



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:12 AM UTC

PDB ID : 4D8C / pdb_00004d8c
Title : Crystal Structure of Human Beta Secretase in Complex with NVP-BXD552,
derived from a co-crystallization experiment
Authors : Rondeau, J.M.; Bourgier, E.
Deposited on : 2012-01-10
Resolution : 2.07 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

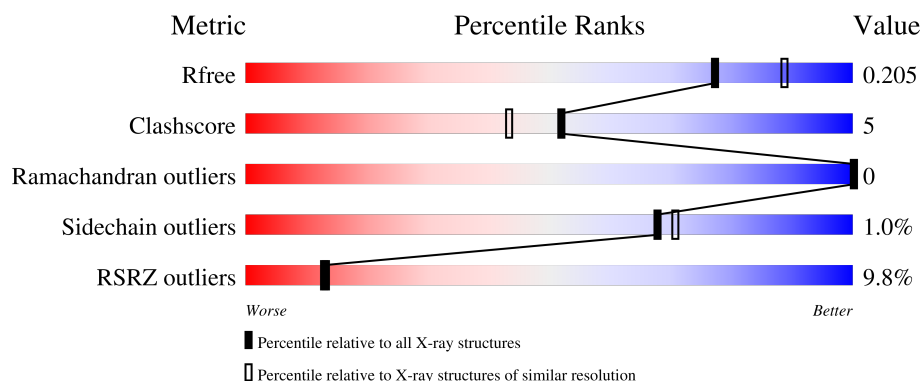
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

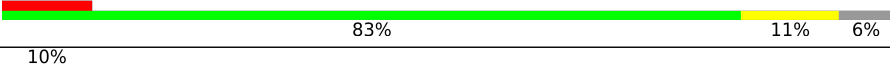
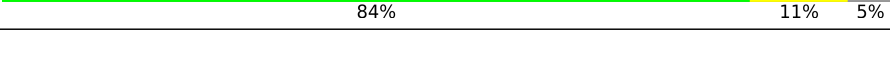
The reported resolution of this entry is 2.07 Å.

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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	402	
1	B	402	
1	C	402	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9759 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.

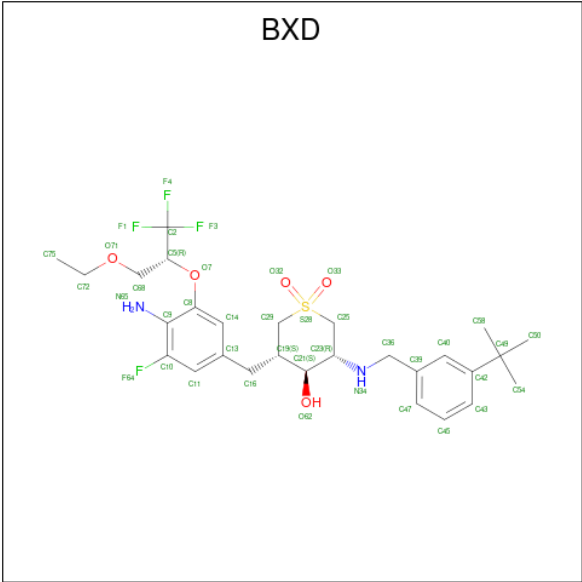
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2966	1898	493	561	14			
1	B	377	Total	C	N	O	S	0	0	0
			2966	1898	493	561	14			
1	C	381	Total	C	N	O	S	0	0	0
			2993	1917	497	565	14			

There are 6 discrepancies between the modelled and reference sequences:

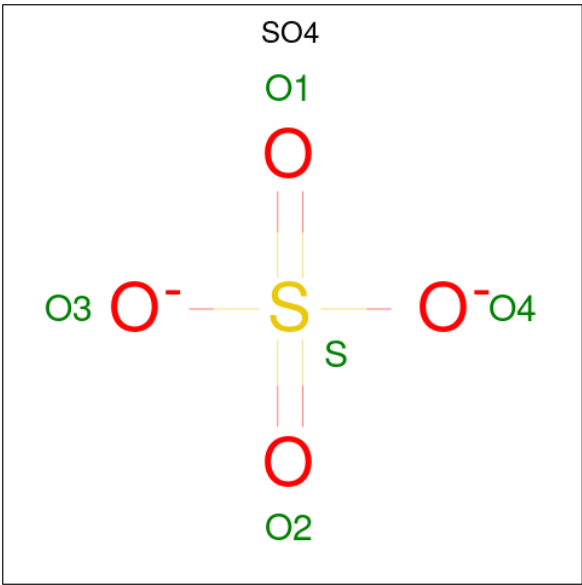
Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	GLY	-	expression tag	UNP P56817
A	-14	PRO	-	expression tag	UNP P56817
B	-15	GLY	-	expression tag	UNP P56817
B	-14	PRO	-	expression tag	UNP P56817
C	-15	GLY	-	expression tag	UNP P56817
C	-14	PRO	-	expression tag	UNP P56817

- Molecule 2 is (3S,4S,5R)-3-(4-amino-3-([(2R)-3-ethoxy-1,1,1-trifluoropropan-2-yl]oxy})-5-fluorobenzyl)-5-[(3-tert-butylbenzyl)amino]tetrahydro-2H-thiopyran-4-ol 1,1-dioxide (CCD ID: BXD) (formula: C₂₈H₃₈F₄N₂O₅S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			40	28	4	2	5	1		
2	B	1	Total	C	F	N	O	S	0	0
			40	28	4	2	5	1		
2	C	1	Total	C	F	N	O	S	0	0
			40	28	4	2	5	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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

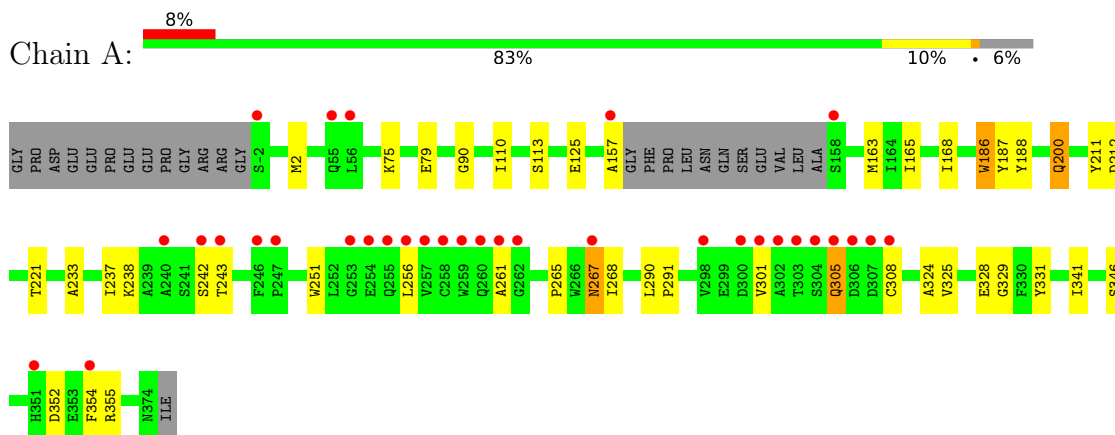
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	244	Total	O	0	0
			244	244		
4	B	215	Total	O	0	0
			215	215		
4	C	245	Total	O	0	0
			245	245		

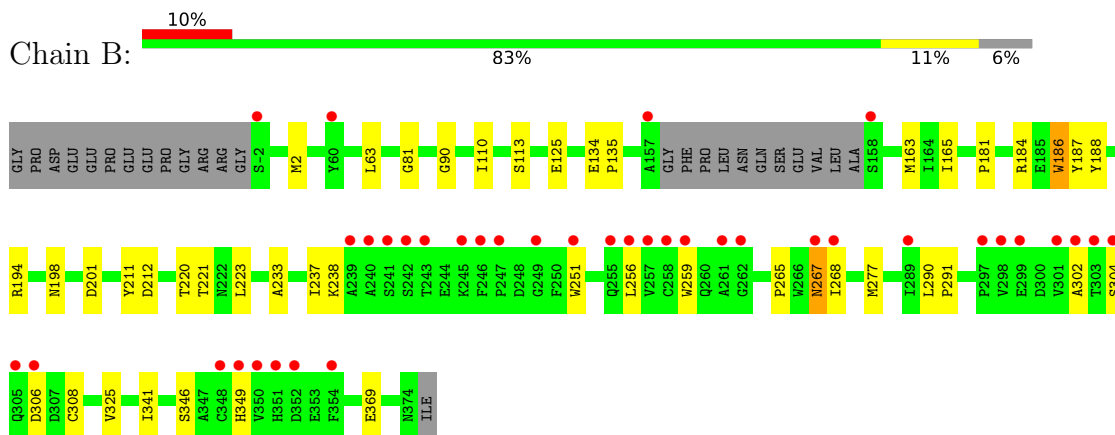
3 Residue-property plots [i](#)

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.

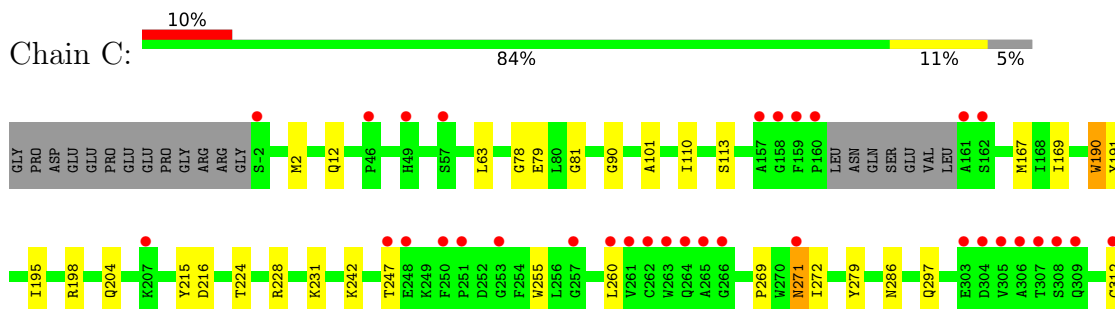
• Molecule 1: Beta-secretase 1



• Molecule 1: Beta-secretase 1



• Molecule 1: Beta-secretase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.13Å 103.50Å 100.41Å 90.00° 103.98° 90.00°	Depositor
Resolution (Å)	70.95 – 2.07 70.95 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.8 (70.95-2.07) 99.9 (70.95-2.07)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 2.07Å)	Xtriage
Refinement program	CNS, CNX 2002	Depositor
R, R_{free}	0.191 , 0.211 0.186 , 0.205	Depositor DCC
R_{free} test set	9956 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9759	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, BXD

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	0.34	0/3041	0.67	0/4133
1	B	0.35	0/3041	0.69	0/4133
1	C	0.35	0/3070	0.68	1/4173 (0.0%)
All	All	0.35	0/9152	0.68	1/12439 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	228	ARG	NE-CZ-NH2	5.43	124.09	119.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2966	0	2878	31	0
1	B	2966	0	2878	30	0
1	C	2993	0	2902	32	0
2	A	40	0	38	0	0
2	B	40	0	38	1	0
2	C	40	0	38	1	0
3	B	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	0	0	0
4	A	244	0	0	3	0
4	B	215	0	0	2	0
4	C	245	0	0	4	0
All	All	9759	0	8772	91	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 5.

All (91) 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:267:ASN:HD22	1:B:267:ASN:N	1.59	1.00
1:B:267:ASN:H	1:B:267:ASN:ND2	1.59	1.00
1:C:271:ASN:H	1:C:271:ASN:HD22	1.07	0.98
1:A:267:ASN:HD22	1:A:267:ASN:H	1.02	0.98
1:A:267:ASN:H	1:A:267:ASN:ND2	1.73	0.82
1:C:271:ASN:H	1:C:271:ASN:ND2	1.74	0.80
1:B:267:ASN:HD22	1:B:267:ASN:H	0.81	0.78
1:A:256:LEU:H	1:A:256:LEU:HD23	1.52	0.75
1:B:256:LEU:H	1:B:256:LEU:HD23	1.52	0.73
1:C:260:LEU:H	1:C:260:LEU:HD23	1.52	0.72
1:A:267:ASN:HD22	1:A:267:ASN:N	1.84	0.71
1:A:243:THR:HG21	1:C:247:THR:HG21	1.74	0.69
1:B:194:ARG:NH2	1:B:201:ASP:HB2	2.09	0.68
1:B:181:PRO:HG2	1:B:277:MET:HE2	1.78	0.65
1:C:204:GLN:HB2	4:C:738:HOH:O	1.96	0.65
1:B:198:ASN:HA	4:B:755:HOH:O	1.98	0.63
1:C:297:GLN:HG3	1:C:354:VAL:HG21	1.84	0.60
1:A:324:ALA:O	1:A:328:GLU:HG3	2.02	0.59
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.84	0.59
1:A:256:LEU:HD12	1:A:308:CYS:HB3	1.85	0.59
1:C:271:ASN:HD22	1:C:271:ASN:N	1.88	0.59
1:B:346:SER:O	1:B:349:HIS:HB3	2.04	0.58
1:A:79:GLU:HG3	4:A:731:HOH:O	2.03	0.58
1:B:256:LEU:HD12	1:B:308:CYS:HB3	1.86	0.57
1:C:328:ALA:O	1:C:332:GLU:HG3	2.06	0.56
1:C:79:GLU:HB3	4:C:712:HOH:O	2.06	0.55
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.88	0.55
1:C:260:LEU:HD12	1:C:312:CYS:HB3	1.88	0.55
1:A:267:ASN:HB3	1:A:354:PHE:CZ	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:PRO:O	1:B:268:ILE:HG12	2.07	0.53
1:B:221:THR:O	1:B:325:VAL:HG13	2.09	0.52
1:A:265:PRO:O	1:A:268:ILE:HG12	2.10	0.52
1:B:163:MET:HE3	1:B:165:ILE:HD11	1.92	0.52
1:C:167:MET:HE3	1:C:169:ILE:HD11	1.91	0.51
1:B:259:TRP:O	1:B:306:ASP:HB3	2.10	0.51
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.92	0.51
1:C:353:HIS:HB2	4:C:704:HOH:O	2.11	0.51
1:C:269:PRO:O	1:C:272:ILE:HG12	2.10	0.51
1:C:190:TRP:CG	1:C:191:TYR:H	2.30	0.50
1:B:223:LEU:H	1:B:325:VAL:HG21	1.77	0.50
1:A:186:TRP:CG	1:A:187:TYR:H	2.29	0.49
1:A:329:GLY:C	1:A:346:SER:HB3	2.37	0.49
1:C:195:ILE:CD1	1:C:372:MET:HG3	2.42	0.49
1:A:267:ASN:ND2	1:A:267:ASN:N	2.47	0.49
1:C:242:LYS:HE2	1:C:255:TRP:CD1	2.48	0.48
1:B:186:TRP:CG	1:B:187:TYR:H	2.32	0.48
1:A:352:ASP:HB3	1:A:355:ARG:O	2.15	0.47
1:C:333:GLY:C	1:C:350:SER:HB3	2.40	0.47
1:B:220:THR:OG1	2:B:501:BXD:H9	2.15	0.47
1:B:238:LYS:HE2	1:B:251:TRP:CD1	2.49	0.47
1:C:271:ASN:ND2	1:C:271:ASN:N	2.49	0.47
1:A:238:LYS:HE2	1:A:251:TRP:CD1	2.51	0.46
1:B:211:TYR:HA	1:B:212:ASP:HA	1.65	0.46
1:B:63:LEU:HG	1:B:81:GLY:HA2	1.97	0.46
1:A:329:GLY:O	1:A:346:SER:HB3	2.16	0.46
1:A:188:TYR:HB3	1:A:341:ILE:HD11	1.98	0.45
1:A:267:ASN:ND2	4:A:829:HOH:O	2.48	0.45
1:A:242:SER:OG	1:C:271:ASN:OD1	2.34	0.45
1:A:110:ILE:HB	1:A:113:SER:HB3	1.99	0.45
1:B:369:GLU:HG3	4:B:792:HOH:O	2.18	0.44
1:B:233:ALA:O	1:B:237:ILE:HG13	2.17	0.44
1:B:290:LEU:HB3	1:B:291:PRO:HD2	1.99	0.44
1:C:286:ASN:HA	1:C:368:VAL:HA	1.99	0.44
1:C:12:GLN:OE1	1:C:113:SER:HA	2.18	0.44
1:A:163:MET:HE3	1:A:165:ILE:HD11	2.00	0.43
1:A:256:LEU:HD11	1:A:301:VAL:HG13	2.00	0.43
1:C:110:ILE:HB	1:C:113:SER:HB3	2.00	0.43
1:C:195:ILE:HD11	1:C:372:MET:HG3	2.01	0.43
1:B:110:ILE:HB	1:B:113:SER:HB3	2.00	0.43
1:B:267:ASN:N	1:B:267:ASN:ND2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:THR:O	1:A:325:VAL:HG13	2.18	0.43
1:A:211:TYR:HA	1:A:212:ASP:HA	1.66	0.42
1:A:168:ILE:HG23	1:A:331:TYR:HE2	1.84	0.42
1:B:125:GLU:CD	1:B:184:ARG:HH21	2.27	0.42
1:C:198:ARG:HB3	1:C:279:TYR:HB2	2.02	0.42
1:B:223:LEU:N	1:B:325:VAL:HG21	2.33	0.42
1:A:290:LEU:HB3	1:A:291:PRO:HD2	2.02	0.42
1:B:302:ALA:C	1:B:304:SER:H	2.28	0.42
1:B:134:GLU:HA	1:B:135:PRO:HD3	1.93	0.42
1:C:215:TYR:HA	1:C:216:ASP:HA	1.65	0.42
1:C:63:LEU:HG	1:C:81:GLY:HA2	2.02	0.41
1:B:188:TYR:HB3	1:B:341:ILE:HD11	2.01	0.41
1:C:224:THR:OG1	2:C:401:BXD:H9	2.20	0.41
1:A:233:ALA:O	1:A:237:ILE:HG13	2.20	0.41
1:A:200:GLN:HE21	1:A:200:GLN:HB2	1.71	0.41
1:A:157:ALA:C	4:A:842:HOH:O	2.63	0.41
1:C:356:ASP:HB3	1:C:359:ARG:O	2.21	0.41
1:A:261:ALA:HB2	1:A:305:GLN:O	2.21	0.41
1:C:231:LYS:HA	1:C:319:GLN:HG3	2.02	0.40
1:C:371:ASP:HB2	4:C:576:HOH:O	2.21	0.40
1:C:78:GLY:HA3	1:C:101:ALA:O	2.21	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	373/402 (93%)	364 (98%)	9 (2%)	0	100	100
1	B	373/402 (93%)	362 (97%)	11 (3%)	0	100	100
1	C	377/402 (94%)	369 (98%)	8 (2%)	0	100	100
All	All	1123/1206 (93%)	1095 (98%)	28 (2%)	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	322/342 (94%)	316 (98%)	6 (2%)	50	49
1	B	322/342 (94%)	320 (99%)	2 (1%)	78	82
1	C	324/342 (95%)	322 (99%)	2 (1%)	78	82
All	All	968/1026 (94%)	958 (99%)	10 (1%)	68	71

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LYS
1	A	125	GLU
1	A	186	TRP
1	A	200	GLN
1	A	267	ASN
1	A	305	GLN
1	B	186	TRP
1	B	267	ASN
1	C	190	TRP
1	C	271	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	114	ASN
1	A	222	ASN
1	A	260	GLN
1	A	267	ASN
1	A	305	GLN
1	A	315	GLN
1	A	374	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	89	HIS
1	B	114	ASN
1	B	170	HIS
1	B	222	ASN
1	B	260	GLN
1	B	267	ASN
1	B	315	GLN
1	B	374	ASN
1	C	89	HIS
1	C	114	ASN
1	C	226	ASN
1	C	319	GLN
1	C	378	ASN

5.3.3 RNA [i](#)

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](#)

5 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	SO4	B	502	-	4,4,4	0.36	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BXD	C	401	-	39,42,42	1.59	8 (20%)	51,63,63	1.03	4 (7%)
3	SO4	C	402	-	4,4,4	0.41	0	6,6,6	0.13	0
2	BXD	B	501	-	39,42,42	1.61	7 (17%)	51,63,63	1.07	3 (5%)
2	BXD	A	501	-	39,42,42	1.63	8 (20%)	51,63,63	1.07	3 (5%)

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	BXD	B	501	-	-	1/29/47/47	0/3/3/3
2	BXD	A	501	-	-	1/29/47/47	0/3/3/3
2	BXD	C	401	-	-	1/29/47/47	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	BXD	C25-S28	3.22	1.80	1.77
2	A	501	BXD	C29-S28	3.18	1.80	1.77
2	A	501	BXD	C16-C19	3.09	1.57	1.53
2	B	501	BXD	C16-C19	2.88	1.57	1.53
2	C	401	BXD	C16-C19	2.88	1.57	1.53
2	B	501	BXD	C29-S28	2.81	1.79	1.77
2	B	501	BXD	C25-S28	2.78	1.79	1.77
2	C	401	BXD	C25-S28	2.73	1.79	1.77
2	B	501	BXD	C40-C42	2.64	1.43	1.39
2	C	401	BXD	C40-C42	2.63	1.43	1.39
2	C	401	BXD	C43-C42	2.61	1.43	1.39
2	C	401	BXD	C29-S28	2.54	1.79	1.77
2	B	501	BXD	C11-C10	2.49	1.41	1.37
2	A	501	BXD	C40-C42	2.46	1.43	1.39
2	A	501	BXD	C11-C10	2.39	1.41	1.37
2	C	401	BXD	C11-C10	2.38	1.41	1.37
2	A	501	BXD	C68-C5	2.34	1.55	1.50
2	A	501	BXD	C43-C42	2.31	1.43	1.39
2	B	501	BXD	C43-C42	2.27	1.43	1.39
2	C	401	BXD	C68-C5	2.24	1.55	1.50
2	B	501	BXD	C68-C5	2.20	1.55	1.50
2	C	401	BXD	C21-C23	2.08	1.56	1.52
2	A	501	BXD	C2-C5	2.07	1.56	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	BXD	C36-N34-C23	3.15	121.37	114.84
2	B	501	BXD	C36-N34-C23	3.07	121.21	114.84
2	C	401	BXD	C36-N34-C23	3.00	121.05	114.84
2	C	401	BXD	C8-C9-C10	2.25	119.59	116.08
2	B	501	BXD	C8-C9-C10	2.21	119.53	116.08
2	B	501	BXD	C54-C49-C42	2.20	115.54	110.35
2	A	501	BXD	C8-C9-C10	2.18	119.48	116.08
2	C	401	BXD	O62-C21-C23	-2.16	104.91	109.40
2	A	501	BXD	C54-C49-C42	2.15	115.43	110.35
2	C	401	BXD	C11-C10-C9	-2.04	120.36	123.36

There are no chirality outliers.

All (3) torsion outliers are listed below:

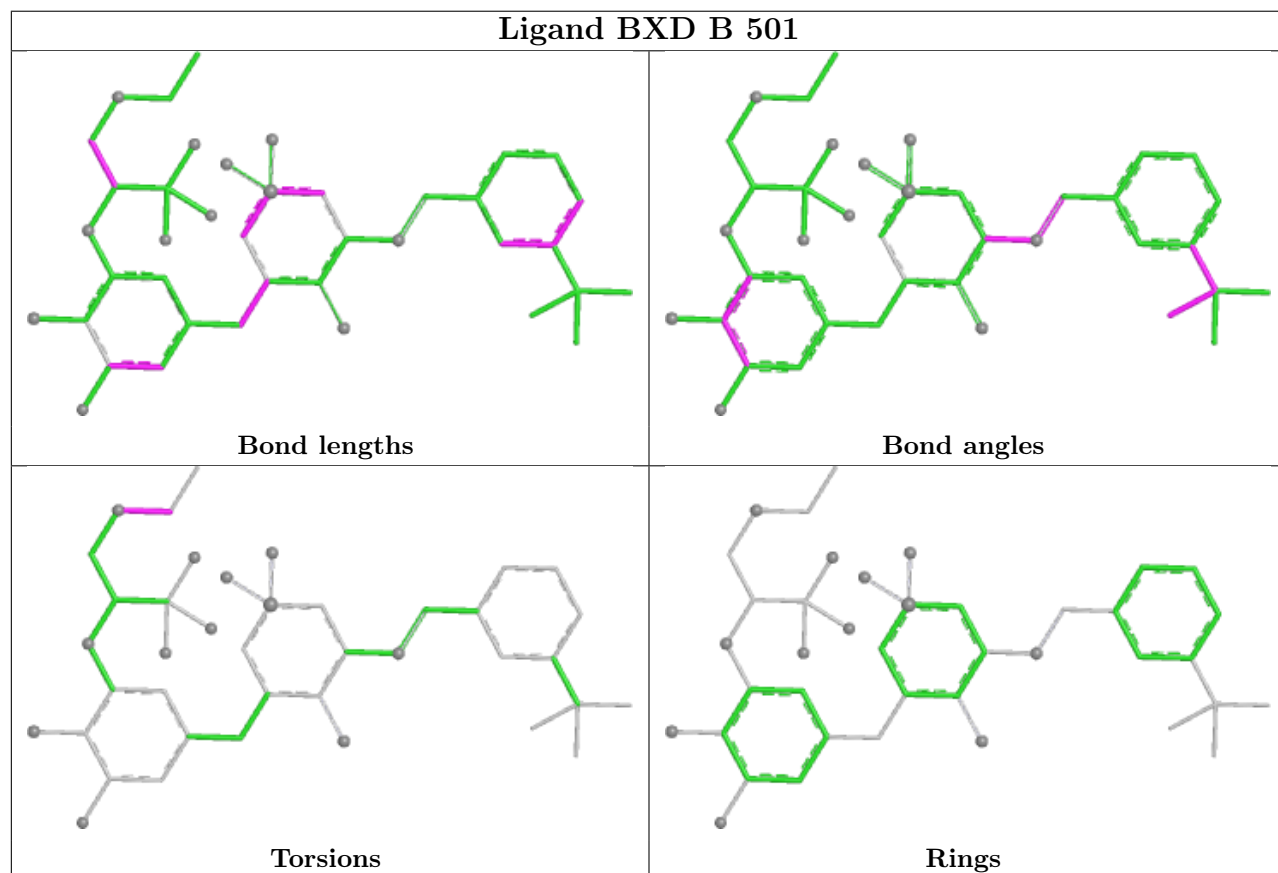
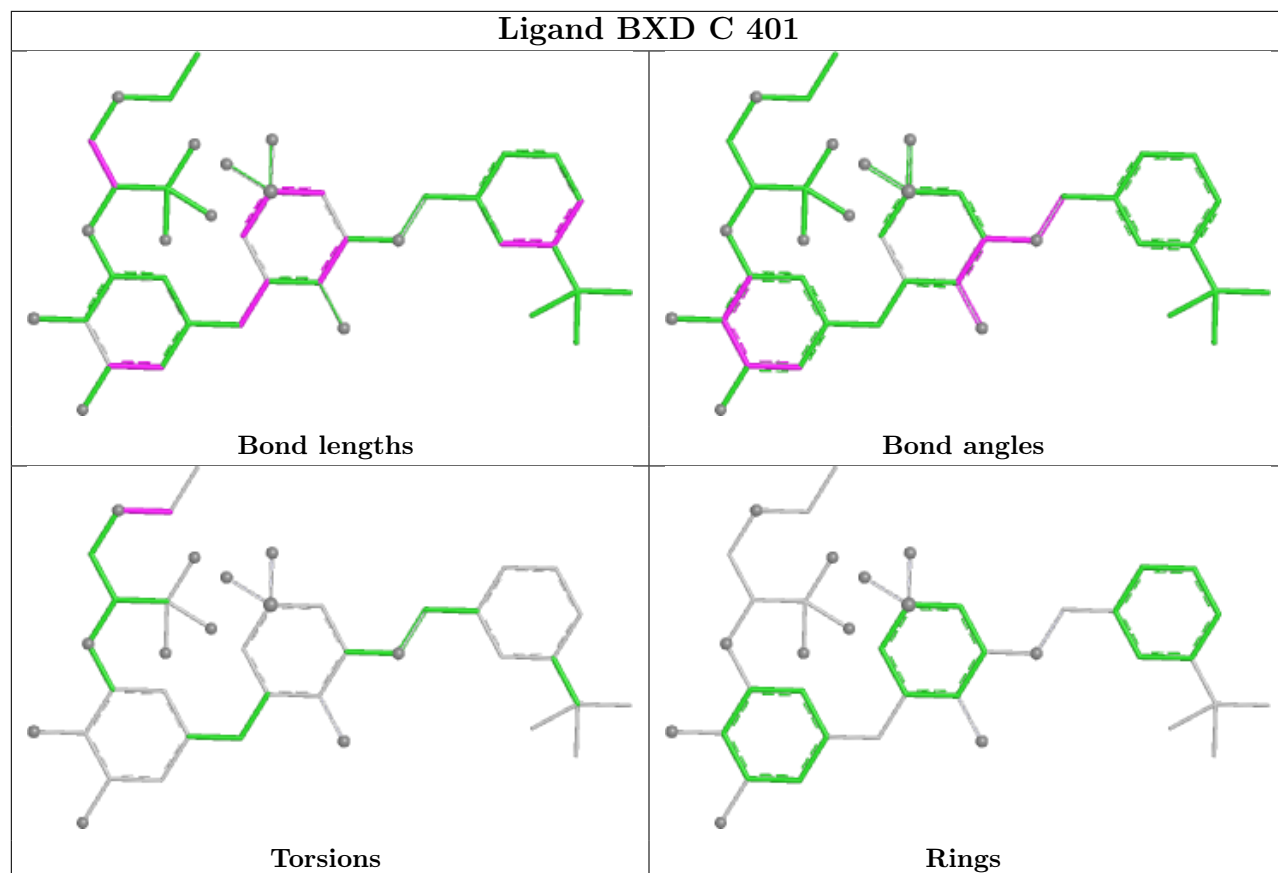
Mol	Chain	Res	Type	Atoms
2	A	501	BXD	C75-C72-O71-C68
2	C	401	BXD	C75-C72-O71-C68
2	B	501	BXD	C75-C72-O71-C68

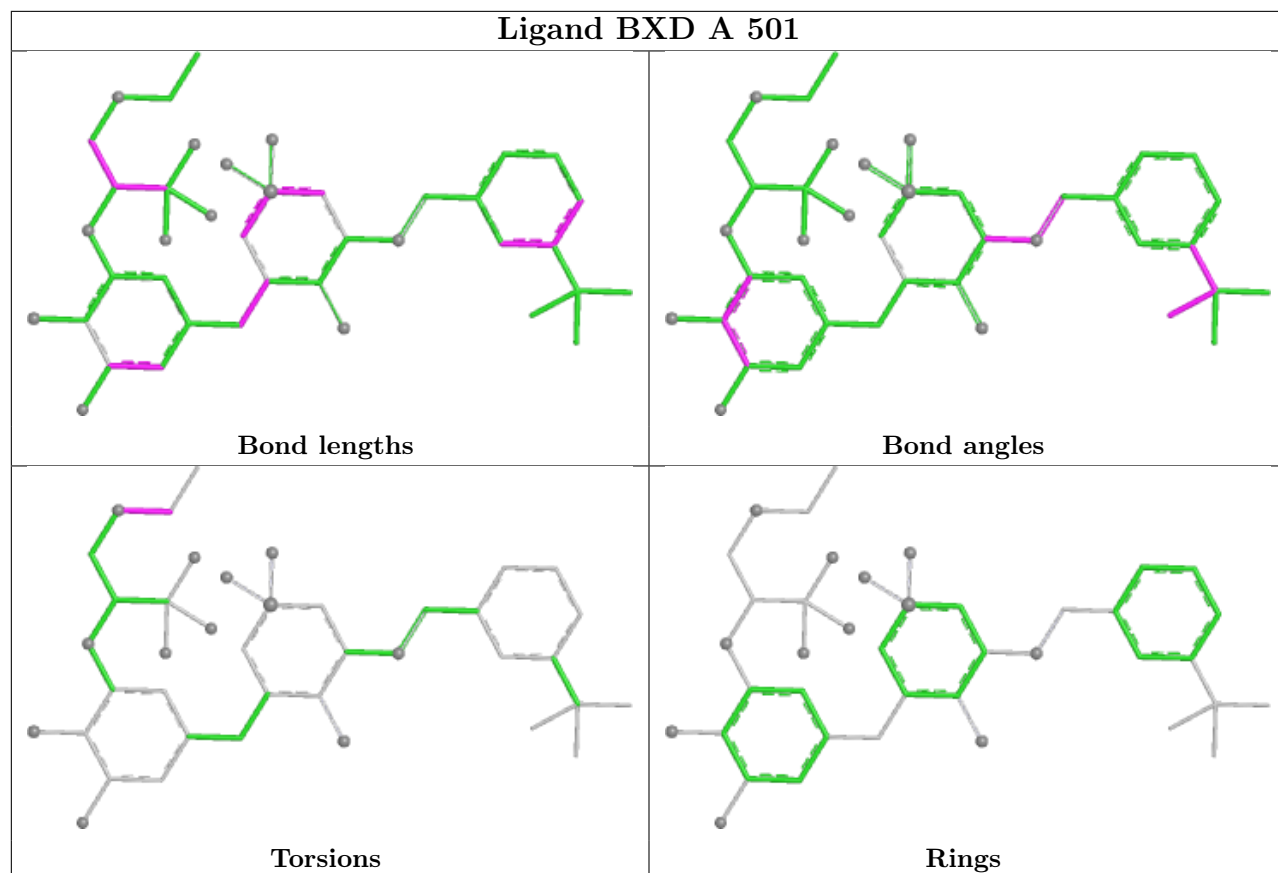
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	BXD	1	0
2	B	501	BXD	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	377/402 (93%)	0.43	33 (8%) 15 16	23, 36, 67, 102	0
1	B	377/402 (93%)	0.52	39 (10%) 12 12	21, 37, 72, 111	0
1	C	381/402 (94%)	0.44	39 (10%) 12 12	23, 37, 71, 104	0
All	All	1135/1206 (94%)	0.46	111 (9%) 13 13	21, 37, 71, 111	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	VAL	7.9
1	B	303	THR	6.5
1	B	302	ALA	5.9
1	C	161	ALA	5.9
1	A	303	THR	5.7
1	C	305	VAL	5.7
1	B	350	VAL	5.6
1	A	354	PHE	5.6
1	B	301	VAL	5.3
1	B	304	SER	5.1
1	B	243	THR	4.8
1	A	302	ALA	4.5
1	B	256	LEU	4.4
1	A	243	THR	4.4
1	C	355	HIS	4.3
1	C	247	THR	4.2
1	C	160	PRO	4.2
1	A	304	SER	4.2
1	B	247	PRO	4.2
1	C	-2	SER	4.2
1	C	354	VAL	4.2
1	C	358	PHE	4.1
1	A	158	SER	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	267	ASN	4.0
1	C	306	ALA	4.0
1	C	304	ASP	4.0
1	B	354	PHE	4.0
1	A	267	ASN	4.0
1	C	265	ALA	3.9
1	A	261	ALA	3.8
1	C	159	PHE	3.8
1	C	307	THR	3.7
1	A	256	LEU	3.7
1	A	247	PRO	3.7
1	B	261	ALA	3.7
1	B	298	VAL	3.5
1	C	271	ASN	3.5
1	C	158	GLY	3.5
1	B	239	ALA	3.5
1	B	-2	SER	3.5
1	B	262	GLY	3.5
1	B	157	ALA	3.4
1	B	351	HIS	3.3
1	A	253	GLY	3.3
1	B	242	SER	3.3
1	A	298	VAL	3.3
1	A	308	CYS	3.2
1	C	251	PRO	3.2
1	B	257	VAL	3.2
1	B	299	GLU	3.2
1	A	306	ASP	3.1
1	B	348	CYS	3.1
1	C	260	LEU	3.1
1	B	241	SER	3.1
1	C	157	ALA	3.0
1	B	240	ALA	2.9
1	B	251	TRP	2.9
1	A	242	SER	2.9
1	C	257	GLY	2.9
1	B	306	ASP	2.9
1	B	246	PHE	2.9
1	A	305	GLN	2.8
1	B	255	GLN	2.8
1	A	246	PHE	2.8
1	A	56	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	312	CYS	2.8
1	C	262	CYS	2.8
1	C	309	GLN	2.7
1	C	248	GLU	2.7
1	A	257	VAL	2.7
1	A	254	GLU	2.7
1	B	268	ILE	2.7
1	A	351	HIS	2.6
1	C	162	SER	2.6
1	C	308	SER	2.6
1	A	258	CYS	2.6
1	C	356	ASP	2.5
1	B	249	GLY	2.5
1	C	360	THR	2.5
1	B	305	GLN	2.4
1	C	250	PHE	2.4
1	C	266	GLY	2.4
1	A	240	ALA	2.4
1	B	259	TRP	2.4
1	C	303	GLU	2.4
1	B	289	ILE	2.4
1	A	307	ASP	2.3
1	B	352	ASP	2.3
1	C	207	LYS	2.3
1	B	245	LYS	2.3
1	C	261	VAL	2.3
1	A	255	GLN	2.3
1	A	259	TRP	2.3
1	C	263	TRP	2.3
1	C	46	PRO	2.3
1	A	262	GLY	2.3
1	B	258	CYS	2.2
1	B	349	HIS	2.2
1	A	157	ALA	2.2
1	B	297	PRO	2.2
1	B	158	SER	2.2
1	C	253	GLY	2.1
1	C	264	GLN	2.1
1	A	-2	SER	2.1
1	B	60	TYR	2.1
1	A	300	ASP	2.1
1	C	57	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	55	GLN	2.1
1	C	49	HIS	2.1
1	A	260	GLN	2.0
1	C	357	GLU	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](#)

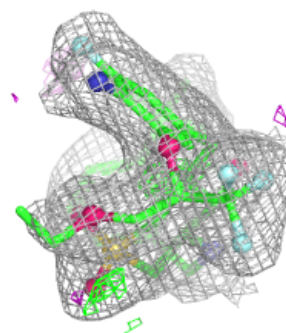
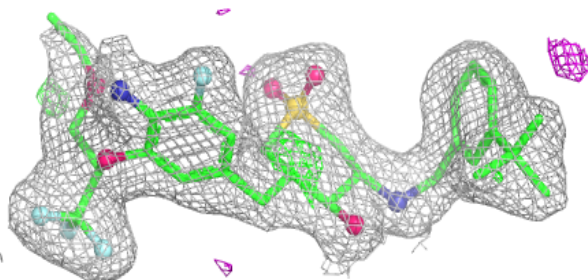
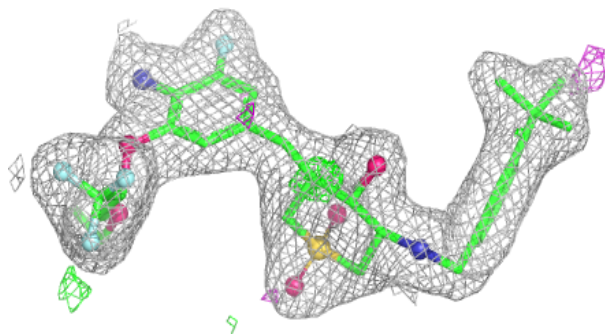
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	B	502	5/5	0.90	0.11	77,77,78,79	0
3	SO4	C	402	5/5	0.90	0.11	57,57,58,59	0
2	BXD	A	501	40/40	0.96	0.08	25,30,48,51	0
2	BXD	B	501	40/40	0.96	0.08	26,30,49,53	0
2	BXD	C	401	40/40	0.97	0.07	26,30,45,50	0

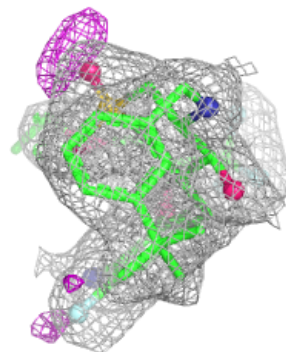
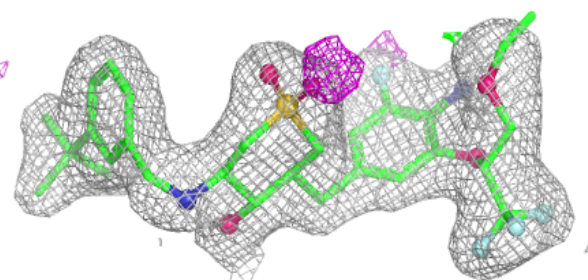
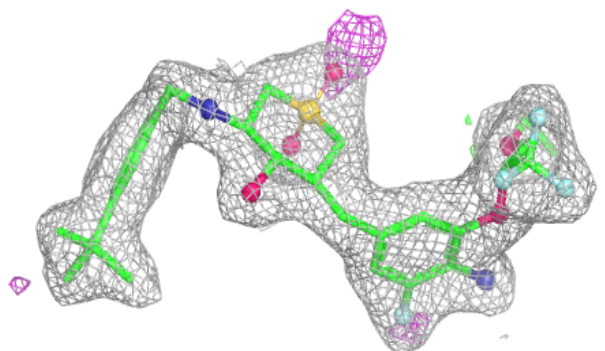
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BXD A 501:

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

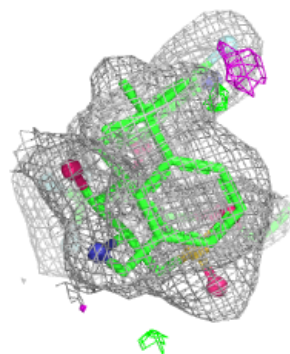
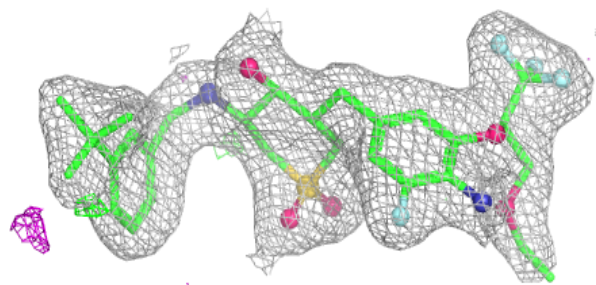
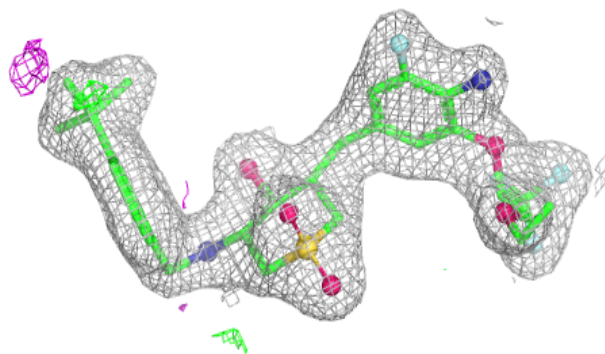
**Electron density around BXD B 501:**

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



Electron density around BXD C 401:

$2mF_o-DF_c$ (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.