Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 07:29 AM EST

PDB ID	:	3PRZ
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 (i) 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 (i)) were used in the production of this report:

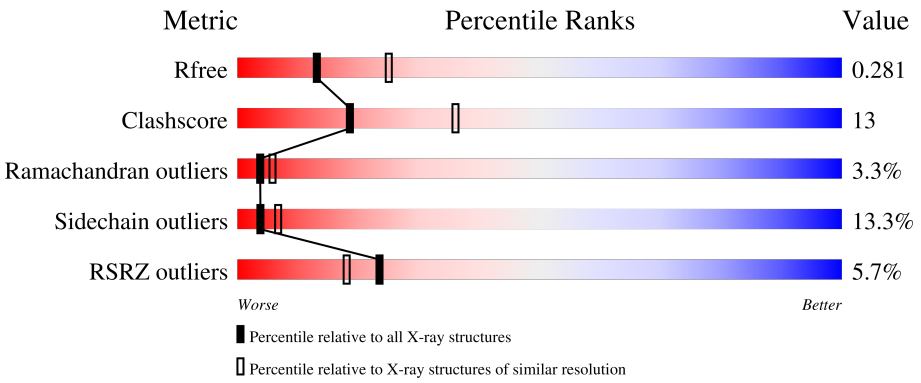
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

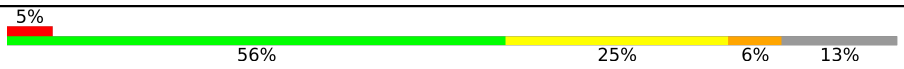
The reported resolution of this entry is 2.60 Å.

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	966	

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.

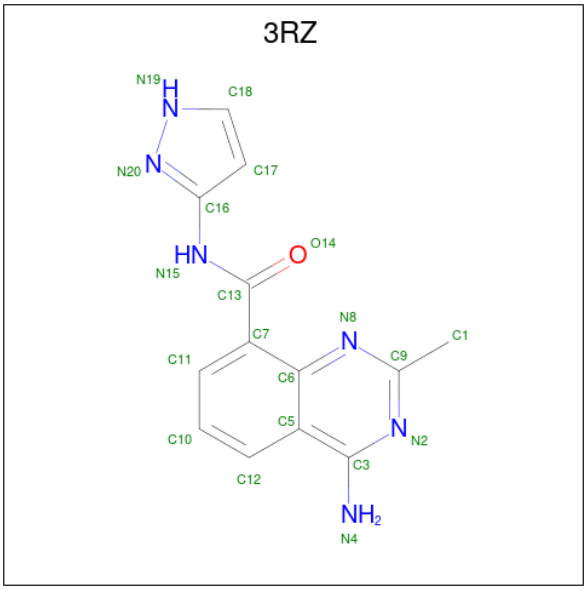
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

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 (three-letter code: 3RZ) (formula: $C_{13}H_{12}N_6O$).



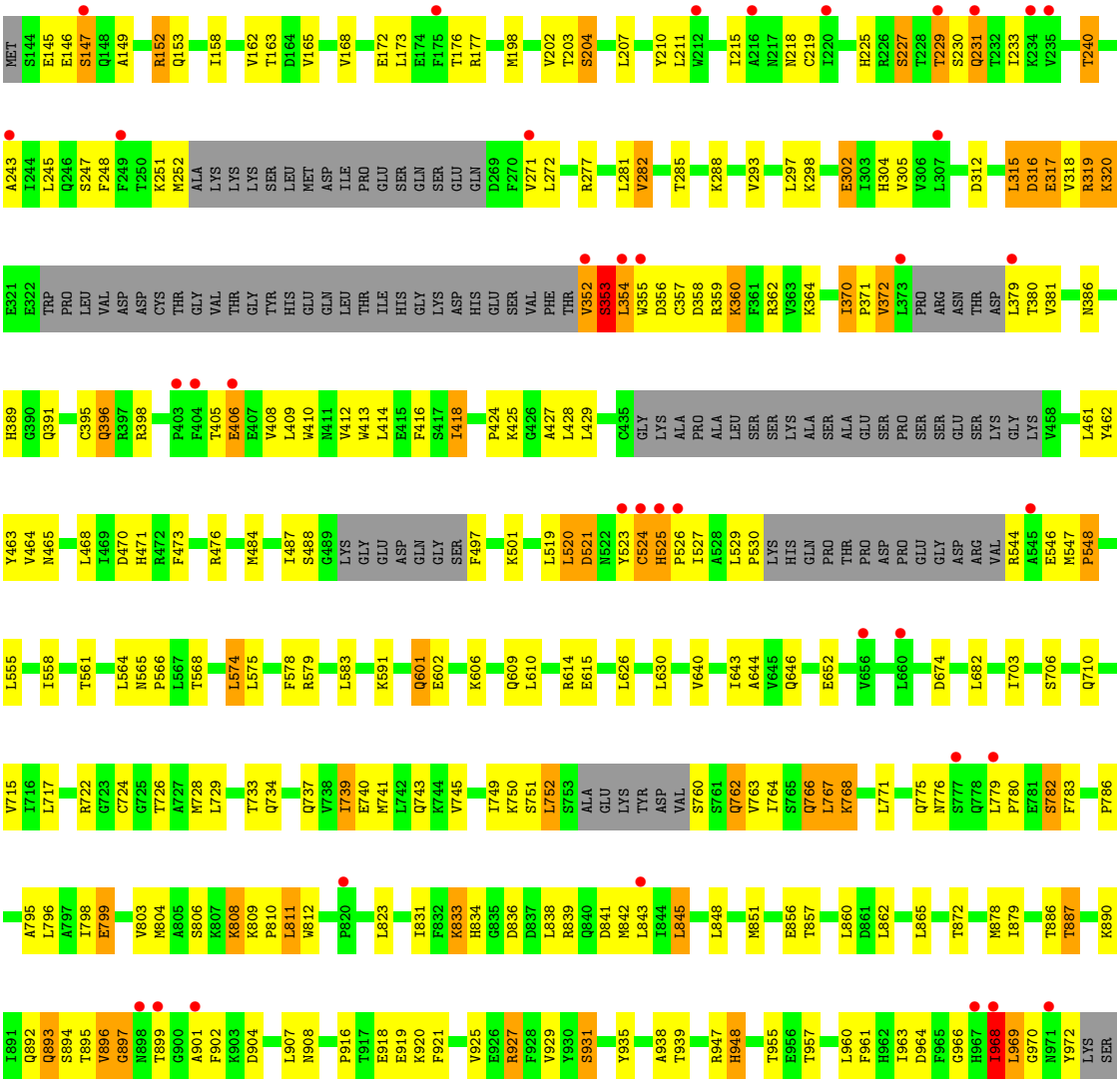
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	20	13	6	1	0	0

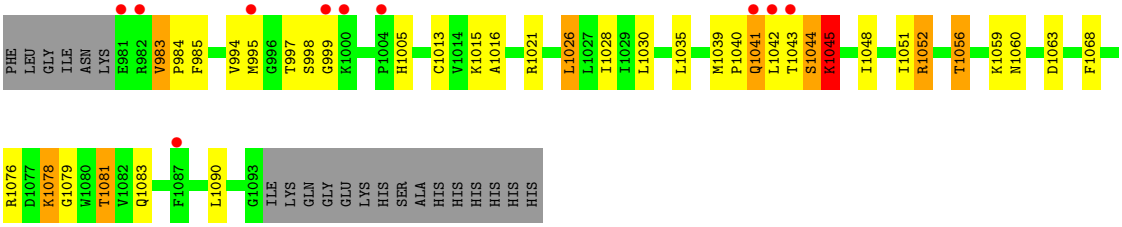
3 Residue-property plots (i)

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

Chain A:




PHE
LEU
GLY
ILE
ASN
LYS
E981
R982
V983
P984
F985
V994
M995
G996
T997
S998
G999
K1000
P1004
H1005
C1013
V1014
K1015
A1016
R1021
L1026
L1027
I1028
I1029
L1030
L1035
M1039
P1040
Q1041
L1042
T1043
S1044
K1045
I1048
I1051
R1052
T1056
K1059
N1060
D1063
F1088
R1076
D1077
K1078
G1079
W1080
T1081
V1082
Q1083
F1087
L1090
G1093
ILE
LYS
GLN
GLY
GLU
LYS
HIS
SER
ALA
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

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 40.80 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.4 (44.73-2.60) 97.4 (40.80-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.61Å)	Xtriage
Refinement program	CNS, BUSTER 2.9.6	Depositor
R, R_{free}	0.250 , 0.281 0.245 , 0.281	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)	0.32 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.46	0/6963	0.78	0/9423

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6816	0	6843	180	0
2	A	20	0	12	0	0
All	All	6836	0	6855	180	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 13.

All (180) 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:352:VAL:N	1:A:526:PRO:O	2.03	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:GLN:HE21	1:A:766:GLN:H	1.20	0.90
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:851:MET:HE1	1:A:938:ALA:HB1	1.65	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:177:ARG:HG2	1:A:715:VAL:HG13	1.76	0.67
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:724:CYS:HB2	1:A:728:MET:HE3	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: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:462:TYR:HB2	1:A:484:MET:HE1	1.82	0.61
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:968:ILE:C	1:A:970:GLY:H	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:786:PRO:HD2	1:A:878:MET:CE	2.42	0.49
1:A:851:MET:CE	1:A:938:ALA:HB1	2.39	0.49
1:A:750:LYS:HZ1	1:A:834:HIS:HD2	1.61	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
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: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: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:786:PRO:HD2	1:A:878:MET:HE2	1.97	0.46
1:A:1028:ILE:HG12	1:A:1051:ILE:HG23	1.97	0.45
1:A:523:TYR:C	1:A:525:HIS:HB2	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:955:THR:C	1:A:957:THR:H	2.19	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:750:LYS:HZ2	1:A:834:HIS:CD2	2.34	0.44
1:A:1043:THR:C	1:A:1045:LYS:H	2.20	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: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:734:GLN:NE2	1:A:782:SER:O	2.51	0.43
1:A:839:ARG:HA	1:A:842:MET:HE2	1.99	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:804:MET:CE	1:A:812:TRP:HB2	2.49	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: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:851:MET:HE2	1:A:851:MET:HB2	1.83	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:851:MET:CE	1:A:938:ALA:CB	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:245:LEU:C	1:A:247:SER:H	2.23	0.41
1:A:405:THR:O	1:A:408:VAL:HG23	2.20	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: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: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 (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	826/966 (86%)	734 (89%)	65 (8%)	27 (3%)	4 6

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

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Mol	Chain	Res	Type
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 (i)

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	753/864 (87%)	653 (87%)	100 (13%)	4 7

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	146	GLU
1	A	147	SER
1	A	152	ARG
1	A	153	GLN
1	A	162	VAL

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Mol	Chain	Res	Type
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	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	319	ARG
1	A	320	LYS
1	A	352	VAL
1	A	353	SER
1	A	354	LEU
1	A	357	CYS
1	A	358	ASP
1	A	359	ARG
1	A	360	LYS
1	A	370	ILE
1	A	379	LEU
1	A	380	THR
1	A	381	VAL
1	A	391	GLN
1	A	396	GLN
1	A	406	GLU
1	A	409	LEU
1	A	418	ILE
1	A	520	LEU
1	A	544	ARG
1	A	568	THR
1	A	574	LEU
1	A	575	LEU
1	A	601	GLN

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Mol	Chain	Res	Type
1	A	602	GLU
1	A	615	GLU
1	A	626	LEU
1	A	682	LEU
1	A	717	LEU
1	A	739	ILE
1	A	740	GLU
1	A	752	LEU
1	A	760	SER
1	A	762	GLN
1	A	766	GLN
1	A	767	LEU
1	A	768	LYS
1	A	779	LEU
1	A	782	SER
1	A	798	ILE
1	A	799	GLU
1	A	808	LYS
1	A	811	LEU
1	A	823	LEU
1	A	833	LYS
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	857	THR
1	A	865	LEU
1	A	886	THR
1	A	887	THR
1	A	893	GLN
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	972	TYR
1	A	983	VAL

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Mol	Chain	Res	Type
1	A	998	SER
1	A	1026	LEU
1	A	1045	LYS
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	304	HIS
1	A	389	HIS
1	A	396	GLN
1	A	498	ASN
1	A	565	ASN
1	A	601	GLN
1	A	609	GLN
1	A	646	GLN
1	A	734	GLN
1	A	737	GLN
1	A	743	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	959	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 monosaccharides 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	-	21,22,22	1.83	2 (9%)	25,31,31	1.56	6 (24%)

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	-	-	0/6/8/8	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	-6.73	1.38	1.45
2	A	1	3RZ	C7-C6	-2.71	1.39	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	3RZ	C7-C6-N8	3.62	122.39	119.53
2	A	1	3RZ	C18-N19-N20	2.56	113.49	107.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	3RZ	C11-C7-C6	2.53	121.48	118.37
2	A	1	3RZ	O14-C13-C7	-2.24	118.63	121.72
2	A	1	3RZ	C17-C18-N19	-2.18	105.84	111.33
2	A	1	3RZ	C16-N15-C13	-2.17	122.07	128.07

There are no chirality outliers.

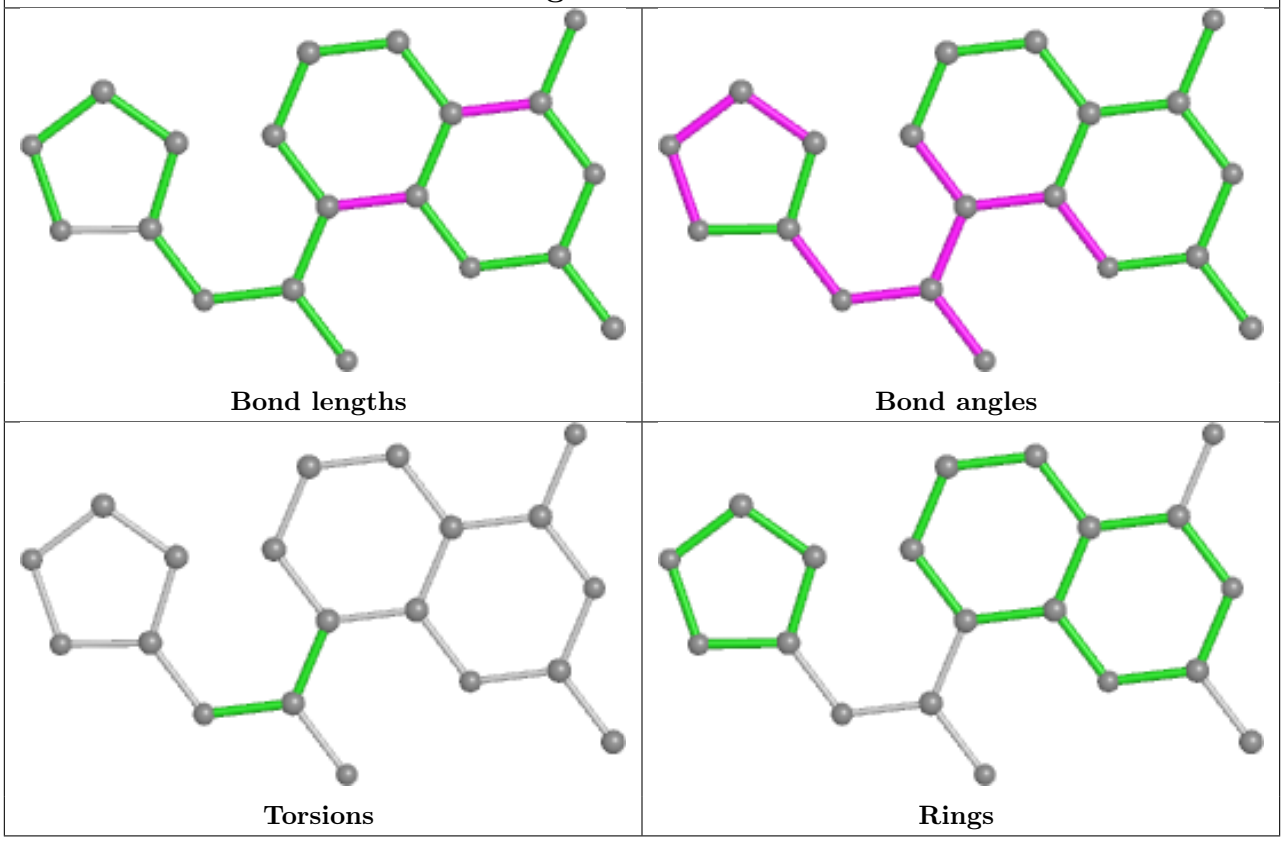
There are no torsion outliers.

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 then 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.

Ligand 3RZ A 1



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	844/966 (87%)	0.38	48 (5%) 23 18	29, 64, 97, 120	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	525	HIS	5.5
1	A	524	CYS	4.7
1	A	234	LYS	4.3
1	A	1041	GLN	4.0
1	A	971	ASN	3.9
1	A	220	ILE	3.9
1	A	981	GLU	3.9
1	A	899	THR	3.6
1	A	898	ASN	3.4
1	A	404	PHE	3.4
1	A	967	HIS	3.4
1	A	354	LEU	3.2
1	A	216	ALA	3.2
1	A	147	SER	3.2
1	A	249	PHE	3.2
1	A	968	ILE	3.1
1	A	545	ALA	2.8
1	A	1000	LYS	2.8
1	A	982	ARG	2.7
1	A	1043	THR	2.7
1	A	523	TYR	2.6
1	A	999	GLY	2.6
1	A	379	LEU	2.5
1	A	526	PRO	2.4
1	A	779	LEU	2.4
1	A	777	SER	2.3
1	A	406	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	271	VAL	2.3
1	A	820	PRO	2.3
1	A	403	PRO	2.3
1	A	1087	PHE	2.3
1	A	995	MET	2.2
1	A	235	VAL	2.2
1	A	901	ALA	2.2
1	A	212	TRP	2.2
1	A	229	THR	2.1
1	A	307	LEU	2.1
1	A	1042	LEU	2.1
1	A	175	PHE	2.1
1	A	355	TRP	2.1
1	A	843	LEU	2.1
1	A	243	ALA	2.1
1	A	231	GLN	2.0
1	A	373	LEU	2.0
1	A	660	LEU	2.0
1	A	352	VAL	2.0
1	A	656	VAL	2.0
1	A	1004	PRO	2.0

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

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

6.3 Carbohydrates (i)

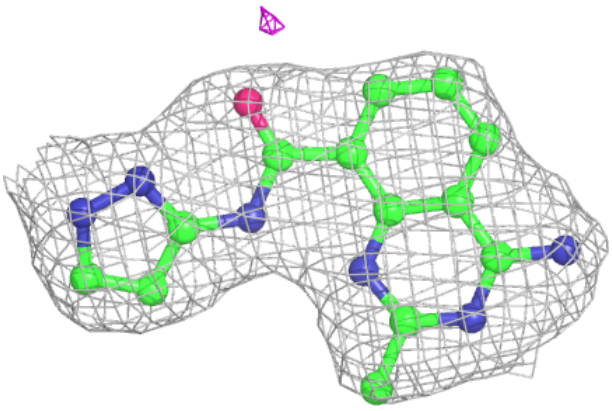
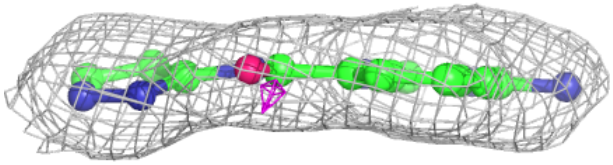
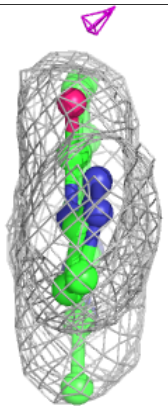
There are no monosaccharides in this entry.

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
2	3RZ	A	1	20/20	0.96	0.15	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.

Electron density around 3RZ 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.