



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:15 PM UTC

PDB ID : 3D4Q / pdb_00003d4q
Title : Pyrazole-based inhibitors of B-Raf kinase
Authors : Morales, T.; Vigers, G.P.A.; Brandhuber, B.J.
Deposited on : 2008-05-14
Resolution : 2.80 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

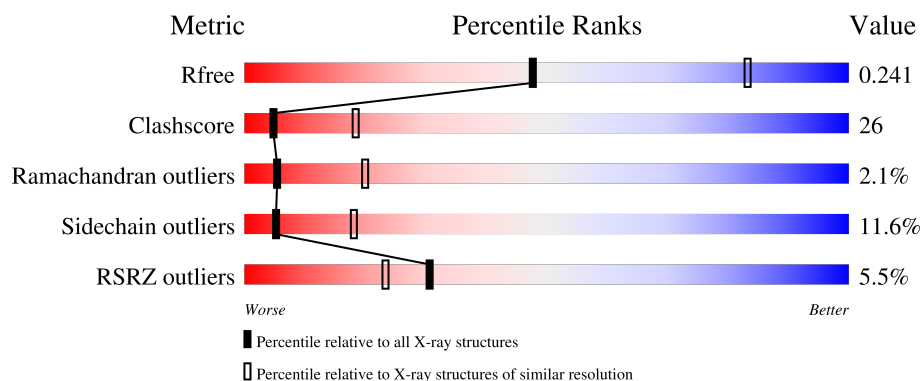
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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% 53% 25% 7% 14%
1	B	307	5% 52% 24% 8% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4293 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	264	Total	C	N	O	S	0	0	0
			2107	1352	366	376	13			
1	B	264	Total	C	N	O	S	0	0	0
			2107	1352	366	376	13			

There are 26 discrepancies between the modelled and reference sequences:

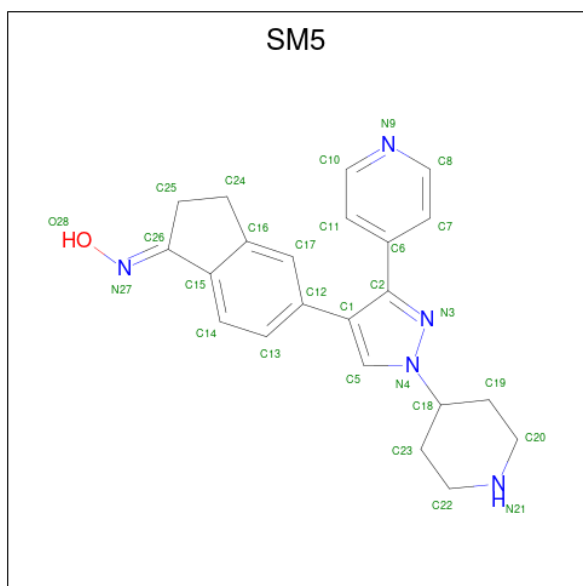
Chain	Residue	Modelled	Actual	Comment	Reference
A	420	MET	-	expression tag	UNP P15056
A	421	ASP	-	expression tag	UNP P15056
A	422	ARG	-	expression tag	UNP P15056
A	423	GLY	-	expression tag	UNP P15056
A	424	SER	-	expression tag	UNP P15056
A	425	HIS	-	expression tag	UNP P15056
A	426	HIS	-	expression tag	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
A	432	SER	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	432	SER	-	expression tag	UNP P15056

- Molecule 2 is (1E)-5-(1-piperidin-4-yl-3-pyridin-4-yl-1H-pyrazol-4-yl)-2,3-dihydro-1H-inden-1-one oxime (CCD ID: SM5) (formula: C₂₂H₂₃N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	22	5	1		
2	B	1	Total	C	N	O	0	0
			28	22	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	14	Total	O	0	0
			14	14		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.34Å 100.34Å 162.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	97.8 (30.00-2.80) 99.0 (30.00-2.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.46 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.250 0.214 , 0.241	Depositor DCC
R_{free} test set	1002 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	65.4	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4293	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: SM5

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	0.90	3/2152 (0.1%)	1.13	12/2905 (0.4%)
1	B	0.87	3/2152 (0.1%)	1.13	12/2905 (0.4%)
All	All	0.89	6/4304 (0.1%)	1.13	24/5810 (0.4%)

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
1	B	0	2
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	666	ILE	CA-CB	9.74	1.65	1.54
1	B	517	MET	SD-CE	9.74	2.03	1.79
1	A	645	VAL	CA-CB	9.16	1.66	1.54
1	A	517	MET	SD-CE	8.85	2.01	1.79
1	B	645	VAL	CA-CB	6.89	1.63	1.54
1	B	484	MET	SD-CE	5.15	1.92	1.79

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	522	LYS	CA-C-N	-11.92	104.94	119.84
1	B	522	LYS	C-N-CA	-11.92	104.94	119.84
1	A	522	LYS	CA-C-N	-10.93	106.17	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	522	LYS	C-N-CA	-10.93	106.17	119.84
1	B	631	ASN	CA-C-N	8.86	128.58	119.19
1	B	631	ASN	C-N-CA	8.86	128.58	119.19
1	A	631	ASN	CA-C-N	8.18	127.86	119.19
1	A	631	ASN	C-N-CA	8.18	127.86	119.19
1	A	452	ILE	CA-C-N	6.82	127.19	119.83
1	A	452	ILE	C-N-CA	6.82	127.19	119.83
1	A	464	GLY	N-CA-C	6.76	118.94	110.29
1	B	668	MET	N-CA-C	6.68	118.64	111.36
1	B	543	ILE	N-CA-C	6.12	116.82	111.56
1	A	631	ASN	N-CA-C	5.98	120.94	108.39
1	B	542	HIS	CA-C-N	-5.87	117.15	123.08
1	B	542	HIS	C-N-CA	-5.87	117.15	123.08
1	B	464	GLY	N-CA-C	5.59	117.44	110.29
1	A	534	GLY	CA-C-N	-5.58	113.24	122.39
1	A	534	GLY	C-N-CA	-5.58	113.24	122.39
1	A	469	GLY	N-CA-C	5.51	118.03	110.69
1	A	543	ILE	N-CA-C	5.45	116.85	111.67
1	B	534	GLY	CA-C-N	-5.40	112.91	122.20
1	B	534	GLY	C-N-CA	-5.40	112.91	122.20
1	B	631	ASN	N-CA-C	5.18	119.26	108.39

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	485	LEU	Peptide
1	A	486	ASN	Peptide
1	B	485	LEU	Peptide
1	B	486	ASN	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	2107	0	2151	107	0
1	B	2107	0	2151	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	28	0	23	6	0
2	B	28	0	23	8	0
3	A	9	0	0	0	0
3	B	14	0	0	0	0
All	All	4293	0	4348	220	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 26.

All (220) 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:A:517:MET:SD	1:A:517:MET:CE	2.01	1.48
1:B:517:MET:SD	1:B:517:MET:CE	2.03	1.47
2:B:1:SM5:C2	2:B:1:SM5:N3	1.75	1.31
2:A:1:SM5:N3	2:A:1:SM5:C2	1.68	1.30
1:A:588:LEU:HD21	1:B:586:GLU:HG3	1.39	1.02
1:B:491:THR:HG22	1:B:493:GLN:H	1.23	1.00
1:A:586:GLU:HG3	1:B:588:LEU:HD21	1.41	0.99
1:A:491:THR:HG22	1:A:493:GLN:H	1.24	0.98
1:A:551:ILE:H	1:A:551:ILE:HD12	1.28	0.95
1:B:551:ILE:HD12	1:B:551:ILE:H	1.31	0.95
1:B:668:MET:HB3	1:B:674:LEU:HB2	1.63	0.81
1:A:684:ASN:H	1:A:684:ASN:HD22	1.28	0.81
1:A:554:ILE:HD12	1:A:721:LEU:HD22	1.63	0.80
1:B:554:ILE:HD12	1:B:721:LEU:HD22	1.64	0.79
1:B:660:ASN:C	1:B:660:ASN:HD22	1.92	0.77
1:A:491:THR:HB	1:A:494:GLN:HG3	1.68	0.76
1:B:454:ASP:HB2	1:B:522:LYS:NZ	2.00	0.76
1:B:491:THR:HB	1:B:494:GLN:HG3	1.66	0.75
1:B:684:ASN:HD22	1:B:684:ASN:H	1.30	0.75
1:A:663:ASP:HA	1:A:666:ILE:HG12	1.68	0.74
1:B:658:ASN:HD22	1:B:658:ASN:H	1.37	0.73
1:A:537:LEU:HD21	1:A:649:LEU:HD21	1.69	0.73
1:A:617:ILE:HA	1:A:620:MET:HB2	1.71	0.72
1:B:491:THR:CG2	1:B:492:PRO:HD2	2.20	0.72
1:B:617:ILE:HG13	1:B:618:LEU:N	2.05	0.71
1:A:666:ILE:HG13	1:A:667:PHE:N	2.06	0.71
1:A:501:GLU:OE1	2:A:1:SM5:O28	2.08	0.71
1:B:617:ILE:HA	1:B:620:MET:HB2	1.72	0.70
1:B:551:ILE:H	1:B:551:ILE:CD1	2.00	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:LEU:HD21	1:B:649:LEU:HD21	1.75	0.69
1:B:616:SER:O	1:B:617:ILE:HG12	1.93	0.68
1:A:486:ASN:O	1:A:487:VAL:HG13	1.92	0.68
1:B:454:ASP:HB2	1:B:522:LYS:HZ3	1.57	0.68
1:B:486:ASN:O	1:B:487:VAL:HG13	1.94	0.67
1:A:491:THR:CG2	1:A:492:PRO:HD2	2.24	0.67
1:A:551:ILE:H	1:A:551:ILE:CD1	2.00	0.66
1:A:660:ASN:C	1:A:660:ASN:HD22	2.03	0.66
1:B:486:ASN:HD22	1:B:487:VAL:HA	1.60	0.66
1:B:487:VAL:O	1:B:489:ALA:N	2.25	0.66
1:B:454:ASP:H	1:B:522:LYS:NZ	1.95	0.65
1:B:660:ASN:C	1:B:660:ASN:ND2	2.53	0.65
1:B:684:ASN:HD22	1:B:684:ASN:N	1.90	0.64
1:A:484:MET:HE2	1:A:524:GLN:CD	2.21	0.64
1:A:626:ARG:O	1:A:628:GLN:N	2.30	0.64
1:A:551:ILE:HD12	1:A:551:ILE:N	2.09	0.64
1:A:718:ALA:O	1:A:722:PRO:HD3	1.99	0.63
1:A:684:ASN:HD22	1:A:684:ASN:N	1.90	0.62
1:B:718:ALA:O	1:B:722:PRO:HD3	1.99	0.62
1:B:464:GLY:HA3	2:B:1:SM5:H119	1.82	0.62
1:A:486:ASN:HD22	1:A:487:VAL:HA	1.65	0.62
1:A:661:ASN:OD1	1:A:664:GLN:HG2	1.99	0.62
1:A:684:ASN:H	1:A:684:ASN:ND2	1.96	0.62
2:A:1:SM5:H11	2:A:1:SM5:C17	2.30	0.62
1:A:454:ASP:HB2	1:A:522:LYS:HZ3	1.64	0.61
1:B:573:ILE:HG22	1:B:575:ARG:HG3	1.82	0.61
1:B:491:THR:HG23	1:B:492:PRO:HD2	1.82	0.61
1:A:666:ILE:HG13	1:A:667:PHE:H	1.65	0.60
1:B:684:ASN:H	1:B:684:ASN:ND2	1.99	0.60
1:B:486:ASN:C	1:B:486:ASN:ND2	2.60	0.60
1:A:616:SER:O	1:A:617:ILE:HG12	2.02	0.59
1:A:523:PRO:O	1:A:524:GLN:HG3	2.03	0.59
1:A:682:ARG:HG3	1:A:684:ASN:ND2	2.16	0.59
1:B:682:ARG:HG3	1:B:684:ASN:ND2	2.17	0.59
2:B:1:SM5:C17	2:B:1:SM5:H11	2.33	0.59
1:B:626:ARG:O	1:B:628:GLN:N	2.35	0.59
1:B:484:MET:HE2	1:B:524:GLN:CD	2.28	0.58
1:A:617:ILE:HG13	1:A:618:LEU:N	2.18	0.58
1:B:486:ASN:CG	1:B:524:GLN:HB3	2.29	0.58
1:A:491:THR:HG23	1:A:492:PRO:HD2	1.85	0.58
1:B:689:MET:HE2	1:B:717:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:LEU:C	1:B:716:LEU:HD23	2.29	0.58
1:A:454:ASP:H	1:A:522:LYS:NZ	2.01	0.58
1:A:717:LEU:C	1:A:717:LEU:HD12	2.29	0.58
1:A:599:THR:HG22	1:A:600:VAL:N	2.19	0.57
1:A:486:ASN:C	1:A:486:ASN:ND2	2.62	0.57
2:B:1:SM5:H11	2:B:1:SM5:C12	2.35	0.56
1:A:486:ASN:CG	1:A:524:GLN:HB3	2.30	0.56
1:B:586:GLU:O	1:B:588:LEU:HD12	2.05	0.56
1:B:491:THR:HG22	1:B:492:PRO:CD	2.36	0.55
1:A:488:THR:O	1:A:489:ALA:HB2	2.07	0.55
2:A:1:SM5:H11	2:A:1:SM5:C12	2.36	0.55
1:A:663:ASP:O	1:A:666:ILE:CG1	2.55	0.55
1:A:465:SER:H	2:A:1:SM5:H120	1.71	0.54
1:B:491:THR:CG2	1:B:493:GLN:H	2.09	0.54
1:B:620:MET:CE	1:B:625:ILE:HA	2.37	0.54
1:B:454:ASP:CB	1:B:522:LYS:NZ	2.68	0.54
1:B:717:LEU:HD12	1:B:717:LEU:C	2.31	0.54
1:A:681:VAL:O	1:A:681:VAL:HG23	2.07	0.54
1:B:488:THR:O	1:B:489:ALA:HB2	2.07	0.54
1:B:717:LEU:HD12	1:B:717:LEU:O	2.07	0.54
1:A:620:MET:HG2	1:A:624:VAL:CG1	2.38	0.54
1:A:689:MET:HE2	1:A:717:LEU:HD21	1.91	0.53
1:A:716:LEU:HD23	1:A:716:LEU:C	2.33	0.53
1:A:488:THR:O	1:A:489:ALA:CB	2.57	0.52
1:A:487:VAL:O	1:A:489:ALA:N	2.37	0.52
1:B:491:THR:HG22	1:B:492:PRO:HD2	1.88	0.52
1:A:586:GLU:O	1:A:588:LEU:HD12	2.09	0.52
1:A:624:VAL:HA	1:A:632:PRO:HB2	1.92	0.52
1:B:502:VAL:O	1:B:506:ARG:HG2	2.09	0.52
1:A:663:ASP:O	1:A:666:ILE:HG13	2.10	0.52
1:B:501:GLU:OE1	2:B:1:SM5:O28	2.26	0.51
1:B:550:MET:O	1:B:554:ILE:HG13	2.10	0.51
1:B:624:VAL:HA	1:B:632:PRO:HB2	1.92	0.51
1:B:658:ASN:HD22	1:B:658:ASN:N	2.05	0.51
1:B:620:MET:HG2	1:B:624:VAL:HG12	1.91	0.51
1:A:484:MET:HB3	1:A:486:ASN:OD1	2.10	0.51
1:B:620:MET:HG2	1:B:624:VAL:CG1	2.41	0.51
1:B:626:ARG:O	1:B:626:ARG:HG3	2.11	0.51
1:A:674:LEU:HD22	1:A:675:SER:N	2.26	0.50
1:A:496:GLN:OE1	1:A:496:GLN:HA	2.10	0.50
1:B:599:THR:HG22	1:B:600:VAL:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:ASN:HD22	1:B:661:ASN:N	2.10	0.50
1:A:454:ASP:HB2	1:A:522:LYS:NZ	2.26	0.50
1:B:532:CYS:H	2:B:1:SM5:C8	2.24	0.50
1:B:537:LEU:HG	1:B:541:LEU:HD22	1.94	0.50
1:B:457:ILE:HG22	1:B:476:TRP:HB2	1.94	0.49
1:B:454:ASP:CB	1:B:522:LYS:HZ1	2.25	0.49
1:B:488:THR:O	1:B:489:ALA:CB	2.60	0.49
1:B:495:LEU:HD22	1:B:525:LEU:HD11	1.95	0.49
1:A:491:THR:HG22	1:A:493:GLN:N	2.09	0.49
1:A:491:THR:HG22	1:A:492:PRO:CD	2.43	0.49
1:A:507:LYS:HG2	1:B:448:ASP:HA	1.94	0.49
1:B:491:THR:HG21	1:B:493:GLN:HB3	1.95	0.48
1:A:495:LEU:HD22	1:A:525:LEU:HD11	1.94	0.48
1:A:626:ARG:O	1:A:626:ARG:HG3	2.13	0.48
1:A:554:ILE:HD12	1:A:721:LEU:CD2	2.39	0.48
1:B:684:ASN:N	1:B:684:ASN:ND2	2.60	0.48
1:B:575:ARG:HG2	1:B:633:TYR:CD2	2.49	0.48
1:A:453:PRO:HG2	1:A:456:GLN:NE2	2.28	0.48
1:A:575:ARG:HG2	1:A:633:TYR:CD2	2.47	0.48
1:B:681:VAL:HG23	1:B:681:VAL:O	2.13	0.48
1:B:484:MET:HB3	1:B:486:ASN:OD1	2.15	0.47
1:B:620:MET:HE2	1:B:625:ILE:CG1	2.45	0.47
1:A:684:ASN:N	1:A:684:ASN:ND2	2.59	0.47
1:B:551:ILE:HD12	1:B:551:ILE:N	2.14	0.47
1:A:510:HIS:HA	1:B:517:MET:HE2	1.96	0.47
1:B:484:MET:HE2	1:B:524:GLN:OE1	2.13	0.47
1:A:454:ASP:H	1:A:522:LYS:HZ3	1.63	0.47
1:A:523:PRO:C	1:A:524:GLN:HG3	2.40	0.47
2:A:1:SM5:C17	2:A:1:SM5:C11	2.93	0.47
1:B:467:SER:OG	1:B:596:GLY:HA3	2.15	0.47
1:A:509:ARG:HD3	1:B:516:PHE:O	2.15	0.47
1:B:520:SER:HB3	1:B:526:ALA:HB3	1.97	0.47
1:A:457:ILE:HG22	1:A:476:TRP:HB2	1.97	0.47
1:A:620:MET:HG2	1:A:624:VAL:HG12	1.96	0.47
1:A:623:GLU:H	1:A:623:GLU:HG3	1.22	0.46
1:B:721:LEU:C	1:B:723:LYS:N	2.73	0.46
1:B:491:THR:CG2	1:B:492:PRO:CD	2.91	0.46
1:A:660:ASN:C	1:A:660:ASN:ND2	2.72	0.46
1:B:491:THR:HG22	1:B:492:PRO:N	2.31	0.46
1:A:502:VAL:O	1:A:506:ARG:HG2	2.15	0.46
1:A:721:LEU:C	1:A:723:LYS:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:THR:HG21	1:A:493:GLN:HB3	1.97	0.46
1:A:589:THR:HG22	1:A:591:LYS:HE2	1.98	0.46
1:A:487:VAL:C	1:A:489:ALA:H	2.22	0.45
1:B:491:THR:HG22	1:B:493:GLN:N	2.08	0.45
1:B:623:GLU:OE1	1:B:704:ARG:NH1	2.47	0.45
1:B:709:GLN:O	1:B:710:ILE:C	2.60	0.45
1:A:623:GLU:OE1	1:A:704:ARG:NH1	2.46	0.45
1:A:663:ASP:O	1:A:666:ILE:HG12	2.16	0.45
1:A:551:ILE:CD1	1:A:551:ILE:N	2.77	0.45
1:A:631:ASN:HA	1:A:632:PRO:HD2	1.80	0.44
1:B:466:GLY:O	1:B:467:SER:C	2.58	0.44
1:B:486:ASN:HD22	1:B:486:ASN:C	2.24	0.44
1:B:588:LEU:CD1	1:B:588:LEU:H	2.30	0.44
1:A:523:PRO:HB2	1:A:524:GLN:HE21	1.82	0.44
1:B:453:PRO:HG2	1:B:456:GLN:NE2	2.32	0.44
1:B:487:VAL:C	1:B:489:ALA:H	2.18	0.44
1:B:541:LEU:HD12	1:B:541:LEU:HA	1.86	0.44
1:A:491:THR:CG2	1:A:493:GLN:H	2.12	0.44
1:A:620:MET:HE2	1:A:625:ILE:HG12	1.99	0.44
1:B:523:PRO:O	1:B:524:GLN:HG3	2.18	0.43
1:A:636:GLN:HG2	1:A:701:ARG:O	2.18	0.43
1:A:475:LYS:HE3	1:A:479:ASP:OD1	2.18	0.43
1:B:491:THR:CG2	1:B:493:GLN:HB3	2.48	0.43
1:B:636:GLN:HG2	1:B:701:ARG:O	2.19	0.43
1:B:639:VAL:HG13	1:B:710:ILE:HD11	2.00	0.43
1:B:555:ASP:OD1	1:B:558:ARG:NH1	2.51	0.43
1:A:620:MET:CE	1:A:625:ILE:HA	2.48	0.43
1:B:448:ASP:O	1:B:449:ASP:O	2.36	0.43
1:B:499:LYS:HD3	1:B:499:LYS:HA	1.72	0.43
1:A:549:GLU:HB3	1:A:551:ILE:HD13	2.01	0.43
1:A:717:LEU:HD12	1:A:717:LEU:O	2.18	0.43
1:B:554:ILE:HD13	1:B:717:LEU:HD11	2.00	0.43
1:B:548:PHE:HB2	1:B:553:LEU:HD21	2.00	0.43
1:B:486:ASN:HD22	1:B:487:VAL:CA	2.27	0.43
1:A:454:ASP:CB	1:A:522:LYS:NZ	2.82	0.43
1:B:677:ASP:OD1	1:B:679:SER:HB2	2.18	0.43
1:A:491:THR:CG2	1:A:492:PRO:CD	2.95	0.42
1:A:516:PHE:O	1:B:509:ARG:HD3	2.19	0.42
1:B:634:SER:OG	1:B:636:GLN:HB2	2.19	0.42
1:A:491:THR:CG2	1:A:493:GLN:HB3	2.50	0.42
1:A:634:SER:OG	1:A:636:GLN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ASN:HA	1:A:590:VAL:O	2.20	0.42
1:A:453:PRO:O	1:A:456:GLN:HG3	2.20	0.42
1:A:693:MET:HE3	1:A:693:MET:HB2	1.83	0.42
1:B:616:SER:O	1:B:617:ILE:CG1	2.65	0.42
1:A:588:LEU:H	1:A:588:LEU:CD1	2.33	0.42
1:A:707:PHE:N	1:A:708:PRO:CD	2.83	0.42
1:B:523:PRO:C	1:B:524:GLN:HG3	2.45	0.42
1:A:448:ASP:HA	1:B:507:LYS:HG2	2.01	0.41
1:B:457:ILE:HG23	1:B:457:ILE:HD13	1.82	0.41
1:B:620:MET:HE2	1:B:625:ILE:HG12	2.02	0.41
1:B:681:VAL:HG22	1:B:690:LYS:NZ	2.36	0.41
1:A:620:MET:HE2	1:A:625:ILE:CG1	2.51	0.41
1:A:682:ARG:HG3	1:A:684:ASN:HD21	1.84	0.41
1:B:496:GLN:OE1	1:B:496:GLN:HA	2.19	0.41
1:A:674:LEU:HD22	1:A:675:SER:H	1.85	0.41
2:B:1:SM5:C17	2:B:1:SM5:C11	2.99	0.41
1:A:537:LEU:HG	1:A:541:LEU:HD22	2.03	0.41
1:A:639:VAL:HG13	1:A:710:ILE:HD11	2.03	0.41
1:B:464:GLY:HA3	2:B:1:SM5:C19	2.49	0.41
1:B:577:LEU:HD23	1:B:577:LEU:HA	1.88	0.41
1:A:486:ASN:HD22	1:A:487:VAL:CA	2.33	0.41
1:A:681:VAL:O	1:A:681:VAL:CG2	2.69	0.40
1:B:486:ASN:O	1:B:486:ASN:ND2	2.54	0.40
1:B:453:PRO:O	1:B:456:GLN:HG3	2.20	0.40
1:B:721:LEU:O	1:B:723:LYS:N	2.55	0.40
1:A:721:LEU:O	1:A:723:LYS:N	2.54	0.40
1:A:573:ILE:HG22	1:A:575:ARG:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/307 (85%)	235 (90%)	20 (8%)	5 (2%)	6	22
1	B	260/307 (85%)	233 (90%)	21 (8%)	6 (2%)	5	18
All	All	520/614 (85%)	468 (90%)	41 (8%)	11 (2%)	5	20

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ALA
1	A	627	MET
1	B	449	ASP
1	B	489	ALA
1	B	627	MET
1	A	449	ASP
1	B	594	ASP
1	A	617	ILE
1	B	617	ILE
1	A	487	VAL
1	B	487	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	232/271 (86%)	207 (89%)	25 (11%)	6	21
1	B	232/271 (86%)	203 (88%)	29 (12%)	4	15
All	All	464/542 (86%)	410 (88%)	54 (12%)	5	18

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

Mol	Chain	Res	Type
1	A	457	ILE
1	A	461	GLN
1	A	484	MET
1	A	485	LEU
1	A	487	VAL

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Mol	Chain	Res	Type
1	A	495	LEU
1	A	496	GLN
1	A	522	LYS
1	A	541	LEU
1	A	544	ILE
1	A	551	ILE
1	A	552	LYS
1	A	577	LEU
1	A	588	LEU
1	A	616	SER
1	A	618	LEU
1	A	620	MET
1	A	623	GLU
1	A	628	GLN
1	A	631	ASN
1	A	645	VAL
1	A	660	ASN
1	A	674	LEU
1	A	684	ASN
1	A	687	LYS
1	B	457	ILE
1	B	484	MET
1	B	485	LEU
1	B	486	ASN
1	B	487	VAL
1	B	495	LEU
1	B	496	GLN
1	B	522	LYS
1	B	541	LEU
1	B	544	ILE
1	B	551	ILE
1	B	552	LYS
1	B	577	LEU
1	B	584	LEU
1	B	588	LEU
1	B	616	SER
1	B	618	LEU
1	B	620	MET
1	B	623	GLU
1	B	628	GLN
1	B	631	ASN
1	B	645	VAL

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Mol	Chain	Res	Type
1	B	658	ASN
1	B	660	ASN
1	B	662	ARG
1	B	674	LEU
1	B	675	SER
1	B	684	ASN
1	B	687	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	486	ASN
1	A	524	GLN
1	A	628	GLN
1	A	660	ASN
1	A	684	ASN
1	B	461	GLN
1	B	486	ASN
1	B	524	GLN
1	B	628	GLN
1	B	658	ASN
1	B	660	ASN
1	B	664	GLN
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	SM5	A	1	-	31,32,32	6.58	15 (48%)	41,45,45	2.19	15 (36%)
2	SM5	B	1	-	31,32,32	7.40	16 (51%)	41,45,45	1.99	11 (26%)

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	SM5	A	1	-	-	2/14/31/31	0/5/5/5
2	SM5	B	1	-	-	2/14/31/31	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	SM5	C2-N3	27.60	1.75	1.33
2	A	1	SM5	C2-N3	22.81	1.68	1.33
2	B	1	SM5	C5-C1	16.69	1.69	1.37
2	B	1	SM5	C26-N27	-15.10	1.14	1.28
2	A	1	SM5	C5-C1	12.58	1.61	1.37
2	A	1	SM5	C24-C25	11.92	1.68	1.54
2	A	1	SM5	C17-C12	10.97	1.55	1.39
2	A	1	SM5	C6-C2	-10.90	1.32	1.48
2	B	1	SM5	C24-C25	10.50	1.66	1.54
2	B	1	SM5	C7-C8	8.97	1.55	1.38
2	B	1	SM5	C17-C12	8.51	1.52	1.39
2	A	1	SM5	C7-C8	8.02	1.54	1.38
2	A	1	SM5	C23-C18	-6.96	1.35	1.52
2	A	1	SM5	C11-C6	6.61	1.49	1.39
2	A	1	SM5	C26-N27	-5.97	1.23	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	SM5	C23-C18	-5.18	1.39	1.52
2	B	1	SM5	C23-C22	5.12	1.66	1.52
2	B	1	SM5	C17-C16	5.03	1.47	1.39
2	B	1	SM5	C11-C6	4.91	1.46	1.39
2	A	1	SM5	C15-C16	4.05	1.45	1.39
2	A	1	SM5	N4-N3	3.52	1.41	1.36
2	A	1	SM5	C12-C1	-3.41	1.43	1.48
2	B	1	SM5	N4-N3	3.36	1.41	1.36
2	B	1	SM5	C11-C10	3.34	1.45	1.38
2	A	1	SM5	C5-N4	3.23	1.40	1.34
2	B	1	SM5	C5-N4	3.10	1.39	1.34
2	A	1	SM5	C17-C16	2.82	1.43	1.39
2	A	1	SM5	C11-C10	2.75	1.43	1.38
2	B	1	SM5	C6-C2	-2.62	1.44	1.48
2	B	1	SM5	C15-C26	-2.21	1.40	1.45
2	B	1	SM5	C7-C6	-2.03	1.36	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	SM5	C13-C12-C1	-5.53	113.04	120.98
2	B	1	SM5	C24-C25-C26	-4.96	103.03	105.42
2	A	1	SM5	C17-C12-C1	4.32	127.24	120.65
2	A	1	SM5	C24-C25-C26	-4.04	103.48	105.42
2	B	1	SM5	C16-C15-C26	4.03	113.74	108.98
2	A	1	SM5	C16-C15-C26	4.02	113.73	108.98
2	B	1	SM5	C23-C18-N4	3.96	116.38	110.95
2	B	1	SM5	C6-C2-N3	3.72	124.55	118.99
2	A	1	SM5	C12-C1-C5	-3.72	117.73	124.47
2	A	1	SM5	C18-N4-C5	-3.70	122.64	128.77
2	B	1	SM5	C18-N4-C5	-3.41	123.12	128.77
2	A	1	SM5	C6-C2-N3	3.25	123.85	118.99
2	B	1	SM5	C13-C12-C1	-3.23	116.34	120.98
2	A	1	SM5	C23-C18-N4	3.20	115.33	110.95
2	A	1	SM5	C12-C17-C16	-2.90	117.14	121.47
2	A	1	SM5	C18-N4-N3	2.78	123.02	119.76
2	A	1	SM5	C14-C15-C26	-2.73	122.72	132.50
2	B	1	SM5	C12-C17-C16	-2.59	117.59	121.47
2	B	1	SM5	C14-C15-C26	-2.58	123.27	132.50
2	B	1	SM5	C17-C12-C1	2.57	124.57	120.65
2	B	1	SM5	C12-C1-C5	-2.43	120.07	124.47
2	A	1	SM5	C24-C16-C15	-2.38	109.66	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	SM5	C8-C7-C6	-2.37	116.46	119.05
2	A	1	SM5	C17-C16-C15	-2.23	118.24	120.65
2	B	1	SM5	C25-C24-C16	-2.20	102.69	104.30
2	A	1	SM5	C14-C15-C16	2.15	123.55	120.88

There are no chirality outliers.

All (4) torsion outliers are listed below:

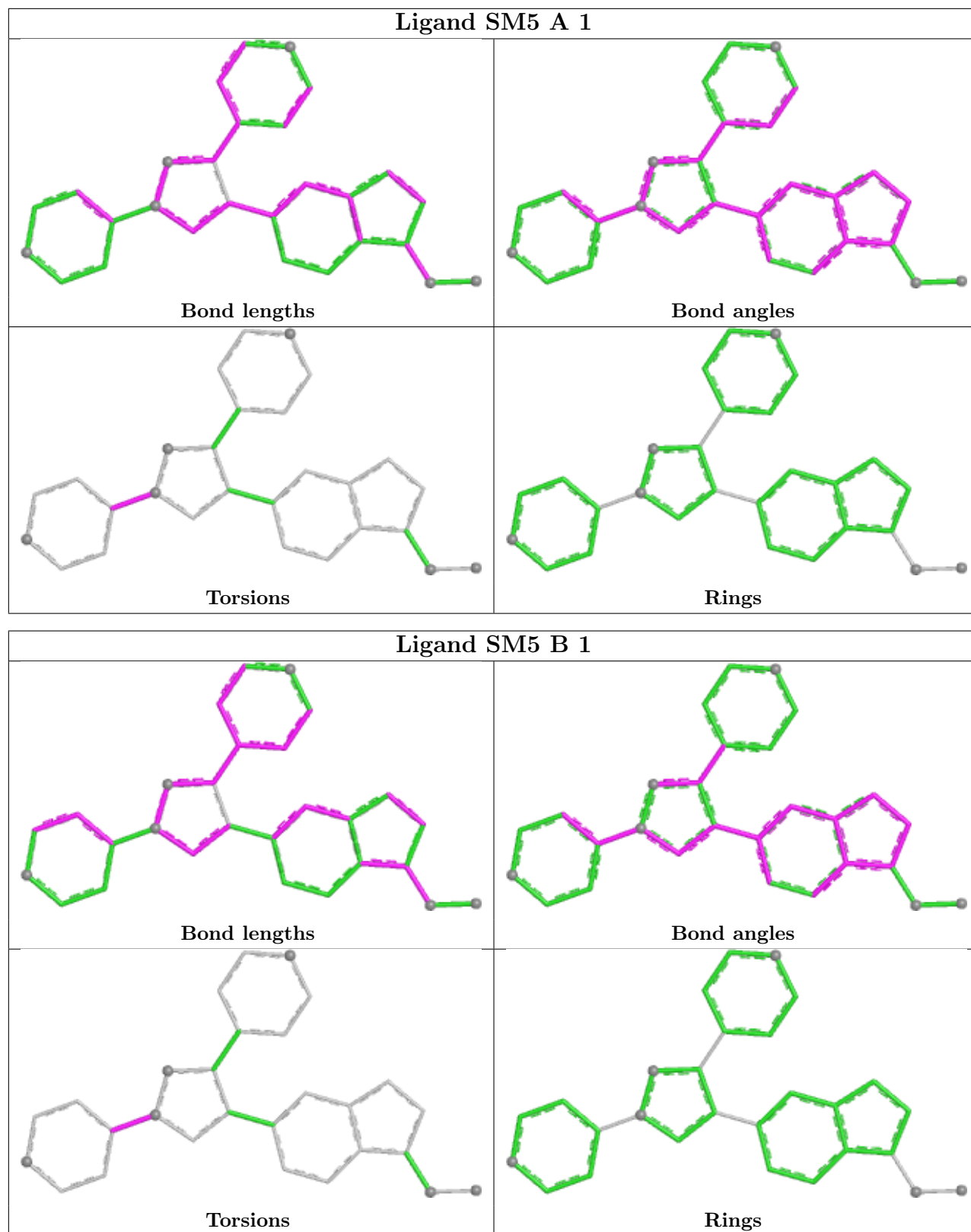
Mol	Chain	Res	Type	Atoms
2	A	1	SM5	C23-C18-N4-N3
2	A	1	SM5	C23-C18-N4-C5
2	B	1	SM5	C23-C18-N4-N3
2	B	1	SM5	C23-C18-N4-C5

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	SM5	6	0
2	B	1	SM5	8	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 ⓘ

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	264/307 (85%)	-0.04	14 (5%) 32 24	38, 52, 89, 123	0
1	B	264/307 (85%)	0.02	15 (5%) 29 22	38, 53, 89, 123	0
All	All	528/614 (85%)	-0.01	29 (5%) 30 23	38, 53, 90, 123	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	613	LEU	6.1
1	A	486	ASN	4.9
1	B	486	ASN	4.6
1	B	613	LEU	4.3
1	A	614	SER	3.8
1	B	722	PRO	3.7
1	A	448	ASP	3.6
1	B	614	SER	3.2
1	B	454	ASP	3.1
1	B	448	ASP	3.0
1	B	488	THR	3.0
1	B	600	VAL	2.9
1	B	721	LEU	2.8
1	B	629	ASP	2.7
1	B	474	GLY	2.7
1	B	630	LYS	2.6
1	A	615	GLY	2.4
1	A	522	LYS	2.4
1	B	616	SER	2.3
1	A	457	ILE	2.3
1	A	616	SER	2.2
1	B	723	LYS	2.2
1	A	489	ALA	2.2
1	A	487	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	523	PRO	2.1
1	A	722	PRO	2.1
1	B	631	ASN	2.1
1	A	485	LEU	2.1
1	A	723	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](#)

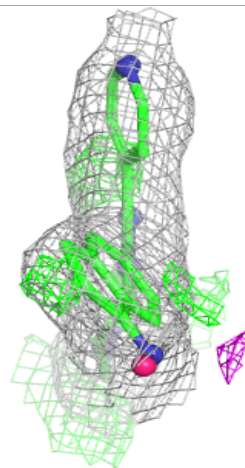
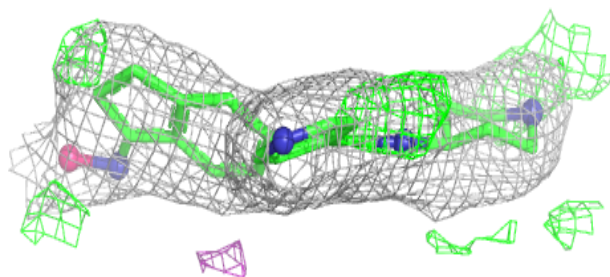
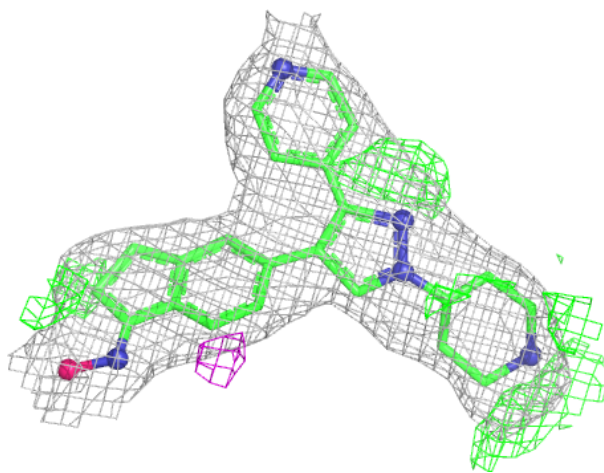
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

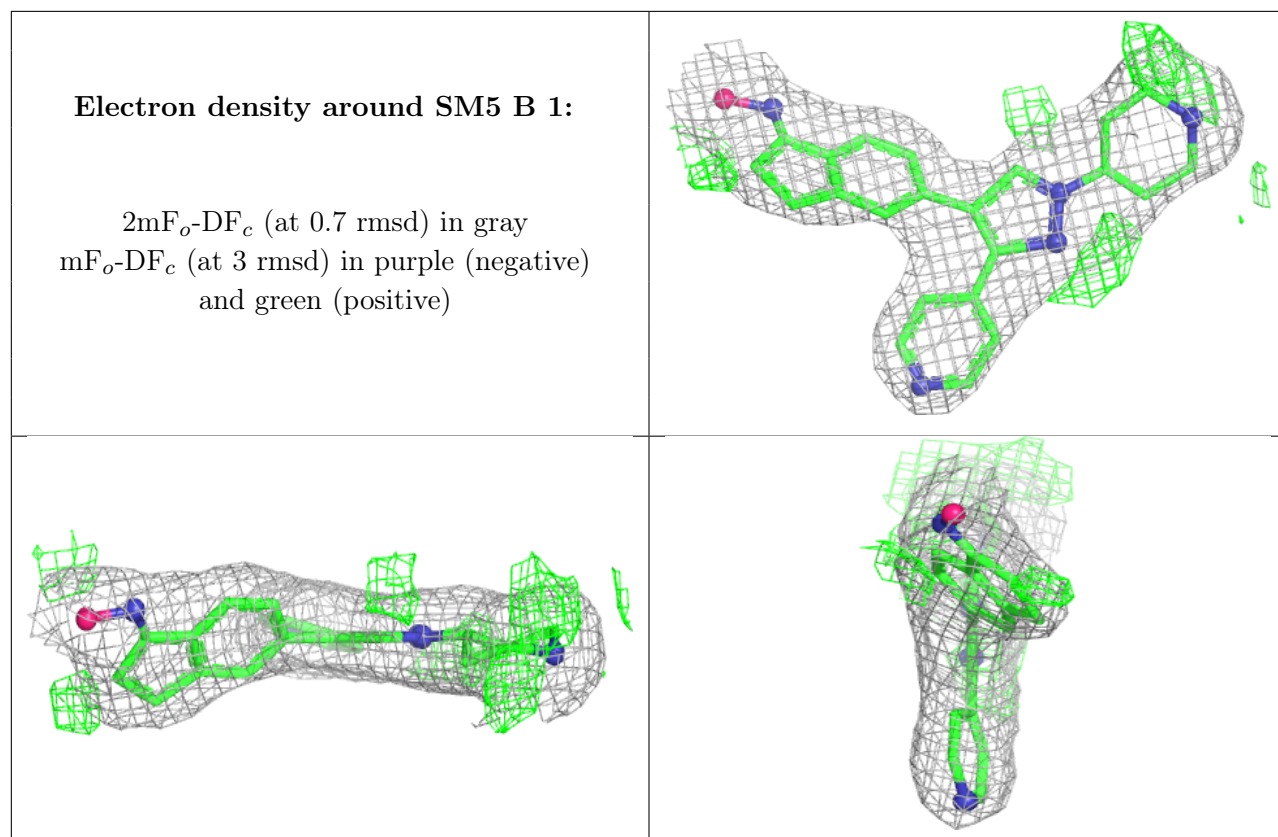
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SM5	A	1	28/28	0.88	0.12	41,44,49,56	0
2	SM5	B	1	28/28	0.88	0.13	39,44,46,48	0

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 SM5 A 1:

$2mF_o-DF_c$ (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.