



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:29 PM UTC

PDB ID : 7FNM / pdb_00007fnm
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P07D05 from the F2X-Universal Library
Authors : Barthel, T.; Wollenhaupt, J.; Lima, G.M.A.; Wahl, M.C.; Weiss, M.S.
Deposited on : 2022-08-26
Resolution : 1.72 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

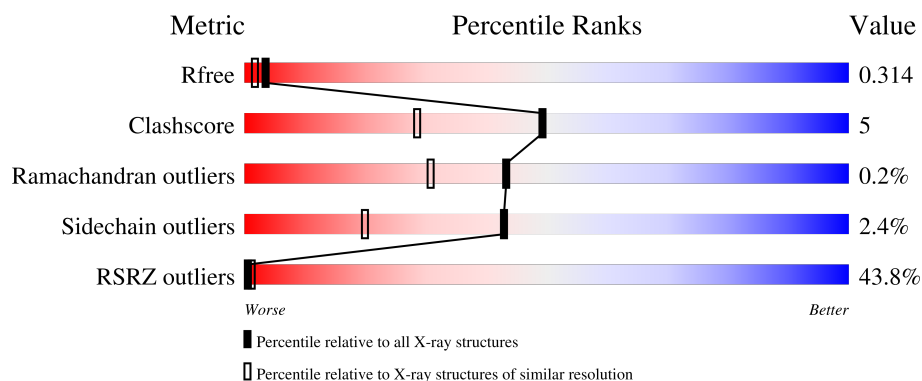
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	258	40% 78% 13% 8%
2	B	308	43% 80% 16% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9225 atoms, of which 4524 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 Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	237	4068	1287	2060	336	373	12	18	21	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1833	GLY	-	expression tag	UNP P33334
A	1834	ALA	-	expression tag	UNP P33334
A	1835	MET	-	expression tag	UNP P33334

- Molecule 2 is a protein called A1 cistron-splicing factor AAR2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	300	5044	1654	2464	421	485	20	11	17	0

There are 20 discrepancies between the modelled and reference sequences:

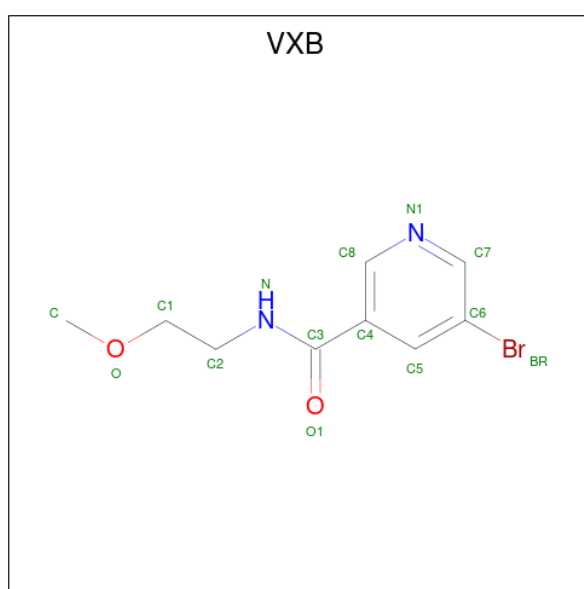
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357
B	?	-	ALA	deletion	UNP P32357
B	?	-	GLY	deletion	UNP P32357
B	?	-	SER	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	MET	deletion	UNP P32357
B	?	-	GLU	deletion	UNP P32357
B	?	-	ALA	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357
B	?	-	ASN	deletion	UNP P32357
B	?	-	GLU	deletion	UNP P32357
B	170	SER	ASP	conflict	UNP P32357

- Molecule 3 is 5-bromo-N-(2-methoxyethyl)pyridine-3-carboxamide (CCD ID: VXB) (formula: C₉H₁₁BrN₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	Br	C	N	O	0	0
			14	1	9	2	2		
3	B	1	Total	Br	C	N	O	0	0
			14	1	9	2	2		
3	B	1	Total	Br	C	N	O	0	0
			14	1	9	2	2		

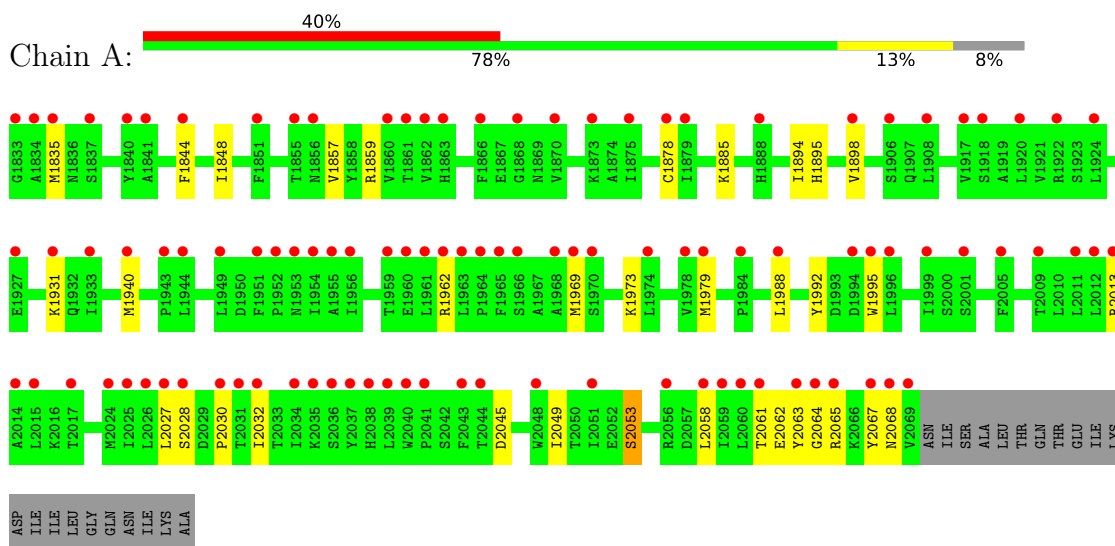
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	39	Total	O	0	0
			39	39		

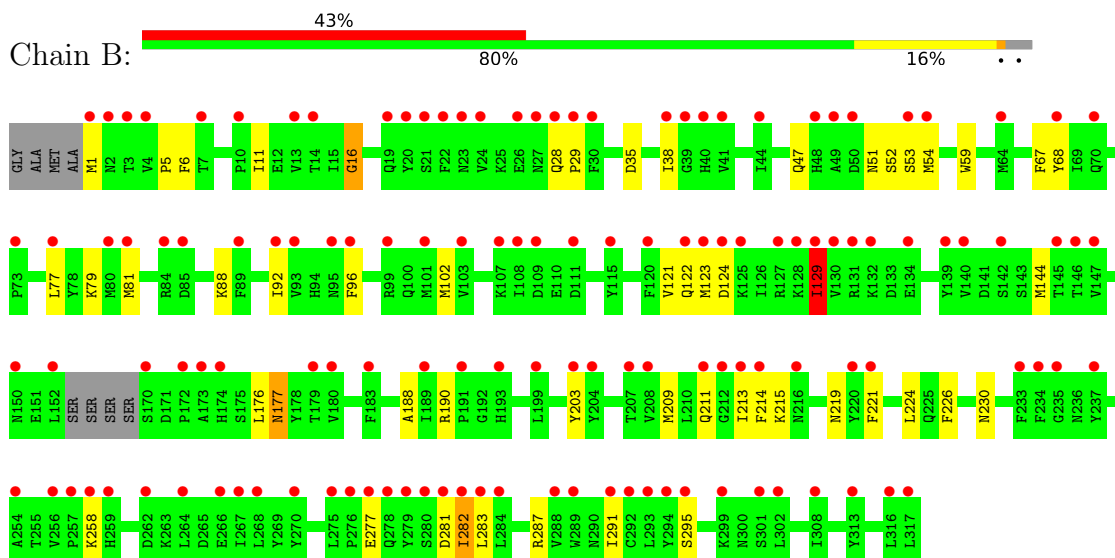
3 Residue-property plots

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: Pre-mRNA-splicing factor 8



• Molecule 2: A1 cistron-splicing factor AAR2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.27Å 81.49Å 93.23Å 90.00° 108.76° 90.00°	Depositor
Resolution (Å)	37.05 – 1.72 37.05 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.05-1.72) 99.8 (37.05-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.72Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.261 , 0.284 0.294 , 0.314	Depositor DCC
R_{free} test set	2098 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9225	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.70	1/2149 (0.0%)	0.75	0/2911
2	B	0.94	12/2739 (0.4%)	1.19	26/3699 (0.7%)
All	All	0.84	13/4888 (0.3%)	1.02	26/6610 (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
2	B	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	PRO	C-O	-8.01	1.14	1.23
2	B	123[A]	MET	N-CA	7.60	1.55	1.46
2	B	123[B]	MET	N-CA	7.60	1.55	1.46
2	B	230[A]	ASN	C-O	7.47	1.32	1.24
2	B	230[B]	ASN	C-O	7.47	1.32	1.24
2	B	16	GLY	CA-C	-7.25	1.47	1.52
2	B	177[A]	ASN	C-N	-7.01	1.23	1.33
2	B	177[B]	ASN	C-N	-7.01	1.23	1.33
2	B	211[A]	GLN	C-N	6.41	1.42	1.33
2	B	211[B]	GLN	C-N	6.41	1.42	1.33
2	B	122[A]	GLN	C-N	5.72	1.41	1.33
2	B	122[B]	GLN	C-N	5.72	1.41	1.33
1	A	1940	MET	SD-CE	-5.30	1.66	1.79

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	211[A]	GLN	CA-C-N	-10.09	101.64	121.41
2	B	211[A]	GLN	C-N-CA	-10.09	101.64	121.41
2	B	211[B]	GLN	CA-C-N	-10.09	101.64	121.41
2	B	211[B]	GLN	C-N-CA	-10.09	101.64	121.41
2	B	230[A]	ASN	CA-C-O	9.61	130.74	120.55
2	B	230[B]	ASN	CA-C-O	9.61	130.74	120.55
2	B	177[A]	ASN	O-C-N	8.35	133.50	122.56
2	B	177[B]	ASN	O-C-N	8.35	133.50	122.56
2	B	122[A]	GLN	CA-C-N	-7.30	109.92	120.29
2	B	122[A]	GLN	C-N-CA	-7.30	109.92	120.29
2	B	122[B]	GLN	CA-C-N	-7.30	109.92	120.29
2	B	122[B]	GLN	C-N-CA	-7.30	109.92	120.29
2	B	221	PHE	CA-C-N	6.68	127.36	119.94
2	B	221	PHE	C-N-CA	6.68	127.36	119.94
2	B	177[A]	ASN	CA-C-N	-6.23	108.11	121.45
2	B	177[A]	ASN	C-N-CA	-6.23	108.11	121.45
2	B	177[B]	ASN	CA-C-N	-6.23	108.11	121.45
2	B	177[B]	ASN	C-N-CA	-6.23	108.11	121.45
2	B	214	PHE	CA-C-N	5.95	132.91	121.54
2	B	214	PHE	C-N-CA	5.95	132.91	121.54
2	B	230[A]	ASN	N-CA-C	5.75	117.55	111.28
2	B	230[B]	ASN	N-CA-C	5.75	117.55	111.28
2	B	129	ILE	N-CA-C	-5.33	106.47	111.48
2	B	6	PHE	CA-CB-CG	5.31	119.11	113.80
2	B	214	PHE	CB-CA-C	5.12	119.55	110.85
2	B	67	PHE	CA-C-O	-5.00	114.96	120.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	121	VAL	Mainchain

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	2008	2060	1974	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2580	2464	2398	26	0
3	B	42	0	0	2	0
4	A	32	0	0	3	0
4	B	39	0	0	1	0
All	All	4701	4524	4372	49	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (49) 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:1962:ARG:O	1:A:2013:ARG:NH1	2.21	0.73
1:A:1885:LYS:HB2	4:A:2101:HOH:O	1.87	0.73
1:A:1885:LYS:HD3	4:A:2101:HOH:O	1.93	0.69
1:A:1878:CYS:SG	1:A:1969:MET:HE3	2.33	0.68
1:A:1962:ARG:HD3	1:A:1962:ARG:H	1.64	0.62
1:A:2061:THR:O	1:A:2064:GLY:N	2.31	0.62
1:A:2064:GLY:O	1:A:2068:ASN:N	2.33	0.60
2:B:129:ILE:HD13	2:B:177[B]:ASN:O	2.02	0.59
2:B:1:MET:N	4:B:503:HOH:O	2.36	0.57
2:B:277:GLU:CD	2:B:277:GLU:H	2.13	0.56
2:B:129:ILE:HD13	2:B:177[A]:ASN:O	2.07	0.55
3:B:403:VXB:C8	3:B:403:VXB:C2	2.85	0.55
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.56	0.54
2:B:219:ASN:HB3	3:B:402:VXB:O1	2.07	0.54
2:B:1:MET:HB3	2:B:35:ASP:HA	1.89	0.53
2:B:209:MET:HA	2:B:213:ILE:HD12	1.91	0.53
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.92	0.51
1:A:2049:ILE:O	1:A:2053[A]:SER:OG	2.28	0.51
2:B:28:GLN:HG3	2:B:29:PRO:HD2	1.93	0.51
2:B:258:LYS:HD2	2:B:258:LYS:H	1.76	0.51
1:A:1895:HIS:O	1:A:1898[A]:VAL:HG22	2.13	0.48
2:B:287:ARG:O	2:B:291:ILE:HD13	2.13	0.48
1:A:1844:PHE:O	1:A:1885:LYS:NZ	2.32	0.47
1:A:2063:TYR:O	1:A:2067:TYR:HD1	1.98	0.47
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.99	0.45
1:A:2062:GLU:OE1	1:A:2065:ARG:NH1	2.50	0.43
1:A:1859:ARG:HH12	1:A:1979[A]:MET:CE	2.31	0.43
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.43	0.43
2:B:53:SER:O	2:B:54[A]:MET:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2045:ASP:O	1:A:2049:ILE:HG12	2.19	0.43
2:B:47:GLN:NE2	2:B:52:SER:O	2.43	0.43
2:B:59:TRP:CE2	2:B:226:PHE:HE1	2.37	0.43
2:B:190:ARG:HG3	2:B:203[B]:TYR:CZ	2.54	0.42
1:A:1973:LYS:NZ	4:A:2102:HOH:O	2.52	0.42
2:B:144:MET:HE2	2:B:176:LEU:HG	2.01	0.42
2:B:68:TYR:CE1	2:B:81:MET:HB2	2.55	0.42
1:A:1835:MET:HE3	1:A:1835:MET:HB3	1.94	0.42
1:A:2028:SER:O	1:A:2030:PRO:HD3	2.20	0.42
2:B:224:LEU:C	2:B:224:LEU:HD23	2.45	0.41
1:A:1857:VAL:HG13	1:A:1894:ILE:HG13	2.03	0.41
2:B:11:ILE:O	2:B:11:ILE:HG13	2.21	0.41
2:B:277:GLU:CD	2:B:277:GLU:N	2.78	0.41
2:B:282:ILE:H	2:B:282:ILE:HG12	1.67	0.41
2:B:1:MET:N	2:B:38:ILE:HD11	2.35	0.41
1:A:1992:TYR:O	1:A:1995:TRP:CG	2.74	0.41
2:B:51:ASN:HD21	2:B:53:SER:HB2	1.87	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	258/258 (100%)	248 (96%)	10 (4%)	0	100	100
2	B	315/308 (102%)	301 (96%)	13 (4%)	1 (0%)	36	24
All	All	573/566 (101%)	549 (96%)	23 (4%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	215	LYS

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	237/233 (102%)	232 (98%)	5 (2%)	47	23
2	B	294/284 (104%)	286 (97%)	8 (3%)	39	17
All	All	531/517 (103%)	518 (98%)	13 (2%)	43	20

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1988	LEU
1	A	2027	LEU
1	A	2032	ILE
1	A	2053[A]	SER
1	A	2053[B]	SER
2	B	88	LYS
2	B	92	ILE
2	B	124	ASP
2	B	129	ILE
2	B	281	ASP
2	B	282	ILE
2	B	283	LEU
2	B	295	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1863	HIS
1	A	1869	ASN
2	B	259	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	VXB	B	403	-	14,14,14	1.01	0	17,17,17	1.84	7 (41%)
3	VXB	B	401	-	14,14,14	3.31	6 (42%)	17,17,17	2.95	7 (41%)
3	VXB	B	402	-	14,14,14	1.04	0	17,17,17	1.18	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	VXB	B	403	-	-	2/9/9/9	0/1/1/1
3	VXB	B	401	-	-	1/9/9/9	0/1/1/1
3	VXB	B	402	-	-	2/9/9/9	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	VXB	C5-C6	6.81	1.51	1.38
3	B	401	VXB	C8-C4	6.14	1.48	1.39
3	B	401	VXB	O1-C3	-5.88	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	VXB	C7-C6	-3.35	1.32	1.38
3	B	401	VXB	BR-C6	2.57	1.95	1.90
3	B	401	VXB	C4-C3	-2.02	1.45	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	VXB	BR-C6-C5	-6.42	110.15	119.23
3	B	401	VXB	BR-C6-C7	5.62	127.61	119.68
3	B	401	VXB	C5-C4-C8	-5.47	112.31	117.92
3	B	403	VXB	O1-C3-N	-3.36	116.04	122.59
3	B	401	VXB	C1-C2-N	3.35	119.80	111.82
3	B	401	VXB	O1-C3-N	-3.11	116.54	122.59
3	B	403	VXB	C2-N-C3	3.10	129.11	122.11
3	B	403	VXB	C1-C2-N	-3.09	104.47	111.82
3	B	402	VXB	C2-N-C3	3.03	128.97	122.11
3	B	401	VXB	C8-N1-C7	2.87	121.41	117.51
3	B	403	VXB	BR-C6-C5	2.51	122.79	119.23
3	B	403	VXB	C4-C3-N	2.28	121.86	117.12
3	B	403	VXB	BR-C6-C7	-2.26	116.50	119.68
3	B	403	VXB	C4-C5-C6	-2.17	116.22	118.94
3	B	401	VXB	C4-C3-N	2.08	121.45	117.12

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	VXB	C4-C3-N-C2
3	B	402	VXB	O1-C3-N-C2
3	B	403	VXB	O1-C3-N-C2
3	B	403	VXB	C4-C3-N-C2
3	B	401	VXB	C2-C1-O-C

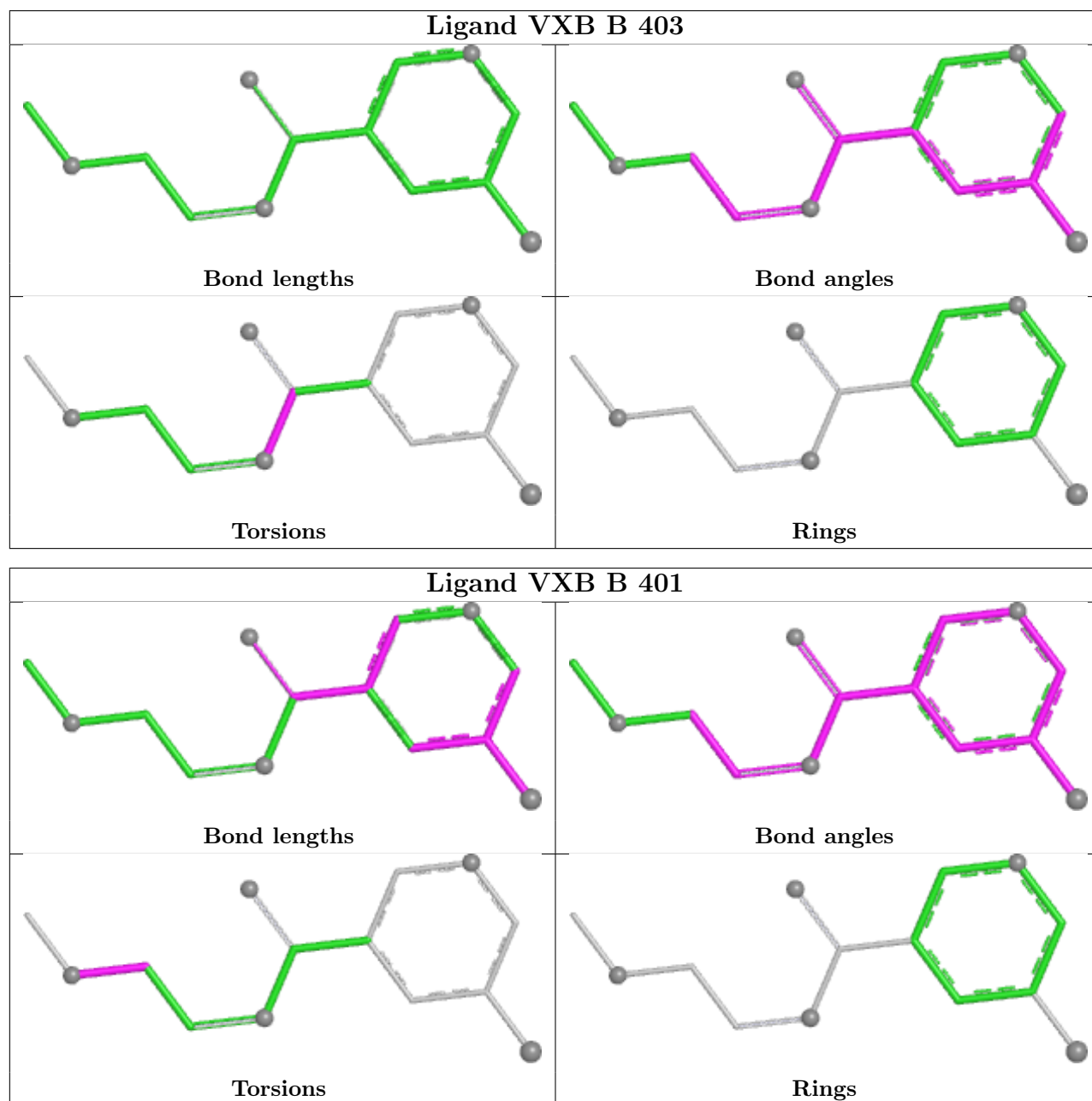
There are no ring outliers.

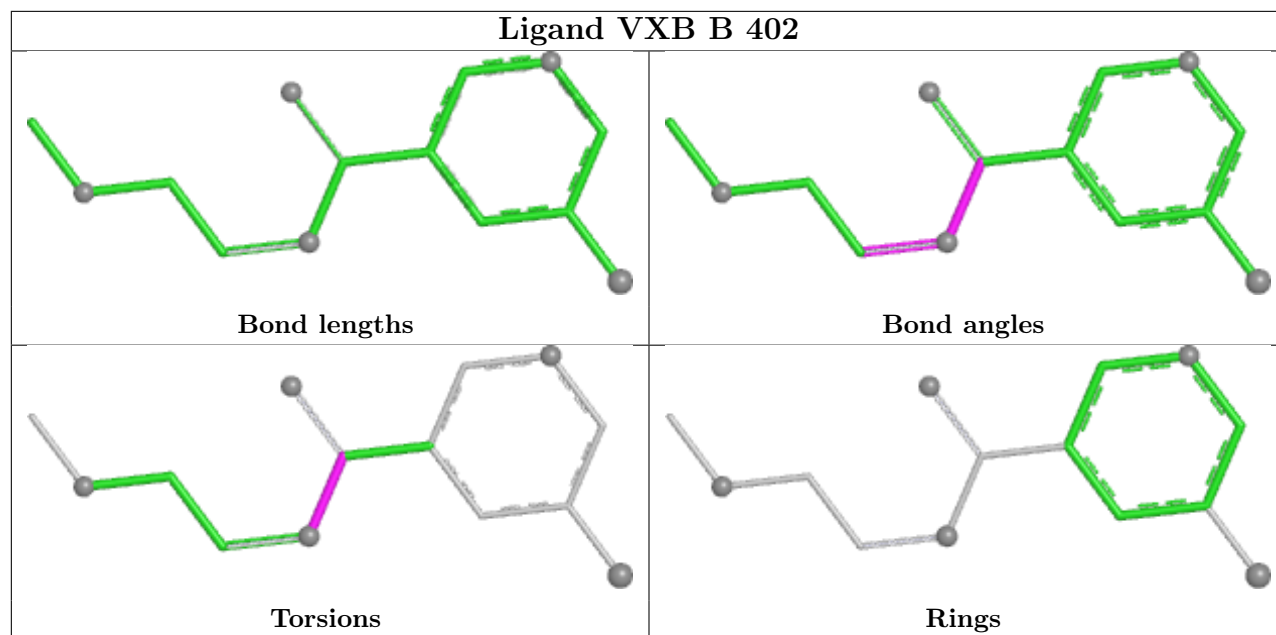
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	VXB	1	0
3	B	402	VXB	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/258 (91%)	2.20	103 (43%) 0 1	29, 73, 121, 184	12 (5%)
2	B	300/308 (97%)	2.00	132 (44%) 0 1	24, 67, 118, 178	9 (3%)
All	All	537/566 (94%)	2.09	235 (43%) 0 1	24, 71, 119, 184	21 (3%)

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1878	CYS	9.6
1	A	2039	LEU	8.0
1	A	2069	VAL	7.6
2	B	284	LEU	6.7
1	A	1979[A]	MET	6.7
2	B	54[A]	MET	6.5
1	A	2040	TRP	6.4
1	A	1860	VAL	6.3
1	A	2037	TYR	6.2
2	B	80	MET	6.2
2	B	152	LEU	5.8
1	A	1862	VAL	5.8
2	B	140	VAL	5.7
2	B	282	ILE	5.5
2	B	129	ILE	5.4
1	A	2038	HIS	5.3
1	A	2064	GLY	5.2
2	B	283	LEU	5.1
2	B	275	LEU	5.0
1	A	2026	LEU	5.0
2	B	208	VAL	5.0
2	B	213	ILE	4.9
1	A	2027	LEU	4.8
1	A	2063	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	203[A]	TYR	4.8
2	B	145	THR	4.8
2	B	122[A]	GLN	4.7
1	A	1866	PHE	4.7
2	B	170	SER	4.6
2	B	316	LEU	4.6
1	A	2034	ILE	4.6
1	A	1840	TYR	4.5
1	A	2051	ILE	4.5
2	B	193	HIS	4.5
2	B	220	TYR	4.5
1	A	2061	THR	4.5
2	B	214	PHE	4.5
1	A	2060	LEU	4.5
1	A	1940	MET	4.5
2	B	101	MET	4.5
1	A	2067	TYR	4.4
2	B	293	LEU	4.4
1	A	2001[A]	SER	4.3
2	B	108	ILE	4.2
1	A	2068	ASN	4.1
1	A	1968	ALA	4.1
2	B	1	MET	4.1
1	A	2065	ARG	4.1
2	B	81	MET	4.1
1	A	1956	ILE	4.1
1	A	1924	LEU	4.0
2	B	146	THR	4.0
1	A	1834	ALA	4.0
2	B	189	ILE	3.9
1	A	2059	ILE	3.9
2	B	279	TYR	3.9
2	B	22	PHE	3.9
2	B	24	VAL	3.8
1	A	1984	PRO	3.8
2	B	172	PRO	3.8
2	B	317	LEU	3.8
2	B	266	GLU	3.8
1	A	2028	SER	3.8
2	B	174	HIS	3.8
2	B	39	GLY	3.7
2	B	291	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	280	SER	3.7
2	B	289	TRP	3.7
1	A	2058	LEU	3.7
1	A	1969	MET	3.7
1	A	1963	LEU	3.6
2	B	92	ILE	3.6
2	B	134	GLU	3.6
2	B	295	SER	3.6
2	B	264	LEU	3.6
2	B	234	PHE	3.5
1	A	1906	SER	3.5
1	A	1943	PRO	3.5
1	A	2043	PHE	3.5
1	A	1944	LEU	3.5
1	A	1965	PHE	3.4
1	A	1835	MET	3.4
2	B	73	PRO	3.4
1	A	2025	ILE	3.4
2	B	124	ASP	3.4
2	B	38	ILE	3.4
2	B	130	VAL	3.4
1	A	1955	ALA	3.3
1	A	1855[A]	THR	3.3
1	A	1995	TRP	3.3
1	A	1875	ILE	3.3
1	A	1970	SER	3.3
2	B	267	ILE	3.3
1	A	2011	LEU	3.3
2	B	259	HIS	3.3
1	A	2014	ALA	3.3
2	B	313	TYR	3.2
1	A	2012	LEU	3.2
2	B	21	SER	3.2
2	B	48	HIS	3.2
2	B	89	PHE	3.1
2	B	258	LYS	3.1
1	A	1856[A]	ASN	3.1
2	B	13	VAL	3.1
2	B	191	PRO	3.1
1	A	1966	SER	3.1
1	A	2024[A]	MET	3.1
2	B	49	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	292	CYS	3.1
2	B	64[A]	MET	3.0
2	B	204[A]	TYR	3.0
2	B	26	GLU	3.0
1	A	1870	VAL	3.0
2	B	23	ASN	3.0
2	B	308	ILE	3.0
2	B	257	PRO	3.0
1	A	2017[A]	THR	2.9
1	A	1996	LEU	2.9
1	A	2041	PRO	2.9
2	B	131	ARG	2.9
2	B	173	ALA	2.9
2	B	150	ASN	2.9
2	B	294	TYR	2.9
2	B	77	LEU	2.9
2	B	29	PRO	2.9
1	A	2056[A]	ARG	2.9
2	B	96	PHE	2.9
1	A	1917	VAL	2.9
2	B	281	ASP	2.9
1	A	1931[A]	LYS	2.9
2	B	179	THR	2.8
2	B	111	ASP	2.8
2	B	262	ASP	2.8
2	B	180	VAL	2.8
1	A	2015	LEU	2.8
2	B	128	LYS	2.8
2	B	53	SER	2.8
2	B	237	TYR	2.8
2	B	268	LEU	2.8
1	A	1954	ILE	2.8
1	A	1833	GLY	2.8
1	A	1927	GLU	2.7
2	B	278	GLN	2.7
1	A	1994	ASP	2.7
1	A	1868	GLY	2.7
2	B	107	LYS	2.7
2	B	109	ASP	2.7
2	B	41[A]	VAL	2.7
1	A	1920	LEU	2.7
2	B	68	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1861	THR	2.7
1	A	2044	THR	2.7
2	B	3	THR	2.7
2	B	120	PHE	2.7
2	B	28	GLN	2.7
2	B	123[A]	MET	2.7
2	B	10	PRO	2.6
1	A	1918[A]	SER	2.6
1	A	1949	LEU	2.6
2	B	20	TYR	2.6
2	B	30	PHE	2.6
2	B	212[A]	GLY	2.6
2	B	84	ARG	2.6
2	B	103	VAL	2.6
1	A	1953	ASN	2.6
2	B	99	ARG	2.6
1	A	1961[A]	LEU	2.6
1	A	1879	ILE	2.6
2	B	183	PHE	2.5
2	B	199	LEU	2.5
1	A	1960[A]	GLU	2.5
1	A	1999	ILE	2.5
2	B	19	GLN	2.5
1	A	2032	ILE	2.5
1	A	1888	HIS	2.5
1	A	2031	THR	2.5
1	A	2030	PRO	2.5
2	B	276	PRO	2.5
2	B	132	LYS	2.5
1	A	1974	LEU	2.4
2	B	221	PHE	2.4
1	A	2013	ARG	2.4
1	A	1841	ALA	2.4
2	B	211[A]	GLN	2.4
2	B	40	HIS	2.4
1	A	1951	PHE	2.4
2	B	115	TYR	2.4
2	B	27	ASN	2.3
2	B	125	LYS	2.3
1	A	1844	PHE	2.3
1	A	2048	TRP	2.3
2	B	70	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1952	PRO	2.3
1	A	1964	PRO	2.3
1	A	2009	THR	2.3
1	A	2036	SER	2.3
1	A	1898[A]	VAL	2.3
2	B	93	VAL	2.3
2	B	301	SER	2.3
2	B	235	GLY	2.2
2	B	4	VAL	2.2
2	B	256	VAL	2.2
2	B	277	GLU	2.2
2	B	288	VAL	2.2
1	A	1922	ARG	2.2
1	A	1988	LEU	2.2
2	B	302	LEU	2.2
1	A	1851	PHE	2.2
1	A	2035	LYS	2.2
2	B	270	TYR	2.2
1	A	1933	ILE	2.2
2	B	7	THR	2.2
2	B	147	VAL	2.1
2	B	127	ARG	2.1
2	B	50	ASP	2.1
2	B	207	THR	2.1
2	B	233	PHE	2.1
2	B	44[A]	ILE	2.1
1	A	1962	ARG	2.1
1	A	1978	VAL	2.1
2	B	254	ALA	2.1
1	A	1863	HIS	2.1
2	B	142	SER	2.1
1	A	2005	PHE	2.1
1	A	1908	LEU	2.1
2	B	95	ASN	2.0
2	B	216	ASN	2.0
2	B	85	ASP	2.0
1	A	1959	THR	2.0
2	B	14	THR	2.0
1	A	1873	LYS	2.0
2	B	2	ASN	2.0
2	B	139	TYR	2.0
1	A	1837	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	299	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](#)

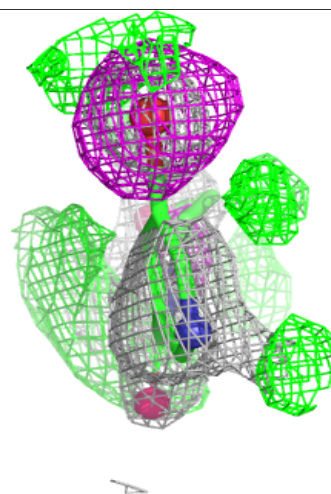
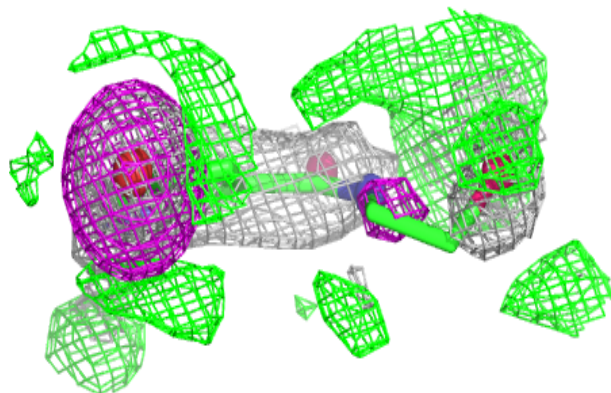
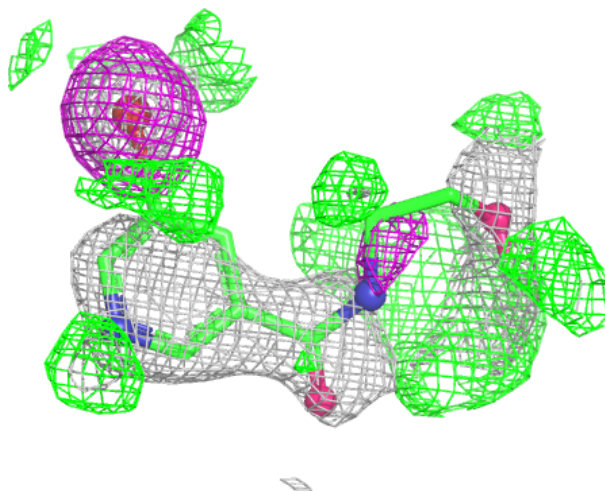
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	VXB	B	402	14/14	0.74	0.28	20,20,20,20	14
3	VXB	B	403	14/14	0.91	0.21	20,20,20,20	14
3	VXB	B	401	14/14	0.95	0.17	20,20,20,20	14

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.

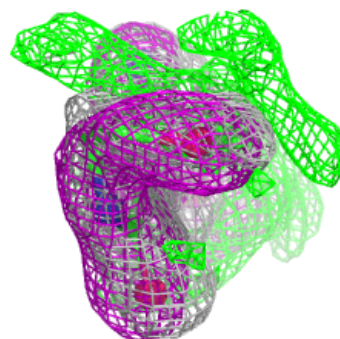
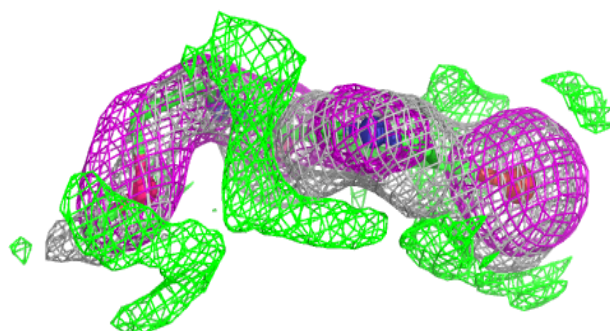
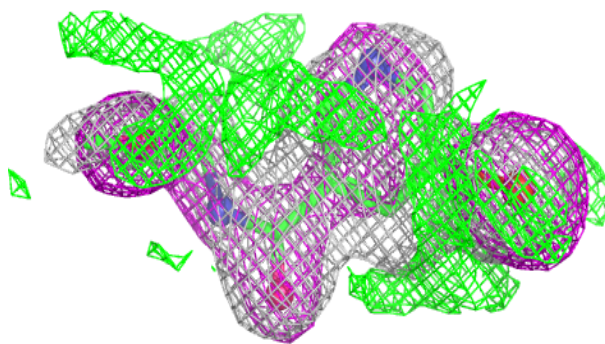
Electron density around VXB B 402:

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

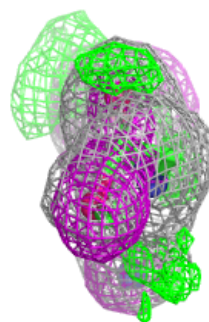
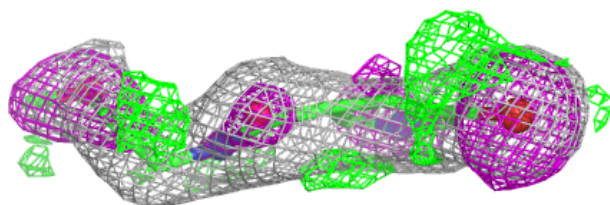
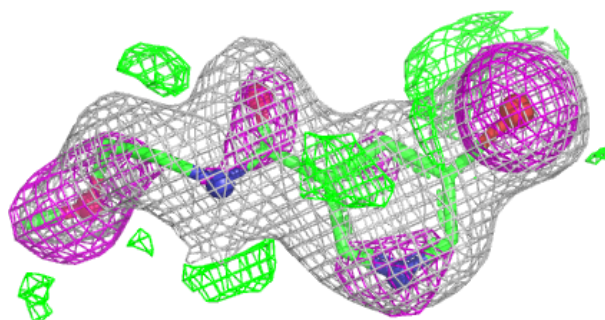


Electron density around VXB B 403:

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

**Electron density around VXB B 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.