 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	PRO	N-CD	7.74	1.58	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	458	VAL	CB-CA-C	-7.93	98.29	111.29
1	A	531	LYS	N-CA-C	-7.35	101.76	111.24
1	A	529	LYS	CB-CA-C	-7.22	97.96	110.45
1	C	533	VAL	N-CA-C	7.19	117.27	110.30
1	A	332	ASP	N-CA-C	6.47	124.12	109.81
1	D	457	GLY	N-CA-C	-5.68	100.99	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	ASP	N-CA-C	5.54	122.06	109.81
1	B	458	VAL	CB-CA-C	-5.07	105.22	112.22
1	A	308	LEU	N-CA-C	-5.01	107.12	113.18

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331	TYR	Peptide
1	B	330	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1771	0	1767	26	0
1	B	1804	0	1795	21	1
1	C	1794	0	1774	28	0
1	D	1659	0	1628	30	1
2	A	35	0	30	7	0
2	B	35	0	30	9	0
2	C	35	0	32	7	0
2	D	35	0	31	9	0
3	A	16	0	0	0	0
3	B	6	0	0	0	0
3	C	7	0	0	0	0
3	D	10	0	0	0	0
All	All	7207	0	7087	121	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (121) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:LEU:O	1:C:481:LYS:NZ	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ILE:HG21	2:A:601:29S:H32	1.62	0.81
1:D:413:ASN:N	1:D:413:ASN:OD1	2.12	0.80
2:C:601:29S:H22	2:C:601:29S:H31	1.73	0.71
1:B:424:ILE:HG21	2:B:601:29S:H34	1.73	0.69
1:D:316:VAL:HG21	1:D:489:LEU:HD21	1.76	0.67
1:C:458:VAL:O	1:C:458:VAL:HG22	1.93	0.66
1:D:424:ILE:HG21	2:D:601:29S:H34	1.78	0.66
1:C:412:ARG:NH2	1:C:426:ASP:OD2	2.30	0.64
1:A:498:GLN:HA	1:A:501[A]:HIS:CE1	2.35	0.62
1:B:368:VAL:HA	1:B:375:GLN:NE2	2.15	0.62
2:C:601:29S:H19	2:C:601:29S:CAV	2.30	0.60
2:D:601:29S:CAQ	2:D:601:29S:H31	2.31	0.60
1:B:525:LEU:HD21	2:B:601:29S:H32	1.82	0.60
1:C:528:MET:HE3	1:C:530:CYS:SG	2.42	0.60
1:C:425:PHE:HE2	1:C:429:LEU:HD11	1.67	0.59
1:B:423:GLU:OE1	1:B:423:GLU:N	2.29	0.59
1:A:488:HIS:CE1	1:A:492:LYS:HE2	2.38	0.59
1:C:534:VAL:HG12	1:C:535:PRO:O	2.03	0.58
1:C:539:LEU:HD11	1:C:543:MET:HE3	1.86	0.57
2:B:601:29S:H31	2:B:601:29S:CAN	2.35	0.56
1:D:525:LEU:HD21	2:D:601:29S:H32	1.88	0.55
1:C:537:TYR:CE2	1:C:541:LEU:HD22	2.42	0.54
1:A:538:ASP:O	1:A:542:GLU:N	2.37	0.54
1:A:316:VAL:HG21	1:A:489:LEU:HD21	1.89	0.54
2:A:601:29S:CAQ	2:A:601:29S:H35	2.38	0.54
1:B:501[A]:HIS:HE1	1:D:484:ASP:OD1	1.90	0.54
2:A:601:29S:H35	2:A:601:29S:CAN	2.38	0.53
1:D:403:LEU:HD23	1:D:409:LEU:HD13	1.90	0.53
1:C:468:SER:O	1:C:472:LYS:HG3	2.08	0.53
1:C:425:PHE:CE2	1:C:429:LEU:HD11	2.43	0.53
1:B:338:SER:H	1:B:341:SER:HB3	1.74	0.52
1:A:319:LEU:HB3	1:A:446:VAL:HG13	1.92	0.52
1:C:412:ARG:HA	1:C:425:PHE:CE2	2.44	0.52
2:D:601:29S:H31	2:D:601:29S:H22	1.92	0.52
1:C:331:TYR:C	1:C:333:PRO:HD3	2.34	0.51
2:C:601:29S:H31	2:C:601:29S:CAQ	2.40	0.51
1:A:373:HIS:HD2	1:A:537:TYR:CE1	2.28	0.51
1:A:368:VAL:HA	1:A:375:GLN:NE2	2.25	0.51
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.91	0.51
1:C:323:GLU:OE2	1:C:449:LYS:NZ	2.41	0.50
1:A:427:MET:HE1	1:A:520:LYS:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:PHE:CE1	1:A:510:ILE:HG21	2.47	0.50
1:C:448:LEU:HD11	1:C:507:LEU:HD22	1.94	0.50
1:A:385:GLU:HG2	1:A:514:ILE:HG22	1.94	0.50
1:D:435:PHE:CE1	1:D:510:ILE:HG21	2.47	0.49
1:A:424:ILE:CG2	2:A:601:29S:H32	2.38	0.49
1:D:350:ALA:HB2	2:D:601:29S:H24	1.94	0.49
1:D:358:ILE:HD12	1:D:379:LEU:HD13	1.94	0.49
1:A:343:MET:HE2	1:A:528:MET:HE1	1.95	0.49
1:D:354:LEU:HD22	2:D:601:29S:H5	1.95	0.49
1:C:315:MET:SD	1:C:365:PRO:HG2	2.53	0.48
1:A:373:HIS:HD2	1:A:537:TYR:OH	1.97	0.48
1:B:421:MET:HE3	1:B:524:HIS:HE1	1.79	0.48
1:C:389:ILE:HA	1:C:392:VAL:HG22	1.95	0.48
1:C:319:LEU:HB3	1:C:446:VAL:CG1	2.43	0.48
1:A:320:LEU:HD23	1:A:446:VAL:HG21	1.95	0.48
1:D:312:ALA:HB3	1:D:488:HIS:ND1	2.29	0.48
1:B:458:VAL:HG12	1:B:472:LYS:HE3	1.96	0.47
1:C:342:MET:HE1	1:C:414:GLN:O	2.15	0.47
1:A:467:LYS:O	1:A:471:GLU:HG2	2.13	0.47
1:D:396:MET:HE3	1:D:436:ARG:HA	1.95	0.47
1:D:354:LEU:HD22	2:D:601:29S:CAC	2.44	0.47
1:B:498:GLN:HA	1:B:501[A]:HIS:CD2	2.49	0.47
1:C:422:VAL:HA	1:C:425:PHE:HB3	1.97	0.47
1:A:347:THR:HG23	2:A:601:29S:H15	1.96	0.47
1:A:435:PHE:HE1	1:A:510:ILE:HG21	1.80	0.47
2:C:601:29S:H35	2:C:601:29S:H30	1.97	0.46
1:A:448:LEU:HD21	1:A:507:LEU:HB3	1.96	0.46
2:B:601:29S:OAJ	2:B:601:29S:H11	2.16	0.46
1:D:534:VAL:HG22	1:D:535:PRO:O	2.15	0.46
1:B:498:GLN:HA	1:B:501[A]:HIS:NE2	2.31	0.46
1:C:329:SER:HB2	1:C:408:LEU:HD22	1.98	0.46
1:C:403:LEU:HD13	1:C:409:LEU:HD12	1.98	0.45
1:D:383:TRP:HE1	1:D:522:MET:HE1	1.81	0.45
2:C:601:29S:H35	2:C:601:29S:CBH	2.46	0.45
1:B:403:LEU:HD13	1:B:409:LEU:HD13	1.99	0.45
1:C:533:VAL:O	2:C:601:29S:H11	2.17	0.45
2:C:601:29S:H20	2:C:601:29S:H17	1.48	0.45
1:B:435:PHE:HE1	1:B:510:ILE:HD13	1.82	0.45
1:C:421:MET:HE3	1:C:524:HIS:HE1	1.81	0.45
1:D:329:SER:C	1:D:331:TYR:H	2.25	0.44
1:B:435:PHE:CE1	1:B:510:ILE:HG21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:29S:OAJ	2:A:601:29S:H11	2.16	0.44
1:D:349:LEU:O	1:D:353:GLU:HG3	2.18	0.44
1:D:418:VAL:HG12	1:D:528:MET:HE1	1.99	0.44
1:D:474:HIS:O	1:D:478:VAL:HG23	2.17	0.44
1:D:435:PHE:HE1	1:D:510:ILE:HD13	1.82	0.44
1:D:525:LEU:CD2	2:D:601:29S:H32	2.47	0.44
1:D:457:GLY:O	1:D:458:VAL:HG12	2.16	0.44
1:D:323:GLU:HA	1:D:324:PRO:HD3	1.88	0.44
2:D:601:29S:OAJ	2:D:601:29S:H1	2.18	0.43
1:D:439:ASN:O	1:D:441:GLN:NE2	2.48	0.43
1:A:545:ASP:OD1	1:A:545:ASP:C	2.62	0.43
1:B:347:THR:HG23	2:B:601:29S:H15	2.00	0.43
1:A:528:MET:HE3	1:A:528:MET:HB2	1.65	0.43
1:B:354:LEU:HD22	2:B:601:29S:H7	2.01	0.43
1:D:328:TYR:O	1:D:352:ARG:NH2	2.44	0.42
2:B:601:29S:CBH	2:B:601:29S:H35	2.49	0.42
1:A:424:ILE:HG21	2:A:601:29S:CAY	2.41	0.42
1:C:376:VAL:HG11	1:C:537:TYR:CD1	2.55	0.42
1:C:343:MET:SD	1:C:421:MET:HE1	2.59	0.42
1:B:418:VAL:HG12	1:B:421:MET:HB2	2.01	0.42
1:C:458:VAL:O	1:C:458:VAL:CG2	2.64	0.42
1:D:528:MET:H	1:D:528:MET:HG2	1.71	0.42
1:D:525:LEU:O	1:D:528:MET:O	2.38	0.41
1:C:328:TYR:CE2	1:C:406:PRO:HB2	2.55	0.41
1:D:528:MET:HE2	1:D:528:MET:HB3	1.84	0.41
1:B:424:ILE:HA	1:B:427:MET:HE3	2.02	0.41
1:B:520:LYS:HD3	1:B:520:LYS:HA	1.81	0.41
1:A:435:PHE:HE1	1:A:510:ILE:HD13	1.86	0.41
1:A:525:LEU:HA	1:A:528:MET:HE2	2.03	0.41
1:D:435:PHE:CE1	1:D:510:ILE:HD13	2.56	0.41
1:C:335:ARG:HA	1:C:336:PRO:C	2.46	0.40
1:A:321:ASP:O	1:A:363:ARG:NH2	2.55	0.40
1:B:368:VAL:HA	1:B:375:GLN:HE21	1.82	0.40
1:B:435:PHE:CE1	1:B:510:ILE:HD13	2.56	0.40
1:A:402:LEU:HD11	1:A:428:LEU:CB	2.51	0.40
2:B:601:29S:H31	2:B:601:29S:CAM	2.52	0.40
1:D:396:MET:HE2	1:D:396:MET:HB3	1.89	0.40
2:B:601:29S:H31	2:B:601:29S:CAQ	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ARG:NH2	1:D:493:ALA:O[1_465]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/243 (93%)	222 (98%)	5 (2%)	0	100	100
1	B	228/243 (94%)	221 (97%)	5 (2%)	2 (1%)	14	27
1	C	232/243 (96%)	223 (96%)	8 (3%)	1 (0%)	30	49
1	D	215/243 (88%)	209 (97%)	6 (3%)	0	100	100
All	All	902/972 (93%)	875 (97%)	24 (3%)	3 (0%)	36	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	333	PRO
1	B	332	ASP
1	C	333	PRO

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	190/219 (87%)	188 (99%)	2 (1%)	65	84
1	B	195/219 (89%)	190 (97%)	5 (3%)	40	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	191/219 (87%)	188 (98%)	3 (2%)	55	79
1	D	174/219 (80%)	173 (99%)	1 (1%)	78	91
All	All	750/876 (86%)	739 (98%)	11 (2%)	57	80

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	446	VAL
1	A	492	LYS
1	B	408	LEU
1	B	418	VAL
1	B	436	ARG
1	B	458	VAL
1	B	492	LYS
1	C	339	GLU
1	C	424	ILE
1	C	492	LYS
1	D	387	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	373	HIS
1	A	414	GLN
1	A	474	HIS
1	A	488	HIS
1	A	516	HIS
1	A	519	ASN
1	B	414	GLN
1	B	455	ASN
1	B	474	HIS
1	B	513	HIS
1	C	356	HIS
1	C	375	GLN
1	C	519	ASN
1	D	356	HIS
1	D	500	GLN
1	D	513	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	29S	B	601	-	39,39,39	2.77	16 (41%)	52,54,54	4.04	19 (36%)
2	29S	D	601	-	39,39,39	2.28	11 (28%)	52,54,54	6.42	31 (59%)
2	29S	C	601	-	39,39,39	2.64	15 (38%)	52,54,54	3.62	20 (38%)
2	29S	A	601	-	39,39,39	2.66	15 (38%)	52,54,54	4.23	20 (38%)

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	29S	B	601	-	-	5/14/23/23	0/5/5/5
2	29S	D	601	-	-	9/14/23/23	0/5/5/5
2	29S	C	601	-	-	3/14/23/23	1/5/5/5
2	29S	A	601	-	-	5/14/23/23	0/5/5/5

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	29S	CAW-CAV	-8.52	1.35	1.48
2	C	601	29S	CAW-CAV	-7.91	1.36	1.48
2	A	601	29S	CAW-CAV	-7.86	1.36	1.48
2	D	601	29S	CAT-CAS	-7.16	1.31	1.41
2	D	601	29S	CAQ-CAN	-7.11	1.38	1.51
2	B	601	29S	CAQ-CAN	-6.98	1.38	1.51
2	A	601	29S	CAQ-CAN	-6.71	1.39	1.51
2	C	601	29S	CAT-CAU	-6.19	1.32	1.44
2	B	601	29S	CAT-CAU	-6.14	1.32	1.44
2	A	601	29S	CAT-CAS	-5.91	1.33	1.41
2	B	601	29S	CAT-CAS	-5.83	1.33	1.41
2	C	601	29S	CAT-CAS	-5.82	1.33	1.41
2	A	601	29S	CAT-CAU	-5.79	1.33	1.44
2	C	601	29S	CAQ-CAN	-5.54	1.41	1.51
2	D	601	29S	CAT-CAU	-4.52	1.35	1.44
2	B	601	29S	CBG-CAT	-3.93	1.33	1.39
2	C	601	29S	CBG-CAT	-3.88	1.33	1.39
2	B	601	29S	CBD-CAS	-3.72	1.33	1.39
2	A	601	29S	CBD-CAS	-3.72	1.33	1.39
2	A	601	29S	CBG-CAT	-3.69	1.34	1.39
2	C	601	29S	CAG-NAF	3.67	1.55	1.46
2	C	601	29S	CBD-CAS	-3.61	1.34	1.39
2	C	601	29S	CAE-NAF	3.30	1.54	1.46
2	A	601	29S	CAS-NAR	-3.25	1.33	1.39
2	A	601	29S	CAA-CAB	3.24	1.64	1.51
2	B	601	29S	CAA-CAB	3.15	1.64	1.51
2	D	601	29S	CAA-CAB	3.10	1.64	1.51
2	C	601	29S	CAD-CAE	3.07	1.61	1.51
2	B	601	29S	CAS-NAR	-3.04	1.34	1.39
2	C	601	29S	CAS-NAR	-2.98	1.34	1.39
2	D	601	29S	CBD-CAS	-2.90	1.35	1.39
2	D	601	29S	CAW-CAV	-2.84	1.44	1.48
2	C	601	29S	CAQ-NAR	2.79	1.51	1.46
2	D	601	29S	CAG-NAF	2.79	1.53	1.46
2	B	601	29S	CAV-NAR	-2.67	1.35	1.39
2	D	601	29S	CAA-CAG	2.65	1.59	1.51
2	A	601	29S	CAA-CAG	2.57	1.59	1.51
2	C	601	29S	CAV-CAU	-2.56	1.35	1.37
2	A	601	29S	CAV-NAR	-2.53	1.35	1.39
2	B	601	29S	CAV-CAU	-2.49	1.35	1.37
2	A	601	29S	CAG-NAF	2.45	1.52	1.46
2	B	601	29S	CAE-NAF	-2.43	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	29S	CAG-NAF	2.39	1.52	1.46
2	B	601	29S	CAH-CAI	2.34	1.57	1.50
2	B	601	29S	CAA-CAG	2.33	1.58	1.51
2	C	601	29S	CAV-NAR	-2.31	1.35	1.39
2	D	601	29S	CAE-NAF	-2.30	1.39	1.46
2	C	601	29S	CAC-CAD	-2.28	1.42	1.51
2	B	601	29S	CAQ-NAR	2.28	1.50	1.46
2	A	601	29S	CBH-CAU	2.28	1.54	1.50
2	A	601	29S	CAQ-NAR	2.27	1.50	1.46
2	B	601	29S	CBH-CAU	2.25	1.54	1.50
2	A	601	29S	CAE-NAF	-2.23	1.40	1.46
2	D	601	29S	CBB-CAW	2.11	1.42	1.39
2	A	601	29S	CAH-CAI	2.08	1.57	1.50
2	D	601	29S	CBG-CBF	2.03	1.42	1.39
2	C	601	29S	CBH-CAU	2.00	1.53	1.50

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	29S	CAU-CAV-NAR	-31.16	99.91	109.82
2	A	601	29S	CAU-CAV-NAR	-15.42	104.92	109.82
2	B	601	29S	CAU-CAV-NAR	-15.29	104.96	109.82
2	D	601	29S	CAG-NAF-CAE	-15.14	72.57	113.22
2	A	601	29S	CAG-NAF-CAE	-15.13	72.59	113.22
2	B	601	29S	CAG-NAF-CAE	-15.12	72.60	113.22
2	D	601	29S	CAT-CAU-CAV	14.92	114.25	107.08
2	C	601	29S	CAU-CAV-NAR	-14.82	105.11	109.82
2	D	601	29S	CAQ-NAR-CAS	-9.87	109.60	124.79
2	D	601	29S	CBB-CAW-CAV	9.45	134.84	120.56
2	C	601	29S	CAG-NAF-CAE	-8.40	90.66	113.22
2	A	601	29S	CAQ-NAR-CAS	-8.16	112.24	124.79
2	A	601	29S	CAQ-NAR-CAV	8.10	138.12	126.44
2	D	601	29S	CAB-CAA-CAG	8.03	139.62	114.64
2	D	601	29S	CAQ-NAR-CAV	7.99	137.98	126.44
2	A	601	29S	CAB-CAA-CAG	7.87	139.10	114.64
2	B	601	29S	CAB-CAA-CAG	7.74	138.72	114.64
2	D	601	29S	CAY-CAX-CAW	7.39	128.69	120.80
2	D	601	29S	CBB-CAW-CAX	-7.10	109.54	118.57
2	C	601	29S	CAC-CAD-CAE	-7.07	92.66	114.64
2	C	601	29S	CAT-CAU-CAV	6.33	110.12	107.08
2	A	601	29S	CAT-CAU-CAV	6.09	110.01	107.08
2	B	601	29S	CAT-CAU-CAV	6.08	110.00	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	29S	CAQ-NAR-CAS	-5.88	115.75	124.79
2	C	601	29S	CAQ-NAR-CAV	5.87	134.91	126.44
2	C	601	29S	CAA-CAB-CAC	-5.85	92.40	116.25
2	C	601	29S	CAQ-NAR-CAS	-5.84	115.81	124.79
2	B	601	29S	CAA-CAG-NAF	5.83	126.36	115.35
2	A	601	29S	CAA-CAG-NAF	5.69	126.09	115.35
2	D	601	29S	CAD-CAE-NAF	5.68	126.08	115.35
2	A	601	29S	CAA-CAB-CAC	-5.65	93.21	116.25
2	B	601	29S	CAA-CAB-CAC	-5.57	93.53	116.25
2	B	601	29S	CAQ-NAR-CAV	5.46	134.32	126.44
2	A	601	29S	CAC-CAD-CAE	5.41	131.45	114.64
2	C	601	29S	CAB-CAC-CAD	5.26	137.71	116.25
2	B	601	29S	CAC-CAD-CAE	5.25	130.95	114.64
2	C	601	29S	CAD-CAE-NAF	-5.04	105.83	115.35
2	A	601	29S	CAI-CAH-NAF	5.03	127.56	113.36
2	C	601	29S	CAB-CAA-CAG	4.98	130.13	114.64
2	B	601	29S	CAI-CAH-NAF	4.95	127.36	113.36
2	D	601	29S	CAA-CAB-CAC	-4.85	96.47	116.25
2	A	601	29S	OAJ-CAI-CAH	4.68	119.59	107.79
2	D	601	29S	CBE-CBF-CBG	-4.52	115.23	120.19
2	D	601	29S	CBA-CBB-CAW	4.44	125.54	120.80
2	B	601	29S	OAJ-CAI-CAH	4.39	118.86	107.79
2	D	601	29S	CAS-NAR-CAV	4.34	111.84	108.37
2	C	601	29S	CAA-CAG-NAF	-4.26	107.30	115.35
2	C	601	29S	CAI-OAJ-CAK	-4.25	106.89	117.93
2	D	601	29S	CAC-CAD-CAE	4.15	127.53	114.64
2	D	601	29S	CAW-CAV-NAR	3.85	127.69	121.44
2	B	601	29S	CAD-CAE-NAF	3.83	122.59	115.35
2	D	601	29S	CAI-OAJ-CAK	3.83	127.88	117.93
2	A	601	29S	CAD-CAE-NAF	3.73	122.39	115.35
2	D	601	29S	CBD-CAS-CAT	-3.50	118.05	121.95
2	D	601	29S	CBE-CBD-CAS	3.44	126.00	119.10
2	D	601	29S	CAT-CBG-CBF	3.43	124.75	120.11
2	C	601	29S	CBH-CAU-CAT	-3.37	118.81	124.76
2	D	601	29S	CAX-CAW-CAV	-3.35	115.50	120.56
2	D	601	29S	CAB-CAC-CAD	-3.35	102.59	116.25
2	A	601	29S	CBB-CAW-CAX	-3.28	114.39	118.57
2	A	601	29S	CBA-CBB-CAW	3.27	124.29	120.80
2	D	601	29S	CBD-CBE-CBF	-3.07	116.63	119.88
2	B	601	29S	CAW-CAV-NAR	3.07	126.43	121.44
2	C	601	29S	CBH-CAU-CAV	3.02	131.01	127.85
2	C	601	29S	CBB-CAW-CAX	-3.00	114.75	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	29S	CBH-CAU-CAT	-2.97	119.51	124.76
2	D	601	29S	CBH-CAU-CAT	-2.96	119.52	124.76
2	A	601	29S	CAB-CAC-CAD	-2.87	104.54	116.25
2	B	601	29S	CBB-CAW-CAX	-2.87	114.92	118.57
2	B	601	29S	CAB-CAC-CAD	-2.82	104.73	116.25
2	C	601	29S	CAY-CAX-CAW	2.81	123.80	120.80
2	A	601	29S	CBH-CAU-CAT	-2.74	119.92	124.76
2	D	601	29S	OAJ-CAI-CAH	2.72	114.65	107.79
2	A	601	29S	CAW-CAV-NAR	2.64	125.74	121.44
2	B	601	29S	CBB-CAW-CAV	2.64	124.55	120.56
2	C	601	29S	CAW-CAV-NAR	2.59	125.65	121.44
2	C	601	29S	CBB-CAW-CAV	2.44	124.25	120.56
2	B	601	29S	CBH-CAU-CAV	2.41	130.36	127.85
2	D	601	29S	CAA-CAG-NAF	2.39	119.86	115.35
2	D	601	29S	CAP-CAO-CAN	-2.39	117.86	121.00
2	D	601	29S	OBI-CBF-CBG	2.35	126.01	119.85
2	D	601	29S	CAS-CAT-CAU	-2.30	105.58	107.87
2	D	601	29S	CAW-CAV-CAU	2.27	131.95	128.68
2	C	601	29S	OAJ-CAI-CAH	2.25	113.46	107.79
2	C	601	29S	CAN-CAQ-NAR	-2.21	109.87	113.46
2	A	601	29S	CBD-CBE-CBF	-2.14	117.61	119.88
2	D	601	29S	CAQ-CAN-CAM	-2.13	116.82	120.75
2	B	601	29S	CAY-CAX-CAW	2.12	123.07	120.80
2	A	601	29S	CBH-CAU-CAV	2.07	130.01	127.85
2	A	601	29S	CAX-CAW-CAV	2.05	123.66	120.56

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	29S	CAI-CAH-NAF-CAG
2	B	601	29S	CAI-CAH-NAF-CAG
2	D	601	29S	CAI-CAH-NAF-CAE
2	D	601	29S	CAI-CAH-NAF-CAG
2	A	601	29S	NAR-CAV-CAW-CBB
2	D	601	29S	NAR-CAV-CAW-CAX
2	D	601	29S	NAR-CAV-CAW-CBB
2	C	601	29S	NAR-CAV-CAW-CBB
2	B	601	29S	NAR-CAV-CAW-CBB
2	C	601	29S	NAR-CAV-CAW-CAX
2	A	601	29S	NAR-CAV-CAW-CAX
2	D	601	29S	CAU-CAV-CAW-CBB

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Mol	Chain	Res	Type	Atoms
2	D	601	29S	CAU-CAV-CAW-CAX
2	B	601	29S	NAR-CAV-CAW-CAX
2	A	601	29S	CAU-CAV-CAW-CBB
2	D	601	29S	CAH-CAI-OAJ-CAK
2	B	601	29S	CAI-CAH-NAF-CAE
2	C	601	29S	CAU-CAV-CAW-CBB
2	D	601	29S	CAO-CAN-CAQ-NAR
2	A	601	29S	CAH-CAI-OAJ-CAK
2	B	601	29S	CAH-CAI-OAJ-CAK
2	D	601	29S	CAM-CAN-CAQ-NAR

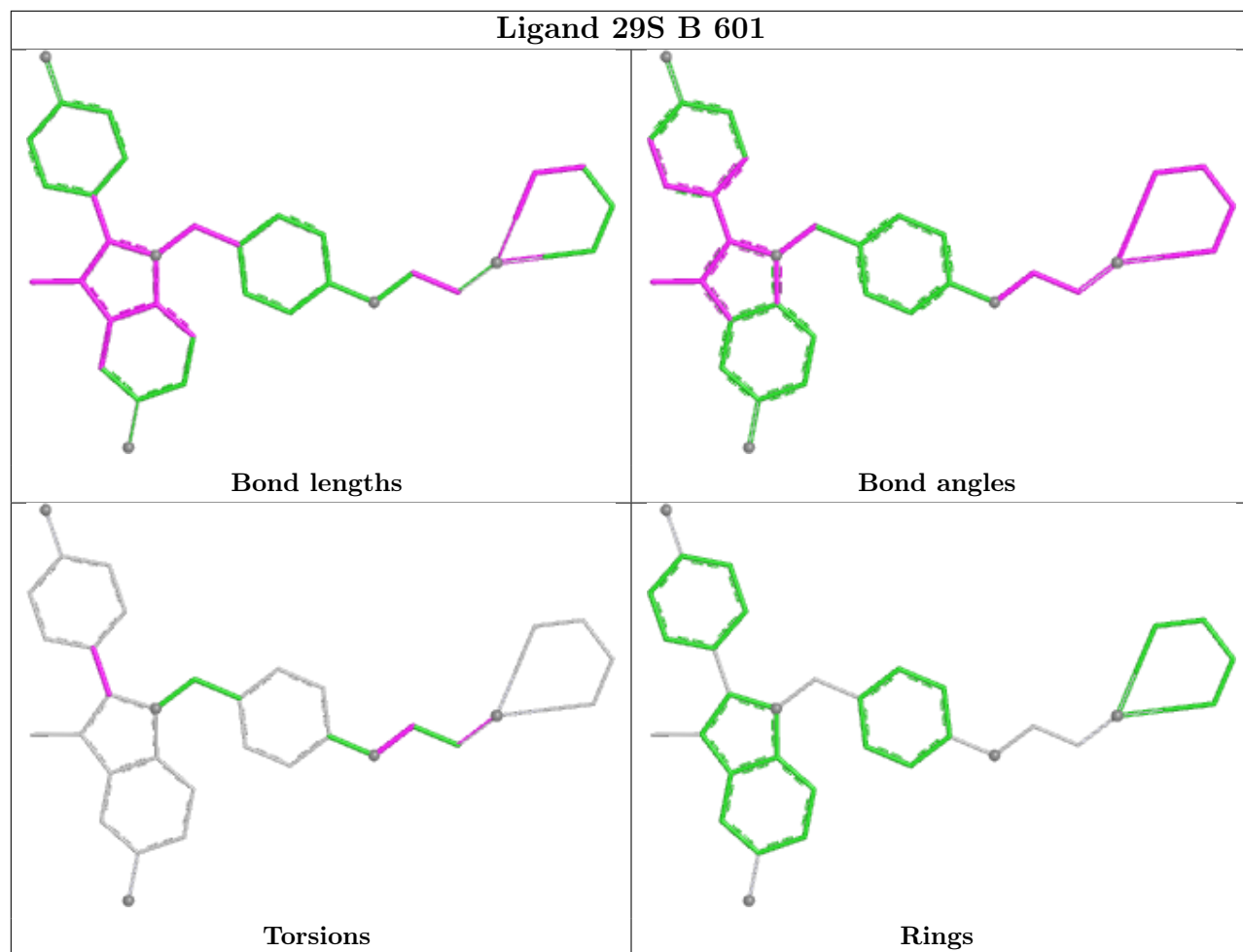
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	29S	CAA-CAB-CAC-CAD-CAE-CAG-NAF

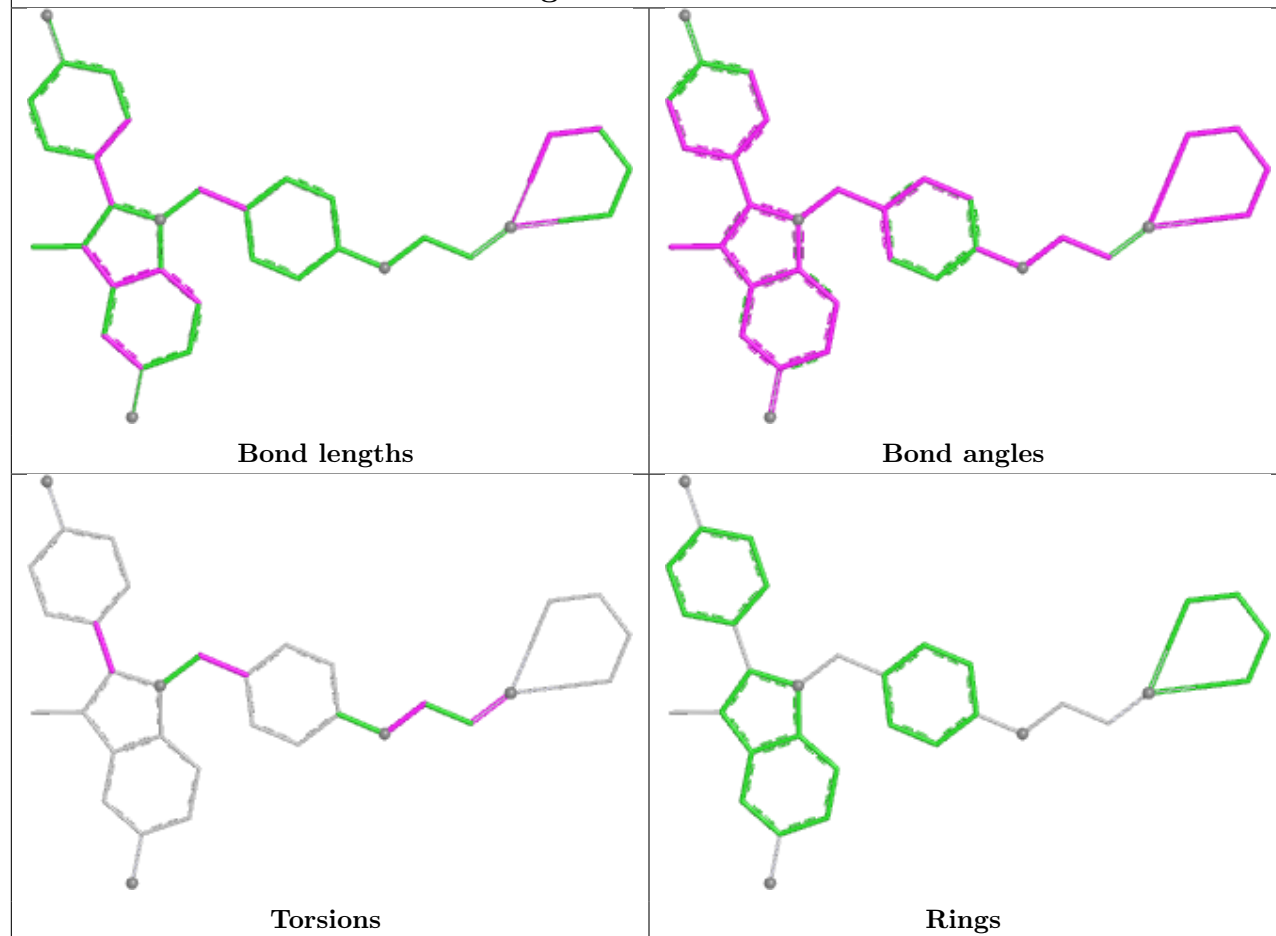
4 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	29S	9	0
2	D	601	29S	9	0
2	C	601	29S	7	0
2	A	601	29S	7	0

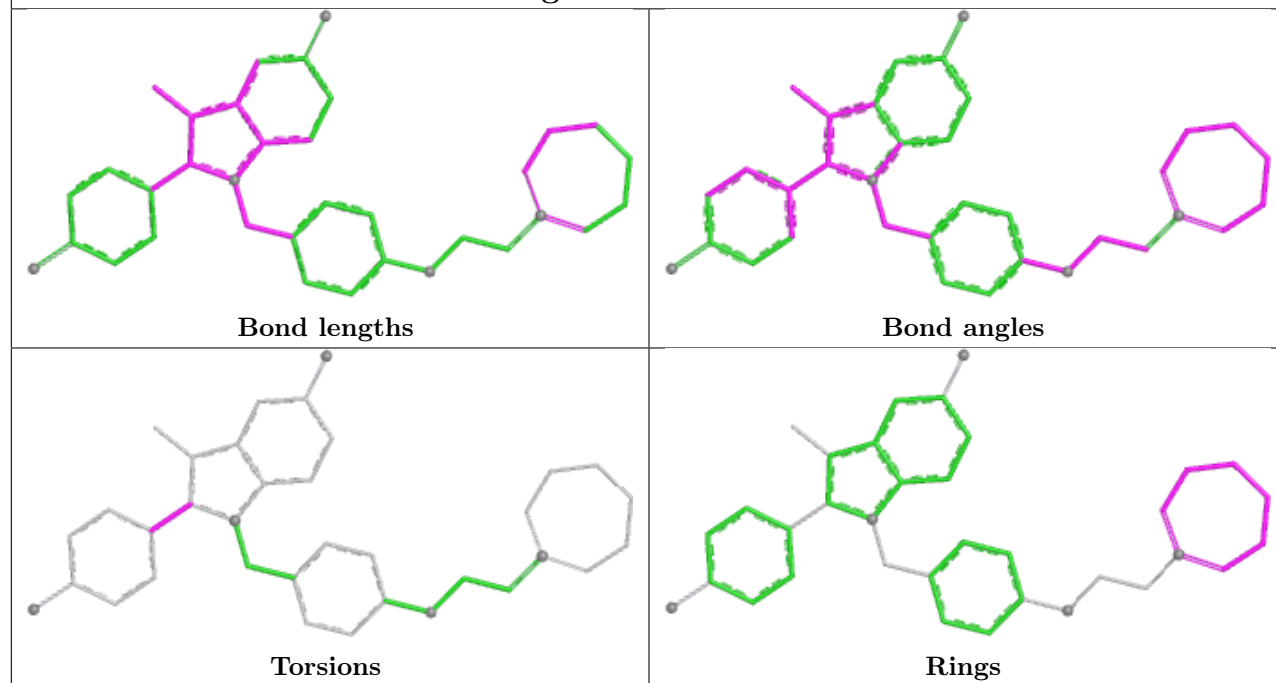
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

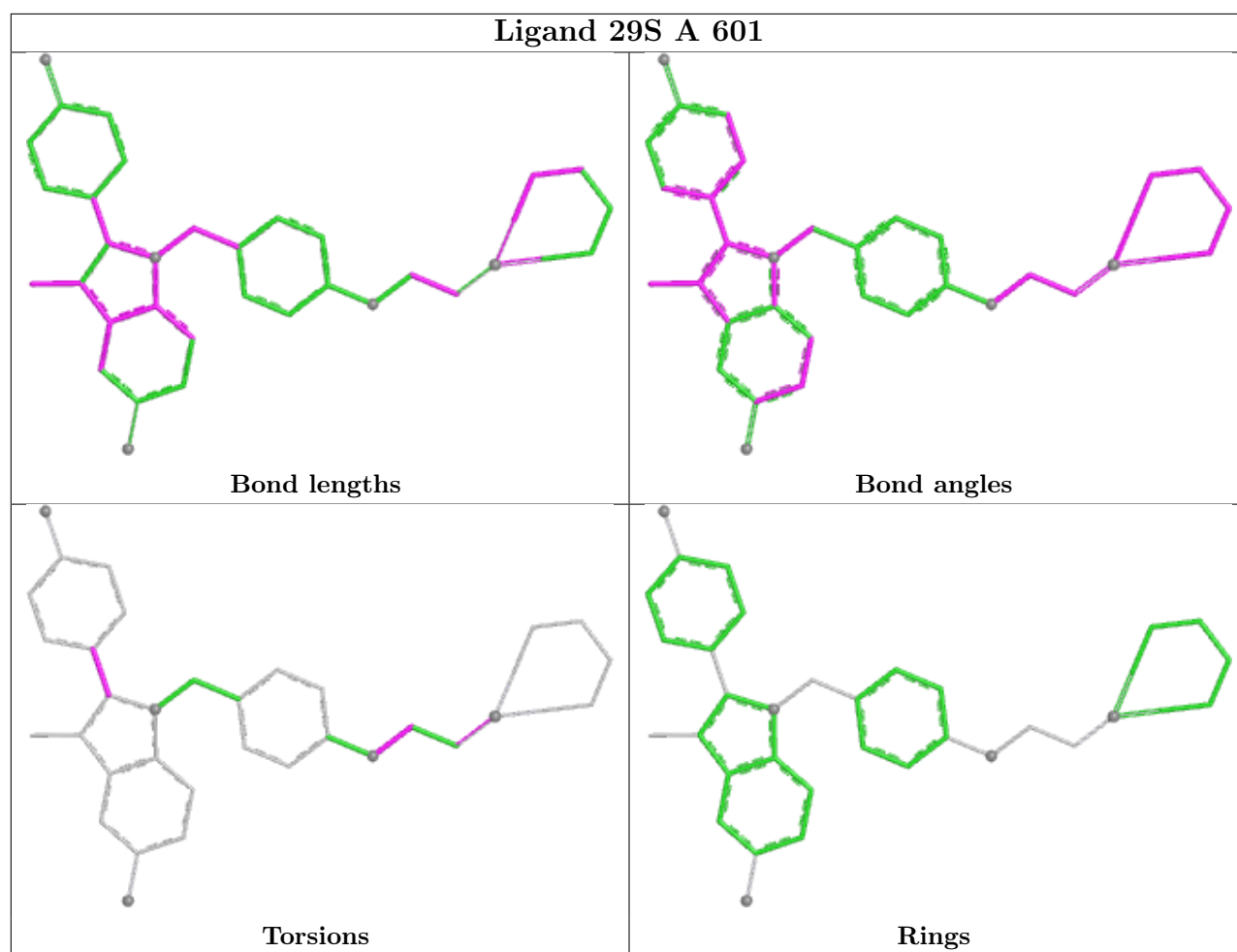


Ligand 29S D 601



Ligand 29S C 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	230/243 (94%)	0.36	7 (3%) 52 48	25, 57, 89, 153	4 (1%)
1	B	233/243 (95%)	0.29	4 (1%) 69 65	26, 56, 87, 102	1 (0%)
1	C	236/243 (97%)	0.26	6 (2%) 58 54	37, 61, 92, 129	0
1	D	219/243 (90%)	0.42	11 (5%) 34 30	27, 58, 110, 156	3 (1%)
All	All	918/972 (94%)	0.33	28 (3%) 51 47	25, 58, 93, 156	8 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	425	PHE	4.2
1	A	331	TYR	3.8
1	B	501[A]	HIS	3.3
1	C	307	ALA	3.1
1	C	460	THR	2.9
1	D	501[A]	HIS	2.7
1	A	332	ASP	2.7
1	C	331	TYR	2.6
1	D	332	ASP	2.6
1	D	533	VAL	2.5
1	B	331	TYR	2.5
1	D	331	TYR	2.4
1	D	537	TYR	2.4
1	D	333	PRO	2.3
1	A	328	TYR	2.3
1	D	306	LEU	2.2
1	D	519	ASN	2.2
1	B	460	THR	2.2
1	C	425	PHE	2.2
1	A	460	THR	2.1
1	B	410	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	536	SER	2.1
1	C	533	VAL	2.1
1	C	334	THR	2.1
1	D	530	CYS	2.1
1	A	333	PRO	2.1
1	A	532	ASN	2.0
1	D	531	LYS	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](#)

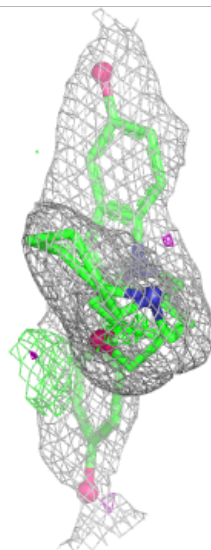
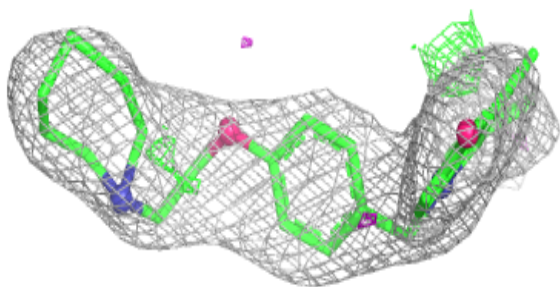
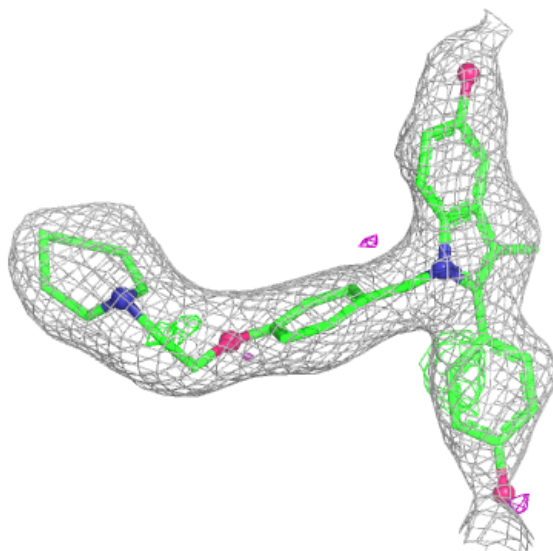
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	29S	A	601	35/35	0.87	0.13	31,57,75,82	0
2	29S	B	601	35/35	0.89	0.13	33,55,83,84	0
2	29S	D	601	35/35	0.89	0.14	42,64,88,104	0
2	29S	C	601	35/35	0.91	0.12	36,54,80,84	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.

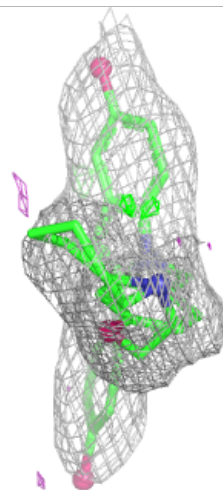
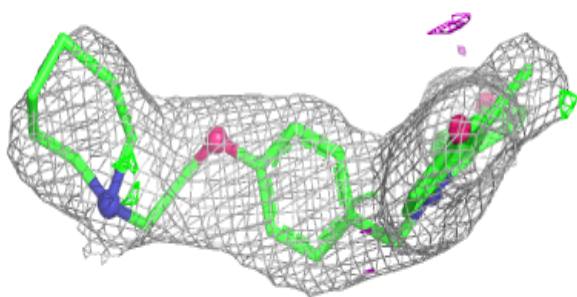
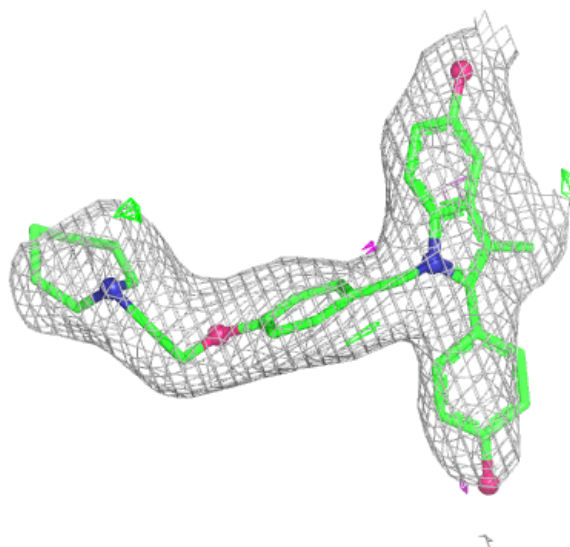
Electron density around 29S A 601:

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



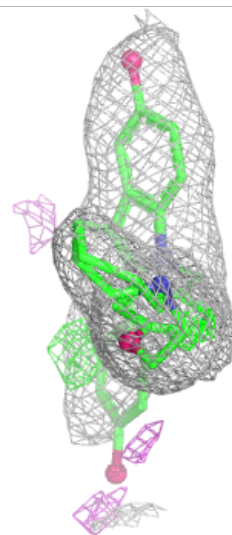
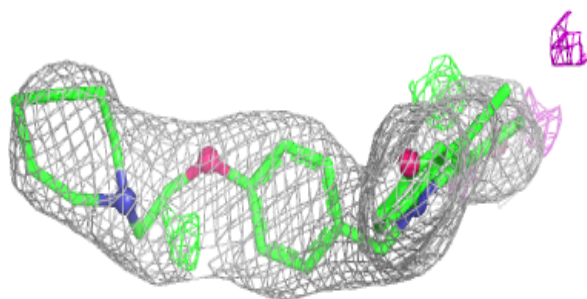
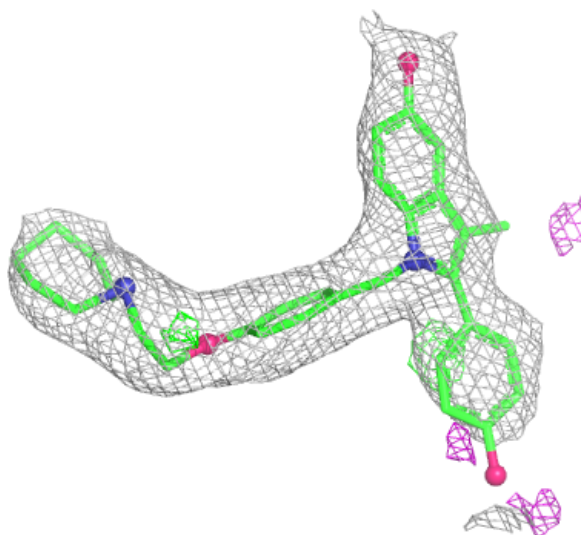
Electron density around 29S B 601:

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



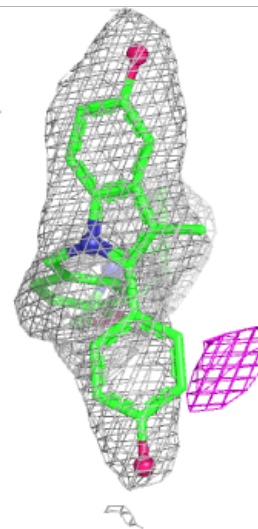
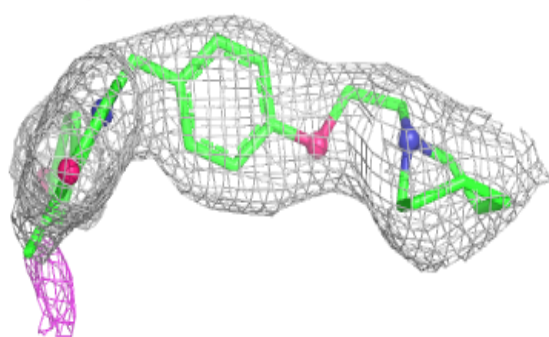
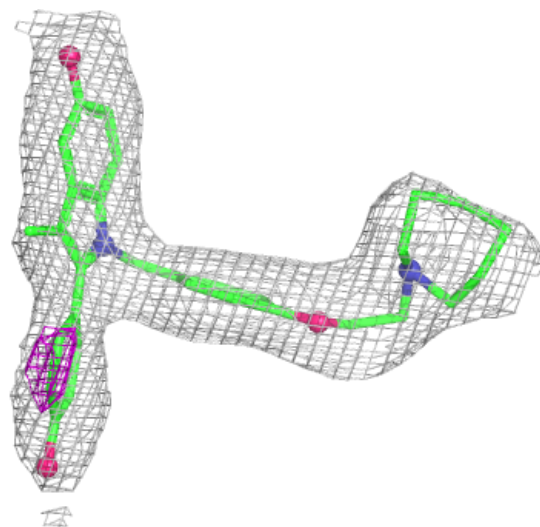
Electron density around 29S D 601:

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



Electron density around 29S 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.