



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:32 AM UTC

PDB ID : 3PRZ / pdb_00003prz
Title : Quinazolines with intra-molecular hydrogen bonding scaffold (iMHBS) as PI3K/mTOR dual inhibitors.
Authors : Knighton, D.R.; Greasley, S.E.; Rodgers, C.M.-L.
Deposited on : 2010-11-30
Resolution : 2.60 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

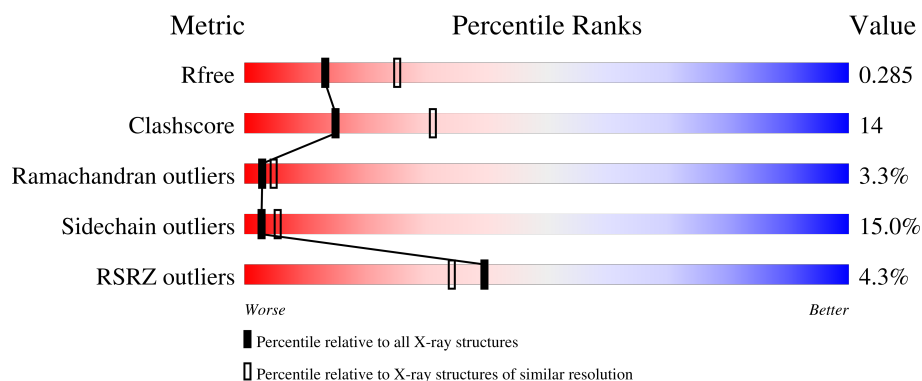
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	626	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6836 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.

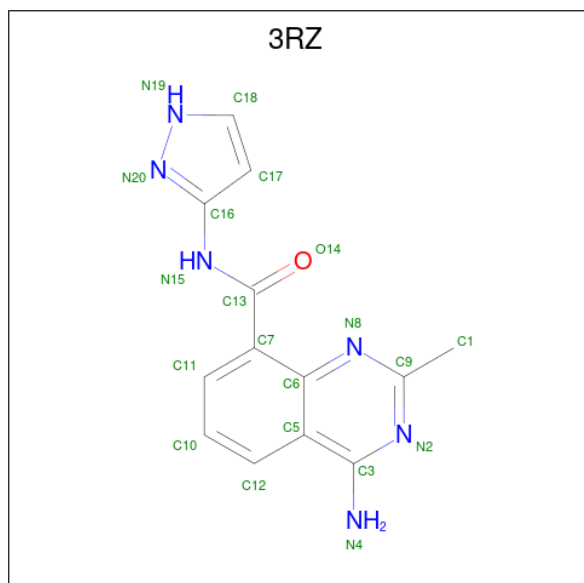
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	844	6816	4385	1158	1238	35	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	initiating methionine	UNP P48736
A	1103	HIS	-	expression tag	UNP P48736
A	1104	HIS	-	expression tag	UNP P48736
A	1105	HIS	-	expression tag	UNP P48736
A	1106	HIS	-	expression tag	UNP P48736
A	1107	HIS	-	expression tag	UNP P48736
A	1108	HIS	-	expression tag	UNP P48736

- Molecule 2 is 4-amino-2-methyl-N-(1H-pyrazol-3-yl)quinazoline-8-carboxamide (CCD ID: 3RZ) (formula: C₁₃H₁₂N₆O).

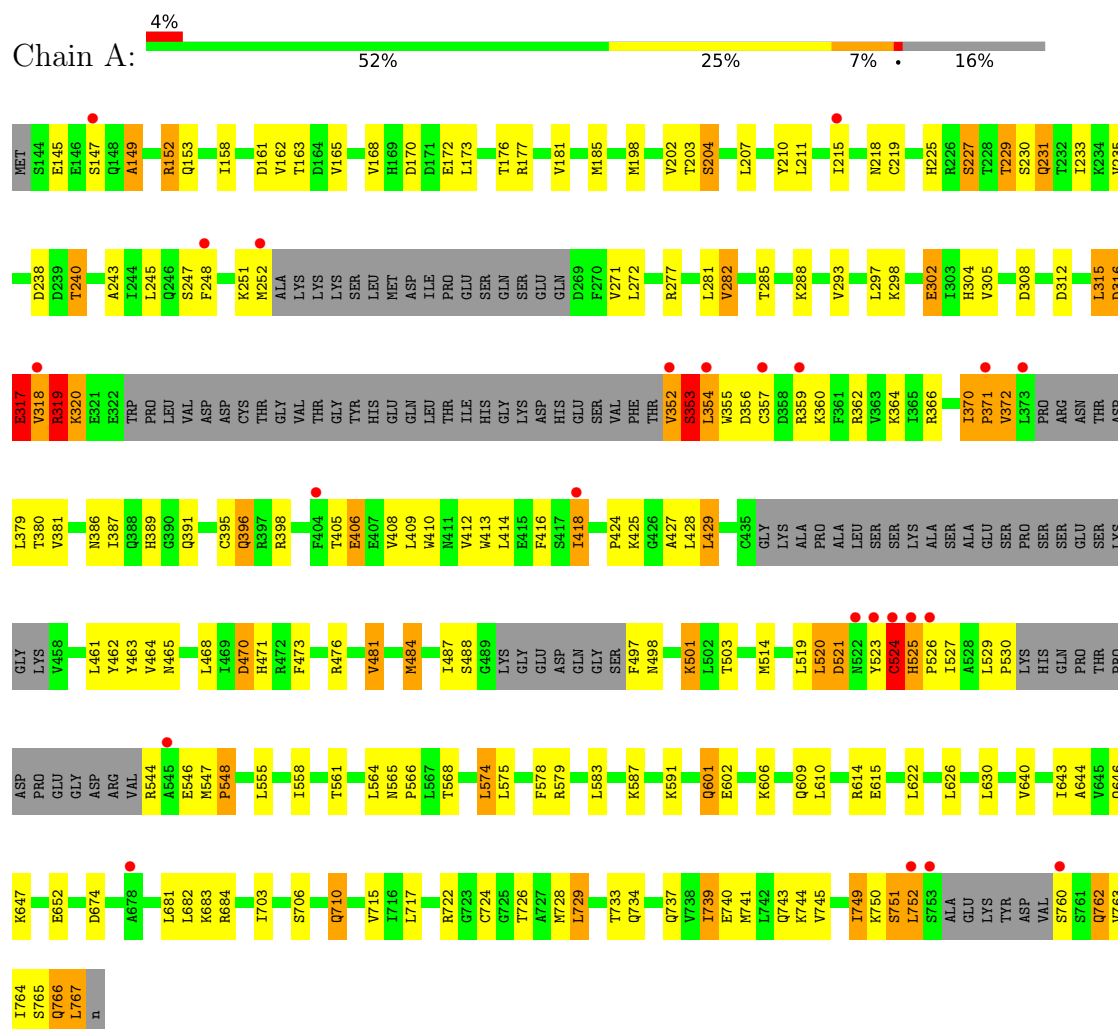


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	13	6	1		

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: Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.87Å 67.19Å 106.44Å 90.00° 95.65° 90.00°	Depositor
Resolution (Å)	44.73 – 2.60 44.73 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.4 (44.73-2.60) 97.3 (44.73-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.61Å)	Xtriage
Refinement program	CNS, BUSTER 2.9.6	Depositor
R, R_{free}	0.250 , 0.281 0.250 , 0.285	Depositor DCC
R_{free} test set	1529 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.9	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	6836	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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: 3RZ

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	0.81	1/6963 (0.0%)	1.48	48/9423 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	804	MET	SD-CE	-7.22	1.61	1.79

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	906	VAL	N-CA-C	11.01	121.68	110.23
1	A	524	CYS	CA-C-N	6.75	133.86	121.70
1	A	524	CYS	C-N-CA	6.75	133.86	121.70
1	A	429	LEU	N-CA-C	-6.72	98.97	109.25
1	A	1078	LYS	N-CA-C	6.62	119.50	111.82
1	A	971	ASN	CA-CB-CG	6.42	119.02	112.60
1	A	905	GLU	CA-C-N	6.15	128.82	120.77
1	A	905	GLU	C-N-CA	6.15	128.82	120.77
1	A	514	MET	N-CA-C	-6.00	101.60	110.48
1	A	470	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	681	LEU	CA-C-N	5.70	128.18	120.65
1	A	681	LEU	C-N-CA	5.70	128.18	120.65
1	A	498	ASN	CA-C-N	5.60	128.56	120.38
1	A	498	ASN	C-N-CA	5.60	128.56	120.38
1	A	308	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	481	VAL	N-CA-CB	5.55	119.21	112.10
1	A	947	ARG	CA-C-N	5.53	129.62	120.94
1	A	947	ARG	C-N-CA	5.53	129.62	120.94
1	A	744	LYS	CA-C-N	5.51	127.71	120.60
1	A	744	LYS	C-N-CA	5.51	127.71	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	ALA	CA-C-N	5.50	127.64	120.28
1	A	149	ALA	C-N-CA	5.50	127.64	120.28
1	A	161	ASP	CA-C-N	5.38	127.34	120.56
1	A	161	ASP	C-N-CA	5.38	127.34	120.56
1	A	1044	SER	CA-C-N	5.37	131.79	121.54
1	A	1044	SER	C-N-CA	5.37	131.79	121.54
1	A	684	ARG	N-CA-C	5.36	117.21	111.36
1	A	484	MET	N-CA-C	5.36	118.84	110.32
1	A	319	ARG	CA-C-N	5.31	131.69	121.54
1	A	319	ARG	C-N-CA	5.31	131.69	121.54
1	A	1056	THR	CB-CA-C	5.31	119.91	111.95
1	A	470	ASP	CA-C-N	5.31	129.09	120.60
1	A	470	ASP	C-N-CA	5.31	129.09	120.60
1	A	1012	ILE	CA-C-N	5.25	127.62	120.54
1	A	1012	ILE	C-N-CA	5.25	127.62	120.54
1	A	170	ASP	CA-CB-CG	5.24	117.83	112.60
1	A	1008	LYS	N-CA-C	-5.17	105.64	111.28
1	A	503	THR	N-CA-C	5.17	117.53	110.24
1	A	765	SER	CA-C-N	5.15	127.43	120.38
1	A	765	SER	C-N-CA	5.15	127.43	120.38
1	A	923	ALA	N-CA-C	-5.14	105.13	111.40
1	A	836	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	937	VAL	CA-C-N	5.10	127.43	120.54
1	A	937	VAL	C-N-CA	5.10	127.43	120.54
1	A	843	LEU	CA-C-N	5.07	126.95	120.56
1	A	843	LEU	C-N-CA	5.07	126.95	120.56
1	A	884	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	904	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

There are no planarity outliers.

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	6816	0	6843	188	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	20	0	12	0	0
All	All	6836	0	6855	188	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 14.

All (188) 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:997:THR:HG21	1:A:1076:ARG:HH12	1.27	1.00
1:A:851:MET:HE1	1:A:938:ALA:HB1	1.48	0.92
1:A:352:VAL:N	1:A:526:PRO:O	2.03	0.92
1:A:766:GLN:HE21	1:A:766:GLN:H	1.20	0.90
1:A:804:MET:HE2	1:A:812:TRP:HB2	1.54	0.89
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.53	0.88
1:A:966:GLY:O	1:A:970:GLY:HA3	1.73	0.88
1:A:470:ASP:HB3	1:A:476:ARG:NH2	1.95	0.82
1:A:786:PRO:HD2	1:A:878:MET:HE1	1.63	0.79
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.64	0.78
1:A:916:PRO:HD2	1:A:920:LYS:HD2	1.65	0.77
1:A:775:GLN:HE22	1:A:796:LEU:H	1.32	0.77
1:A:997:THR:HG21	1:A:1076:ARG:NH1	1.98	0.76
1:A:558:ILE:O	1:A:561:THR:HG22	1.87	0.75
1:A:470:ASP:HB3	1:A:476:ARG:HH21	1.51	0.74
1:A:862:LEU:HD11	1:A:1016:ALA:HB2	1.70	0.73
1:A:147:SER:HB3	1:A:319:ARG:HH21	1.54	0.73
1:A:908:ASN:HD22	1:A:994:VAL:HA	1.54	0.72
1:A:762:GLN:O	1:A:766:GLN:NE2	2.24	0.70
1:A:487:ILE:HG22	1:A:488:SER:H	1.57	0.69
1:A:152:ARG:HH11	1:A:152:ARG:HB2	1.57	0.69
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.76	0.68
1:A:750:LYS:HZ1	1:A:834:HIS:HD2	1.42	0.68
1:A:177:ARG:HG2	1:A:715:VAL:HG13	1.76	0.67
1:A:851:MET:HE1	1:A:938:ALA:CB	2.22	0.66
1:A:461:LEU:HB3	1:A:462:TYR:CD2	2.31	0.65
1:A:887:THR:HB	1:A:890:LYS:HD2	1.76	0.65
1:A:462:TYR:HB2	1:A:484:MET:HE2	1.78	0.65
1:A:931:SER:OG	1:A:960:LEU:HB3	1.99	0.63
1:A:947:ARG:HH22	1:A:964:ASP:HB3	1.62	0.63
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.63	0.63
1:A:462:TYR:CB	1:A:484:MET:HE2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LEU:HD12	1:A:527:ILE:HG22	1.81	0.62
1:A:887:THR:HG22	1:A:890:LYS:H	1.65	0.62
1:A:808:LYS:O	1:A:810:PRO:HD3	1.99	0.62
1:A:734:GLN:HE21	1:A:780:PRO:HG2	1.64	0.61
1:A:271:VAL:HG23	1:A:282:VAL:CG1	2.30	0.61
1:A:546:GLU:HG3	1:A:547:MET:H	1.65	0.61
1:A:741:MET:O	1:A:745:VAL:HG23	2.01	0.61
1:A:529:LEU:HD12	1:A:530:PRO:HD2	1.82	0.60
1:A:752:LEU:HD12	1:A:763:VAL:HG22	1.82	0.60
1:A:804:MET:HE1	1:A:831:ILE:HG12	1.84	0.59
1:A:360:LYS:HG3	1:A:416:PHE:O	2.02	0.59
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.84	0.59
1:A:995:MET:O	1:A:1005:HIS:HB2	2.02	0.58
1:A:233:ILE:HD11	1:A:248:PHE:HD1	1.69	0.58
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.86	0.58
1:A:739:ILE:O	1:A:743:GLN:HG3	2.04	0.57
1:A:947:ARG:NH1	1:A:948:HIS:CE1	2.72	0.57
1:A:966:GLY:O	1:A:970:GLY:CA	2.49	0.57
1:A:546:GLU:HG3	1:A:547:MET:N	2.20	0.57
1:A:1035:LEU:HD12	1:A:1048:ILE:HG12	1.86	0.57
1:A:706:SER:O	1:A:710:GLN:HB3	2.05	0.57
1:A:810:PRO:HB3	1:A:833:LYS:HD3	1.87	0.56
1:A:833:LYS:HE3	1:A:836:ASP:OD2	2.06	0.56
1:A:395:CYS:HB2	1:A:418:ILE:HD11	1.87	0.56
1:A:750:LYS:NZ	1:A:834:HIS:HD2	2.03	0.56
1:A:766:GLN:H	1:A:766:GLN:NE2	1.97	0.56
1:A:204:SER:HB2	1:A:652:GLU:OE2	2.07	0.55
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.89	0.55
1:A:775:GLN:HE22	1:A:796:LEU:N	2.01	0.55
1:A:968:ILE:C	1:A:970:GLY:H	2.15	0.55
1:A:860:LEU:HD21	1:A:1015:LYS:HD2	1.87	0.55
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.72	0.55
1:A:165:VAL:HG12	1:A:165:VAL:O	2.08	0.54
1:A:370:ILE:O	1:A:372:VAL:N	2.41	0.54
1:A:487:ILE:HG22	1:A:488:SER:N	2.20	0.54
1:A:579:ARG:HB2	1:A:610:LEU:HD11	1.88	0.54
1:A:614:ARG:HH11	1:A:646:GLN:HE22	1.55	0.54
1:A:726:THR:HA	1:A:729:LEU:HB2	1.90	0.54
1:A:564:LEU:HB2	1:A:1052:ARG:HD2	1.90	0.53
1:A:293:VAL:O	1:A:297:LEU:HG	2.08	0.53
1:A:947:ARG:HH11	1:A:968:ILE:HG23	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:ASP:O	1:A:845:LEU:HD22	2.10	0.52
1:A:947:ARG:HH11	1:A:948:HIS:CE1	2.28	0.52
1:A:935:TYR:O	1:A:939:THR:HG22	2.10	0.52
1:A:173:LEU:O	1:A:177:ARG:HG3	2.10	0.51
1:A:947:ARG:HD3	1:A:968:ILE:HG21	1.91	0.51
1:A:803:VAL:CG1	1:A:809:LYS:HB3	2.40	0.51
1:A:225:HIS:CE1	1:A:304:HIS:CD2	2.99	0.51
1:A:983:VAL:HG13	1:A:985:PHE:O	2.11	0.51
1:A:271:VAL:CG2	1:A:282:VAL:CG1	2.88	0.51
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.46	0.51
1:A:519:LEU:HD12	1:A:520:LEU:N	2.26	0.50
1:A:833:LYS:HG3	1:A:834:HIS:N	2.27	0.50
1:A:927:ARG:O	1:A:931:SER:HB3	2.12	0.50
1:A:487:ILE:CG2	1:A:488:SER:H	2.22	0.50
1:A:523:TYR:C	1:A:525:HIS:HB2	2.37	0.50
1:A:955:THR:C	1:A:957:THR:H	2.19	0.49
1:A:547:MET:O	1:A:548:PRO:O	2.30	0.49
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.46	0.49
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.47	0.49
1:A:766:GLN:HE21	1:A:766:GLN:N	1.99	0.49
1:A:862:LEU:HD11	1:A:1016:ALA:CB	2.40	0.49
1:A:947:ARG:NH2	1:A:963:ILE:O	2.41	0.49
1:A:410:TRP:HB3	1:A:412:VAL:HG22	1.95	0.49
1:A:1043:THR:C	1:A:1045:LYS:H	2.20	0.49
1:A:739:ILE:HD13	1:A:872:THR:HG21	1.94	0.49
1:A:210:TYR:OH	1:A:856:GLU:HG3	2.12	0.49
1:A:921:PHE:O	1:A:925:VAL:HG23	2.13	0.48
1:A:355:TRP:CE2	1:A:601:GLN:NE2	2.78	0.48
1:A:614:ARG:HH11	1:A:646:GLN:NE2	2.12	0.48
1:A:893:GLN:O	1:A:897:GLY:HA2	2.14	0.48
1:A:1060:ASN:H	1:A:1060:ASN:ND2	2.12	0.48
1:A:149:ALA:HA	1:A:152:ARG:HD3	1.95	0.48
1:A:240:THR:HG23	1:A:243:ALA:HB3	1.96	0.48
1:A:519:LEU:HD12	1:A:520:LEU:H	1.79	0.48
1:A:524:CYS:N	1:A:525:HIS:HB2	2.28	0.48
1:A:775:GLN:NE2	1:A:795:ALA:HB1	2.29	0.48
1:A:1040:PRO:O	1:A:1041:GLN:HB2	2.13	0.48
1:A:749:ILE:HD13	1:A:811:LEU:HD21	1.94	0.47
1:A:892:GLN:OE1	1:A:902:PHE:HA	2.14	0.47
1:A:1035:LEU:HD23	1:A:1039:MET:HG3	1.95	0.47
1:A:750:LYS:NZ	1:A:834:HIS:CD2	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:SER:HB3	1:A:808:LYS:O	2.14	0.47
1:A:247:SER:HA	1:A:251:LYS:HB2	1.97	0.47
1:A:198:MET:SD	1:A:271:VAL:HG21	2.55	0.47
1:A:497:PHE:CE1	1:A:1044:SER:HA	2.50	0.47
1:A:929:VAL:HG22	1:A:995:MET:HG2	1.97	0.47
1:A:389:HIS:CD2	1:A:424:PRO:HG2	2.50	0.47
1:A:640:VAL:O	1:A:643:ILE:HG12	2.14	0.46
1:A:1056:THR:O	1:A:1056:THR:HG23	2.16	0.46
1:A:245:LEU:C	1:A:247:SER:H	2.23	0.46
1:A:565:ASN:HA	1:A:566:PRO:HD3	1.86	0.46
1:A:734:GLN:HE21	1:A:780:PRO:CG	2.29	0.46
1:A:839:ARG:HA	1:A:842:MET:HE2	1.98	0.46
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.98	0.46
1:A:1044:SER:O	1:A:1045:LYS:HB3	2.15	0.46
1:A:968:ILE:C	1:A:970:GLY:N	2.74	0.45
1:A:1028:ILE:HG12	1:A:1051:ILE:HG23	1.97	0.45
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.52	0.45
1:A:353:SER:HB3	1:A:356:ASP:OD2	2.16	0.45
1:A:230:SER:O	1:A:231:GLN:HB2	2.17	0.45
1:A:529:LEU:HD12	1:A:530:PRO:CD	2.47	0.45
1:A:606:LYS:O	1:A:609:GLN:HB2	2.17	0.45
1:A:555:LEU:HD13	1:A:574:LEU:HD22	1.99	0.45
1:A:947:ARG:NH1	1:A:948:HIS:HE1	2.15	0.45
1:A:158:ILE:HG23	1:A:703:ILE:HD13	1.99	0.45
1:A:767:LEU:HD12	1:A:803:VAL:HG23	1.99	0.44
1:A:225:HIS:NE2	1:A:304:HIS:HD2	2.14	0.44
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.35	0.44
1:A:561:THR:HG23	1:A:591:LYS:NZ	2.32	0.44
1:A:583:LEU:HD22	1:A:610:LEU:HD22	2.00	0.44
1:A:574:LEU:HD23	1:A:578:PHE:HD1	1.82	0.44
1:A:848:LEU:HA	1:A:851:MET:HE2	2.00	0.44
1:A:1078:LYS:O	1:A:1081:THR:OG1	2.34	0.44
1:A:312:ASP:O	1:A:315:LEU:HB2	2.18	0.44
1:A:240:THR:HG23	1:A:243:ALA:CB	2.47	0.44
1:A:355:TRP:NE1	1:A:601:GLN:HE22	2.16	0.44
1:A:734:GLN:NE2	1:A:782:SER:O	2.51	0.43
1:A:763:VAL:HA	1:A:766:GLN:HE22	1.83	0.43
1:A:386:ASN:OD1	1:A:396:GLN:NE2	2.51	0.43
1:A:318:VAL:HG11	1:A:722:ARG:O	2.19	0.43
1:A:764:ILE:O	1:A:768:LYS:HG2	2.17	0.43
1:A:786:PRO:HD2	1:A:878:MET:CE	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:LEU:O	1:A:1030:LEU:HG	2.19	0.43
1:A:799:GLU:H	1:A:799:GLU:HG3	1.52	0.43
1:A:207:LEU:HB2	1:A:288:LYS:HD2	2.01	0.43
1:A:302:GLU:HB2	1:A:304:HIS:HE1	1.83	0.43
1:A:352:VAL:O	1:A:527:ILE:HA	2.19	0.43
1:A:364:LYS:HB2	1:A:413:TRP:CZ3	2.54	0.43
1:A:935:TYR:CE1	1:A:961:PHE:HA	2.53	0.42
1:A:767:LEU:HD13	1:A:768:LYS:HE2	2.01	0.42
1:A:831:ILE:HB	1:A:879:ILE:HB	2.01	0.42
1:A:163:THR:O	1:A:165:VAL:HG23	2.19	0.42
1:A:464:VAL:HB	1:A:484:MET:HG2	2.02	0.42
1:A:630:LEU:HB2	1:A:644:ALA:HB2	2.01	0.42
1:A:733:THR:HG22	1:A:737:GLN:HE21	1.84	0.42
1:A:172:GLU:HG3	1:A:471:HIS:ND1	2.34	0.42
1:A:462:TYR:HB3	1:A:484:MET:HE2	2.01	0.42
1:A:899:THR:HG22	1:A:901:ALA:H	1.84	0.41
1:A:895:THR:O	1:A:896:VAL:HG23	2.20	0.41
1:A:947:ARG:HD3	1:A:968:ILE:CG2	2.50	0.41
1:A:1050:TYR:CD2	1:A:1050:TYR:C	2.99	0.41
1:A:405:THR:O	1:A:408:VAL:HG23	2.20	0.41
1:A:900:GLY:C	1:A:902:PHE:H	2.27	0.41
1:A:207:LEU:HD11	1:A:211:LEU:HB2	2.02	0.41
1:A:424:PRO:HD2	1:A:427:ALA:HB2	2.01	0.41
1:A:767:LEU:O	1:A:771:LEU:HG	2.21	0.41
1:A:181:VAL:HG12	1:A:185:MET:HE2	2.02	0.41
1:A:370:ILE:O	1:A:371:PRO:C	2.64	0.41
1:A:398:ARG:O	1:A:414:LEU:HD21	2.21	0.41
1:A:425:LYS:HD2	1:A:473:PHE:CE2	2.55	0.41
1:A:355:TRP:NE1	1:A:601:GLN:NE2	2.70	0.40
1:A:751:SER:C	1:A:752:LEU:HD23	2.47	0.40
1:A:316:ASP:O	1:A:317:GLU:O	2.40	0.40
1:A:362:ARG:NH2	1:A:521:ASP:OD1	2.53	0.40
1:A:1083:GLN:NE2	1:A:1083:GLN:HA	2.35	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	826/626 (132%)	734 (89%)	65 (8%)	27 (3%)	3 5

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	GLU
1	A	320	LYS
1	A	524	CYS
1	A	548	PRO
1	A	776	ASN
1	A	1042	LEU
1	A	231	GLN
1	A	371	PRO
1	A	406	GLU
1	A	897	GLY
1	A	1041	GLN
1	A	1045	LYS
1	A	227	SER
1	A	229	THR
1	A	896	VAL
1	A	999	GLY
1	A	316	ASP
1	A	968	ILE
1	A	969	LEU
1	A	1044	SER
1	A	353	SER
1	A	751	SER
1	A	783	PHE
1	A	521	ASP
1	A	372	VAL
1	A	1079	GLY
1	A	525	HIS

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	753/564 (134%)	640 (85%)	113 (15%)	3 5

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	152	ARG
1	A	153	GLN
1	A	162	VAL
1	A	168	VAL
1	A	202	VAL
1	A	203	THR
1	A	204	SER
1	A	215	ILE
1	A	218	ASN
1	A	219	CYS
1	A	227	SER
1	A	229	THR
1	A	235	VAL
1	A	238	ASP
1	A	240	THR
1	A	252	MET
1	A	277	ARG
1	A	281	LEU
1	A	282	VAL
1	A	285	THR
1	A	298	LYS
1	A	302	GLU
1	A	315	LEU
1	A	317	GLU
1	A	318	VAL
1	A	319	ARG
1	A	320	LYS
1	A	352	VAL
1	A	353	SER

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Mol	Chain	Res	Type
1	A	354	LEU
1	A	357	CYS
1	A	359	ARG
1	A	366	ARG
1	A	370	ILE
1	A	379	LEU
1	A	380	THR
1	A	381	VAL
1	A	387	ILE
1	A	391	GLN
1	A	396	GLN
1	A	406	GLU
1	A	409	LEU
1	A	418	ILE
1	A	481	VAL
1	A	501	LYS
1	A	520	LEU
1	A	544	ARG
1	A	568	THR
1	A	574	LEU
1	A	575	LEU
1	A	587	LYS
1	A	601	GLN
1	A	602	GLU
1	A	615	GLU
1	A	622	LEU
1	A	626	LEU
1	A	647	LYS
1	A	682	LEU
1	A	683	LYS
1	A	710	GLN
1	A	717	LEU
1	A	729	LEU
1	A	739	ILE
1	A	740	GLU
1	A	749	ILE
1	A	752	LEU
1	A	760	SER
1	A	762	GLN
1	A	766	GLN
1	A	767	LEU
1	A	768	LYS

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Mol	Chain	Res	Type
1	A	779	LEU
1	A	782	SER
1	A	798	ILE
1	A	799	GLU
1	A	802	LYS
1	A	808	LYS
1	A	811	LEU
1	A	823	LEU
1	A	830	ILE
1	A	838	LEU
1	A	839	ARG
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	857	THR
1	A	865	LEU
1	A	875	LYS
1	A	886	THR
1	A	887	THR
1	A	894	SER
1	A	904	ASP
1	A	907	LEU
1	A	918	GLU
1	A	919	GLU
1	A	927	ARG
1	A	931	SER
1	A	948	HIS
1	A	968	ILE
1	A	969	LEU
1	A	983	VAL
1	A	998	SER
1	A	1026	LEU
1	A	1045	LYS
1	A	1051	ILE
1	A	1052	ARG
1	A	1056	THR
1	A	1059	LYS
1	A	1063	ASP
1	A	1078	LYS
1	A	1081	THR
1	A	1090	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	A	218	ASN
1	A	291	GLN
1	A	304	HIS
1	A	389	HIS
1	A	396	GLN
1	A	498	ASN
1	A	601	GLN
1	A	629	GLN
1	A	646	GLN
1	A	734	GLN
1	A	737	GLN
1	A	762	GLN
1	A	766	GLN
1	A	775	GLN
1	A	834	HIS
1	A	893	GLN
1	A	908	ASN
1	A	948	HIS
1	A	1007	GLN
1	A	1060	ASN
1	A	1083	GLN
1	A	1085	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	$\# Z > 2$
2	3RZ	A	1	-	22,22,22	1.79	2 (9%)	27,31,31	1.81	8 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3RZ	A	1	-	-	6/8/8/8	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	3RZ	C3-C5	-6.87	1.38	1.45
2	A	1	3RZ	C7-C6	-2.67	1.39	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	3RZ	N15-C16-N20	4.65	125.30	117.50
2	A	1	3RZ	C7-C6-N8	3.59	122.39	119.56
2	A	1	3RZ	C13-N15-C16	-2.56	122.07	126.41
2	A	1	3RZ	C17-C16-N15	-2.44	123.71	128.90
2	A	1	3RZ	O14-C13-C7	-2.41	118.63	121.73
2	A	1	3RZ	O14-C13-N15	2.28	125.60	122.27
2	A	1	3RZ	C11-C7-C6	2.20	121.48	118.48
2	A	1	3RZ	C12-C5-C3	-2.00	120.28	123.01

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	3RZ	C17-C16-N15-C13

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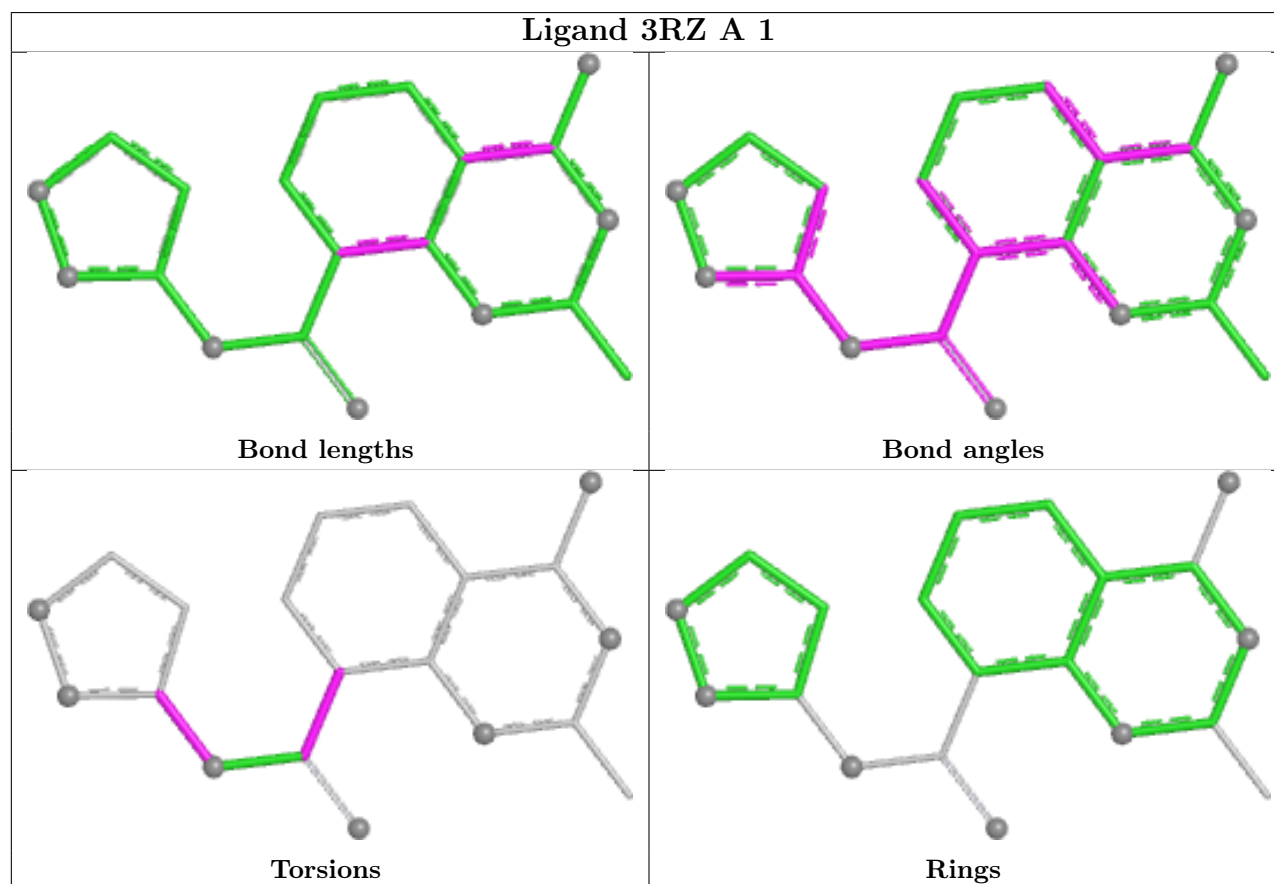
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Mol	Chain	Res	Type	Atoms
2	A	1	3RZ	N20-C16-N15-C13
2	A	1	3RZ	O14-C13-C7-C11
2	A	1	3RZ	O14-C13-C7-C6
2	A	1	3RZ	N15-C13-C7-C11
2	A	1	3RZ	N15-C13-C7-C6

There are no ring outliers.

No monomer is involved in short contacts.

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

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	526/626 (84%)	0.48	23 (4%) 39 33	29, 63, 98, 120	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	523	TYR	3.6
1	A	524	CYS	3.1
1	A	252	MET	2.9
1	A	526	PRO	2.8
1	A	354	LEU	2.8
1	A	318	VAL	2.8
1	A	352	VAL	2.8
1	A	525	HIS	2.8
1	A	545	ALA	2.7
1	A	760	SER	2.5
1	A	357	CYS	2.5
1	A	404	PHE	2.4
1	A	752	LEU	2.3
1	A	418	ILE	2.3
1	A	753	SER	2.3
1	A	147	SER	2.3
1	A	373	LEU	2.2
1	A	359	ARG	2.2
1	A	215	ILE	2.2
1	A	522	ASN	2.1
1	A	248	PHE	2.1
1	A	678	ALA	2.1
1	A	371	PRO	2.1

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](#)

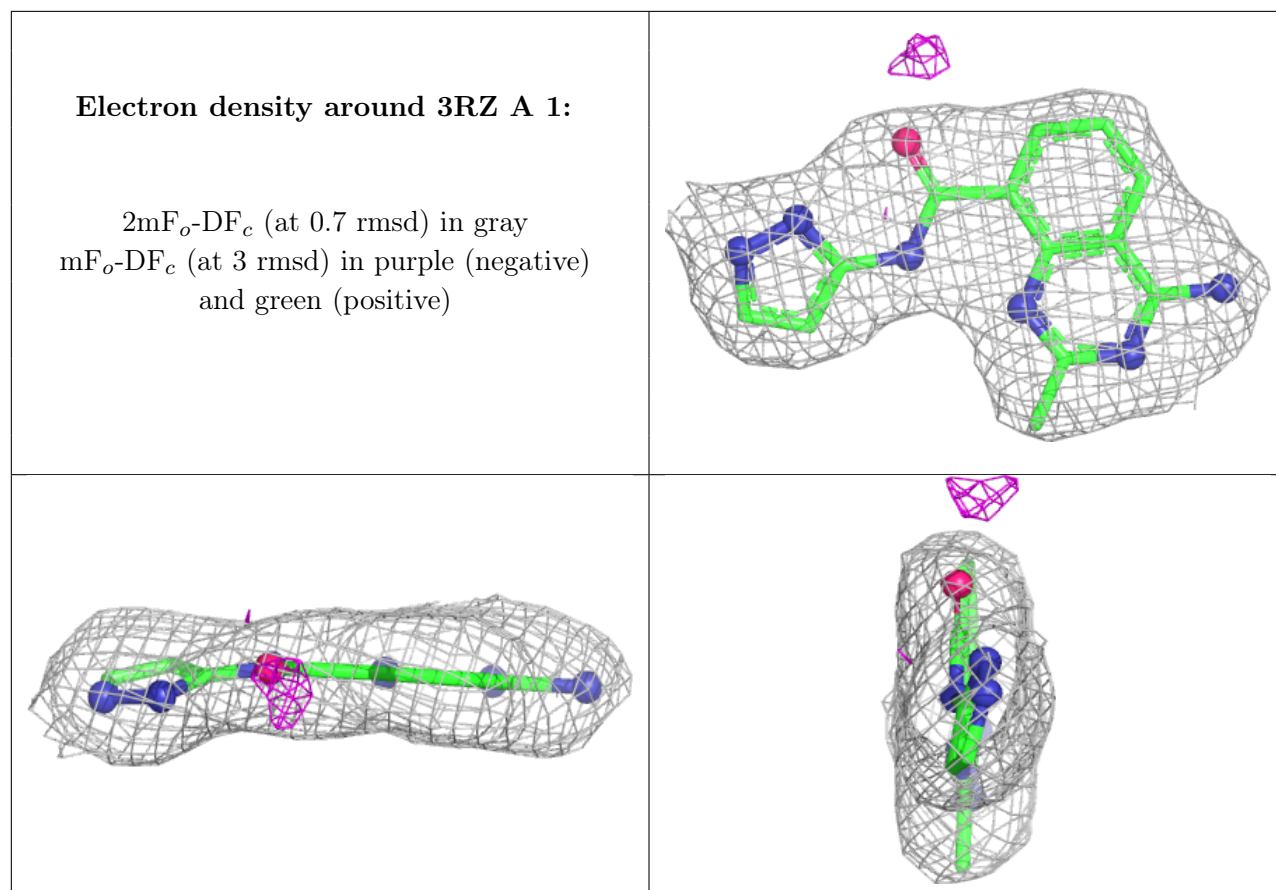
There are no oligosaccharides in this entry.

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	3RZ	A	1	20/20	0.95	0.07	40,46,47,48	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.