



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:00 PM EDT

PDB ID : 3SKC / pdb_00003skc
Title : Human B-Raf Kinase in Complex with an Amide Linked Pyrazolopyridine Inhibitor
Authors : Voegtli, W.C.; Sturgis, H.L.
Deposited on : 2011-06-22
Resolution : 3.20 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

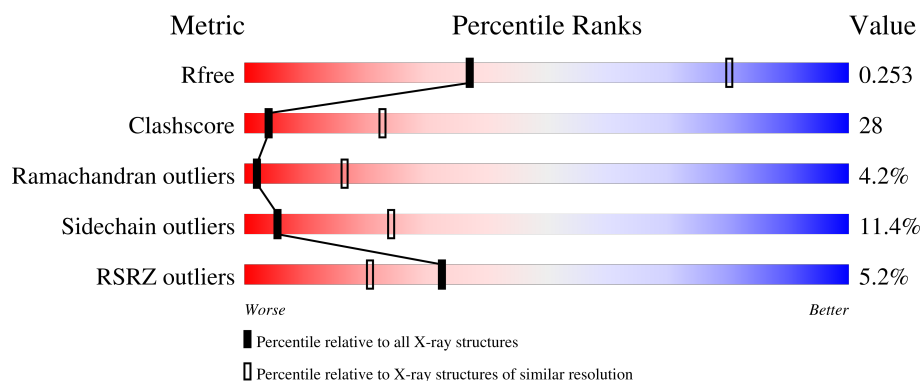
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	307	5% 45% 32% 7% 15%
1	B	307	4% 48% 33% 9% 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	BR2	A	801	X	-	-	-
2	BR2	B	801	X	-	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4355 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.

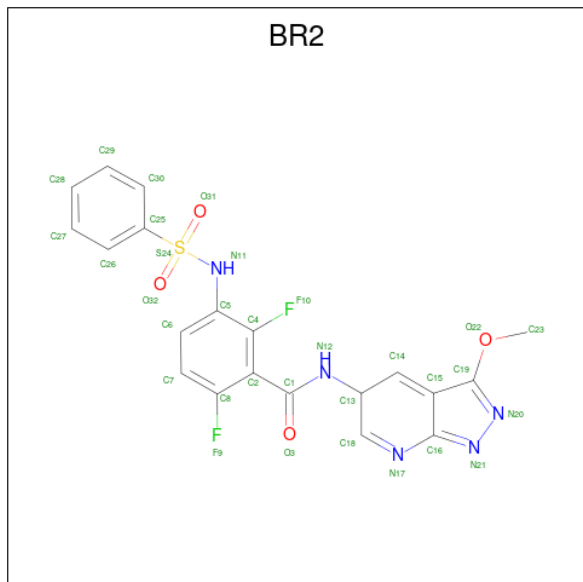
- Molecule 1 is a protein called Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2080	1334	362	371	13			
1	B	276	Total	C	N	O	S	0	0	0
			2211	1416	387	395	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	MET	-	expression tag	UNP P15056
A	421	ASP	-	expression tag	UNP P15056
A	422	ARG	-	expression tag	UNP P15056
A	423	GLY	-	expression tag	UNP P15056
A	424	SER	-	expression tag	UNP P15056
A	425	HIS	-	expression tag	UNP P15056
A	426	HIS	-	expression tag	UNP P15056
A	427	HIS	-	expression tag	UNP P15056
A	428	HIS	-	expression tag	UNP P15056
A	429	HIS	-	expression tag	UNP P15056
A	430	HIS	-	expression tag	UNP P15056
A	431	GLY	-	expression tag	UNP P15056
B	420	MET	-	expression tag	UNP P15056
B	421	ASP	-	expression tag	UNP P15056
B	422	ARG	-	expression tag	UNP P15056
B	423	GLY	-	expression tag	UNP P15056
B	424	SER	-	expression tag	UNP P15056
B	425	HIS	-	expression tag	UNP P15056
B	426	HIS	-	expression tag	UNP P15056
B	427	HIS	-	expression tag	UNP P15056
B	428	HIS	-	expression tag	UNP P15056
B	429	HIS	-	expression tag	UNP P15056
B	430	HIS	-	expression tag	UNP P15056
B	431	GLY	-	expression tag	UNP P15056

- Molecule 2 is 2,6-difluoro-N-[(5S)-3-methoxy-5H-pyrazolo[3,4-b]pyridin-5-yl]-3-[(phenylsulfonyl)amino]benzamide (CCD ID: BR2) (formula: $C_{20}H_{15}F_2N_5O_4S$).

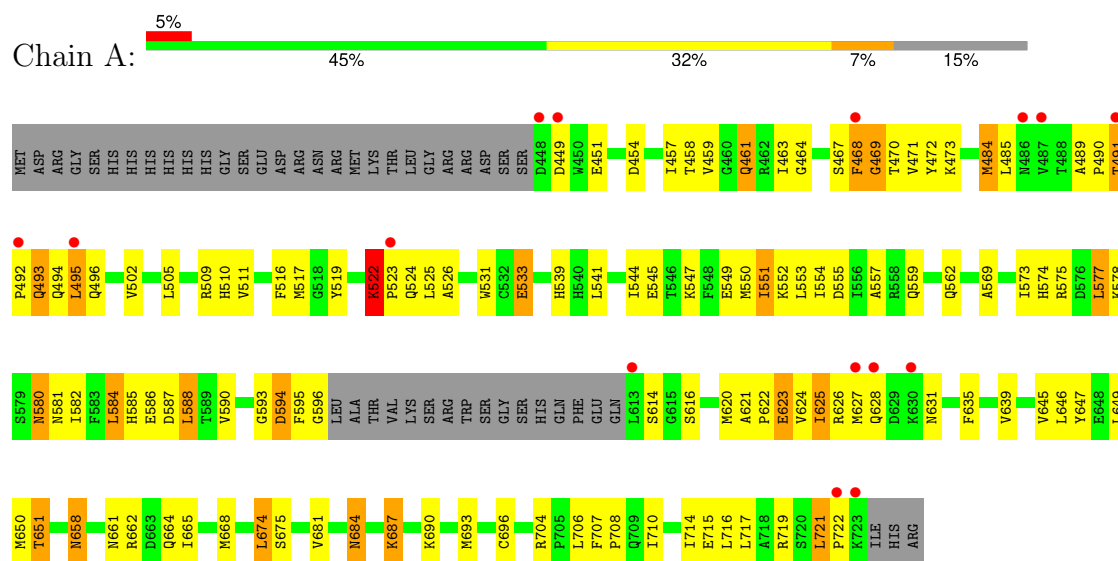


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			32	20	2	5	4	1		
2	B	1	Total	C	F	N	O	S	0	0
			32	20	2	5	4	1		

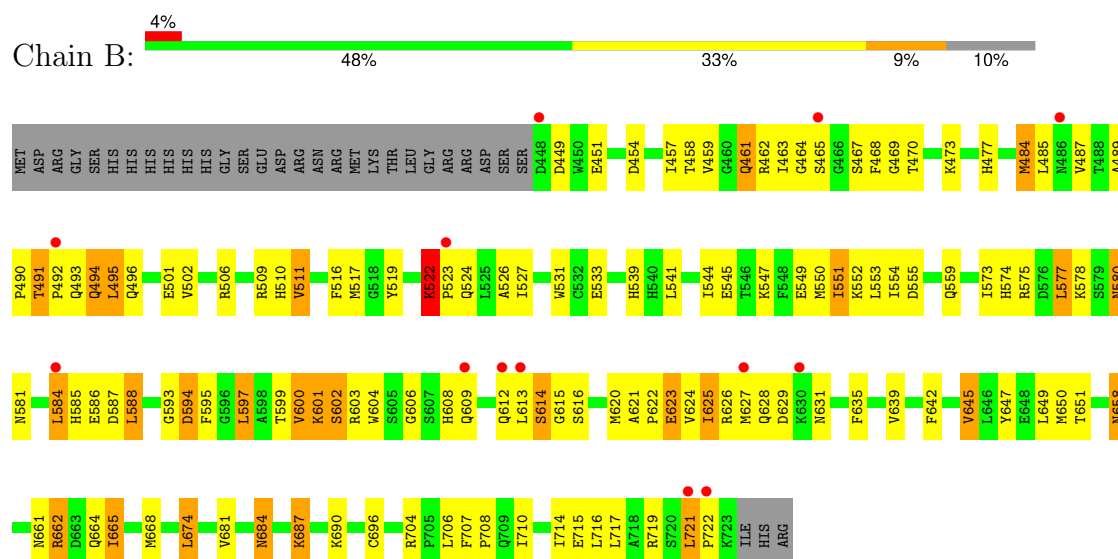
3 Residue-property plots

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: Serine/threonine-protein kinase B-raf



• Molecule 1: Serine/threonine-protein kinase B-raf



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.90Å 107.90Å 151.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.30 – 3.20 29.30 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.30-3.20) 99.3 (29.30-3.20)	Depositor EDS
R_{merge}	0.86	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 3.18Å)	Xtriage
Refinement program	CNS, CNX 2005	Depositor
R, R_{free}	0.233 , 0.271 0.221 , 0.253	Depositor DCC
R_{free} test set	905 reflections (5.94%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4355	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: BR2

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	0.54	0/2125	0.89	6/2867 (0.2%)
1	B	0.51	0/2261	0.88	6/3052 (0.2%)
All	All	0.53	0/4386	0.88	12/5919 (0.2%)

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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	469	GLY	N-CA-C	6.45	118.68	111.85
1	B	494	GLN	N-CA-C	-5.76	105.09	111.36
1	A	522	LYS	CA-C-N	-5.64	112.79	119.84
1	A	522	LYS	C-N-CA	-5.64	112.79	119.84
1	B	522	LYS	CA-C-N	-5.42	113.06	119.84
1	B	522	LYS	C-N-CA	-5.42	113.06	119.84
1	A	631	ASN	CA-C-N	5.33	125.42	119.87
1	A	631	ASN	C-N-CA	5.33	125.42	119.87
1	B	631	ASN	CA-C-N	5.15	125.22	119.87
1	B	631	ASN	C-N-CA	5.15	125.22	119.87
1	B	615	GLY	N-CA-C	-5.09	107.17	115.46
1	A	651	THR	N-CA-C	-5.05	107.29	113.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	493	GLN	Peptide

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	2080	0	2119	120	0
1	B	2211	0	2244	129	1
2	A	32	0	14	4	0
2	B	32	0	14	2	0
All	All	4355	0	4391	245	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 28.

All (245) 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:684:ASN:HD22	1:B:684:ASN:H	1.14	0.94
1:B:454:ASP:HB2	1:B:522:LYS:HD3	1.52	0.90
1:A:684:ASN:H	1:A:684:ASN:HD22	1.16	0.90
1:B:684:ASN:H	1:B:684:ASN:ND2	1.69	0.88
1:A:454:ASP:HB2	1:A:522:LYS:HD3	1.55	0.88
1:B:551:ILE:HD12	1:B:551:ILE:H	1.38	0.88
1:A:551:ILE:H	1:A:551:ILE:HD12	1.39	0.87
1:A:620:MET:HE3	1:A:624:VAL:HG12	1.56	0.85
1:B:462:ARG:HH22	1:B:465:SER:HA	1.39	0.85
1:A:490:PRO:HA	1:A:491:THR:CB	2.07	0.85
1:B:490:PRO:HA	1:B:491:THR:CB	2.07	0.85
1:A:684:ASN:H	1:A:684:ASN:ND2	1.71	0.84
1:B:462:ARG:NH2	1:B:465:SER:HA	1.94	0.82
1:B:681:VAL:HG21	1:B:690:LYS:HD2	1.61	0.82
1:B:501:GLU:HG3	1:B:597:LEU:HA	1.61	0.80
1:B:620:MET:HE3	1:B:624:VAL:HG12	1.65	0.77
1:A:658:ASN:HD22	1:A:658:ASN:H	1.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:ILE:HG22	1:B:575:ARG:HG3	1.67	0.77
1:B:658:ASN:HD22	1:B:658:ASN:H	1.33	0.76
1:A:490:PRO:HA	1:A:491:THR:OG1	1.85	0.76
1:A:573:ILE:HG22	1:A:575:ARG:HG3	1.67	0.75
1:A:464:GLY:O	1:A:470:THR:HG23	1.86	0.74
1:A:681:VAL:HG21	1:A:690:LYS:HD2	1.67	0.73
1:A:493:GLN:HB2	1:A:496:GLN:HB3	1.71	0.73
1:A:551:ILE:HD12	1:A:551:ILE:N	2.02	0.73
1:A:550:MET:HE2	1:A:553:LEU:HD12	1.71	0.73
1:B:487:VAL:HG11	1:B:604:TRP:HZ3	1.55	0.71
1:A:459:VAL:HG21	1:A:484:MET:HE1	1.72	0.71
1:B:490:PRO:HA	1:B:491:THR:OG1	1.89	0.71
1:B:487:VAL:HG11	1:B:604:TRP:CZ3	2.25	0.71
1:B:551:ILE:HD12	1:B:551:ILE:N	2.04	0.71
1:B:493:GLN:HB2	1:B:496:GLN:HB3	1.73	0.71
1:B:459:VAL:HG21	1:B:484:MET:HE1	1.74	0.70
1:B:454:ASP:H	1:B:522:LYS:HD3	1.57	0.69
1:B:490:PRO:HA	1:B:491:THR:HB	1.74	0.69
1:B:588:LEU:H	1:B:588:LEU:HD22	1.58	0.69
1:A:454:ASP:H	1:A:522:LYS:HD3	1.58	0.69
1:A:584:LEU:HD22	1:A:587:ASP:HA	1.75	0.69
1:B:468:PHE:CE2	1:B:485:LEU:HD12	2.28	0.68
1:B:584:LEU:HD22	1:B:587:ASP:HA	1.76	0.68
1:B:551:ILE:H	1:B:551:ILE:CD1	2.06	0.68
1:A:539:HIS:CE1	1:A:544:ILE:HD13	2.28	0.68
1:A:522:LYS:HB2	1:A:523:PRO:CD	2.23	0.67
1:A:516:PHE:HB2	2:A:801:BR2:H29	1.75	0.67
1:A:490:PRO:HA	1:A:491:THR:HB	1.77	0.66
1:A:551:ILE:H	1:A:551:ILE:CD1	2.06	0.66
1:B:600:VAL:O	1:B:600:VAL:HG12	1.96	0.66
1:A:491:THR:HB	1:A:494:GLN:OE1	1.96	0.65
1:B:550:MET:HE2	1:B:553:LEU:HD12	1.79	0.65
1:B:494:GLN:HB3	1:B:604:TRP:CZ2	2.32	0.65
1:A:493:GLN:HB2	1:A:496:GLN:CB	2.27	0.64
1:A:510:HIS:HA	1:B:517:MET:HE2	1.78	0.64
1:A:588:LEU:H	1:A:588:LEU:HD22	1.62	0.64
1:B:491:THR:HB	1:B:494:GLN:OE1	1.98	0.62
1:B:468:PHE:CZ	1:B:485:LEU:HD12	2.34	0.62
1:B:522:LYS:HB2	1:B:523:PRO:CD	2.29	0.62
1:B:620:MET:CE	1:B:624:VAL:HG12	2.30	0.61
1:B:493:GLN:HB2	1:B:496:GLN:CB	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:ARG:O	1:B:628:GLN:N	2.34	0.61
2:B:801:BR2:O31	2:B:801:BR2:H6	1.99	0.61
1:A:505:LEU:HD22	2:A:801:BR2:C30	2.30	0.60
1:B:684:ASN:HD22	1:B:684:ASN:N	1.92	0.60
1:B:600:VAL:HG13	1:B:604:TRP:CE2	2.37	0.60
1:A:502:VAL:HG11	1:A:519:TYR:CD2	2.37	0.60
1:A:687:LYS:HE3	1:A:687:LYS:HA	1.82	0.60
1:B:687:LYS:HE3	1:B:687:LYS:HA	1.83	0.60
1:B:539:HIS:CE1	1:B:544:ILE:HD13	2.36	0.59
1:B:602:SER:O	1:B:603:ARG:HG2	2.02	0.59
1:A:620:MET:CE	1:A:624:VAL:HG12	2.28	0.59
1:B:491:THR:N	1:B:492:PRO:HD3	2.18	0.58
1:B:550:MET:O	1:B:554:ILE:HG13	2.03	0.58
1:A:626:ARG:O	1:A:628:GLN:N	2.37	0.57
1:B:550:MET:HE2	1:B:550:MET:HA	1.86	0.57
1:A:490:PRO:CA	1:A:491:THR:CB	2.81	0.57
1:B:647:TYR:CE1	1:B:651:THR:HG21	2.39	0.57
1:A:491:THR:N	1:A:492:PRO:HD3	2.19	0.57
1:A:578:LYS:HD2	1:A:580:ASN:ND2	2.19	0.57
2:A:801:BR2:H6	2:A:801:BR2:O31	2.05	0.56
1:B:469:GLY:HA2	1:B:484:MET:O	2.05	0.56
1:B:664:GLN:O	1:B:668:MET:HG3	2.06	0.56
1:B:588:LEU:HD22	1:B:588:LEU:N	2.21	0.56
1:B:580:ASN:H	1:B:580:ASN:HD22	1.53	0.56
1:B:601:LYS:C	1:B:603:ARG:H	2.14	0.56
1:A:550:MET:HE2	1:A:550:MET:HA	1.88	0.55
1:A:661:ASN:OD1	1:A:664:GLN:HG2	2.05	0.55
1:B:485:LEU:HD11	1:B:597:LEU:HD13	1.88	0.55
1:A:647:TYR:CE1	1:A:651:THR:HG21	2.41	0.55
1:A:575:ARG:HD3	1:A:596:GLY:HA3	1.87	0.55
1:A:626:ARG:O	1:A:626:ARG:HG3	2.07	0.55
1:B:635:PHE:O	1:B:639:VAL:HG23	2.06	0.55
1:A:580:ASN:ND2	1:A:580:ASN:H	2.05	0.55
1:A:467:SER:C	1:A:469:GLY:H	2.15	0.55
1:B:696:CYS:O	1:B:704:ARG:HD3	2.07	0.55
1:A:580:ASN:H	1:A:580:ASN:HD22	1.55	0.55
1:B:620:MET:HE2	1:B:625:ILE:HA	1.88	0.55
1:A:509:ARG:HD3	1:B:516:PHE:O	2.07	0.54
1:A:464:GLY:HA3	1:A:471:VAL:HB	1.90	0.54
1:B:555:ASP:O	1:B:559:GLN:HG3	2.07	0.54
1:A:550:MET:O	1:A:554:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:MET:HE2	1:A:625:ILE:HA	1.88	0.54
1:A:716:LEU:HD23	1:A:716:LEU:C	2.32	0.54
1:B:580:ASN:H	1:B:580:ASN:ND2	2.04	0.54
1:B:502:VAL:HG11	1:B:519:TYR:CD2	2.43	0.54
1:B:716:LEU:C	1:B:716:LEU:HD23	2.33	0.53
1:A:555:ASP:O	1:A:559:GLN:HG3	2.09	0.53
1:A:522:LYS:HB2	1:A:523:PRO:HD3	1.90	0.53
1:A:588:LEU:HD22	1:A:588:LEU:N	2.24	0.53
1:B:681:VAL:HG23	1:B:681:VAL:O	2.08	0.53
1:B:490:PRO:CA	1:B:491:THR:CB	2.81	0.53
1:B:484:MET:HE2	1:B:524:GLN:NE2	2.24	0.52
1:B:721:LEU:HB3	1:B:722:PRO:HD3	1.92	0.52
1:B:661:ASN:OD1	1:B:664:GLN:HG2	2.10	0.51
1:A:684:ASN:HD22	1:A:684:ASN:N	1.94	0.51
1:B:574:HIS:O	1:B:575:ARG:HB2	2.10	0.51
1:A:681:VAL:O	1:A:681:VAL:HG23	2.09	0.51
1:B:585:HIS:CE1	1:B:586:GLU:HG2	2.45	0.51
1:A:721:LEU:HB3	1:A:722:PRO:HD3	1.93	0.51
1:A:491:THR:HG21	1:A:494:GLN:CD	2.36	0.51
1:B:706:LEU:O	1:B:710:ILE:HG13	2.10	0.51
1:A:621:ALA:HB1	1:A:623:GLU:OE1	2.11	0.51
1:B:461:GLN:HE21	1:B:461:GLN:C	2.19	0.51
1:A:635:PHE:O	1:A:639:VAL:HG23	2.11	0.51
1:A:706:LEU:O	1:A:710:ILE:HG13	2.11	0.51
1:B:586:GLU:O	1:B:588:LEU:HD13	2.11	0.51
1:B:612:GLN:C	1:B:614:SER:H	2.19	0.51
1:B:522:LYS:HB2	1:B:523:PRO:HD3	1.93	0.50
1:B:639:VAL:HG13	1:B:710:ILE:HD11	1.92	0.50
1:B:490:PRO:HG2	1:B:495:LEU:HD23	1.93	0.50
1:B:574:HIS:CD2	1:B:595:PHE:HB3	2.47	0.50
1:A:491:THR:N	1:A:492:PRO:CD	2.75	0.49
1:B:595:PHE:CZ	2:B:801:BR2:H27	2.47	0.49
1:B:491:THR:N	1:B:492:PRO:CD	2.75	0.49
1:B:626:ARG:O	1:B:626:ARG:HG3	2.13	0.49
1:A:490:PRO:HG2	1:A:495:LEU:HD23	1.94	0.49
1:B:578:LYS:HD2	1:B:580:ASN:ND2	2.27	0.49
1:B:501:GLU:OE1	1:B:599:THR:HB	2.13	0.49
1:A:616:SER:O	1:A:620:MET:HG3	2.14	0.48
1:A:575:ARG:NH1	1:A:575:ARG:HG2	2.29	0.48
1:A:664:GLN:O	1:A:668:MET:HG3	2.12	0.48
1:A:484:MET:HE2	1:A:524:GLN:NE2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:LEU:HD13	1:A:495:LEU:O	2.13	0.48
1:B:491:THR:HG21	1:B:494:GLN:CD	2.37	0.48
1:B:495:LEU:HD13	1:B:495:LEU:O	2.12	0.48
1:A:461:GLN:C	1:A:461:GLN:HE21	2.22	0.48
1:B:574:HIS:CG	1:B:595:PHE:HB3	2.49	0.48
1:A:551:ILE:N	1:A:551:ILE:CD1	2.71	0.48
1:A:715:GLU:HB3	1:A:719:ARG:HH12	1.78	0.48
1:B:550:MET:HA	1:B:553:LEU:HD12	1.95	0.48
1:B:600:VAL:HG13	1:B:604:TRP:CZ2	2.48	0.48
1:B:622:PRO:O	1:B:626:ARG:HG2	2.13	0.48
1:B:454:ASP:HB2	1:B:522:LYS:CD	2.34	0.48
1:B:612:GLN:C	1:B:614:SER:N	2.71	0.48
1:B:623:GLU:OE1	1:B:704:ARG:NH2	2.45	0.47
1:A:517:MET:HE2	1:B:510:HIS:HA	1.97	0.47
1:A:658:ASN:HD22	1:A:658:ASN:N	2.09	0.47
1:A:696:CYS:O	1:A:704:ARG:HD3	2.14	0.47
1:A:574:HIS:O	1:A:575:ARG:HB2	2.14	0.47
1:B:501:GLU:CB	1:B:597:LEU:HD23	2.44	0.47
1:A:473:LYS:HD2	1:A:531:TRP:CZ2	2.49	0.47
1:A:585:HIS:CE1	1:A:586:GLU:HG2	2.50	0.47
1:B:527:ILE:HD11	1:B:597:LEU:HD21	1.97	0.47
1:A:485:LEU:HD22	1:A:485:LEU:H	1.79	0.47
1:A:553:LEU:HB3	1:A:650:MET:HE1	1.96	0.46
1:A:467:SER:C	1:A:469:GLY:N	2.73	0.46
1:A:586:GLU:O	1:A:588:LEU:HD13	2.15	0.46
1:B:464:GLY:O	1:B:470:THR:HG23	2.16	0.46
1:B:553:LEU:HB3	1:B:650:MET:HE1	1.96	0.46
1:A:581:ASN:HB3	1:A:593:GLY:O	2.15	0.46
1:A:623:GLU:H	1:A:623:GLU:HG3	1.40	0.46
1:B:468:PHE:HB2	1:B:608:HIS:CB	2.45	0.46
1:B:490:PRO:CA	1:B:491:THR:HB	2.43	0.46
1:A:650:MET:HG3	1:A:693:MET:HE1	1.98	0.46
1:B:715:GLU:HB3	1:B:719:ARG:HH12	1.78	0.46
1:A:710:ILE:O	1:A:714:ILE:HG13	2.16	0.46
1:B:551:ILE:N	1:B:551:ILE:CD1	2.72	0.46
1:A:485:LEU:HD22	1:A:485:LEU:N	2.30	0.46
1:A:491:THR:CG2	1:A:494:GLN:CD	2.89	0.46
1:B:485:LEU:N	1:B:485:LEU:HD22	2.31	0.45
1:B:491:THR:CG2	1:B:494:GLN:CD	2.90	0.45
1:A:539:HIS:ND1	1:A:544:ILE:HD13	2.31	0.45
1:A:522:LYS:CB	1:A:523:PRO:CD	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:VAL:HG13	1:A:710:ILE:HD11	1.99	0.45
1:B:457:ILE:HG22	1:B:458:THR:N	2.32	0.45
1:A:684:ASN:ND2	1:A:684:ASN:N	2.49	0.45
1:B:545:GLU:O	1:B:547:LYS:HD2	2.17	0.45
1:B:501:GLU:HG2	1:B:600:VAL:HG23	2.00	0.44
1:B:602:SER:HA	1:B:609:GLN:HE22	1.81	0.44
1:A:569:ALA:HB2	1:B:477:HIS:CE1	2.52	0.44
1:B:628:GLN:HG3	1:B:629:ASP:H	1.83	0.44
1:B:606:GLY:C	1:B:608:HIS:H	2.25	0.44
1:A:491:THR:O	1:A:491:THR:HG22	2.18	0.44
1:A:505:LEU:HD22	2:A:801:BR2:C29	2.48	0.44
1:A:533:GLU:H	1:A:585:HIS:HD2	1.65	0.44
1:A:545:GLU:O	1:A:547:LYS:HD2	2.18	0.44
1:A:717:LEU:O	1:A:717:LEU:HD12	2.17	0.44
1:B:581:ASN:HB3	1:B:593:GLY:O	2.18	0.44
1:A:516:PHE:O	1:B:509:ARG:HD3	2.18	0.43
1:A:457:ILE:HG22	1:A:458:THR:N	2.34	0.43
1:A:578:LYS:HD2	1:A:580:ASN:HD22	1.84	0.43
1:A:550:MET:HA	1:A:553:LEU:HD12	2.00	0.43
1:A:646:LEU:HA	1:A:646:LEU:HD23	1.77	0.43
1:B:628:GLN:HG3	1:B:629:ASP:N	2.33	0.43
1:B:491:THR:HG22	1:B:491:THR:O	2.19	0.43
1:A:492:PRO:HA	1:A:493:GLN:HA	1.50	0.43
1:B:649:LEU:C	1:B:650:MET:HE2	2.44	0.43
1:B:717:LEU:HD12	1:B:717:LEU:O	2.18	0.43
1:A:707:PHE:N	1:A:708:PRO:CD	2.82	0.43
1:A:490:PRO:CA	1:A:491:THR:HB	2.45	0.43
1:A:539:HIS:O	1:A:544:ILE:HG12	2.18	0.43
1:B:501:GLU:HG2	1:B:600:VAL:CG2	2.49	0.43
1:B:668:MET:HB3	1:B:674:LEU:HB2	2.01	0.43
1:A:484:MET:HG3	1:A:526:ALA:HB2	2.01	0.42
1:A:582:ILE:HG23	1:A:590:VAL:HG13	2.02	0.42
1:A:559:GLN:O	1:A:562:GLN:HB3	2.20	0.42
1:B:485:LEU:HD22	1:B:485:LEU:H	1.84	0.42
1:B:621:ALA:HB1	1:B:623:GLU:OE1	2.19	0.42
1:B:577:LEU:O	1:B:578:LYS:HB3	2.19	0.42
1:B:642:PHE:O	1:B:645:VAL:HG22	2.20	0.42
1:B:721:LEU:H	1:B:722:PRO:CD	2.33	0.42
1:A:454:ASP:HB2	1:A:522:LYS:CD	2.37	0.42
1:A:668:MET:HB3	1:A:674:LEU:HB2	2.02	0.42
1:B:707:PHE:N	1:B:708:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:SER:O	1:B:620:MET:HG3	2.20	0.42
1:A:459:VAL:HG13	1:A:472:TYR:CB	2.50	0.41
1:A:577:LEU:HD23	1:A:577:LEU:HA	1.84	0.41
1:B:467:SER:OG	1:B:468:PHE:N	2.51	0.41
1:B:658:ASN:H	1:B:658:ASN:ND2	2.10	0.41
1:A:495:LEU:HD22	1:A:525:LEU:HD21	2.02	0.41
1:B:710:ILE:O	1:B:714:ILE:HG13	2.21	0.41
1:A:467:SER:O	1:A:468:PHE:CD2	2.74	0.41
1:A:620:MET:HE3	1:A:624:VAL:CG1	2.38	0.41
1:A:658:ASN:H	1:A:658:ASN:ND2	2.09	0.41
1:B:623:GLU:H	1:B:623:GLU:HG3	1.38	0.41
1:B:662:ARG:HA	1:B:665:ILE:HG13	2.03	0.41
1:A:557:ALA:HB2	1:A:649:LEU:HD13	2.02	0.41
1:A:577:LEU:O	1:A:578:LYS:HB3	2.20	0.41
1:A:622:PRO:O	1:A:626:ARG:HG2	2.20	0.41
1:B:577:LEU:HA	1:B:577:LEU:HD23	1.87	0.41
1:A:467:SER:O	1:A:469:GLY:N	2.54	0.41
1:A:517:MET:CE	1:B:511:VAL:HG12	2.51	0.41
1:A:674:LEU:HD22	1:A:675:SER:N	2.36	0.41
1:B:473:LYS:HD2	1:B:531:TRP:CZ2	2.55	0.41
1:B:484:MET:HG3	1:B:526:ALA:HB2	2.02	0.41
1:B:612:GLN:O	1:B:614:SER:N	2.47	0.41
1:A:485:LEU:H	1:A:485:LEU:CD2	2.35	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:662:ARG:NH2	1:B:662:ARG:NH2[7_645]	2.17	0.03

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	256/307 (83%)	225 (88%)	21 (8%)	10 (4%)	2	18
1	B	274/307 (89%)	242 (88%)	20 (7%)	12 (4%)	2	15
All	All	530/614 (86%)	467 (88%)	41 (8%)	22 (4%)	2	16

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	PHE
1	A	522	LYS
1	A	594	ASP
1	A	627	MET
1	B	627	MET
1	A	491	THR
1	B	491	THR
1	B	522	LYS
1	A	449	ASP
1	B	594	ASP
1	B	613	LEU
1	B	614	SER
1	A	595	PHE
1	A	614	SER
1	B	602	SER
1	A	489	ALA
1	A	721	LEU
1	B	449	ASP
1	B	489	ALA
1	B	601	LYS
1	B	721	LEU
1	B	600	VAL

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	229/271 (84%)	203 (89%)	26 (11%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	243/271 (90%)	215 (88%)	28 (12%)	5	24
All	All	472/542 (87%)	418 (89%)	54 (11%)	5	24

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	451	GLU
1	A	461	GLN
1	A	463	ILE
1	A	484	MET
1	A	495	LEU
1	A	511	VAL
1	A	522	LYS
1	A	533	GLU
1	A	541	LEU
1	A	549	GLU
1	A	551	ILE
1	A	552	LYS
1	A	577	LEU
1	A	580	ASN
1	A	584	LEU
1	A	588	LEU
1	A	594	ASP
1	A	623	GLU
1	A	625	ILE
1	A	645	VAL
1	A	658	ASN
1	A	662	ARG
1	A	665	ILE
1	A	674	LEU
1	A	684	ASN
1	A	687	LYS
1	B	451	GLU
1	B	461	GLN
1	B	463	ILE
1	B	484	MET
1	B	495	LEU
1	B	506	ARG
1	B	511	VAL
1	B	522	LYS
1	B	533	GLU
1	B	541	LEU

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Mol	Chain	Res	Type
1	B	549	GLU
1	B	551	ILE
1	B	552	LYS
1	B	577	LEU
1	B	580	ASN
1	B	584	LEU
1	B	588	LEU
1	B	594	ASP
1	B	597	LEU
1	B	623	GLU
1	B	625	ILE
1	B	645	VAL
1	B	658	ASN
1	B	662	ARG
1	B	665	ILE
1	B	674	LEU
1	B	684	ASN
1	B	687	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	500	ASN
1	A	512	ASN
1	A	524	GLN
1	A	539	HIS
1	A	562	GLN
1	A	580	ASN
1	A	585	HIS
1	A	658	ASN
1	A	684	ASN
1	B	461	GLN
1	B	477	HIS
1	B	500	ASN
1	B	512	ASN
1	B	524	GLN
1	B	580	ASN
1	B	585	HIS
1	B	609	GLN
1	B	658	ASN
1	B	684	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 oligosaccharides 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	BR2	B	801	-	31,35,35	3.76	9 (29%)	40,51,51	4.00	11 (27%)
2	BR2	A	801	-	31,35,35	2.98	12 (38%)	40,51,51	4.07	12 (30%)

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	BR2	B	801	-	1/1/6/10	4/21/43/43	0/4/4/4
2	BR2	A	801	-	1/1/6/10	4/21/43/43	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	BR2	C2-C1	-12.93	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	BR2	C13-C14	-11.61	1.39	1.50
2	A	801	BR2	C13-C14	-10.48	1.40	1.50
2	A	801	BR2	C5-N11	-6.81	1.31	1.42
2	B	801	BR2	C18-N17	5.66	1.35	1.28
2	B	801	BR2	C5-N11	-5.63	1.33	1.42
2	A	801	BR2	C18-N17	5.25	1.34	1.28
2	B	801	BR2	C19-N20	3.43	1.32	1.29
2	A	801	BR2	C19-N20	3.33	1.32	1.29
2	B	801	BR2	O31-S24	3.32	1.47	1.43
2	A	801	BR2	O31-S24	3.18	1.47	1.43
2	A	801	BR2	C2-C8	3.13	1.44	1.39
2	B	801	BR2	C13-C18	-3.00	1.42	1.50
2	B	801	BR2	S24-N11	2.92	1.68	1.63
2	A	801	BR2	O32-S24	2.85	1.46	1.43
2	A	801	BR2	S24-N11	2.80	1.68	1.63
2	A	801	BR2	C5-C4	2.71	1.43	1.38
2	A	801	BR2	C13-C18	-2.57	1.43	1.50
2	A	801	BR2	C15-C16	-2.34	1.39	1.44
2	B	801	BR2	C15-C16	-2.33	1.39	1.44
2	A	801	BR2	C28-C27	2.06	1.42	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	BR2	C16-N21-N20	15.38	112.80	105.75
2	A	801	BR2	C16-N21-N20	15.16	112.70	105.75
2	A	801	BR2	C15-C16-N21	-14.43	105.01	112.09
2	B	801	BR2	C15-C16-N21	-13.59	105.42	112.09
2	A	801	BR2	C14-C13-N12	8.19	122.61	111.10
2	B	801	BR2	C14-C13-N12	8.08	122.45	111.10
2	B	801	BR2	C25-S24-N11	-6.41	98.92	106.88
2	B	801	BR2	C18-C13-N12	5.77	119.21	111.10
2	A	801	BR2	C25-S24-N11	-5.72	99.78	106.88
2	A	801	BR2	C18-C13-N12	5.68	119.08	111.10
2	B	801	BR2	C8-C2-C4	4.42	120.00	115.66
2	B	801	BR2	C13-N12-C1	4.02	129.91	121.63
2	A	801	BR2	C13-N12-C1	4.00	129.85	121.63
2	A	801	BR2	C8-C2-C4	3.86	119.46	115.66
2	A	801	BR2	C4-C2-C1	-3.63	116.09	121.82
2	B	801	BR2	C19-N20-N21	-2.85	103.80	106.03
2	A	801	BR2	C4-C5-N11	-2.64	117.68	120.73
2	A	801	BR2	C19-N20-N21	-2.61	103.99	106.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	BR2	C4-C2-C1	-2.28	118.22	121.82
2	A	801	BR2	C6-C5-C4	2.12	120.66	117.72
2	B	801	BR2	C6-C5-C4	2.10	120.64	117.72
2	A	801	BR2	C5-N11-S24	2.08	130.00	123.34
2	B	801	BR2	O31-S24-C25	2.01	110.51	107.98

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	801	BR2	C13
2	B	801	BR2	C13

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	BR2	C14-C13-N12-C1
2	B	801	BR2	C14-C13-N12-C1
2	A	801	BR2	C5-N11-S24-O31
2	B	801	BR2	C5-N11-S24-O31
2	A	801	BR2	C5-N11-S24-O32
2	A	801	BR2	C5-N11-S24-C25
2	B	801	BR2	C5-N11-S24-C25
2	B	801	BR2	C5-N11-S24-O32

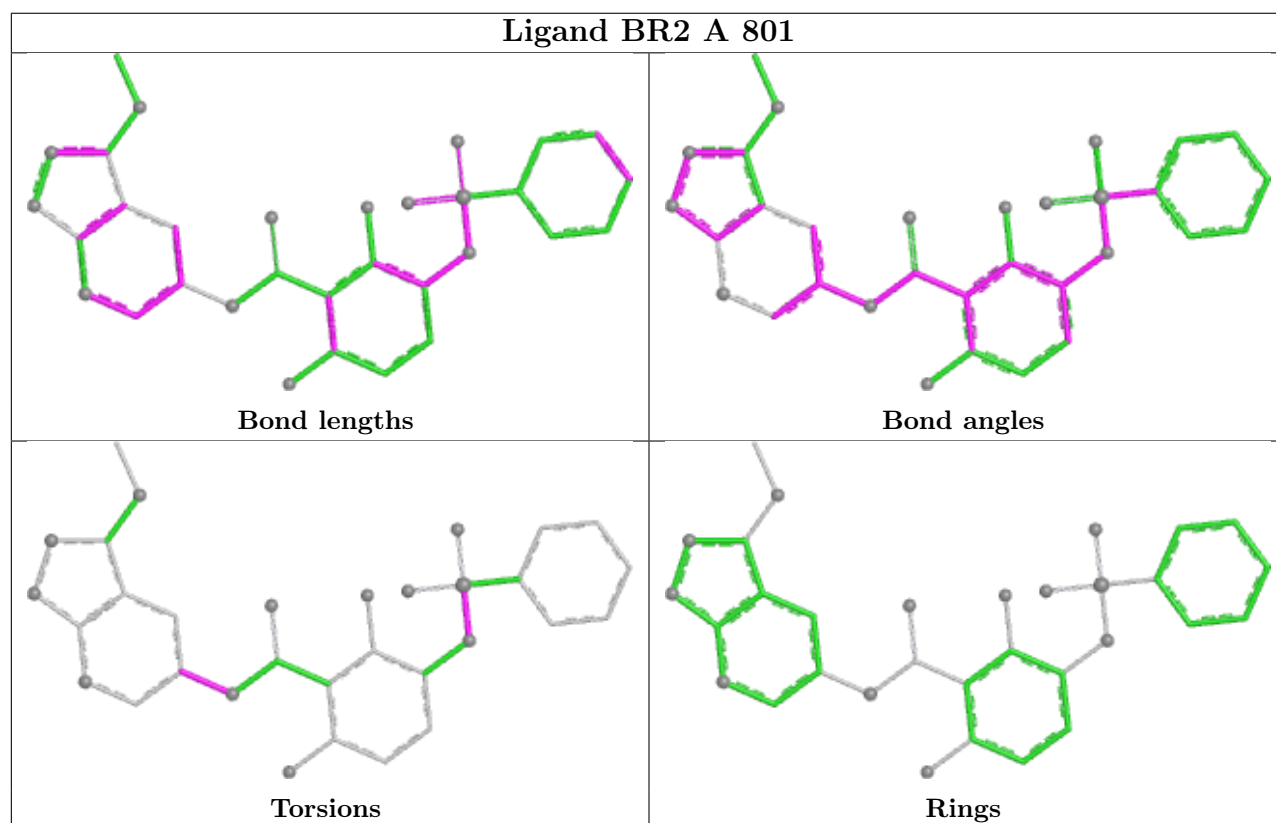
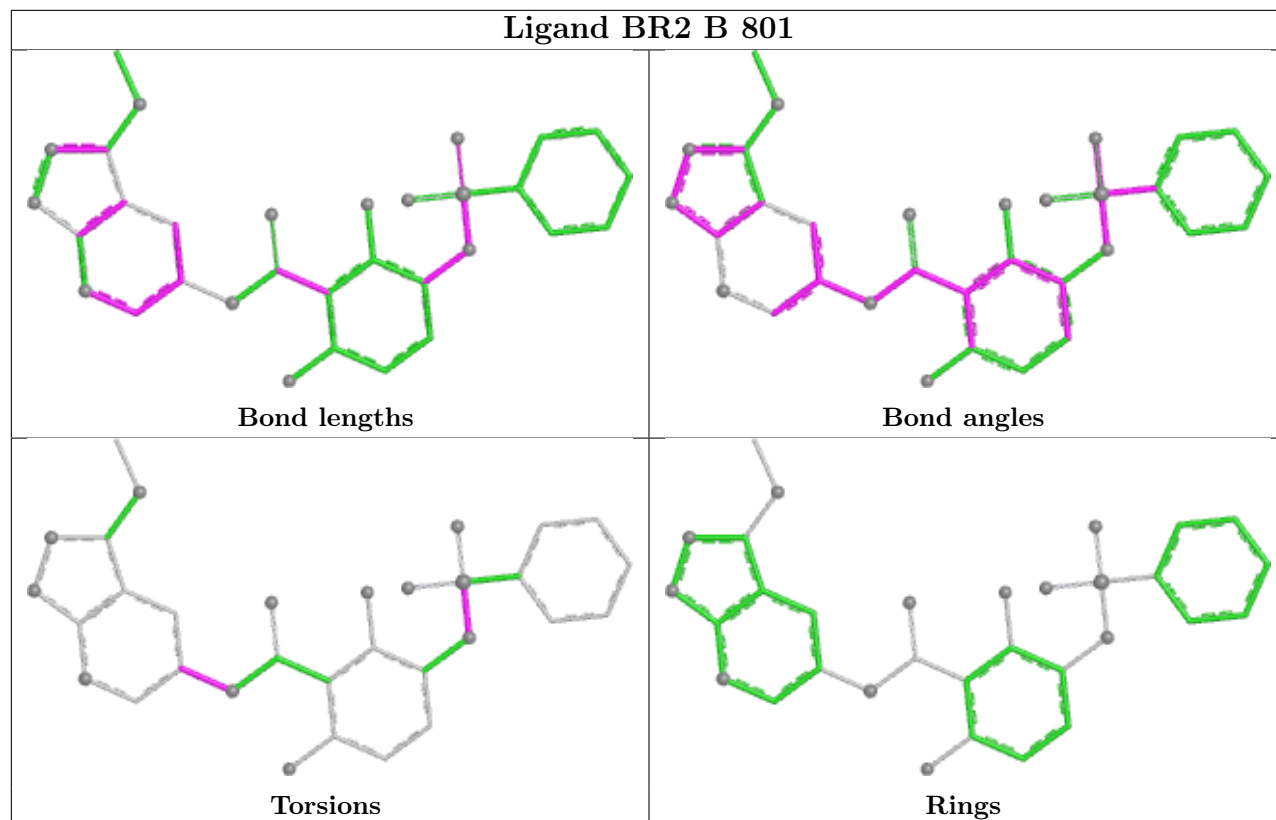
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	BR2	2	0
2	A	801	BR2	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 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 [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	260/307 (84%)	0.23	15 (5%) 29 18	20, 39, 90, 102	0
1	B	276/307 (89%)	0.26	13 (4%) 36 23	21, 41, 88, 102	0
All	All	536/614 (87%)	0.24	28 (5%) 33 21	20, 40, 88, 102	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	628	GLN	4.1
1	A	448	ASP	3.9
1	B	722	PRO	3.5
1	A	613	LEU	3.4
1	B	492	PRO	3.3
1	A	468	PHE	3.2
1	A	492	PRO	3.1
1	B	627	MET	3.1
1	A	491	THR	3.0
1	A	627	MET	2.9
1	B	612	GLN	2.9
1	A	523	PRO	2.8
1	A	486	ASN	2.7
1	B	613	LEU	2.6
1	A	495	LEU	2.6
1	A	723	LYS	2.5
1	B	609	GLN	2.4
1	B	523	PRO	2.4
1	B	630	LYS	2.2
1	B	465	SER	2.2
1	A	449	ASP	2.2
1	B	486	ASN	2.2
1	A	630	LYS	2.2
1	B	448	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	721	LEU	2.1
1	B	584	LEU	2.1
1	A	487	VAL	2.1
1	A	722	PRO	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](#)

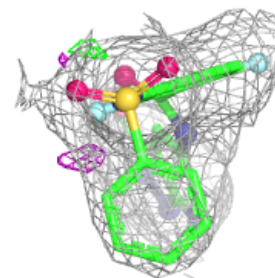
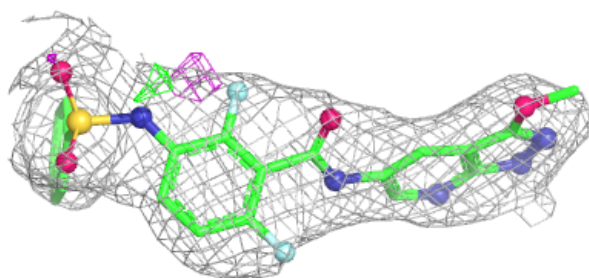
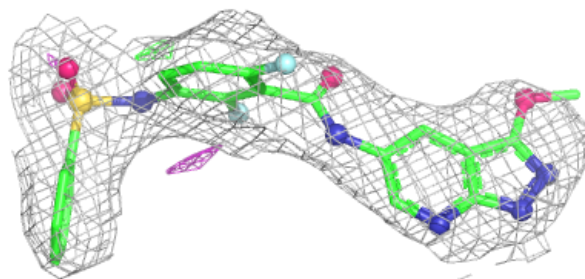
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	BR2	A	801	32/32	0.94	0.12	41,43,47,47	0
2	BR2	B	801	32/32	0.95	0.10	34,38,42,43	0

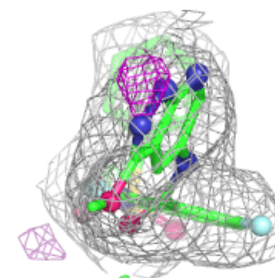
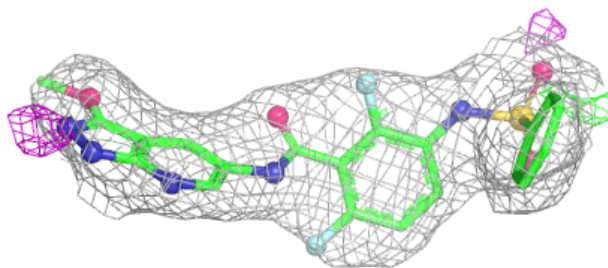
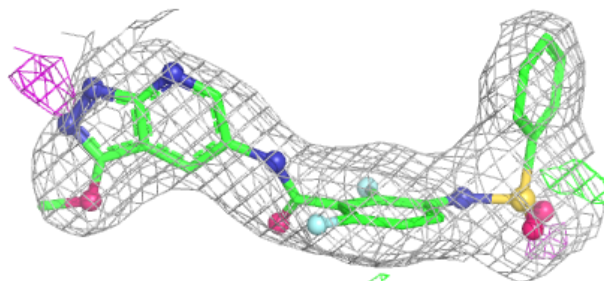
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BR2 A 801:

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

**Electron density around BR2 B 801:**

$2mF_o-DF_c$ (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.