



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:59 AM UTC

PDB ID : 7FNA / pdb_00007fna
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P07A11 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 : 1.69 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

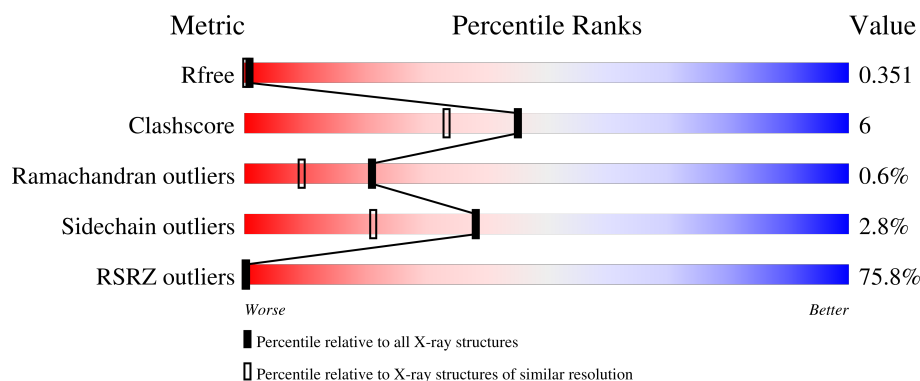
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	70% 76% 15% 8%
2	B	308	74% 80% 16% ..

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
3	VZ3	B	401	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9172 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	0	17	0

There are 20 discrepancies between the modelled and reference sequences:

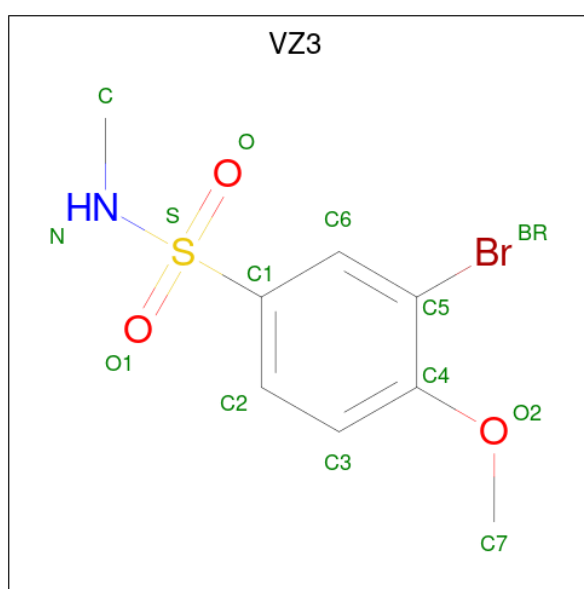
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	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 3-bromo-4-methoxy-N-methylbenzene-1-sulfonamide (CCD ID: VZ3) (formula: $C_8H_{10}BrNO_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	Br	C	N	O	S	0	0
			14	1	8	1	3	1		

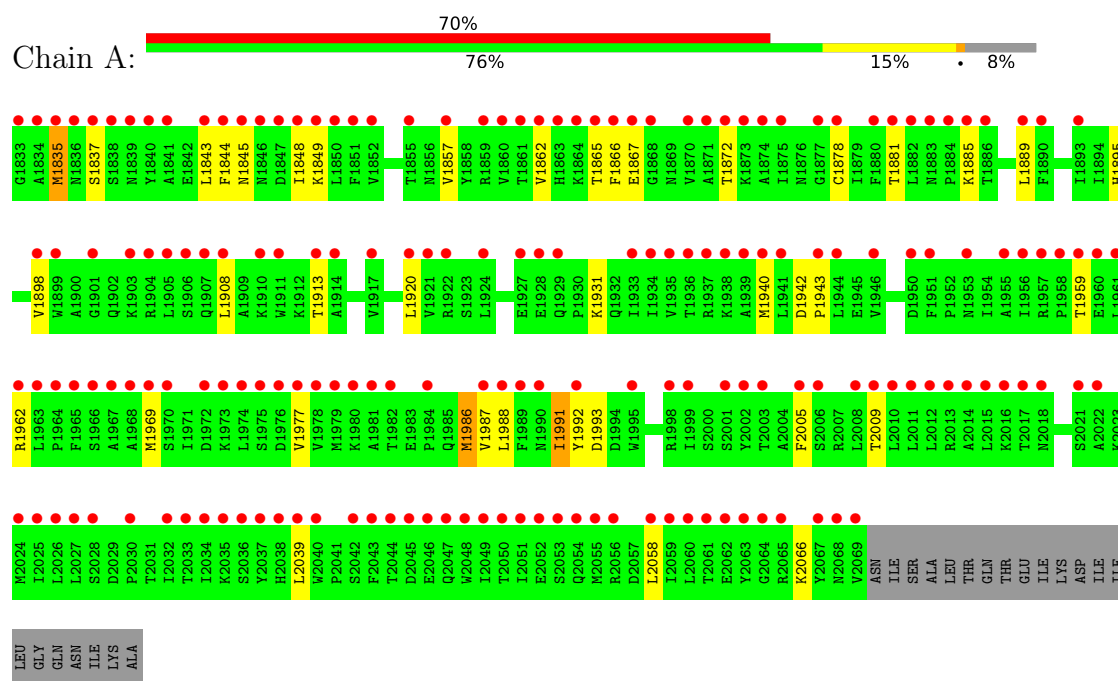
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	23	Total	O	0	0
			23	23		

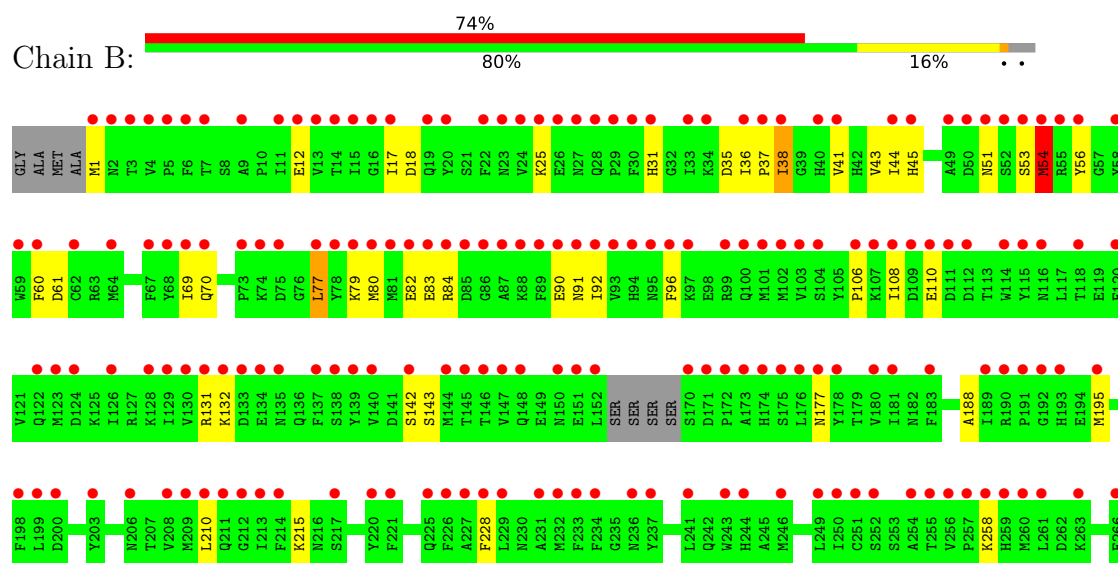
3 Residue-property plots

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



L267	L268	Y269	Y270	Q271	L272	K273	T274	L275	F276	E277	Q278	Y279	S280	D281	I282	L283	L284	M285	E286	R287	V288	W289	M290	I291	G292	L293	Y294	S295	S296	F297	Q298	R299	M300	S301	L302	H303	M304	T305	E306	K307	I308	M309	E310	M311	K312	Y313	P314	E315	L316	L317
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.14Å 81.28Å 93.19Å 90.00° 108.47° 90.00°	Depositor
Resolution (Å)	44.20 – 1.69 44.20 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.20-1.69) 99.6 (44.20-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.300 , 0.330 0.321 , 0.351	Depositor DCC
R_{free} test set	2091 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9172	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: VZ3

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	0.75	1/2149 (0.0%)	0.87	1/2911 (0.0%)
2	B	0.85	4/2739 (0.1%)	0.93	2/3699 (0.1%)
All	All	0.80	5/4888 (0.1%)	0.91	3/6610 (0.0%)

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	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1940	MET	SD-CE	-7.11	1.61	1.79
2	B	90	GLU	C-O	-5.83	1.17	1.24
2	B	31	HIS	CE1-NE2	-5.78	1.26	1.32
2	B	31	HIS	C-O	-5.19	1.16	1.24
2	B	70	GLN	C-O	-5.11	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	96	PHE	CA-CB-CG	7.63	121.43	113.80
2	B	31	HIS	CB-CA-C	7.43	123.06	111.02
1	A	1991	ILE	N-CA-C	5.92	120.28	112.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	54[A]	MET	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	2008	2060	1974	20	0
2	B	2580	2464	2398	35	0
3	B	14	0	0	1	0
4	A	23	0	0	0	0
4	B	23	0	0	2	0
All	All	4648	4524	4372	54	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 6.

All (54) 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)
2:B:12:GLU:HG3	2:B:25:LYS:HA	1.69	0.75
2:B:1:MET:N	4:B:501:HOH:O	2.23	0.72
2:B:54[B]:MET:HE1	2:B:143:SER:HB3	1.78	0.66
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.80	0.63
2:B:258:LYS:HD2	2:B:258:LYS:H	1.67	0.59
1:A:1878:CYS:SG	1:A:1969:MET:HE3	2.44	0.57
1:A:1895:HIS:O	1:A:1898[A]:VAL:HG22	2.06	0.56
1:A:1920:LEU:HD13	1:A:1986:MET:HE1	1.86	0.56
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.88	0.56
2:B:277:GLU:CD	2:B:277:GLU:H	2.15	0.55
1:A:1908:LEU:HA	2:B:195:MET:HE1	1.90	0.54
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.34	0.53
2:B:56:TYR:CZ	2:B:77:LEU:HB2	2.44	0.53
2:B:228:PHE:CD2	2:B:271:GLN:HG2	2.43	0.53
2:B:287:ARG:O	2:B:291:ILE:HD13	2.09	0.53
2:B:43:VAL:HG13	2:B:43:VAL:O	2.09	0.52
1:A:1844:PHE:O	1:A:1885:LYS:NZ	2.35	0.51
2:B:69:ILE:HD13	2:B:80:MET:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:LEU:N	2:B:77:LEU:HD23	2.26	0.50
2:B:1:MET:H2	2:B:38:ILE:HD11	1.78	0.48
2:B:91:ASN:HD22	2:B:91:ASN:C	2.22	0.48
1:A:1857:VAL:HG21	1:A:1913:THR:OG1	2.14	0.47
2:B:77:LEU:HD23	2:B:77:LEU:H	1.79	0.47
2:B:1:MET:N	2:B:38:ILE:HD11	2.28	0.47
2:B:92:ILE:HG21	3:B:401:VZ3:BR	2.70	0.46
1:A:2005:PHE:O	1:A:2009:THR:HG23	2.16	0.46
2:B:41[A]:VAL:HG12	4:B:521:HOH:O	2.15	0.45
2:B:44[B]:ILE:HG13	2:B:60:PHE:HE1	1.80	0.45
1:A:1992:TYR:O	1:A:1993:ASP:C	2.58	0.45
1:A:1881:THR:O	1:A:1889:LEU:HD12	2.17	0.45
2:B:77:LEU:N	2:B:77:LEU:CD2	2.80	0.44
2:B:1:MET:HB3	2:B:35:ASP:HA	2.00	0.44
2:B:51:ASN:HD21	2:B:53:SER:HB2	1.81	0.44
2:B:91:ASN:C	2:B:91:ASN:ND2	2.74	0.44
1:A:1991:ILE:HA	1:A:2039:LEU:HD12	2.00	0.44
1:A:1865:THR:O	1:A:1866:PHE:C	2.60	0.44
2:B:110:GLU:HG2	2:B:110:GLU:O	2.17	0.44
1:A:1867:GLU:OE1	1:A:1867:GLU:N	2.46	0.43
1:A:1977:VAL:HG21	1:A:1987:VAL:HG21	2.01	0.43
1:A:1942:ASP:O	1:A:1943:PRO:C	2.59	0.43
2:B:210:LEU:O	2:B:215:LYS:N	2.51	0.43
2:B:131:ARG:HG3	2:B:177[A]:ASN:ND2	2.34	0.42
2:B:300:ASN:O	2:B:303:HIS:NE2	2.52	0.42
2:B:38:ILE:H	2:B:38:ILE:HG13	1.66	0.42
2:B:36:ILE:HA	2:B:37:PRO:HD3	1.87	0.42
2:B:108:ILE:HG22	2:B:110:GLU:H	1.84	0.41
1:A:1845:ASN:OD1	1:A:1845:ASN:C	2.63	0.41
1:A:1862:VAL:HG22	1:A:1872:THR:HG22	2.03	0.41
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.69	0.41
2:B:17:ILE:O	2:B:18:ASP:C	2.63	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%)	254 (98%)	4 (2%)	0	100	100
2	B	315/308 (102%)	303 (96%)	8 (2%)	4 (1%)	9	2
All	All	573/566 (101%)	557 (97%)	12 (2%)	4 (1%)	21	7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	132	LYS
2	B	106	PRO
2	B	54[A]	MET
2	B	54[B]	MET

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%)	230 (97%)	7 (3%)	36	19
2	B	294/284 (104%)	286 (97%)	8 (3%)	39	23
All	All	531/517 (103%)	516 (97%)	15 (3%)	38	21

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1835	MET
1	A	1837	SER
1	A	1959	THR
1	A	1962	ARG
1	A	1986	MET
1	A	1988	LEU
1	A	2066	LYS
2	B	38	ILE

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Mol	Chain	Res	Type
2	B	45[A]	HIS
2	B	45[B]	HIS
2	B	77	LEU
2	B	83	GLU
2	B	84	ARG
2	B	142	SER
2	B	295	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1869	ASN
1	A	1947	HIS
2	B	23	ASN
2	B	40	HIS
2	B	91	ASN
2	B	135	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	VZ3	B	401	-	14,14,14	4.15	8 (57%)	20,20,20	3.55	14 (70%)

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	VZ3	B	401	-	-	4/11/11/11	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	VZ3	BR-C5	-9.89	1.67	1.89
3	B	401	VZ3	C1-S	-6.09	1.67	1.76
3	B	401	VZ3	C2-C3	-5.21	1.30	1.38
3	B	401	VZ3	S-N	-4.96	1.54	1.61
3	B	401	VZ3	O-S	-4.94	1.37	1.43
3	B	401	VZ3	O2-C7	-3.35	1.33	1.42
3	B	401	VZ3	C4-C5	-3.34	1.32	1.39
3	B	401	VZ3	O1-S	-2.43	1.40	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	VZ3	C6-C1-S	7.47	126.70	119.06
3	B	401	VZ3	O2-C4-C5	6.63	126.82	116.84
3	B	401	VZ3	O2-C4-C3	-4.73	116.33	124.30
3	B	401	VZ3	C3-C2-C1	4.57	123.89	119.44
3	B	401	VZ3	C1-S-N	3.70	112.63	107.55
3	B	401	VZ3	C6-C5-C4	3.68	125.61	121.14
3	B	401	VZ3	C1-C6-C5	-3.65	116.38	119.13
3	B	401	VZ3	BR-C5-C4	-3.62	115.15	119.62
3	B	401	VZ3	O1-S-C1	-3.38	103.72	107.98
3	B	401	VZ3	C2-C1-S	-3.22	116.21	119.76
3	B	401	VZ3	C2-C1-C6	-3.05	116.90	120.68
3	B	401	VZ3	O-S-N	2.79	112.21	107.06
3	B	401	VZ3	C-N-S	2.27	122.16	119.16
3	B	401	VZ3	O1-S-N	-2.22	102.97	107.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

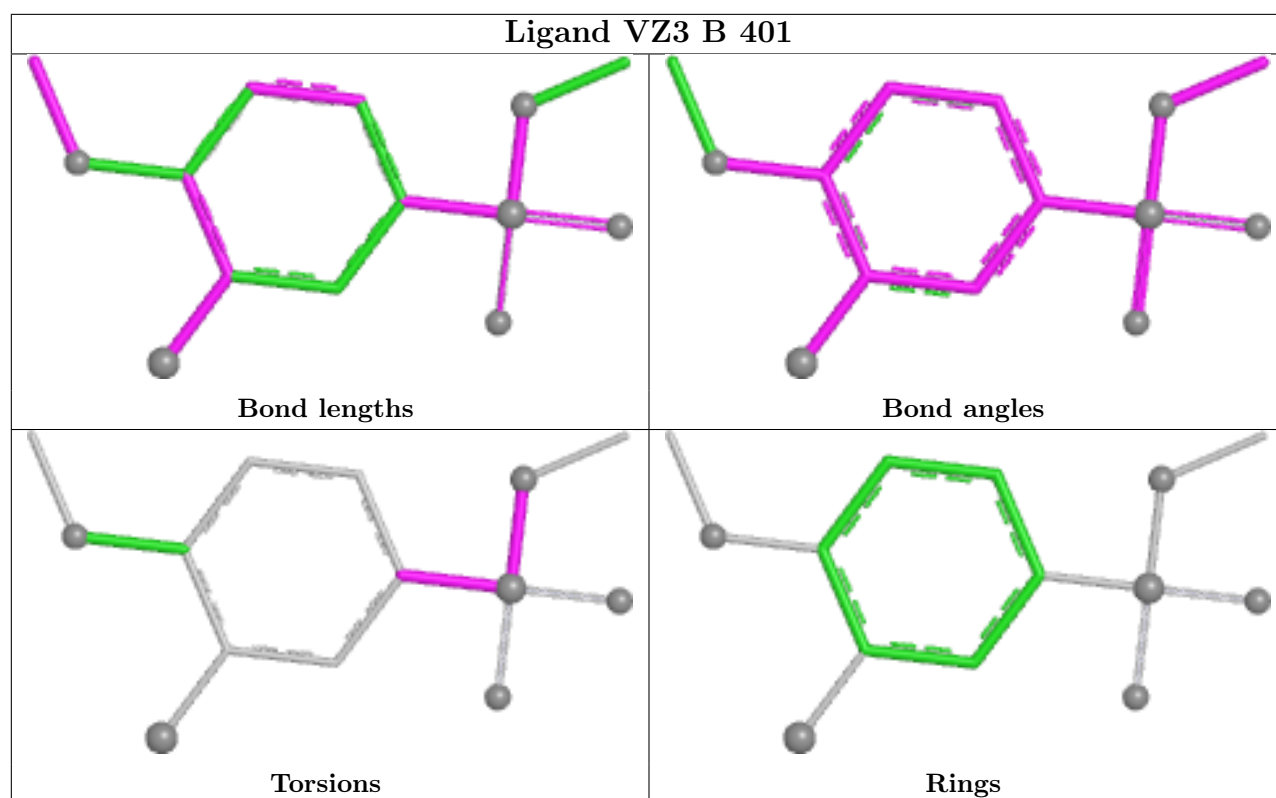
Mol	Chain	Res	Type	Atoms
3	B	401	VZ3	C-N-S-O1
3	B	401	VZ3	C-N-S-C1
3	B	401	VZ3	C-N-S-O
3	B	401	VZ3	C2-C1-S-O

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	VZ3	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%)	3.06	180 (75%) 0 0	22, 66, 116, 185	12 (5%)
2	B	300/308 (97%)	2.90	227 (75%) 0 0	18, 64, 129, 230	9 (3%)
All	All	537/566 (94%)	2.97	407 (75%) 0 0	18, 65, 122, 230	21 (3%)

All (407) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2040	TRP	10.4
2	B	54[A]	MET	9.7
2	B	31	HIS	9.4
1	A	1979[A]	MET	9.4
2	B	246	MET	8.9
2	B	152	LEU	8.0
1	A	2063	TYR	8.0
1	A	2048	TRP	7.6
2	B	316	LEU	7.2
1	A	1840	TYR	7.0
2	B	41[A]	VAL	7.0
1	A	2039	LEU	6.9
1	A	1878	CYS	6.6
2	B	203[A]	TYR	6.6
1	A	2069	VAL	6.5
1	A	1834	ALA	6.5
1	A	1861	THR	6.4
1	A	1898[A]	VAL	6.3
1	A	2059	ILE	6.3
1	A	1920	LEU	6.2
2	B	170	SER	6.2
2	B	1	MET	6.0
1	A	2037	TYR	5.9
2	B	103	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
2	B	22	PHE	5.9
2	B	89	PHE	5.9
2	B	92	ILE	5.9
1	A	1881	THR	5.9
1	A	1924	LEU	5.9
1	A	2043	PHE	5.9
2	B	232	MET	5.7
2	B	68	TYR	5.6
1	A	2017[A]	THR	5.6
2	B	272	ILE	5.6
1	A	1967	ALA	5.5
2	B	174	HIS	5.4
2	B	289	TRP	5.3
1	A	2067	TYR	5.3
2	B	16	GLY	5.3
1	A	1863	HIS	5.3
1	A	2060	LEU	5.2
2	B	283	LEU	5.2
2	B	284	LEU	5.2
2	B	97	LYS	5.1
1	A	1940	MET	5.1
2	B	213	ILE	5.1
2	B	172	PRO	5.1
2	B	101	MET	5.0
1	A	2009	THR	5.0
2	B	276	PRO	5.0
2	B	313	TYR	5.0
2	B	87	ALA	4.9
1	A	2028	SER	4.9
2	B	173	ALA	4.8
1	A	1950	ASP	4.8
2	B	237	TYR	4.7
1	A	2049	ILE	4.7
1	A	1988	LEU	4.7
2	B	176	LEU	4.7
2	B	11	ILE	4.7
2	B	282	ILE	4.7
1	A	1837	SER	4.7
2	B	290	ASN	4.7
1	A	1875	ILE	4.7
1	A	1841	ALA	4.7
1	A	1977	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	2061	THR	4.6
1	A	1966	SER	4.6
1	A	1866	PHE	4.5
1	A	2027	LEU	4.5
2	B	254	ALA	4.5
2	B	288	VAL	4.5
1	A	2038	HIS	4.5
2	B	302	LEU	4.5
2	B	291	ILE	4.5
1	A	1871	ALA	4.4
1	A	1865	THR	4.4
2	B	292	CYS	4.4
2	B	95	ASN	4.4
2	B	217	SER	4.4
2	B	212[A]	GLY	4.4
1	A	1978	VAL	4.3
2	B	24	VAL	4.3
2	B	263	LYS	4.3
2	B	269	TYR	4.3
2	B	13	VAL	4.3
1	A	1868	GLY	4.3
2	B	96	PHE	4.2
2	B	279	TYR	4.2
1	A	2058	LEU	4.2
1	A	1870	VAL	4.2
2	B	150	ASN	4.2
1	A	1927	GLU	4.2
2	B	14	THR	4.2
1	A	1852	VAL	4.2
2	B	88	LYS	4.1
1	A	1833	GLY	4.1
1	A	2002[A]	TYR	4.1
2	B	108	ILE	4.1
1	A	1953	ASN	4.1
1	A	1908	LEU	4.0
2	B	130	VAL	4.0
1	A	2021	SER	4.0
1	A	1886	THR	4.0
2	B	80	MET	4.0
1	A	2065	ARG	4.0
2	B	181	ILE	3.9
1	A	2015	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	233	PHE	3.9
2	B	114	TRP	3.9
1	A	1965	PHE	3.9
1	A	2022	ALA	3.9
2	B	293	LEU	3.8
2	B	317	LEU	3.8
2	B	234	PHE	3.8
1	A	1835	MET	3.8
2	B	275	LEU	3.8
1	A	1958	PRO	3.8
1	A	2056[A]	ARG	3.8
2	B	211[A]	GLN	3.8
2	B	145	THR	3.8
2	B	267	ILE	3.8
2	B	278	GLN	3.8
1	A	2032	ILE	3.7
2	B	50	ASP	3.7
1	A	1974	LEU	3.7
1	A	2044	THR	3.7
2	B	109	ASP	3.7
1	A	2051	ILE	3.7
2	B	15	ILE	3.7
1	A	1836	ASN	3.7
1	A	1951	PHE	3.7
2	B	6	PHE	3.7
2	B	17	ILE	3.7
2	B	256	VAL	3.7
1	A	1984	PRO	3.7
2	B	120	PHE	3.6
1	A	1943	PRO	3.6
2	B	86	GLY	3.6
2	B	53	SER	3.6
1	A	1941	LEU	3.6
1	A	1963	LEU	3.6
2	B	122[A]	GLN	3.6
2	B	20	TYR	3.6
2	B	73	PRO	3.6
1	A	2053[A]	SER	3.5
1	A	1904	ARG	3.5
1	A	2025	ILE	3.5
2	B	221	PHE	3.5
1	A	1937	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1957	ARG	3.5
2	B	297	PHE	3.5
1	A	1862	VAL	3.5
2	B	90	GLU	3.5
2	B	29	PRO	3.5
2	B	131	ARG	3.5
2	B	171	ASP	3.4
1	A	1867	GLU	3.4
2	B	178[A]	TYR	3.4
2	B	27	ASN	3.4
2	B	112	ASP	3.4
1	A	1969	MET	3.4
2	B	111	ASP	3.4
1	A	1921	VAL	3.4
1	A	2068	ASN	3.4
2	B	33	ILE	3.3
2	B	126	ILE	3.3
1	A	1889	LEU	3.3
1	A	2010	LEU	3.3
1	A	1860	VAL	3.3
1	A	1914	ALA	3.3
1	A	2064	GLY	3.3
1	A	1933	ILE	3.3
2	B	268	LEU	3.3
2	B	280	SER	3.3
2	B	301	SER	3.3
1	A	1857	VAL	3.3
1	A	1968	ALA	3.3
2	B	49	ALA	3.3
2	B	99	ARG	3.3
2	B	249	LEU	3.3
2	B	124	ASP	3.3
2	B	4	VAL	3.3
1	A	2012	LEU	3.2
2	B	84	ARG	3.2
2	B	129	ILE	3.2
2	B	307	LYS	3.2
1	A	1874	ALA	3.2
2	B	55[A]	ARG	3.2
1	A	1960[A]	GLU	3.2
1	A	1956	ILE	3.2
2	B	128	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1906	SER	3.2
1	A	1981	ALA	3.2
2	B	191	PRO	3.1
1	A	1893	ILE	3.1
2	B	85	ASP	3.1
2	B	83	GLU	3.1
1	A	1911	TRP	3.1
1	A	1936	THR	3.1
1	A	2035	LYS	3.1
1	A	1970	SER	3.1
1	A	1846	ASN	3.1
1	A	1880	PHE	3.1
2	B	305	THR	3.1
2	B	147	VAL	3.1
2	B	106	PRO	3.1
2	B	209	MET	3.1
1	A	2046	GLU	3.1
1	A	2042	SER	3.1
1	A	2030	PRO	3.0
2	B	257	PRO	3.0
2	B	193	HIS	3.0
1	A	2055	MET	3.0
2	B	140	VAL	3.0
2	B	59	TRP	3.0
2	B	82	GLU	3.0
2	B	294	TYR	3.0
2	B	94	HIS	3.0
2	B	19	GLN	3.0
1	A	1962	ARG	3.0
1	A	1939	ALA	3.0
1	A	1928	GLU	3.0
2	B	52	SER	2.9
1	A	2024[A]	MET	2.9
2	B	144	MET	2.9
1	A	2033	THR	2.9
2	B	56	TYR	2.9
1	A	2062	GLU	2.9
2	B	110	GLU	2.9
2	B	38	ILE	2.9
2	B	69	ILE	2.9
1	A	1859	ARG	2.9
2	B	67	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1838	SER	2.9
1	A	1873	LYS	2.9
2	B	45[A]	HIS	2.9
1	A	2052	GLU	2.9
2	B	220	TYR	2.9
1	A	2013	ARG	2.9
1	A	1844	PHE	2.9
1	A	1959	THR	2.9
1	A	1944	LEU	2.9
1	A	2026	LEU	2.9
2	B	295	SER	2.9
2	B	214	PHE	2.8
2	B	226	PHE	2.8
1	A	2047	GLN	2.8
1	A	2014	ALA	2.8
1	A	1872	THR	2.8
2	B	7	THR	2.8
2	B	40	HIS	2.8
2	B	190	ARG	2.8
2	B	287	ARG	2.8
2	B	277	GLU	2.8
1	A	2001[A]	SER	2.8
2	B	9	ALA	2.8
2	B	60	PHE	2.8
2	B	183	PHE	2.8
1	A	2018[A]	ASN	2.8
1	A	1907	GLN	2.7
1	A	1990	ASN	2.7
1	A	1843	LEU	2.7
2	B	286	GLU	2.7
2	B	51	ASN	2.7
2	B	123[A]	MET	2.7
2	B	198	PHE	2.7
1	A	1917	VAL	2.7
2	B	93	VAL	2.7
2	B	208	VAL	2.7
1	A	2006	SER	2.7
2	B	70	GLN	2.7
1	A	1955	ALA	2.7
1	A	1989	PHE	2.7
1	A	1882	LEU	2.7
2	B	285	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	312	LYS	2.7
1	A	1972	ASP	2.7
2	B	281	ASP	2.7
1	A	2005	PHE	2.6
2	B	299	LYS	2.6
2	B	102	MET	2.6
1	A	1975	SER	2.6
1	A	1849	LYS	2.6
1	A	1982	THR	2.6
1	A	1905	LEU	2.6
1	A	2008	LEU	2.6
2	B	259	HIS	2.6
1	A	2016	LYS	2.6
2	B	5	PRO	2.6
2	B	74	LYS	2.6
2	B	310	GLU	2.6
1	A	1847	ASP	2.6
1	A	1976	ASP	2.6
2	B	210	LEU	2.6
2	B	251	CYS	2.6
2	B	308	ILE	2.6
2	B	135	ASN	2.6
2	B	274	THR	2.5
1	A	1839	ASN	2.5
2	B	227	ALA	2.5
1	A	1913	THR	2.5
2	B	3	THR	2.5
2	B	25	LYS	2.5
2	B	104	SER	2.5
1	A	1883	ASN	2.5
1	A	1998	ARG	2.5
2	B	2	ASN	2.5
2	B	311	ASN	2.5
1	A	2011	LEU	2.5
2	B	241	LEU	2.5
2	B	133	ASP	2.5
1	A	2050	THR	2.5
2	B	142	SER	2.5
2	B	229	LEU	2.5
2	B	115	TYR	2.5
2	B	231	ALA	2.5
1	A	1885	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	180	VAL	2.5
2	B	12	GLU	2.5
2	B	81	MET	2.5
2	B	266	GLU	2.5
2	B	175	SER	2.5
2	B	243	TRP	2.4
2	B	30	PHE	2.4
2	B	77	LEU	2.4
2	B	132	LYS	2.4
2	B	26	GLU	2.4
2	B	270	TYR	2.4
2	B	300	ASN	2.4
2	B	79	LYS	2.4
2	B	151	GLU	2.4
2	B	62	CYS	2.4
2	B	199	LEU	2.4
2	B	236	ASN	2.4
2	B	36	ILE	2.4
2	B	189	ILE	2.4
2	B	309	MET	2.4
2	B	296	SER	2.4
2	B	134	GLU	2.4
2	B	107	LYS	2.4
2	B	91	ASN	2.3
1	A	1855[A]	THR	2.3
2	B	255	THR	2.3
1	A	1910	LYS	2.3
1	A	1938	LYS	2.3
2	B	137	PHE	2.3
2	B	260	MET	2.3
2	B	78	TYR	2.3
1	A	1999	ILE	2.3
1	A	2045	ASP	2.3
1	A	1964	PRO	2.3
1	A	1980[A]	LYS	2.3
2	B	37	PRO	2.3
2	B	146	THR	2.3
1	A	1890	PHE	2.3
2	B	192	GLY	2.3
2	B	34	LYS	2.3
2	B	195	MET	2.3
2	B	244	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	28	GLN	2.3
2	B	100	GLN	2.3
1	A	1961[A]	LEU	2.3
2	B	138	SER	2.3
1	A	1992	TYR	2.3
2	B	258	LYS	2.3
2	B	314	PRO	2.2
2	B	200	ASP	2.2
1	A	1929	GLN	2.2
1	A	1922	ARG	2.2
1	A	1903	LYS	2.2
1	A	2036	SER	2.2
1	A	1850	LEU	2.2
2	B	58	TYR	2.2
1	A	2034	ILE	2.2
1	A	1884	PRO	2.2
2	B	118	THR	2.2
1	A	1935	VAL	2.2
1	A	1946	VAL	2.1
1	A	1987	VAL	2.1
1	A	1901	GLY	2.1
1	A	1899[A]	TRP	2.1
2	B	261	LEU	2.1
1	A	1851	PHE	2.1
2	B	75	ASP	2.1
2	B	228	PHE	2.1
2	B	148	GLN	2.1
1	A	1877	GLY	2.1
1	A	1845	ASN	2.1
2	B	64[A]	MET	2.1
2	B	298	GLN	2.1
2	B	250	ILE	2.1
2	B	116	ASN	2.1
2	B	206	ASN	2.1
2	B	225	GLN	2.1
1	A	1973	LYS	2.1
1	A	1934	ILE	2.1
2	B	44[A]	ILE	2.1
2	B	23	ASN	2.0
1	A	2054[A]	GLN	2.0
1	A	2003	THR	2.0
1	A	1864	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	177[A]	ASN	2.0
1	A	1995	TRP	2.0
1	A	1848	ILE	2.0
2	B	139	TYR	2.0
2	B	252	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

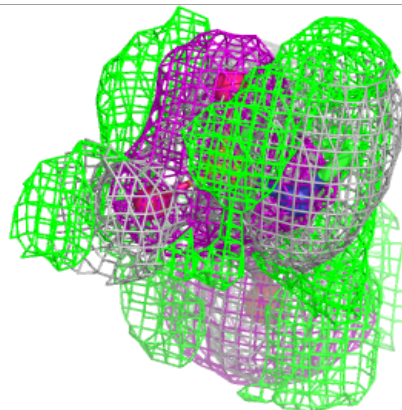
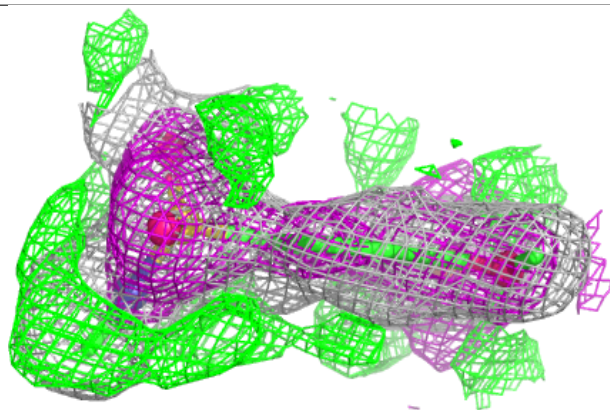
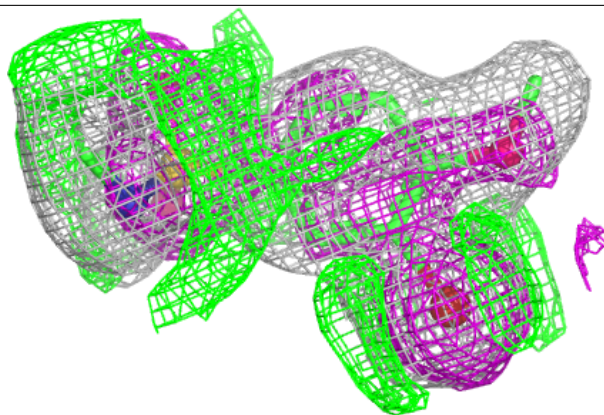
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	VZ3	B	401	14/14	0.85	0.26	20,20,20,20	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 VZ3 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.