



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:35 AM UTC

PDB ID : 3PRE / pdb\_00003pre  
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 : 2010-11-29  
Resolution : 2.91 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](mailto: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>.

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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)  
Xtrriage (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

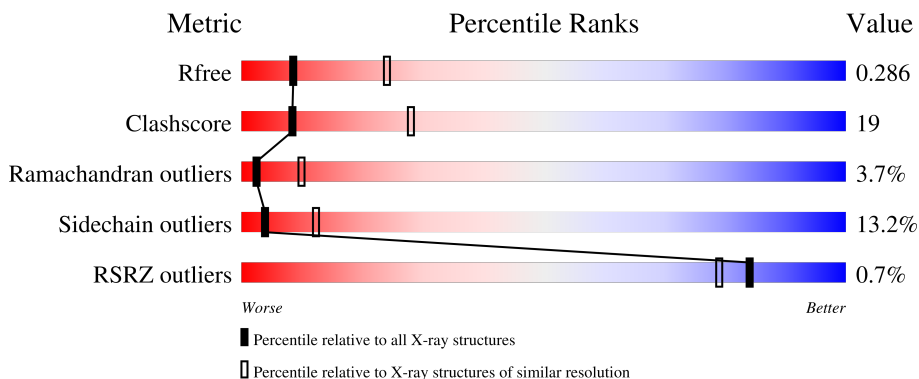
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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  $\geq 3$ , 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	966	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6813 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.

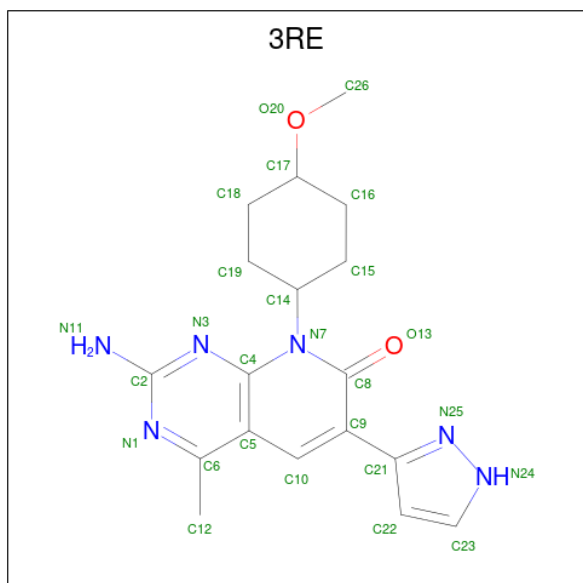
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	839	6787	4364	1154	1234	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 2-amino-8-(trans-4-methoxycyclohexyl)-4-methyl-6-(1H-pyrazol-3-yl)pyrido[2,3-d]pyrimidin-7(8H)-one (CCD ID: 3RE) (formula: C<sub>18</sub>H<sub>22</sub>N<sub>6</sub>O<sub>2</sub>).

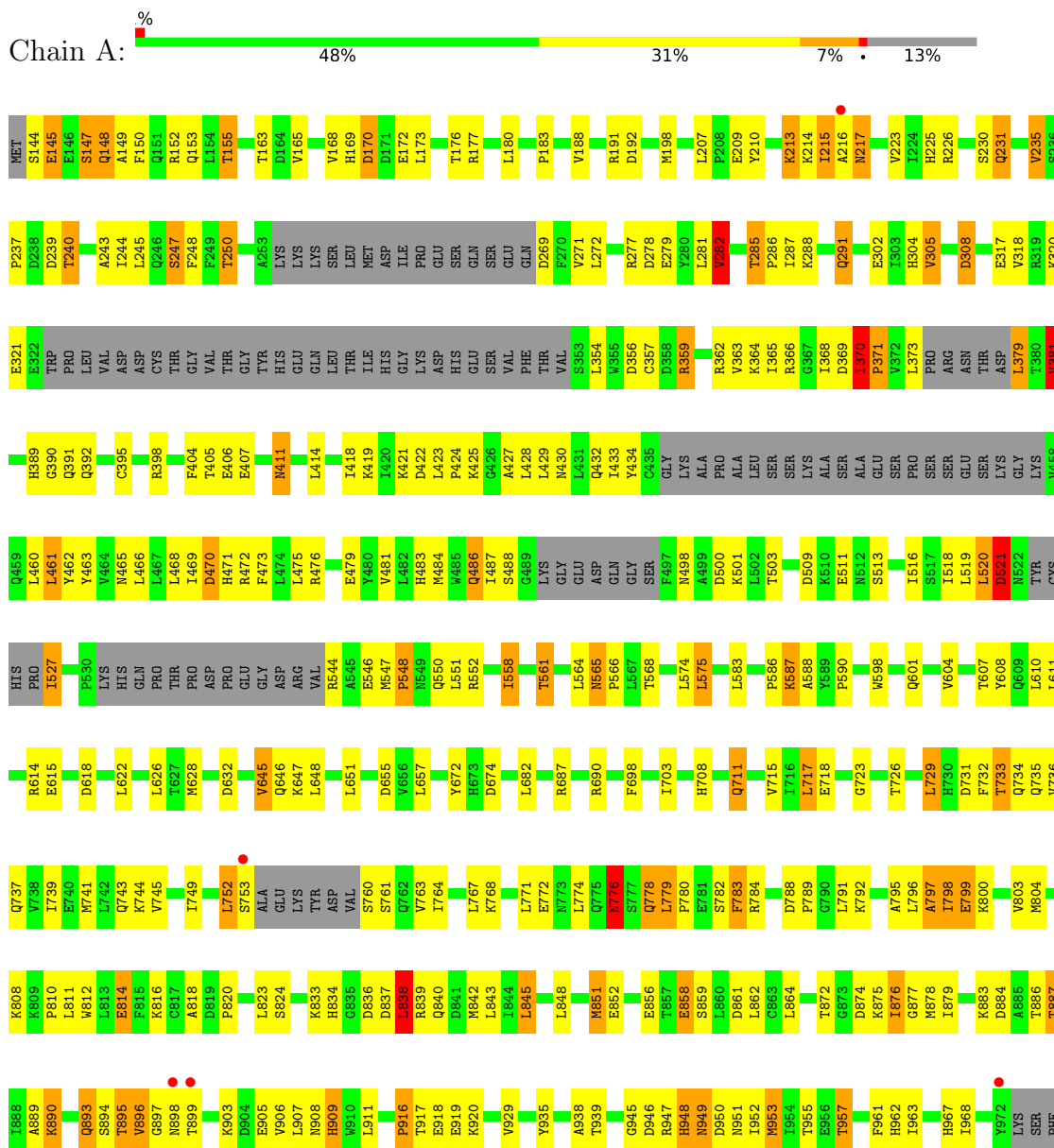


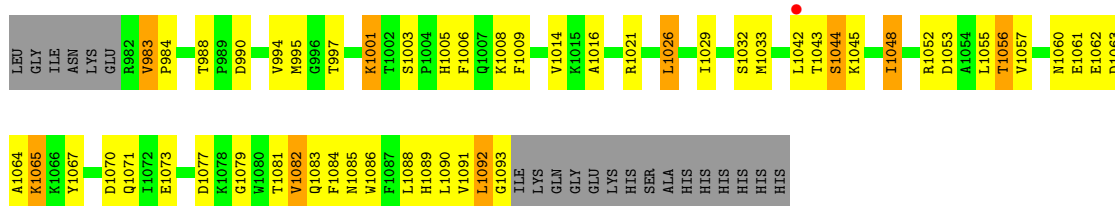
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	26	18	6	2	0	0

### 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, $\alpha$ , $\beta$ , $\gamma$	143.54Å 67.28Å 106.53Å 90.00° 95.77° 90.00°	Depositor
Resolution (Å)	50.00 – 2.91 50.00 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.91) 99.5 (50.00-2.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.90Å)	Xtrriage
Refinement program	REFMAC 5.5.0072, CNS	Depositor
R, $R_{free}$	0.232 , 0.295 0.223 , 0.286	Depositor DCC
$R_{free}$ test set	1151 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.1	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6813	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 3RE

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	0/6931	1.03	14/9375 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	SER	N-CA-C	-7.90	105.61	114.62
1	A	906	VAL	N-CA-C	7.62	118.39	110.62
1	A	550	GLN	N-CA-C	-7.14	106.48	114.62
1	A	308	ASP	N-CA-C	6.66	117.04	108.24
1	A	370	ILE	CA-C-N	6.19	127.58	119.84
1	A	370	ILE	C-N-CA	6.19	127.58	119.84
1	A	798	ILE	N-CA-C	5.86	117.30	110.62
1	A	381	VAL	N-CA-C	5.44	116.20	108.42
1	A	282	VAL	N-CA-C	5.38	115.09	108.53
1	A	698	PHE	N-CA-C	-5.26	105.19	111.03
1	A	919	GLU	N-CA-C	-5.18	105.63	111.28
1	A	565	ASN	CA-C-N	5.18	125.38	120.31
1	A	565	ASN	C-N-CA	5.18	125.38	120.31
1	A	148	GLN	N-CA-C	-5.07	105.75	111.28

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	6787	0	6826	260	0
2	A	26	0	22	1	0
All	All	6813	0	6848	261	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 19.

All (261) 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:939:THR:CG2	1:A:945:GLY:HA2	1.72	1.19
1:A:149:ALA:HA	1:A:152:ARG:NH1	1.77	0.97
1:A:558:ILE:O	1:A:561:THR:HG22	1.72	0.88
1:A:476:ARG:O	1:A:520:LEU:HD23	1.73	0.88
1:A:149:ALA:HA	1:A:152:ARG:HH11	1.35	0.87
1:A:359:ARG:HB2	1:A:359:ARG:HH11	1.43	0.83
1:A:851:MET:HE1	1:A:938:ALA:HB1	1.59	0.83
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.60	0.83
1:A:949:ASN:OD1	1:A:1083:GLN:NE2	2.13	0.81
1:A:887:THR:HG22	1:A:890:LYS:H	1.46	0.81
1:A:939:THR:CG2	1:A:945:GLY:CA	2.57	0.81
1:A:223:VAL:HB	1:A:304:HIS:HD2	1.47	0.78
1:A:812:TRP:NE1	1:A:814:GLU:OE2	2.16	0.77
1:A:173:LEU:O	1:A:177:ARG:HG3	1.84	0.77
1:A:172:GLU:HG3	1:A:471:HIS:ND1	1.99	0.77
1:A:1088:LEU:O	1:A:1093:GLY:N	2.20	0.74
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.70	0.74
1:A:948:HIS:CE1	1:A:950:ASP:HB2	2.22	0.73
1:A:893:GLN:HA	1:A:896:VAL:O	1.87	0.73
1:A:546:GLU:HG3	1:A:547:MET:H	1.53	0.72
1:A:939:THR:HG22	1:A:945:GLY:HA2	1.71	0.72
1:A:726:THR:HA	1:A:729:LEU:HB2	1.71	0.72
1:A:558:ILE:O	1:A:561:THR:CG2	2.37	0.71
1:A:776:ASN:HD22	1:A:778:GLN:HE22	1.36	0.71
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.74	0.70
1:A:939:THR:HG21	1:A:945:GLY:HA2	1.70	0.70
1:A:357:CYS:SG	1:A:359:ARG:NH1	2.64	0.69
1:A:732:PHE:O	1:A:736:VAL:HG23	1.94	0.68
1:A:362:ARG:HE	1:A:521:ASP:HB3	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.75	0.67
1:A:1055:LEU:O	1:A:1056:THR:HG22	1.95	0.67
1:A:657:LEU:HD11	1:A:690:ARG:HG2	1.77	0.66
1:A:947:ARG:NH2	1:A:963:ILE:O	2.28	0.66
1:A:546:GLU:CG	1:A:547:MET:H	2.08	0.66
1:A:271:VAL:HG12	1:A:308:ASP:O	1.96	0.66
1:A:1056:THR:HG23	1:A:1056:THR:O	1.96	0.66
1:A:223:VAL:HB	1:A:304:HIS:CD2	2.30	0.66
1:A:177:ARG:HG2	1:A:715:VAL:HG13	1.76	0.66
1:A:804:MET:HB2	1:A:810:PRO:HD2	1.77	0.66
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.76	0.65
1:A:948:HIS:NE2	1:A:950:ASP:HB2	2.12	0.65
1:A:169:HIS:O	1:A:170:ASP:HB3	1.97	0.65
1:A:734:GLN:HE21	1:A:780:PRO:HB2	1.63	0.64
1:A:359:ARG:HB2	1:A:359:ARG:NH1	2.12	0.63
1:A:165:VAL:HG12	1:A:165:VAL:O	1.98	0.62
1:A:878:MET:C	1:A:879:ILE:HD12	2.25	0.62
1:A:564:LEU:HB2	1:A:1052:ARG:HD2	1.81	0.62
1:A:939:THR:HG22	1:A:945:GLY:CA	2.26	0.62
1:A:782:SER:O	1:A:783:PHE:HB3	1.99	0.62
1:A:470:ASP:HB2	1:A:476:ARG:NH2	2.14	0.61
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.80	0.61
1:A:1091:VAL:HG12	1:A:1092:LEU:HD23	1.82	0.61
1:A:291:GLN:HE21	1:A:291:GLN:HA	1.65	0.61
1:A:277:ARG:NH2	1:A:791:LEU:HG	2.16	0.60
1:A:808:LYS:O	1:A:810:PRO:HD3	2.01	0.60
1:A:172:GLU:HG3	1:A:471:HIS:HD1	1.64	0.60
1:A:737:GLN:O	1:A:741:MET:HG3	2.01	0.60
1:A:935:TYR:O	1:A:939:THR:HB	2.02	0.60
1:A:743:GLN:HE21	1:A:876:ILE:HG12	1.67	0.59
1:A:461:LEU:HB2	1:A:462:TYR:CD2	2.38	0.59
1:A:948:HIS:O	1:A:950:ASP:N	2.36	0.59
1:A:519:LEU:HD12	1:A:520:LEU:H	1.68	0.59
1:A:519:LEU:HD12	1:A:520:LEU:N	2.18	0.59
1:A:405:THR:O	1:A:407:GLU:N	2.36	0.58
1:A:851:MET:CE	1:A:938:ALA:HB1	2.33	0.58
1:A:207:LEU:HD12	1:A:288:LYS:HB2	1.84	0.58
1:A:645:VAL:HA	1:A:648:LEU:HD12	1.86	0.58
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.68	0.57
1:A:207:LEU:HD12	1:A:288:LYS:HD2	1.86	0.57
1:A:487:ILE:HG22	1:A:488:SER:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.85	0.57
1:A:837:ASP:HB3	1:A:840:GLN:NE2	2.20	0.56
1:A:487:ILE:CG2	1:A:488:SER:N	2.68	0.56
1:A:235:VAL:HG11	1:A:244:ILE:HG12	1.86	0.56
1:A:145:GLU:C	1:A:147:SER:H	2.13	0.56
1:A:897:GLY:C	1:A:899:THR:H	2.14	0.55
1:A:188:VAL:HG11	1:A:318:VAL:HG21	1.88	0.55
1:A:424:PRO:HD2	1:A:427:ALA:HB2	1.88	0.55
1:A:240:THR:HG23	1:A:243:ALA:CB	2.36	0.55
1:A:547:MET:HB3	1:A:552:ARG:HH12	1.73	0.54
1:A:818:ALA:O	1:A:820:PRO:HD3	2.07	0.54
1:A:905:GLU:HG2	1:A:909:HIS:CE1	2.43	0.54
1:A:997:THR:HG23	1:A:1001:LYS:HB2	1.90	0.54
1:A:277:ARG:HH21	1:A:791:LEU:HG	1.74	0.53
1:A:365:ILE:HD13	1:A:518:ILE:HG22	1.89	0.53
1:A:509:ASP:O	1:A:513:SER:HB3	2.08	0.53
1:A:607:THR:O	1:A:610:LEU:HB2	2.08	0.53
1:A:608:TYR:HD2	1:A:608:TYR:N	2.05	0.53
1:A:837:ASP:HB3	1:A:840:GLN:HE21	1.72	0.53
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.09	0.53
1:A:285:THR:HG22	1:A:286:PRO:HD2	1.90	0.53
1:A:767:LEU:HG	1:A:803:VAL:HG23	1.91	0.53
1:A:240:THR:HG23	1:A:243:ALA:HB2	1.92	0.52
1:A:608:TYR:N	1:A:608:TYR:CD2	2.76	0.52
1:A:191:ARG:NH2	1:A:723:GLY:O	2.39	0.52
1:A:1043:THR:O	1:A:1044:SER:C	2.52	0.52
1:A:144:SER:HB3	1:A:147:SER:HB3	1.91	0.52
1:A:476:ARG:C	1:A:520:LEU:HD23	2.35	0.52
1:A:929:VAL:HG22	1:A:995:MET:HG2	1.91	0.52
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.90	0.52
1:A:784:ARG:HG2	1:A:792:LYS:HE3	1.92	0.51
1:A:317:GLU:O	1:A:726:THR:HG23	2.11	0.51
1:A:862:LEU:HD11	1:A:1016:ALA:HB2	1.92	0.51
1:A:861:ASP:OD1	1:A:861:ASP:C	2.54	0.51
1:A:990:ASP:O	1:A:994:VAL:HG23	2.11	0.51
1:A:379:LEU:N	1:A:404:PHE:HB3	2.26	0.51
1:A:1086:TRP:HE3	1:A:1090:LEU:CD2	2.23	0.51
1:A:237:PRO:HA	1:A:287:ILE:HD11	1.92	0.51
1:A:800:LYS:HB2	1:A:814:GLU:HG3	1.92	0.51
1:A:144:SER:O	1:A:148:GLN:HG2	2.09	0.51
1:A:248:PHE:C	1:A:250:THR:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LEU:O	1:A:487:ILE:HG12	2.11	0.51
1:A:800:LYS:CB	1:A:814:GLU:HG3	2.41	0.50
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.11	0.50
1:A:845:LEU:HD12	1:A:848:LEU:HD22	1.92	0.50
1:A:462:TYR:CE1	1:A:486:GLN:HG3	2.45	0.50
1:A:889:ALA:HA	1:A:949:ASN:HD22	1.76	0.50
1:A:731:ASP:O	1:A:735:GLN:HG3	2.11	0.50
1:A:834:HIS:HA	1:A:875:LYS:O	2.11	0.50
1:A:419:LYS:O	1:A:422:ASP:N	2.42	0.50
1:A:734:GLN:NE2	1:A:780:PRO:HB2	2.25	0.50
1:A:213:LYS:C	1:A:215:ILE:H	2.20	0.50
1:A:796:LEU:O	1:A:798:ILE:HG13	2.11	0.50
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.47	0.49
1:A:430:ASN:OD1	1:A:432:GLN:NE2	2.46	0.49
1:A:955:THR:C	1:A:957:THR:H	2.18	0.49
1:A:245:LEU:C	1:A:247:SER:H	2.21	0.49
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.44	0.48
1:A:564:LEU:CB	1:A:1052:ARG:HD2	2.43	0.48
1:A:188:VAL:HG13	1:A:191:ARG:NH2	2.28	0.48
1:A:953:MET:HB2	1:A:961:PHE:CZ	2.48	0.48
1:A:1052:ARG:O	1:A:1057:VAL:HG23	2.14	0.48
1:A:604:VAL:O	1:A:607:THR:HB	2.14	0.48
1:A:622:LEU:HD13	1:A:647:LYS:O	2.13	0.48
1:A:739:ILE:O	1:A:743:GLN:HG3	2.14	0.48
1:A:879:ILE:HD12	1:A:879:ILE:N	2.29	0.47
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.44	0.47
1:A:180:LEU:O	1:A:183:PRO:HD2	2.14	0.47
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.96	0.47
1:A:225:HIS:HE1	1:A:304:HIS:CD2	2.32	0.47
1:A:1070:ASP:O	1:A:1073:GLU:HB2	2.15	0.47
1:A:703:ILE:HD12	1:A:717:LEU:HD12	1.97	0.47
1:A:916:PRO:HG2	1:A:920:LYS:HD3	1.96	0.47
1:A:149:ALA:HA	1:A:152:ARG:HH12	1.72	0.47
1:A:858:GLU:O	1:A:859:SER:C	2.58	0.47
1:A:155:THR:HG22	1:A:155:THR:O	2.14	0.46
1:A:248:PHE:C	1:A:250:THR:N	2.73	0.46
1:A:291:GLN:HA	1:A:291:GLN:NE2	2.29	0.46
1:A:1089:HIS:CD2	1:A:1090:LEU:HD22	2.51	0.46
1:A:277:ARG:HH22	1:A:788:ASP:CG	2.23	0.46
1:A:1084:PHE:O	1:A:1088:LEU:HG	2.15	0.46
1:A:188:VAL:HG13	1:A:191:ARG:HH21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ASP:HB3	1:A:1033:MET:HE3	1.96	0.46
1:A:897:GLY:C	1:A:899:THR:N	2.74	0.46
1:A:398:ARG:O	1:A:414:LEU:HD21	2.15	0.46
1:A:1060:ASN:ND2	1:A:1063:ASP:HB2	2.31	0.46
1:A:947:ARG:NH1	1:A:951:ASN:OD1	2.49	0.46
1:A:741:MET:O	1:A:745:VAL:HG23	2.15	0.46
1:A:434:TYR:CE1	1:A:460:LEU:HB2	2.51	0.45
1:A:291:GLN:HE21	1:A:291:GLN:CA	2.25	0.45
1:A:425:LYS:HE2	1:A:672:TYR:CE1	2.51	0.45
1:A:611:LEU:O	1:A:614:ARG:HB2	2.17	0.45
1:A:764:ILE:O	1:A:768:LYS:HG2	2.16	0.45
1:A:768:LYS:O	1:A:772:GLU:HG2	2.17	0.45
1:A:433:ILE:HG13	1:A:484:MET:HE1	1.99	0.45
1:A:711:GLN:HE21	1:A:711:GLN:HB3	1.50	0.45
1:A:848:LEU:HA	1:A:851:MET:HE2	1.98	0.45
1:A:1005:HIS:O	1:A:1008:LYS:HB3	2.16	0.45
1:A:354:LEU:C	1:A:356:ASP:H	2.24	0.45
1:A:239:ASP:O	1:A:287:ILE:HG23	2.16	0.45
1:A:799:GLU:CD	1:A:799:GLU:H	2.23	0.45
1:A:470:ASP:CB	1:A:476:ARG:NH2	2.80	0.45
1:A:887:THR:HG22	1:A:890:LYS:N	2.23	0.45
1:A:1053:ASP:O	1:A:1056:THR:N	2.48	0.45
1:A:833:LYS:HE3	1:A:836:ASP:HB2	1.99	0.44
1:A:1026:LEU:O	1:A:1029:ILE:HG22	2.17	0.44
1:A:896:VAL:HG21	1:A:899:THR:HB	2.00	0.44
1:A:1056:THR:O	1:A:1056:THR:CG2	2.64	0.44
1:A:1086:TRP:HE3	1:A:1090:LEU:HD23	1.82	0.44
1:A:895:THR:O	1:A:896:VAL:HB	2.17	0.44
1:A:774:LEU:O	1:A:779:LEU:HB2	2.18	0.44
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.98	0.44
1:A:272:LEU:HD22	1:A:305:VAL:HG11	1.99	0.44
1:A:363:VAL:O	1:A:363:VAL:HG13	2.16	0.44
1:A:423:LEU:HA	1:A:424:PRO:HD3	1.86	0.44
1:A:558:ILE:HG21	1:A:575:LEU:HD21	2.00	0.44
1:A:839:ARG:O	1:A:842:MET:HB2	2.18	0.44
1:A:395:CYS:HB2	1:A:418:ILE:HG13	2.00	0.44
1:A:797:ALA:HA	1:A:816:LYS:HE2	1.98	0.44
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.65	0.44
1:A:734:GLN:NE2	1:A:782:SER:O	2.50	0.44
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.52	0.43
1:A:472:ARG:O	1:A:473:PHE:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ASN:HA	1:A:566:PRO:HD3	1.77	0.43
1:A:795:ALA:O	1:A:816:LYS:HE3	2.18	0.43
1:A:812:TRP:CD1	1:A:812:TRP:C	2.95	0.43
1:A:357:CYS:C	1:A:359:ARG:H	2.26	0.43
1:A:392:GLN:NE2	1:A:598:TRP:HD1	2.16	0.43
1:A:470:ASP:OD1	1:A:470:ASP:C	2.60	0.43
1:A:364:LYS:HE3	1:A:411:ASN:O	2.18	0.43
1:A:354:LEU:O	1:A:421:LYS:HB3	2.19	0.43
1:A:586:PRO:O	1:A:588:ALA:N	2.51	0.43
1:A:210:TYR:CE2	1:A:859:SER:HA	2.53	0.43
1:A:851:MET:CE	1:A:938:ALA:CB	2.97	0.43
1:A:687:ARG:O	1:A:687:ARG:HG2	2.19	0.43
1:A:741:MET:HE1	1:A:778:GLN:O	2.19	0.43
1:A:192:ASP:C	1:A:192:ASP:OD1	2.62	0.42
1:A:209:GLU:O	1:A:210:TYR:C	2.62	0.42
1:A:216:ALA:O	1:A:217:ASN:HB3	2.18	0.42
1:A:487:ILE:CG2	1:A:488:SER:H	2.31	0.42
1:A:952:ILE:HG12	1:A:962:HIS:CD2	2.54	0.42
1:A:1062:GLU:O	1:A:1063:ASP:C	2.61	0.42
1:A:476:ARG:HG2	1:A:520:LEU:HD22	2.02	0.42
1:A:632:ASP:HB3	1:A:1033:MET:CE	2.50	0.42
1:A:883:LYS:O	1:A:884:ASP:HB2	2.20	0.42
1:A:1006:PHE:O	1:A:1009:PHE:HB3	2.20	0.42
1:A:366:ARG:NH1	1:A:479:GLU:OE2	2.53	0.42
1:A:368:ILE:HD13	1:A:433:ILE:HD13	2.01	0.42
1:A:874:ASP:O	1:A:876:ILE:HG22	2.19	0.42
1:A:852:GLU:HG3	1:A:864:LEU:HD12	2.02	0.42
1:A:897:GLY:O	1:A:899:THR:N	2.53	0.42
1:A:483:HIS:HB3	1:A:513:SER:OG	2.20	0.42
1:A:767:LEU:HD13	1:A:771:LEU:HD12	2.01	0.42
1:A:230:SER:OG	1:A:231:GLN:N	2.53	0.41
1:A:743:GLN:NE2	1:A:876:ILE:HG12	2.32	0.41
1:A:466:LEU:HD11	1:A:476:ARG:HD3	2.02	0.41
1:A:856:GLU:C	1:A:858:GLU:H	2.27	0.41
1:A:198:MET:HE3	1:A:282:VAL:HG21	2.03	0.41
1:A:389:HIS:O	1:A:390:GLY:C	2.61	0.41
1:A:772:GLU:C	1:A:774:LEU:H	2.27	0.41
1:A:1061:GLU:O	1:A:1064:ALA:HB3	2.19	0.41
1:A:1086:TRP:CE3	1:A:1090:LEU:HD21	2.55	0.41
1:A:788:ASP:C	1:A:788:ASP:OD1	2.64	0.41
1:A:792:LYS:HB3	1:A:818:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:ASN:OD1	1:A:994:VAL:HA	2.20	0.41
1:A:180:LEU:O	1:A:183:PRO:CD	2.68	0.41
1:A:432:GLN:HB3	1:A:460:LEU:HD11	2.02	0.41
1:A:475:LEU:HD23	1:A:527:ILE:HD12	2.02	0.41
1:A:476:ARG:HG2	1:A:520:LEU:CD2	2.50	0.41
1:A:1048:ILE:H	1:A:1048:ILE:HG12	1.52	0.41
1:A:150:PHE:O	1:A:153:GLN:N	2.54	0.41
1:A:752:LEU:O	1:A:753:SER:HB3	2.20	0.41
2:A:101:3RE:O13	2:A:101:3RE:H19	2.20	0.41
1:A:381:VAL:HG21	1:A:404:PHE:CE1	2.56	0.41
1:A:245:LEU:C	1:A:247:SER:N	2.78	0.41
1:A:363:VAL:CG1	1:A:414:LEU:HB2	2.51	0.41
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.56	0.41
1:A:503:THR:HG23	1:A:503:THR:O	2.20	0.41
1:A:838:LEU:HD12	1:A:838:LEU:HA	1.90	0.41
1:A:1082:VAL:O	1:A:1085:ASN:HB2	2.20	0.41
1:A:618:ASP:OD1	1:A:618:ASP:N	2.51	0.41
1:A:729:LEU:O	1:A:733:THR:OG1	2.39	0.41
1:A:784:ARG:NH1	1:A:789:PRO:O	2.54	0.40
1:A:163:THR:O	1:A:165:VAL:HG23	2.21	0.40
1:A:370:ILE:HA	1:A:371:PRO:HD2	1.65	0.40
1:A:651:LEU:HD22	1:A:655:ASP:HB3	2.04	0.40
1:A:772:GLU:C	1:A:774:LEU:N	2.78	0.40
1:A:929:VAL:HG13	1:A:1009:PHE:HB2	2.04	0.40
1:A:946:ASP:HB2	1:A:983:VAL:O	2.20	0.40
1:A:470:ASP:HB2	1:A:476:ARG:HH21	1.87	0.40
1:A:763:VAL:O	1:A:764:ILE:C	2.64	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	819/966 (85%)	687 (84%)	102 (12%)	30 (4%)	<b>2</b>   <b>10</b>

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	371	PRO
1	A	406	GLU
1	A	548	PRO
1	A	896	VAL
1	A	949	ASN
1	A	1044	SER
1	A	217	ASN
1	A	411	ASN
1	A	521	ASP
1	A	587	LYS
1	A	783	PHE
1	A	838	LEU
1	A	898	ASN
1	A	917	THR
1	A	1045	LYS
1	A	155	THR
1	A	615	GLU
1	A	761	SER
1	A	797	ALA
1	A	916	PRO
1	A	967	HIS
1	A	214	LYS
1	A	558	ILE
1	A	776	ASN
1	A	1077	ASP
1	A	170	ASP
1	A	226	ARG
1	A	590	PRO
1	A	1079	GLY

### 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	751/864 (87%)	652 (87%)	99 (13%)	4 12

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	168	VAL
1	A	213	LYS
1	A	215	ILE
1	A	235	VAL
1	A	240	THR
1	A	247	SER
1	A	250	THR
1	A	269	ASP
1	A	278	ASP
1	A	279	GLU
1	A	281	LEU
1	A	282	VAL
1	A	285	THR
1	A	291	GLN
1	A	305	VAL
1	A	320	LYS
1	A	321	GLU
1	A	359	ARG
1	A	369	ASP
1	A	370	ILE
1	A	373	LEU
1	A	379	LEU
1	A	381	VAL
1	A	391	GLN
1	A	461	LEU
1	A	469	ILE
1	A	470	ASP
1	A	481	VAL
1	A	486	GLN
1	A	498	ASN
1	A	511	GLU
1	A	516	ILE
1	A	520	LEU
1	A	521	ASP
1	A	527	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	544	ARG
1	A	561	THR
1	A	568	THR
1	A	574	LEU
1	A	575	LEU
1	A	587	LYS
1	A	601	GLN
1	A	626	LEU
1	A	628	MET
1	A	645	VAL
1	A	646	GLN
1	A	682	LEU
1	A	711	GLN
1	A	717	LEU
1	A	718	GLU
1	A	729	LEU
1	A	733	THR
1	A	744	LYS
1	A	749	ILE
1	A	752	LEU
1	A	760	SER
1	A	776	ASN
1	A	778	GLN
1	A	779	LEU
1	A	799	GLU
1	A	811	LEU
1	A	814	GLU
1	A	823	LEU
1	A	824	SER
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	851	MET
1	A	858	GLU
1	A	876	ILE
1	A	886	THR
1	A	887	THR
1	A	890	LYS
1	A	893	GLN
1	A	894	SER
1	A	895	THR
1	A	903	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	907	LEU
1	A	909	HIS
1	A	911	LEU
1	A	918	GLU
1	A	948	HIS
1	A	953	MET
1	A	957	THR
1	A	968	ILE
1	A	983	VAL
1	A	988	THR
1	A	1001	LYS
1	A	1003	SER
1	A	1026	LEU
1	A	1032	SER
1	A	1042	LEU
1	A	1048	ILE
1	A	1056	THR
1	A	1065	LYS
1	A	1081	THR
1	A	1082	VAL
1	A	1092	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	153	GLN
1	A	169	HIS
1	A	291	GLN
1	A	295	HIS
1	A	304	HIS
1	A	389	HIS
1	A	391	GLN
1	A	392	GLN
1	A	522	ASN
1	A	550	GLN
1	A	646	GLN
1	A	658	HIS
1	A	711	GLN
1	A	734	GLN
1	A	743	GLN
1	A	778	GLN
1	A	840	GLN

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Mol	Chain	Res	Type
1	A	893	GLN
1	A	922	GLN
1	A	949	ASN
1	A	959	ASN
1	A	1007	GLN
1	A	1060	ASN
1	A	1083	GLN
1	A	1085	ASN
1	A	1089	HIS

### 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	3RE	A	101	-	29,29,29	1.27	3 (10%)	34,42,42	2.14	7 (20%)

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	3RE	A	101	-	-	2/7/20/20	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	3RE	C5-C4	-3.74	1.37	1.42
2	A	101	3RE	C2-N11	2.98	1.39	1.33
2	A	101	3RE	C5-C6	-2.08	1.37	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	101	3RE	C10-C9-C8	-5.89	115.94	120.09
2	A	101	3RE	C21-N25-N24	5.58	106.37	104.28
2	A	101	3RE	C22-C21-N25	-4.80	108.32	111.09
2	A	101	3RE	C26-O20-C17	-3.13	106.25	113.81
2	A	101	3RE	O13-C8-C9	-2.95	118.70	124.96
2	A	101	3RE	C4-C5-C10	2.58	122.18	118.97
2	A	101	3RE	C2-N1-C6	-2.34	114.89	116.79

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	101	3RE	C16-C17-O20-C26
2	A	101	3RE	C18-C17-O20-C26

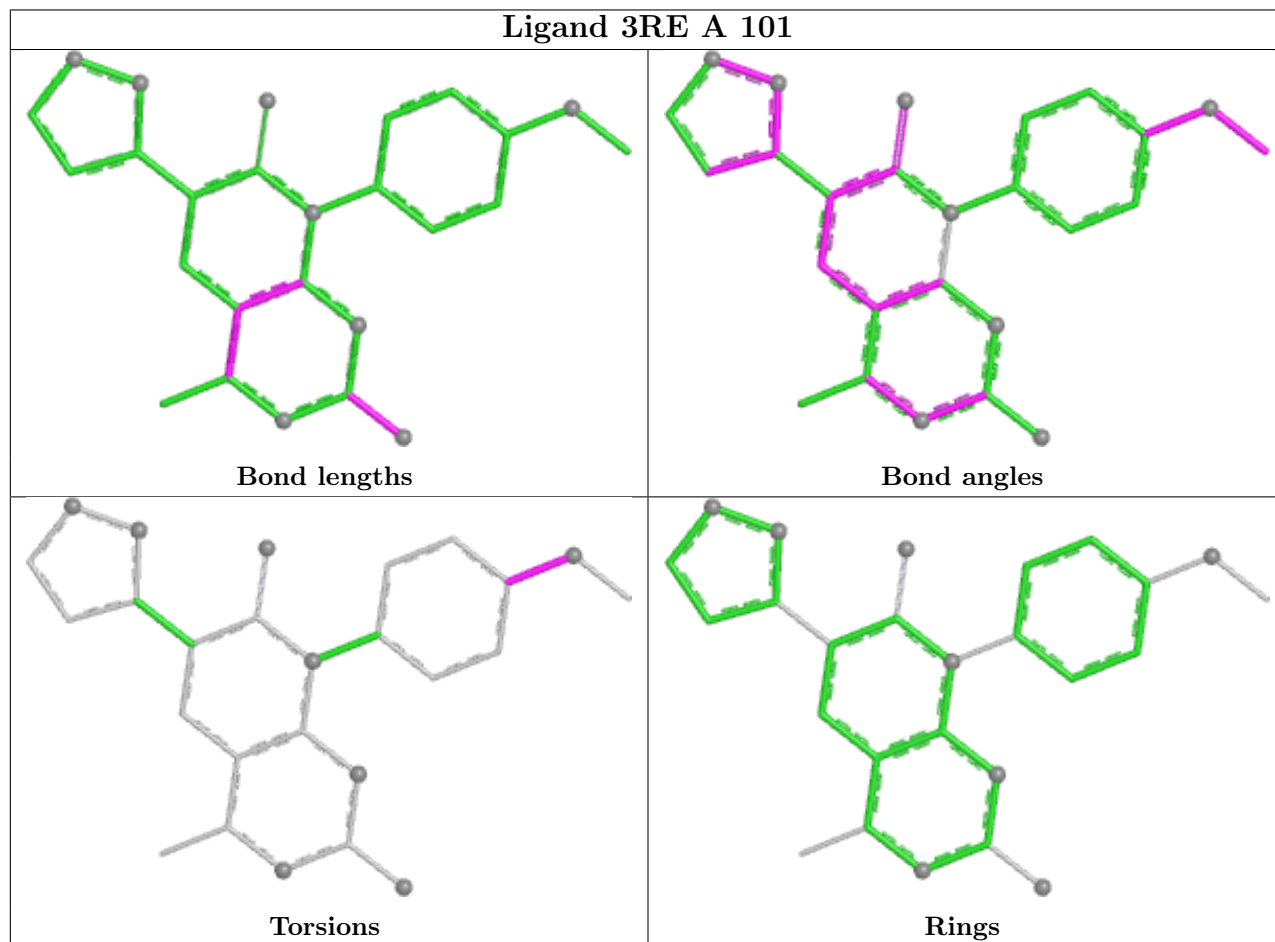
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	101	3RE	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	839/966 (86%)	-0.06	6 (0%) 84 79	27, 62, 92, 105	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	898	ASN	2.8
1	A	899	THR	2.8
1	A	972	TYR	2.5
1	A	216	ALA	2.5
1	A	1042	LEU	2.1
1	A	753	SER	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](#)

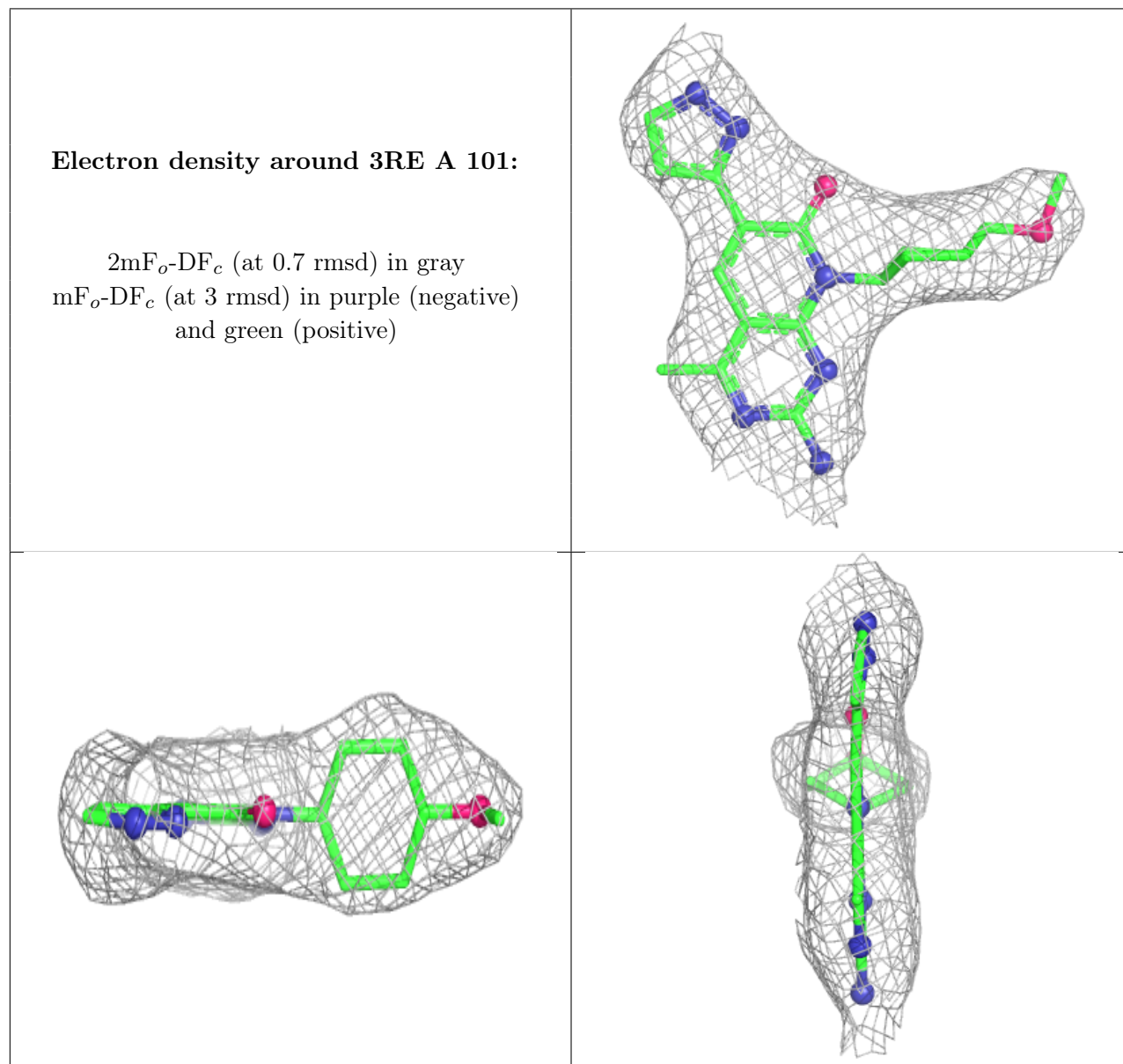
There are no oligosaccharides in this entry.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	3RE	A	101	26/26	0.94	0.08	38,41,49,49	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 [i](#)

There are no such residues in this entry.