Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2024 – 10:32 AM EST

PDB ID	:	2FB8
Title	:	Structure of the B-Raf kinase domain bound to SB-590885
Authors	:	Lougheed, J.C.; Lee, J.; Chau, D.C.; Stout, T.J.
Deposited on	:	2005-12-08
Resolution	:	2.90 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
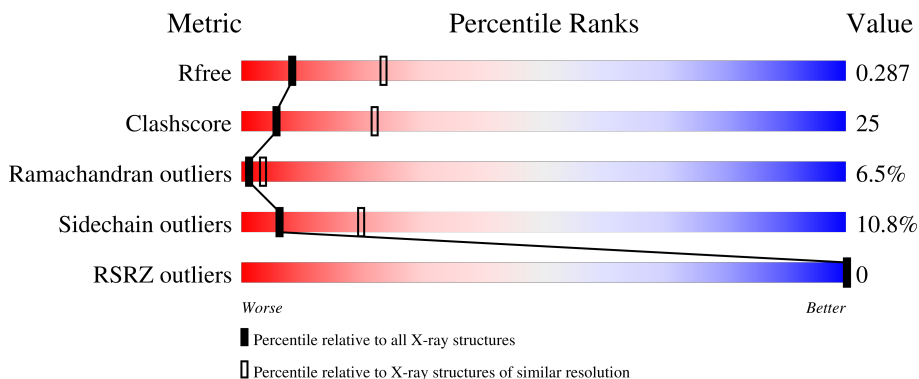http://www.wwpdb.org/validation/2017/FAQs#types.

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 2.90 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	Percentile Ranks	Value
Rfree		0.287
Clashscore		25
Ramachandran outliers		6.5%
Sidechain outliers		10.8%
RSRZ outliers		0

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	281	48% 35% 8% · 8%
1	B	281	46% 36% 9% · 8%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4238 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 B-Raf proto-oncogene serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total 2067	C 1325	N 360	O 369	S 13	0	0	0
1	B	259	Total 2067	C 1325	N 360	O 369	S 13	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	443	GLY	-	cloning artifact	UNP P15056
A	444	SER	-	cloning artifact	UNP P15056
B	443	GLY	-	cloning artifact	UNP P15056
B	444	SER	-	cloning artifact	UNP P15056

- Molecule 2 is (1Z)-5-(2-{4-[2-(DIMETHYLAMINO)ETHOXY]PHENYL}-5-PYRIDIN-4-YL-1H-IMIDAZOL-4-YL)INDAN-1-ONE OXIME (three-letter code: 215) (formula: $C_{27}H_{27}N_5O_2$).
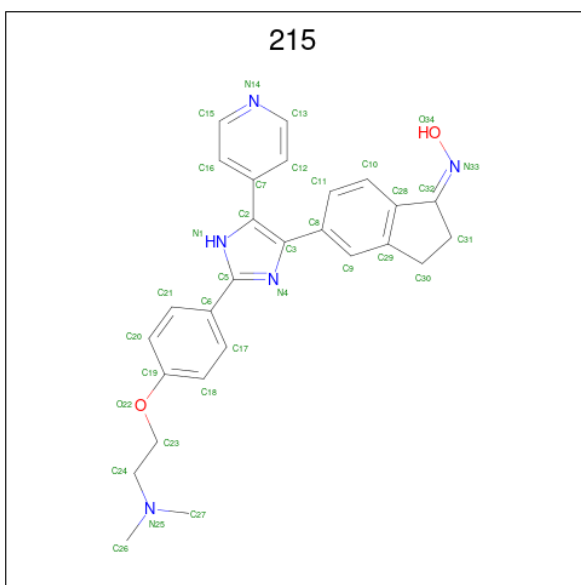
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 34	C 27	N 5	O 2	0	0
2	B	1	Total 34	C 27	N 5	O 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total 22	O 22	0	0
3	B	14	Total 14	O 14	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above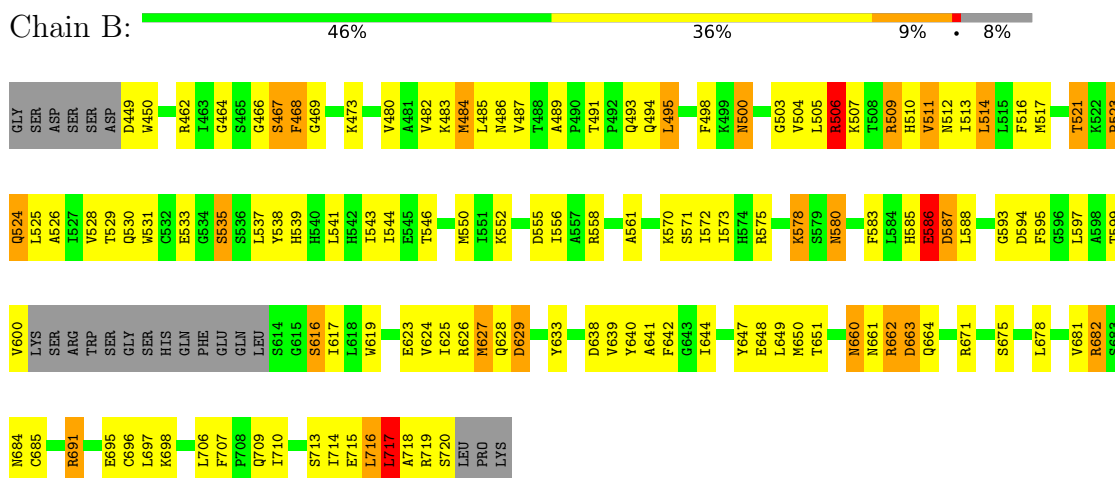 a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: B-Raf proto-oncogene serine/threonine-protein kinase
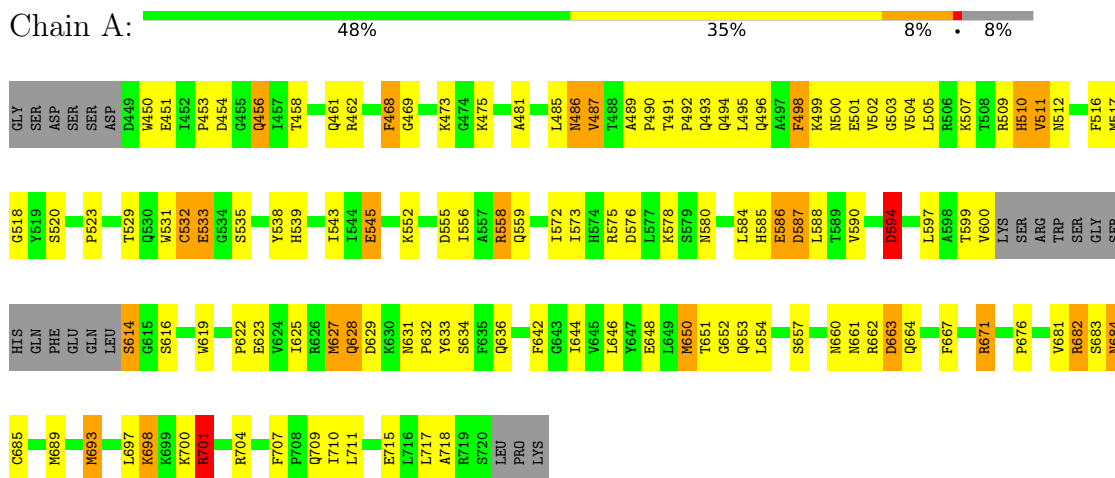
• Molecule 1: B-Raf proto-oncogene serine/threonine-protein kinase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	95.64Å 95.64Å 159.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.42 – 2.90 46.41 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (46.42-2.90) 97.9 (46.41-2.90)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	0.23	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.291 0.198 , 0.287	Depositor DCC
R_{free} test set	840 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	37.4	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.4	EDS
L-test for twinning[2]	$< |L| > = 0.41, < L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4238	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 215

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	0.93	0/2111	1.01	3/2849 (0.1%)
1	B	0.94	1/2111 (0.0%)	1.04	3/2849 (0.1%)
All	All	0.93	1/4222 (0.0%)	1.03	6/5698 (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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	696	CYS	CB-SG	-5.30	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	509	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	A	594	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	A	517	MET	CG-SD-CE	5.47	108.95	100.20
1	B	495	LEU	CA-CB-CG	5.14	127.13	115.30
1	B	696	CYS	CA-CB-SG	-5.13	104.76	114.00
1	A	693	MET	CB-CG-SD	-5.08	97.15	112.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	532	CYS	Peptide
1	A	614	SER	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	2067	0	2105	103	0
1	B	2067	0	2105	110	0
2	A	34	0	27	3	0
2	B	34	0	27	4	0
3	A	22	0	0	2	0
3	B	14	0	0	2	0
All	All	4238	0	4264	210	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 25.

All (210) 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:491:THR:HG22	1:B:493:GLN:H	1.17	1.07
1:A:558:ARG:HG2	1:A:558:ARG:HH21	1.19	1.04
1:B:484:MET:HB3	1:B:526:ALA:HB2	1.41	1.02
1:B:538:TYR:CE2	2:B:101:215:H261	2.07	0.88
1:A:575:ARG:HD2	1:A:599:THR:HG22	1.62	0.82
1:B:491:THR:CG2	1:B:493:GLN:H	1.91	0.82
1:A:491:THR:HG22	1:A:493:GLN:H	1.45	0.80
1:A:516:PHE:O	1:B:509:ARG:HD3	1.81	0.80
1:B:521:THR:HA	1:B:525:LEU:HD23	1.64	0.80
1:B:491:THR:HG22	1:B:493:GLN:N	2.00	0.75
1:B:538:TYR:HE2	2:B:101:215:H261	1.52	0.75
1:B:575:ARG:NH1	1:B:599:THR:HB	2.02	0.75
1:B:661:ASN:O	1:B:662:ARG:C	2.24	0.74
1:A:504:VAL:HG13	1:A:572:ILE:HD12	1.71	0.73
1:A:578:LYS:HD2	1:A:580:ASN:HD22	1.55	0.71
1:A:575:ARG:HD3	1:A:597:LEU:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:THR:HB	1:A:494:GLN:H	1.54	0.71
1:A:485:LEU:HG	1:A:485:LEU:O	1.88	0.71
1:A:501:GLU:HG2	1:A:505:LEU:CD1	2.21	0.71
1:A:682:ARG:HB3	1:A:684:ASN:OD1	1.91	0.71
1:A:501:GLU:HG2	1:A:505:LEU:HD11	1.73	0.70
1:B:468:PHE:HD1	1:B:468:PHE:C	1.94	0.70
1:A:644:ILE:O	1:A:648:GLU:HG3	1.92	0.70
1:B:468:PHE:C	1:B:468:PHE:CD1	2.66	0.69
1:B:467:SER:OG	1:B:483:LYS:NZ	2.26	0.69
1:B:661:ASN:O	1:B:664:GLN:N	2.22	0.68
1:B:466:GLY:O	1:B:467:SER:HB3	1.94	0.68
1:B:500:ASN:O	1:B:504:VAL:HG23	1.94	0.68
1:B:691:ARG:NH1	1:B:691:ARG:HB2	2.08	0.68
1:B:710:ILE:O	1:B:714:ILE:HG13	1.95	0.66
1:B:661:ASN:OD1	1:B:663:ASP:HB3	1.95	0.66
1:A:707:PHE:HA	1:A:710:ILE:HD12	1.79	0.65
1:B:449:ASP:CG	1:B:450:TRP:H	1.99	0.65
1:A:552:LYS:O	1:A:556:ILE:HG13	1.97	0.65
1:B:552:LYS:O	1:B:556:ILE:HG12	1.98	0.64
1:B:578:LYS:NZ	1:B:616:SER:HB2	2.13	0.64
2:A:102:215:C9	2:A:102:215:H16	2.28	0.64
1:A:453:PRO:O	1:A:456:GLN:HB2	1.99	0.61
1:B:650:MET:HE2	1:B:685:CYS:HB2	1.82	0.61
1:B:523:PRO:HG2	1:B:524:GLN:H	1.65	0.61
1:A:584:LEU:HG	1:A:587:ASP:HA	1.81	0.61
1:A:496:GLN:OE1	1:A:496:GLN:HA	2.01	0.60
1:A:619:TRP:CD1	1:A:644:ILE:HB	2.36	0.60
1:B:650:MET:CE	1:B:685:CYS:HB2	2.32	0.60
1:A:509:ARG:HD2	1:B:450:TRP:CH2	2.37	0.59
1:A:533:GLU:HB3	1:A:586:GLU:OE2	2.01	0.59
1:B:491:THR:HB	1:B:494:GLN:H	1.66	0.59
1:B:468:PHE:CE2	1:B:498:PHE:HB2	2.38	0.59
1:A:701:ARG:O	1:A:704:ARG:HG3	2.04	0.58
1:B:510:HIS:CE1	1:B:512:ASN:HB2	2.38	0.58
1:A:450:TRP:HA	1:A:450:TRP:CE3	2.39	0.58
1:A:711:LEU:O	1:A:715:GLU:HG3	2.02	0.58
1:B:647:TYR:O	1:B:651:THR:HG23	2.03	0.58
1:B:691:ARG:HB2	1:B:691:ARG:HH11	1.68	0.57
1:B:449:ASP:CG	1:B:450:TRP:N	2.58	0.57
1:A:512:ASN:HA	1:A:590:VAL:O	2.05	0.56
1:A:532:CYS:SG	1:A:585:HIS:HB2	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:ASP:HB2	1:A:597:LEU:HD12	1.88	0.56
1:A:558:ARG:HG2	1:A:558:ARG:NH2	2.00	0.56
1:A:651:THR:HG22	1:A:681:VAL:HA	1.87	0.56
1:A:575:ARG:HD2	1:A:599:THR:CG2	2.35	0.55
1:A:650:MET:HA	1:A:650:MET:CE	2.35	0.55
1:A:555:ASP:O	1:A:559:GLN:HG3	2.06	0.55
1:A:660:ASN:HB2	3:A:39:HOH:O	2.06	0.55
1:B:660:ASN:H	1:B:660:ASN:HD22	1.54	0.55
1:A:661:ASN:O	1:A:664:GLN:HB2	2.07	0.55
1:A:538:TYR:CG	1:A:580:ASN:OD1	2.60	0.54
1:A:573:ILE:HG22	1:A:575:ARG:HG3	1.88	0.54
1:B:485:LEU:O	1:B:486:ASN:HB2	2.06	0.54
1:B:626:ARG:O	1:B:627:MET:HB2	2.06	0.54
1:A:512:ASN:ND2	1:A:559:GLN:HB3	2.22	0.54
1:B:466:GLY:O	1:B:467:SER:CB	2.54	0.54
1:B:578:LYS:HZ3	1:B:616:SER:HB2	1.72	0.54
1:A:616:SER:HA	3:A:8:HOH:O	2.08	0.54
1:A:586:GLU:O	1:A:588:LEU:N	2.38	0.54
1:B:628:GLN:HG2	1:B:629:ASP:OD1	2.08	0.54
1:A:512:ASN:HD21	1:A:559:GLN:HB3	1.73	0.54
1:A:682:ARG:O	1:A:685:CYS:HB3	2.08	0.53
1:A:625:ILE:C	1:A:627:MET:H	2.11	0.53
1:A:509:ARG:HD3	1:B:516:PHE:O	2.09	0.53
1:A:700:LYS:O	1:A:701:ARG:C	2.46	0.53
1:A:578:LYS:HD3	1:A:616:SER:HB2	1.91	0.53
1:A:632:PRO:HD2	1:A:633:TYR:HD1	1.75	0.52
1:A:681:VAL:O	1:A:682:ARG:C	2.48	0.52
1:A:623:GLU:OE2	1:A:704:ARG:NH2	2.43	0.52
1:B:561:ALA:HB2	1:B:642:PHE:CZ	2.44	0.51
2:A:102:215:C9	2:A:102:215:C16	2.88	0.51
1:B:555:ASP:OD1	1:B:558:ARG:NH1	2.43	0.51
1:B:661:ASN:OD1	1:B:664:GLN:HG2	2.11	0.51
1:A:555:ASP:OD2	1:A:559:GLN:NE2	2.44	0.51
1:A:468:PHE:CE1	1:A:485:LEU:HB2	2.46	0.51
1:A:650:MET:HA	1:A:650:MET:HE3	1.94	0.51
1:B:468:PHE:HE2	1:B:498:PHE:HB2	1.75	0.50
1:A:473:LYS:HD2	1:A:531:TRP:CZ2	2.46	0.50
1:A:683:SER:C	1:A:685:CYS:H	2.15	0.50
1:B:578:LYS:HD3	1:B:580:ASN:ND2	2.26	0.50
1:A:491:THR:HG22	1:A:493:GLN:N	2.20	0.50
1:B:507:LYS:O	1:B:570:LYS:NZ	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:TRP:CH2	1:B:509:ARG:HG3	2.47	0.50
1:A:458:THR:OG1	1:A:475:LYS:HB2	2.12	0.50
1:B:491:THR:HG21	1:B:493:GLN:HB2	1.92	0.49
1:A:501:GLU:HG2	1:A:505:LEU:HD12	1.93	0.49
1:A:503:GLY:O	1:A:507:LYS:NZ	2.28	0.49
1:A:493:GLN:O	1:A:496:GLN:HB3	2.12	0.49
1:B:468:PHE:HE2	1:B:498:PHE:HD1	1.59	0.49
1:B:597:LEU:N	1:B:597:LEU:HD12	2.27	0.49
1:B:682:ARG:CB	1:B:682:ARG:HH11	2.26	0.49
1:B:623:GLU:HG2	1:B:624:VAL:N	2.28	0.49
1:B:468:PHE:HD1	1:B:469:GLY:N	2.11	0.49
1:B:513:ILE:O	1:B:514:LEU:C	2.51	0.49
1:B:714:ILE:HA	1:B:717:LEU:CD2	2.43	0.49
1:A:558:ARG:HH21	1:A:558:ARG:CG	2.06	0.48
1:B:468:PHE:HE2	1:B:498:PHE:CD1	2.31	0.48
1:A:450:TRP:HA	1:A:450:TRP:HE3	1.78	0.48
1:A:509:ARG:O	1:A:510:HIS:HB2	2.13	0.48
1:A:461:GLN:HG2	1:A:462:ARG:N	2.29	0.47
1:B:580:ASN:ND2	1:B:580:ASN:N	2.61	0.47
1:A:622:PRO:O	1:A:625:ILE:HB	2.14	0.47
1:B:715:GLU:O	1:B:716:LEU:C	2.52	0.47
1:A:594:ASP:HA	2:A:102:215:O34	2.14	0.47
1:A:468:PHE:HD1	1:A:485:LEU:HD13	1.79	0.47
1:A:631:ASN:HA	1:A:632:PRO:HD3	1.64	0.47
1:A:632:PRO:HD2	1:A:633:TYR:CD1	2.50	0.47
1:B:533:GLU:HB3	1:B:586:GLU:OE2	2.13	0.47
1:B:462:ARG:NH1	1:B:464:GLY:HA2	2.30	0.47
1:A:485:LEU:O	1:A:485:LEU:CG	2.57	0.47
1:B:550:MET:HE3	1:B:684:ASN:OD1	2.15	0.47
1:B:678:LEU:O	1:B:681:VAL:HG13	2.14	0.47
1:B:505:LEU:O	1:B:507:LYS:N	2.48	0.47
1:B:707:PHE:HA	1:B:710:ILE:HB	1.97	0.47
1:A:532:CYS:HA	1:A:585:HIS:HD2	1.79	0.46
1:A:634:SER:OG	1:A:636:GLN:HB2	2.15	0.46
1:A:501:GLU:CG	1:A:505:LEU:HD11	2.44	0.46
1:A:486:ASN:O	1:A:487:VAL:C	2.53	0.46
1:B:644:ILE:O	1:B:648:GLU:HG3	2.16	0.46
1:B:660:ASN:HD22	1:B:660:ASN:N	2.12	0.46
1:A:586:GLU:C	1:A:588:LEU:H	2.18	0.46
1:B:671:ARG:HD3	3:B:32:HOH:O	2.16	0.46
1:A:676:PRO:HG3	1:A:697:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:THR:CG2	1:A:492:PRO:HD2	2.46	0.45
1:B:484:MET:HB3	1:B:526:ALA:CB	2.28	0.45
1:B:543:ILE:HG22	1:B:544:ILE:HG23	1.98	0.45
1:A:715:GLU:O	1:A:718:ALA:HB3	2.17	0.45
1:B:503:GLY:O	1:B:506:ARG:HG2	2.16	0.45
1:B:541:LEU:HD12	1:B:648:GLU:HB3	1.97	0.45
1:B:639:VAL:O	1:B:640:TYR:C	2.54	0.45
1:A:498:PHE:O	1:A:499:LYS:C	2.53	0.45
1:A:599:THR:OG1	1:A:600:VAL:N	2.50	0.45
1:B:485:LEU:HD12	1:B:525:LEU:HD12	1.99	0.45
1:A:619:TRP:HA	1:A:644:ILE:HG13	1.98	0.45
1:B:580:ASN:H	1:B:580:ASN:HD22	1.65	0.45
1:A:496:GLN:HE21	1:A:500:ASN:HD21	1.64	0.44
1:B:530:GLN:O	1:B:530:GLN:HG3	2.16	0.44
1:A:516:PHE:CE1	1:A:518:GLY:O	2.71	0.44
1:A:697:LEU:O	1:A:698:LYS:C	2.55	0.44
1:B:713:SER:O	1:B:717:LEU:HD23	2.18	0.44
1:B:625:ILE:O	1:B:626:ARG:C	2.54	0.44
1:B:505:LEU:HD21	1:B:595:PHE:CD1	2.53	0.44
1:B:575:ARG:HG2	1:B:633:TYR:CD2	2.53	0.44
1:A:651:THR:O	1:A:653:GLN:N	2.50	0.44
1:B:529:THR:HG23	2:B:101:215:H311	1.99	0.44
1:A:684:ASN:OD1	1:A:684:ASN:N	2.49	0.43
1:B:644:ILE:HD13	1:B:697:LEU:HD21	2.00	0.43
1:A:646:LEU:HD12	1:A:693:MET:HG2	2.00	0.43
1:B:661:ASN:O	1:B:663:ASP:N	2.50	0.43
1:B:473:LYS:HD2	1:B:531:TRP:CZ2	2.53	0.43
1:A:468:PHE:CD1	1:A:485:LEU:HD13	2.54	0.43
1:B:660:ASN:H	1:B:660:ASN:ND2	2.14	0.43
1:B:585:HIS:CG	1:B:586:GLU:N	2.86	0.43
1:B:483:LYS:HB3	2:B:101:215:H312	2.00	0.43
1:B:505:LEU:O	1:B:506:ARG:C	2.56	0.43
1:B:517:MET:HB2	1:B:528:VAL:O	2.19	0.43
1:B:537:LEU:HD21	1:B:649:LEU:HD21	2.01	0.43
1:A:584:LEU:HD11	1:A:587:ASP:O	2.18	0.42
1:A:634:SER:OG	1:A:636:GLN:N	2.52	0.42
1:B:578:LYS:HB3	1:B:619:TRP:CD2	2.55	0.42
1:A:676:PRO:CG	1:A:697:LEU:HD13	2.50	0.42
1:B:523:PRO:CG	1:B:524:GLN:H	2.31	0.42
1:A:578:LYS:NZ	1:A:616:SER:HB2	2.35	0.42
1:A:683:SER:C	1:A:685:CYS:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:GLU:OE2	1:B:586:GLU:HA	2.19	0.42
1:A:468:PHE:CD1	1:A:469:GLY:N	2.88	0.42
1:A:654:LEU:HA	1:A:654:LEU:HD23	1.61	0.42
1:A:619:TRP:HD1	1:A:644:ILE:HB	1.82	0.42
1:A:625:ILE:C	1:A:627:MET:N	2.72	0.42
1:B:660:ASN:N	1:B:660:ASN:ND2	2.68	0.42
1:B:587:ASP:C	1:B:588:LEU:HD23	2.39	0.41
1:B:718:ALA:O	1:B:719:ARG:C	2.59	0.41
1:A:481:ALA:HB3	1:A:529:THR:OG1	2.20	0.41
1:B:571:SER:O	1:B:600:VAL:HA	2.20	0.41
1:B:583:PHE:HE1	1:B:593:GLY:HA3	1.86	0.41
1:B:482:VAL:HG22	1:B:528:VAL:HG22	2.03	0.41
1:A:628:GLN:HE21	1:A:628:GLN:HB3	1.68	0.41
1:B:539:HIS:O	1:B:543:ILE:HB	2.20	0.41
1:B:514:LEU:HD12	1:B:514:LEU:HA	1.80	0.41
1:A:539:HIS:O	1:A:543:ILE:HB	2.20	0.41
1:B:572:ILE:HA	1:B:599:THR:O	2.21	0.41
1:B:535:SER:HB2	1:B:539:HIS:HB3	2.02	0.41
1:B:573:ILE:HG23	1:B:638:ASP:OD2	2.21	0.41
1:B:641:ALA:O	1:B:642:PHE:C	2.58	0.41
1:B:707:PHE:HA	1:B:710:ILE:HD12	2.02	0.41
1:A:642:PHE:CZ	1:A:646:LEU:HD21	2.56	0.41
1:B:504:VAL:O	1:B:505:LEU:C	2.60	0.41
1:B:706:LEU:HD23	1:B:706:LEU:HA	1.79	0.41
1:A:509:ARG:HD2	1:B:450:TRP:CZ2	2.56	0.40
1:B:695:GLU:HG3	3:B:21:HOH:O	2.21	0.40
1:B:578:LYS:HZ2	1:B:616:SER:HB2	1.86	0.40
1:B:682:ARG:HH11	1:B:682:ARG:CG	2.34	0.40
1:A:502:VAL:O	1:A:503:GLY:C	2.59	0.40
1:A:667:PHE:CZ	1:A:671:ARG:HD3	2.55	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	255/281 (91%)	201 (79%)	37 (14%)	17 (7%)	1	3
1	B	255/281 (91%)	215 (84%)	24 (9%)	16 (6%)	1	4
All	All	510/562 (91%)	416 (82%)	61 (12%)	33 (6%)	1	3

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	A	487	VAL
1	A	545	GLU
1	A	587	ASP
1	A	701	ARG
1	B	467	SER
1	B	587	ASP
1	B	629	ASP
1	A	629	ASP
1	A	684	ASN
1	B	487	VAL
1	B	594	ASP
1	B	662	ARG
1	B	663	ASP
1	A	627	MET
1	A	663	ASP
1	B	514	LEU
1	B	586	GLU
1	B	716	LEU
1	A	510	HIS
1	A	652	GLY
1	B	489	ALA
1	B	627	MET
1	B	717	LEU
1	A	489	ALA
1	A	511	VAL
1	A	662	ARG
1	A	682	ARG
1	B	506	ARG
1	B	511	VAL
1	A	594	ASP
1	A	490	PRO
1	B	523	PRO

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	227/247 (92%)	202 (89%)	25 (11%)	6	19
1	B	227/247 (92%)	203 (89%)	24 (11%)	6	20
All	All	454/494 (92%)	405 (89%)	49 (11%)	6	20

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	451	GLU
1	A	454	ASP
1	A	456	GLN
1	A	468	PHE
1	A	495	LEU
1	A	498	PHE
1	A	511	VAL
1	A	520	SER
1	A	523	PRO
1	A	533	GLU
1	A	535	SER
1	A	545	GLU
1	A	558	ARG
1	A	586	GLU
1	A	614	SER
1	A	628	GLN
1	A	650	MET
1	A	657	SER
1	A	663	ASP
1	A	671	ARG
1	A	689	MET
1	A	698	LYS
1	A	701	ARG
1	A	709	GLN
1	A	717	LEU
1	B	468	PHE
1	B	480	VAL

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Mol	Chain	Res	Type
1	B	484	MET
1	B	495	LEU
1	B	500	ASN
1	B	506	ARG
1	B	511	VAL
1	B	521	THR
1	B	524	GLN
1	B	535	SER
1	B	546	THR
1	B	578	LYS
1	B	580	ASN
1	B	586	GLU
1	B	616	SER
1	B	617	ILE
1	B	660	ASN
1	B	675	SER
1	B	682	ARG
1	B	691	ARG
1	B	698	LYS
1	B	709	GLN
1	B	717	LEU
1	B	720	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	496	GLN
1	A	512	ASN
1	A	580	ASN
1	A	585	HIS
1	A	628	GLN
1	B	477	HIS
1	B	512	ASN
1	B	539	HIS
1	B	562	GLN
1	B	580	ASN
1	B	585	HIS
1	B	660	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	215	A	102	-	33,38,38	1.34	5 (15%)	31,53,53	2.39	12 (38%)
2	215	B	101	-	33,38,38	1.28	4 (12%)	31,53,53	2.24	9 (29%)

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	215	A	102	-	-	6/8/29/29	0/5/5/5
2	215	B	101	-	-	6/8/29/29	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	102	215	C21-C20	2.94	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	215	C32-N33	-2.73	1.26	1.28
2	B	101	215	C28-C32	2.60	1.51	1.45
2	A	102	215	C11-C10	2.51	1.41	1.36
2	A	102	215	C17-C18	2.41	1.41	1.36
2	A	102	215	C12-C13	2.30	1.39	1.36
2	A	102	215	C28-C32	2.27	1.50	1.45
2	B	101	215	C17-C18	2.19	1.41	1.36
2	B	101	215	C27-N25	2.18	1.52	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	102	215	O34-N33-C32	8.51	124.17	112.50
2	B	101	215	O34-N33-C32	6.64	121.61	112.50
2	B	101	215	C12-C13-N14	-5.26	116.97	123.81
2	A	102	215	C23-O22-C19	5.04	131.10	117.93
2	A	102	215	C30-C29-C28	4.21	113.58	111.27
2	B	101	215	C11-C10-C28	-3.14	115.68	120.77
2	B	101	215	C30-C29-C9	-2.91	124.71	129.43
2	A	102	215	O22-C23-C24	-2.88	100.57	107.68
2	B	101	215	C13-N14-C15	2.87	123.60	116.85
2	B	101	215	C29-C9-C8	-2.73	116.44	121.28
2	A	102	215	C17-C18-C19	2.56	123.60	120.17
2	A	102	215	C12-C7-C16	-2.50	116.43	118.65
2	A	102	215	C18-C19-C20	-2.44	116.42	120.18
2	A	102	215	C12-C13-N14	-2.41	120.67	123.81
2	B	101	215	C15-C16-C7	-2.29	115.48	119.46
2	A	102	215	C16-C15-N14	-2.29	120.83	123.81
2	B	101	215	C12-C7-C16	2.27	120.67	118.65
2	A	102	215	C21-C6-C17	-2.18	116.71	118.65
2	A	102	215	C27-N25-C24	2.09	119.01	110.74
2	B	101	215	C18-C17-C6	-2.05	117.64	120.82
2	A	102	215	C30-C29-C9	-2.03	126.15	129.43

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	102	215	C31-C32-N33-O34
2	A	102	215	C23-C24-N25-C26
2	B	101	215	C31-C32-N33-O34
2	B	101	215	C23-C24-N25-C27

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Mol	Chain	Res	Type	Atoms
2	B	101	215	C20-C19-O22-C23
2	B	101	215	C18-C19-O22-C23
2	A	102	215	C20-C19-O22-C23
2	A	102	215	C18-C19-O22-C23
2	B	101	215	O22-C23-C24-N25
2	A	102	215	C28-C32-N33-O34
2	B	101	215	C28-C32-N33-O34
2	A	102	215	C23-C24-N25-C27

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	102	215	3	0
2	B	101	215	4	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 then 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 215 A 102

Bond lengths

Bond angles

Torsions

Rings

Ligand 215 B 101

Bond lengths

Bond angles

Torsions

Rings
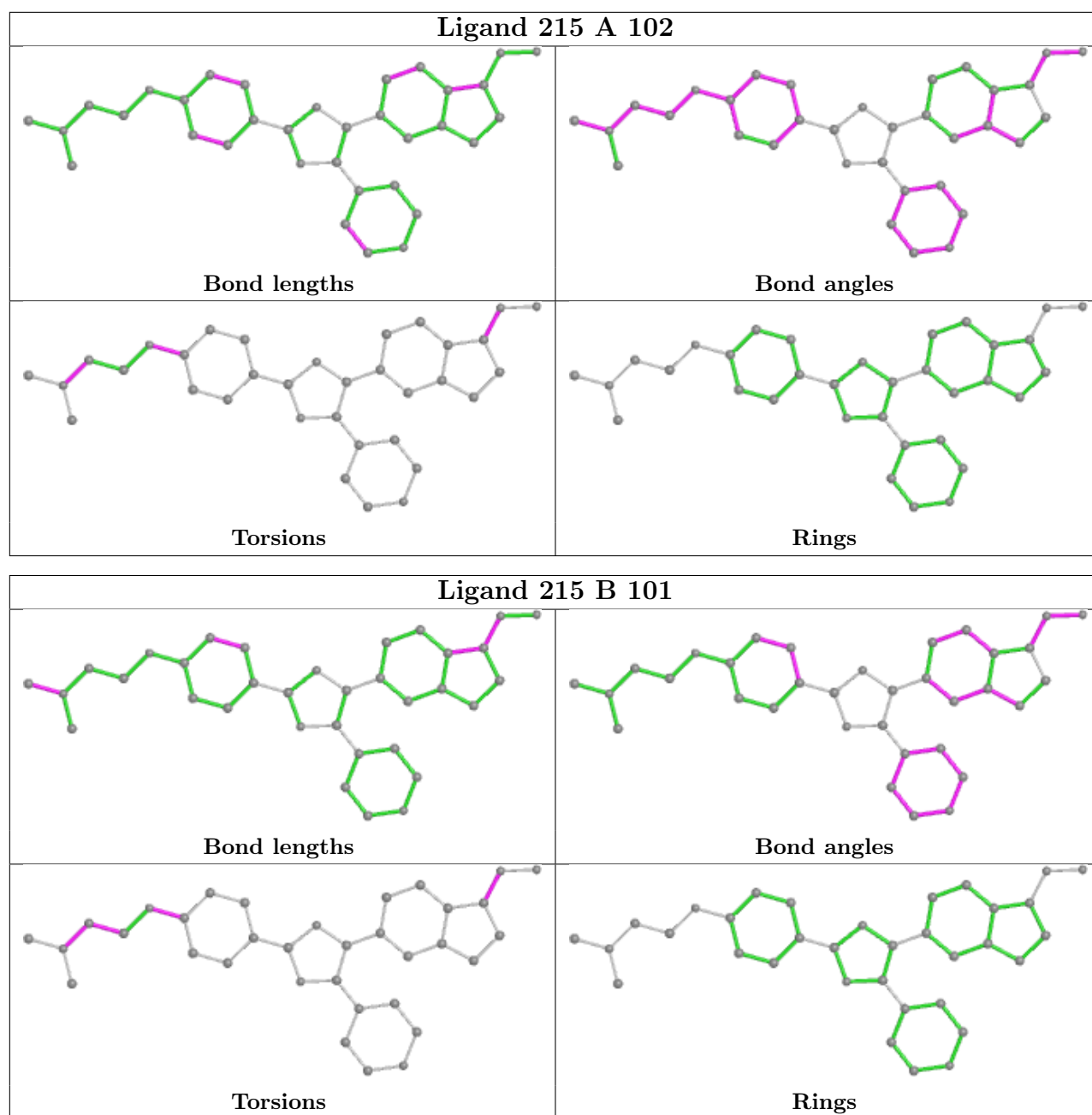
5.7 Other polymers (i)

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	259/281 (92%)	-0.47	0	100	100	9, 26, 49, 61	9 (3%)
1	B	259/281 (92%)	-0.52	0	100	100	8, 24, 40, 55	9 (3%)
All	All	518/562 (92%)	-0.49	0	100	100	8, 25, 45, 61	18 (3%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

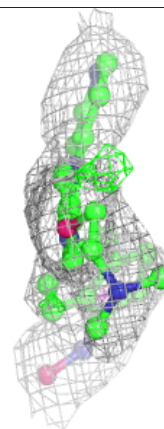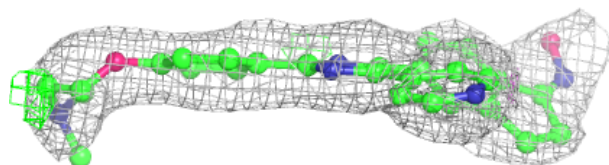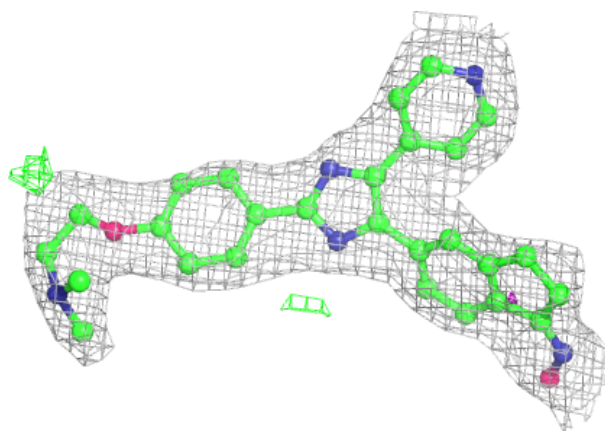There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
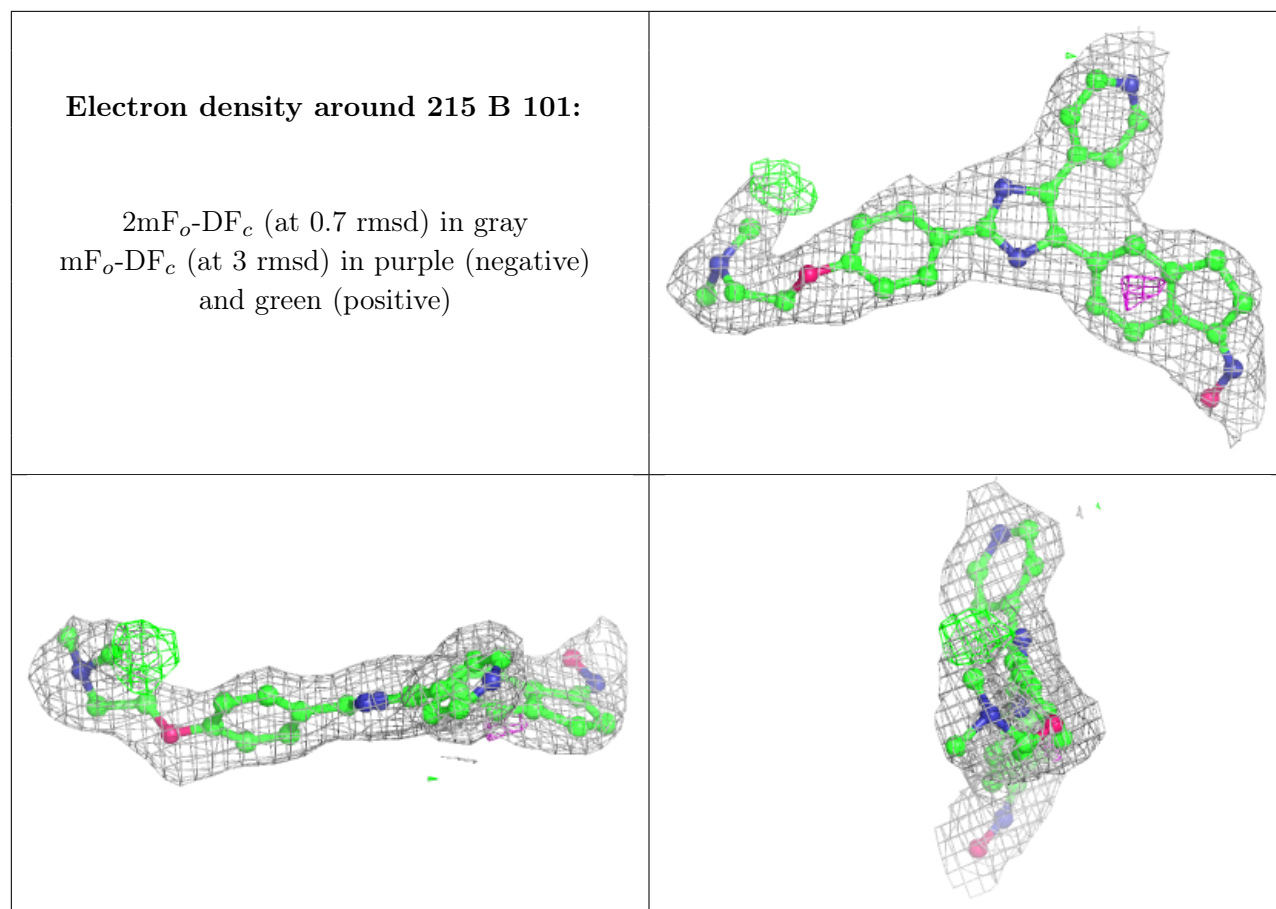
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	215	A	102	34/34	0.94	0.21	18,28,36,38	0
2	215	B	101	34/34	0.95	0.18	19,21,24,32	0

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 215 A 102:

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

Electron density around 215 B 101:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.