



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 10:53 PM EDT

PDB ID : 2A4Z  
Title : Crystal Structure of human PI3Kgamma complexed with AS604850  
Authors : Camps, M.; Ruckle, T.; Ji, H.; Ardisson, V.; Rintelen, F.; Shaw, J.; Ferrandi, C.; Chabert, C.; Gillieron, C.; Francon, B.; Martin, T.; Gretener, D.; Perrin, D.; Leroy, D.; Vitte, P.-A.; Hirsch, E.; Wymann, M.P.; Cirillo, R.; Schwarz, M.K.; Rommel, C.  
Deposited on : 2005-06-30  
Resolution : 2.90 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (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

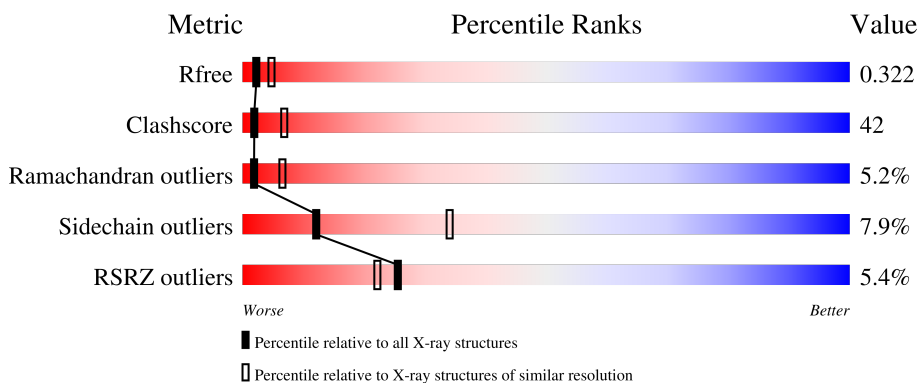
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 3 unique types of molecules in this entry. The entry contains 6273 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.

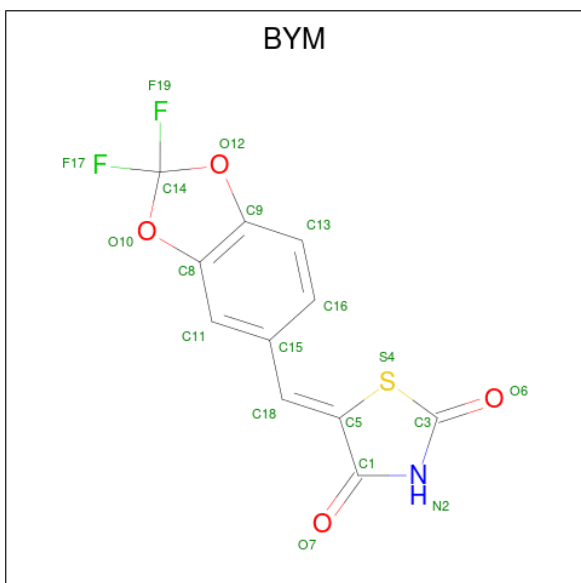
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit, gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	812	6247	4045	1040	1127	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 (5E)-5-[(2,2-DIFLUORO-1,3-BENZODIOXOL-5-YL)METHYLENE]-1,3-THIAZOLIDINE-2,4-DIONE (three-letter code: BYM) (formula: C<sub>11</sub>H<sub>5</sub>F<sub>2</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
2	A	1	19	11	2	1	4	1	0	0

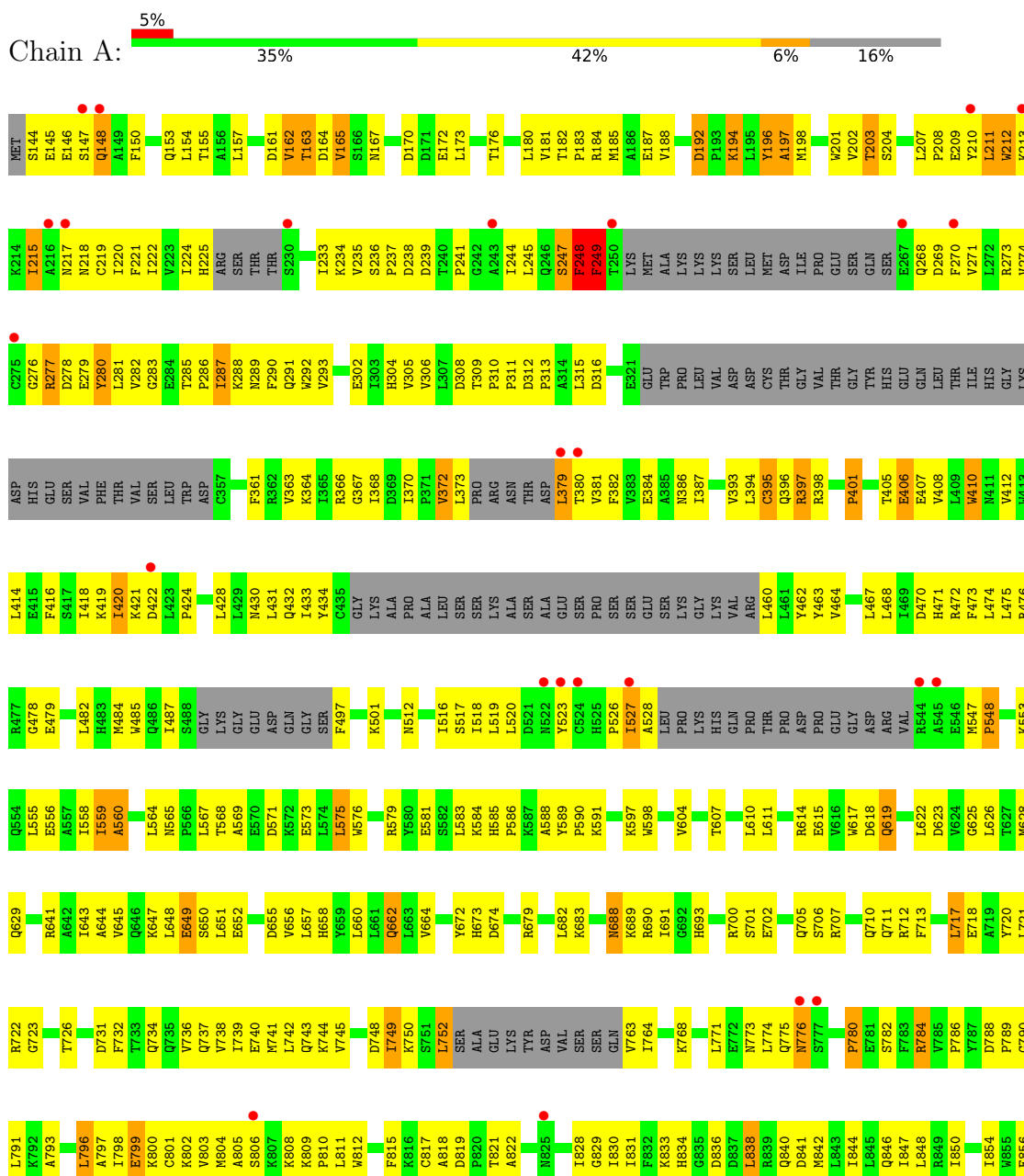
- Molecule 3 is water.

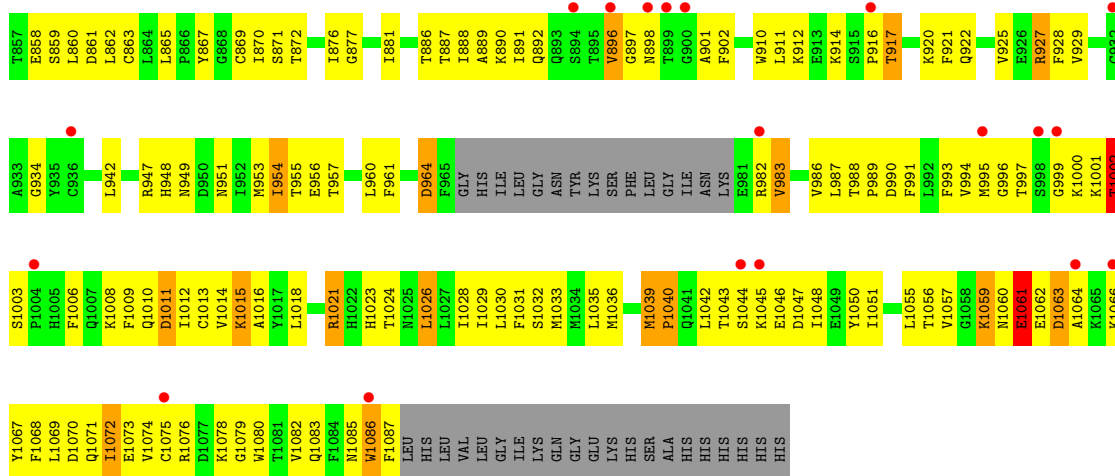
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		

### 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, $\alpha$ , $\beta$ , $\gamma$	142.35Å 67.65Å 106.39Å 90.00° 95.77° 90.00°	Depositor
Resolution (Å)	19.75 – 2.90 19.75 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.2 (19.75-2.90) 96.2 (19.75-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 2.88Å)	Xtrriage
Refinement program	CNS, CNX 2002	Depositor
R, $R_{free}$	0.257 , 0.352 0.232 , 0.322	Depositor DCC
$R_{free}$ test set	2156 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.9	Xtrriage
Anisotropy	0.153	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 117.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6273	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: BYM

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	0.36	0/6385	0.62	1/8692 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	LEU	CA-CB-CG	5.98	129.06	115.30

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	6247	0	6012	510	0
2	A	19	0	5	5	0
3	A	7	0	0	3	0
All	All	6273	0	6017	510	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 42.

All (510) 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:927:ARG:HH11	1:A:927:ARG:HB2	1.10	1.11
1:A:860:LEU:HD22	1:A:1015:LYS:HD3	1.33	1.05
1:A:184:ARG:NH1	1:A:722:ARG:HB2	1.76	1.01
1:A:474:LEU:HA	1:A:526:PRO:HB3	1.45	0.98
1:A:235:VAL:HG11	1:A:244:ILE:HG12	1.46	0.97
1:A:207:LEU:HD12	1:A:208:PRO:HD2	1.45	0.96
1:A:1036:MET:HG2	1:A:1042:LEU:HD23	1.47	0.95
1:A:527:ILE:HD13	1:A:528:ALA:H	1.30	0.92
1:A:657:LEU:HD13	1:A:691:ILE:HG12	1.52	0.92
1:A:144:SER:HB2	1:A:147:SER:HB2	1.52	0.92
1:A:734:GLN:HE21	1:A:780:PRO:HB3	1.37	0.89
1:A:749:ILE:HD12	1:A:811:LEU:HD11	1.52	0.89
1:A:804:MET:HE1	1:A:831:ILE:HG23	1.56	0.87
1:A:833:LYS:NZ	2:A:101:BYM:HN2	1.71	0.87
1:A:558:ILE:HG22	1:A:559:ILE:HD13	1.57	0.86
1:A:474:LEU:HD23	1:A:526:PRO:HG3	1.57	0.85
1:A:397:ARG:HE	1:A:416:PHE:HA	1.41	0.84
1:A:833:LYS:HZ2	2:A:101:BYM:HN2	1.23	0.84
1:A:929:VAL:HG13	1:A:995:MET:SD	2.18	0.83
1:A:476:ARG:HG2	1:A:520:LEU:HD12	1.60	0.83
1:A:410:TRP:HB3	1:A:412:VAL:HG12	1.62	0.81
1:A:688:ASN:ND2	1:A:690:ARG:H	1.78	0.80
1:A:615:GLU:O	1:A:619:GLN:HB2	1.81	0.80
1:A:1008:LYS:HZ3	1:A:1008:LYS:HB2	1.45	0.80
1:A:860:LEU:HD22	1:A:1015:LYS:CD	2.11	0.79
1:A:910:TRP:HE3	1:A:911:LEU:HD12	1.47	0.79
1:A:277:ARG:HG2	1:A:277:ARG:HH11	1.50	0.77
1:A:184:ARG:HH11	1:A:722:ARG:HB2	1.49	0.76
1:A:1008:LYS:HZ3	1:A:1008:LYS:CB	1.99	0.76
1:A:688:ASN:HD22	1:A:690:ARG:H	1.32	0.76
1:A:1031:PHE:HE2	1:A:1048:ILE:HA	1.49	0.76
1:A:527:ILE:CD1	1:A:528:ALA:H	1.97	0.75
1:A:277:ARG:HG2	1:A:277:ARG:NH1	2.02	0.75
1:A:910:TRP:CH2	1:A:956:GLU:HG3	2.22	0.75
1:A:927:ARG:HH11	1:A:927:ARG:CB	1.93	0.75
1:A:547:MET:HE2	1:A:581:GLU:HG2	1.69	0.74
1:A:988:THR:CG2	1:A:1083:GLN:HE21	2.01	0.74
1:A:379:LEU:HD22	1:A:380:THR:H	1.50	0.74
1:A:673:HIS:HD2	1:A:712:ARG:HE	1.36	0.74
1:A:180:LEU:O	1:A:183:PRO:HD2	1.88	0.74
1:A:611:LEU:O	1:A:614:ARG:HG2	1.89	0.73
1:A:184:ARG:NH1	1:A:722:ARG:CB	2.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:CYS:SG	1:A:418:ILE:HG13	2.29	0.72
1:A:379:LEU:HD13	1:A:380:THR:N	2.04	0.72
1:A:910:TRP:O	1:A:914:LYS:HB2	1.90	0.72
1:A:559:ILE:HG21	1:A:588:ALA:HB2	1.72	0.72
1:A:568:THR:HG23	1:A:571:ASP:H	1.55	0.71
1:A:861:ASP:C	1:A:862:LEU:HD22	2.11	0.71
1:A:960:LEU:HD23	1:A:961:PHE:N	2.05	0.71
1:A:184:ARG:HD2	1:A:722:ARG:O	1.90	0.71
1:A:215:ILE:HG12	1:A:215:ILE:O	1.91	0.71
1:A:987:LEU:HA	1:A:991:PHE:HD1	1.56	0.70
1:A:737:GLN:O	1:A:741:MET:HG3	1.91	0.70
1:A:987:LEU:HB3	1:A:1075:CYS:SG	2.32	0.70
1:A:224:ILE:HA	1:A:305:VAL:HG22	1.73	0.70
1:A:568:THR:HG22	1:A:571:ASP:OD1	1.91	0.70
1:A:379:LEU:HD13	1:A:380:THR:H	1.56	0.70
1:A:405:THR:O	1:A:407:GLU:N	2.25	0.70
1:A:431:LEU:HD13	1:A:516:ILE:HD13	1.73	0.70
1:A:625:GLY:O	1:A:629:GLN:HG3	1.92	0.70
1:A:202:VAL:HG11	1:A:285:THR:HG21	1.73	0.69
1:A:222:ILE:HD12	1:A:244:ILE:HD13	1.73	0.69
1:A:233:ILE:HG22	1:A:234:LYS:N	2.08	0.69
1:A:280:TYR:N	1:A:280:TYR:CD1	2.61	0.69
1:A:887:THR:HA	1:A:953:MET:HG2	1.75	0.69
1:A:201:TRP:CE2	1:A:291:GLN:HG3	2.28	0.69
1:A:796:LEU:HD12	1:A:796:LEU:H	1.58	0.68
1:A:474:LEU:CA	1:A:526:PRO:HB3	2.23	0.68
1:A:280:TYR:N	1:A:280:TYR:HD1	1.92	0.68
1:A:872:THR:OG1	1:A:877:GLY:HA2	1.94	0.68
1:A:271:VAL:HB	1:A:310:PRO:HG3	1.76	0.68
1:A:752:LEU:N	1:A:752:LEU:HD23	2.08	0.67
1:A:927:ARG:HB2	1:A:927:ARG:NH1	1.96	0.67
1:A:182:THR:HB	1:A:183:PRO:HD3	1.76	0.67
1:A:567:LEU:HD21	1:A:591:LYS:HD3	1.76	0.67
1:A:947:ARG:NH2	1:A:951:ASN:HB3	2.09	0.67
1:A:929:VAL:HG22	1:A:995:MET:CE	2.25	0.67
1:A:738:VAL:HG12	1:A:742:LEU:HD12	1.77	0.66
1:A:782:SER:HA	1:A:793:ALA:O	1.96	0.66
1:A:1009:PHE:HE2	1:A:1072:ILE:HD11	1.61	0.66
1:A:224:ILE:HA	1:A:305:VAL:CG2	2.26	0.65
1:A:212:TRP:HE3	1:A:215:ILE:HG23	1.61	0.65
1:A:184:ARG:HH12	1:A:722:ARG:HD2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:TYR:HD1	1:A:280:TYR:H	1.45	0.65
1:A:808:LYS:C	1:A:810:PRO:HD3	2.17	0.65
1:A:982:ARG:O	1:A:983:VAL:HG13	1.97	0.65
1:A:474:LEU:CD2	1:A:526:PRO:HG3	2.27	0.64
1:A:282:VAL:HG22	1:A:283:GLY:N	2.11	0.64
1:A:568:THR:CG2	1:A:571:ASP:H	2.11	0.64
1:A:732:PHE:O	1:A:736:VAL:HG23	1.98	0.64
1:A:379:LEU:HD22	1:A:380:THR:N	2.13	0.63
1:A:277:ARG:NH1	1:A:791:LEU:HG	2.14	0.63
1:A:366:ARG:HG2	1:A:366:ARG:HH11	1.63	0.63
1:A:576:TRP:O	1:A:579:ARG:HD3	1.97	0.63
1:A:236:SER:C	1:A:238:ASP:H	2.02	0.63
1:A:519:LEU:HD12	1:A:520:LEU:N	2.13	0.62
1:A:1008:LYS:HG3	1:A:1011:ASP:OD2	1.99	0.62
1:A:277:ARG:HD2	1:A:292:TRP:CH2	2.35	0.62
1:A:212:TRP:CE3	1:A:215:ILE:HG23	2.35	0.62
1:A:312:ASP:O	1:A:315:LEU:HD13	2.00	0.61
1:A:398:ARG:O	1:A:414:LEU:HD21	1.99	0.61
1:A:286:PRO:HD2	1:A:289:ASN:HD22	1.65	0.61
1:A:847:ILE:HG21	1:A:942:LEU:HD21	1.82	0.61
1:A:212:TRP:CE3	1:A:212:TRP:HA	2.36	0.61
1:A:862:LEU:HD12	1:A:934:GLY:N	2.15	0.61
1:A:1068:PHE:O	1:A:1071:GLN:HB2	2.00	0.61
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.83	0.61
1:A:363:VAL:HG23	1:A:520:LEU:CD2	2.30	0.61
1:A:553:LYS:O	1:A:556:GLU:HG3	2.01	0.61
1:A:576:TRP:CE2	1:A:579:ARG:HD2	2.36	0.61
1:A:239:ASP:H	1:A:287:ILE:HG22	1.66	0.61
1:A:1026:LEU:O	1:A:1029:ILE:HG22	2.01	0.61
1:A:641:ARG:O	1:A:645:VAL:HG23	2.01	0.60
1:A:478:GLY:N	1:A:520:LEU:O	2.34	0.60
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.37	0.60
1:A:796:LEU:HD12	1:A:796:LEU:N	2.16	0.60
1:A:922:GLN:HA	1:A:922:GLN:OE1	2.01	0.60
1:A:361:PHE:HA	1:A:420:ILE:HD11	1.83	0.60
1:A:1074:VAL:O	1:A:1078:LYS:HG2	2.02	0.60
1:A:180:LEU:C	1:A:183:PRO:HD2	2.21	0.60
1:A:547:MET:O	1:A:548:PRO:O	2.20	0.60
1:A:688:ASN:HD22	1:A:689:LYS:N	2.00	0.60
1:A:379:LEU:CD2	1:A:380:THR:H	2.15	0.60
1:A:1082:VAL:HG12	1:A:1086:TRP:NE1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:GLN:NE2	1:A:780:PRO:HB3	2.12	0.59
1:A:808:LYS:O	1:A:810:PRO:HD3	2.02	0.59
1:A:470:ASP:HB3	1:A:476:ARG:HH21	1.67	0.59
1:A:1035:LEU:HB3	1:A:1042:LEU:HD13	1.82	0.59
1:A:1006:PHE:O	1:A:1009:PHE:HB3	2.03	0.59
1:A:1014:VAL:HG12	1:A:1018:LEU:HD12	1.85	0.59
1:A:1045:LYS:NZ	1:A:1045:LYS:HB3	2.17	0.59
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.02	0.59
1:A:278:ASP:C	1:A:279:GLU:HG2	2.23	0.59
1:A:802:LYS:HG3	1:A:812:TRP:HB3	1.84	0.59
1:A:768:LYS:HA	1:A:771:LEU:HB2	1.85	0.59
1:A:1001:LYS:O	1:A:1002:THR:HG23	2.01	0.59
1:A:236:SER:O	1:A:287:ILE:HG21	2.03	0.59
1:A:1085:ASN:O	1:A:1087:PHE:N	2.36	0.58
1:A:734:GLN:O	1:A:738:VAL:HG23	2.03	0.58
1:A:1060:ASN:C	1:A:1062:GLU:H	2.05	0.58
1:A:750:LYS:HE3	1:A:834:HIS:O	2.04	0.58
1:A:763:VAL:HG13	1:A:764:ILE:H	1.69	0.58
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.85	0.58
1:A:1082:VAL:HG12	1:A:1086:TRP:CE2	2.39	0.58
1:A:197:ALA:HB2	1:A:316:ASP:OD2	2.04	0.58
1:A:673:HIS:CD2	1:A:712:ARG:HE	2.18	0.57
1:A:144:SER:HB2	1:A:147:SER:CB	2.29	0.57
1:A:1046:GLU:O	1:A:1047:ASP:HB2	2.04	0.57
1:A:784:ARG:O	1:A:786:PRO:HD3	2.04	0.57
1:A:1018:LEU:HD13	1:A:1061:GLU:OE1	2.05	0.57
1:A:763:VAL:HG13	1:A:764:ILE:N	2.18	0.57
1:A:850:ILE:O	1:A:854:ILE:HG13	2.05	0.57
1:A:989:PRO:O	1:A:993:PHE:N	2.36	0.57
1:A:986:VAL:HG12	1:A:991:PHE:HE1	1.69	0.57
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.70	0.57
1:A:1073:GLU:O	1:A:1076:ARG:N	2.33	0.57
1:A:921:PHE:O	1:A:925:VAL:HG23	2.05	0.57
1:A:1024:THR:HG21	1:A:1057:VAL:HG22	1.87	0.57
1:A:916:PRO:O	1:A:920:LYS:HB2	2.05	0.56
1:A:393:VAL:O	1:A:394:LEU:HD23	2.05	0.56
1:A:397:ARG:HG2	1:A:414:LEU:HD22	1.87	0.56
1:A:1012:ILE:HG22	1:A:1013:CYS:N	2.19	0.56
1:A:474:LEU:HA	1:A:526:PRO:CB	2.29	0.56
1:A:236:SER:O	1:A:238:ASP:N	2.38	0.56
1:A:145:GLU:HA	1:A:148:GLN:HE22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLU:O	1:A:212:TRP:N	2.35	0.56
1:A:277:ARG:HH11	1:A:277:ARG:CG	2.16	0.56
1:A:954:ILE:HA	1:A:960:LEU:HA	1.88	0.56
1:A:833:LYS:NZ	2:A:101:BYM:N2	2.50	0.55
1:A:860:LEU:HD12	1:A:861:ASP:H	1.69	0.55
1:A:184:ARG:HH12	1:A:722:ARG:CD	2.18	0.55
1:A:706:SER:O	1:A:710:GLN:HB3	2.06	0.55
1:A:739:ILE:O	1:A:743:GLN:HG3	2.05	0.55
1:A:1082:VAL:CG1	1:A:1086:TRP:CE2	2.89	0.55
1:A:366:ARG:HB2	1:A:517:SER:HB2	1.88	0.55
1:A:497:PHE:O	1:A:1042:LEU:HB3	2.07	0.55
1:A:988:THR:HG21	1:A:1083:GLN:HE21	1.71	0.55
1:A:1083:GLN:HA	1:A:1086:TRP:HD1	1.70	0.55
1:A:287:ILE:HG23	1:A:288:LYS:H	1.71	0.55
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.89	0.55
1:A:367:GLY:HA3	1:A:408:VAL:O	2.06	0.55
1:A:387:ILE:HD12	1:A:468:LEU:HD11	1.88	0.55
1:A:947:ARG:HG3	1:A:947:ARG:HH11	1.71	0.55
1:A:164:ASP:O	1:A:165:VAL:HG13	2.05	0.55
1:A:796:LEU:O	1:A:798:ILE:HD12	2.07	0.55
1:A:225:HIS:HE1	1:A:304:HIS:ND1	2.05	0.54
1:A:614:ARG:HG3	1:A:614:ARG:O	2.07	0.54
1:A:201:TRP:NE1	1:A:291:GLN:HG3	2.21	0.54
1:A:201:TRP:CD1	1:A:291:GLN:HG3	2.42	0.54
1:A:547:MET:HG3	1:A:548:PRO:HD2	1.89	0.54
1:A:618:ASP:HA	1:A:647:LYS:NZ	2.23	0.54
1:A:740:GLU:O	1:A:744:LYS:HG3	2.08	0.54
1:A:1046:GLU:C	1:A:1048:ILE:H	2.11	0.54
1:A:144:SER:CB	1:A:147:SER:HB2	2.30	0.54
1:A:176:THR:O	1:A:180:LEU:HG	2.08	0.54
1:A:527:ILE:HD13	1:A:528:ALA:N	2.11	0.54
1:A:196:TYR:O	1:A:198:MET:N	2.40	0.54
1:A:652:GLU:O	1:A:656:VAL:HG23	2.08	0.54
1:A:282:VAL:HG22	1:A:283:GLY:H	1.72	0.54
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.43	0.54
1:A:1060:ASN:O	1:A:1062:GLU:N	2.40	0.54
1:A:829:GLY:HA3	1:A:881:ILE:HB	1.89	0.54
1:A:833:LYS:NZ	1:A:836:ASP:OD2	2.38	0.54
1:A:842:MET:HG2	1:A:869:CYS:O	2.07	0.53
1:A:910:TRP:CE3	1:A:911:LEU:HD12	2.37	0.53
1:A:277:ARG:HH12	1:A:791:LEU:HG	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:VAL:HG13	1:A:994:VAL:HG12	1.91	0.53
1:A:233:ILE:CG2	1:A:234:LYS:N	2.70	0.53
1:A:914:LYS:HB3	1:A:956:GLU:HG2	1.89	0.53
1:A:996:GLY:O	1:A:1003:SER:HB3	2.07	0.53
1:A:1042:LEU:HD12	1:A:1043:THR:H	1.74	0.53
1:A:475:LEU:HD23	1:A:476:ARG:O	2.08	0.53
1:A:1031:PHE:CE2	1:A:1048:ILE:HA	2.35	0.53
1:A:990:ASP:O	1:A:993:PHE:HB3	2.09	0.53
1:A:366:ARG:HG2	1:A:366:ARG:NH1	2.23	0.53
1:A:379:LEU:CD1	1:A:380:THR:H	2.20	0.53
1:A:397:ARG:HB3	1:A:414:LEU:HD22	1.91	0.53
1:A:688:ASN:HD22	1:A:690:ARG:N	2.05	0.53
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.91	0.53
1:A:1085:ASN:O	1:A:1086:TRP:C	2.47	0.53
1:A:397:ARG:HG3	1:A:397:ARG:HH11	1.74	0.53
1:A:955:THR:OG1	1:A:957:THR:HG22	2.08	0.53
1:A:929:VAL:HG22	1:A:995:MET:HE1	1.90	0.53
1:A:181:VAL:O	1:A:185:MET:HG2	2.09	0.53
1:A:397:ARG:NE	1:A:416:PHE:HA	2.20	0.53
1:A:947:ARG:HG3	3:A:6:HOH:O	2.09	0.53
1:A:889:ALA:O	1:A:892:GLN:N	2.42	0.52
1:A:1009:PHE:CE2	1:A:1072:ILE:HD11	2.43	0.52
1:A:364:LYS:O	1:A:518:ILE:HA	2.09	0.52
1:A:1036:MET:CG	1:A:1042:LEU:HD23	2.30	0.52
1:A:662:GLN:HA	1:A:662:GLN:HE21	1.73	0.52
1:A:833:LYS:O	1:A:876:ILE:HG13	2.09	0.52
1:A:482:LEU:HB2	1:A:516:ILE:HG22	1.92	0.52
1:A:576:TRP:CD2	1:A:579:ARG:HD2	2.45	0.52
1:A:1078:LYS:O	1:A:1080:TRP:N	2.43	0.52
1:A:862:LEU:HB3	1:A:934:GLY:HA3	1.91	0.52
1:A:207:LEU:HD12	1:A:208:PRO:CD	2.31	0.52
1:A:1082:VAL:HG12	1:A:1086:TRP:CD1	2.44	0.52
1:A:809:LYS:N	3:A:4:HOH:O	2.40	0.52
1:A:916:PRO:C	1:A:917:THR:HG23	2.31	0.52
1:A:558:ILE:O	1:A:560:ALA:N	2.41	0.52
1:A:1059:LYS:HD2	1:A:1059:LYS:N	2.25	0.52
1:A:1008:LYS:HA	1:A:1011:ASP:HB3	1.92	0.51
1:A:1035:LEU:CB	1:A:1042:LEU:HD22	2.40	0.51
1:A:576:TRP:O	1:A:579:ARG:CD	2.58	0.51
1:A:749:ILE:O	1:A:749:ILE:HG22	2.10	0.51
1:A:987:LEU:O	1:A:987:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:VAL:HG11	1:A:292:TRP:NE1	2.26	0.51
1:A:910:TRP:CZ2	1:A:956:GLU:HG3	2.45	0.51
1:A:1039:MET:HB3	1:A:1040:PRO:CD	2.40	0.51
1:A:213:LYS:HD3	1:A:213:LYS:C	2.31	0.51
1:A:292:TRP:HA	1:A:292:TRP:CE3	2.45	0.51
1:A:623:ASP:HB3	1:A:626:LEU:HB3	1.93	0.51
1:A:645:VAL:O	1:A:649:GLU:HG2	2.11	0.51
1:A:213:LYS:C	1:A:215:ILE:H	2.13	0.51
1:A:1035:LEU:HB2	1:A:1042:LEU:HD22	1.93	0.51
1:A:628:MET:HE3	1:A:1030:LEU:HD21	1.93	0.50
1:A:803:VAL:HG22	1:A:811:LEU:CD2	2.41	0.50
1:A:430:ASN:OD1	1:A:432:GLN:HG3	2.11	0.50
1:A:170:ASP:OD2	1:A:172:GLU:HB2	2.11	0.50
1:A:432:GLN:HE22	1:A:501:LYS:NZ	2.09	0.50
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.93	0.50
1:A:241:PRO:HD3	1:A:285:THR:O	2.11	0.50
1:A:1043:THR:C	1:A:1045:LYS:H	2.15	0.50
1:A:202:VAL:CG1	1:A:285:THR:HG21	2.39	0.50
1:A:467:LEU:HD13	1:A:672:TYR:CE2	2.47	0.50
1:A:607:THR:O	1:A:610:LEU:HB3	2.11	0.50
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.77	0.50
1:A:161:ASP:CG	1:A:163:THR:HG1	2.16	0.49
1:A:928:PHE:HD2	1:A:995:MET:HE1	1.76	0.49
1:A:209:GLU:O	1:A:211:LEU:N	2.46	0.49
1:A:910:TRP:CZ3	1:A:956:GLU:HA	2.47	0.49
1:A:586:PRO:C	1:A:588:ALA:H	2.16	0.49
1:A:846:GLN:HA	1:A:846:GLN:OE1	2.12	0.49
1:A:387:ILE:CD1	1:A:468:LEU:HD11	2.42	0.49
1:A:558:ILE:HG22	1:A:559:ILE:N	2.27	0.49
1:A:208:PRO:HB3	1:A:856:GLU:HG3	1.95	0.49
1:A:276:GLY:HA2	1:A:822:ALA:HB2	1.95	0.49
1:A:589:TYR:HB2	1:A:590:PRO:HD3	1.93	0.49
1:A:890:LYS:O	1:A:890:LYS:HD3	2.12	0.49
1:A:679:ARG:O	1:A:683:LYS:HG3	2.11	0.49
1:A:274:VAL:HG23	1:A:279:GLU:O	2.12	0.49
1:A:527:ILE:HG23	1:A:528:ALA:N	2.28	0.49
1:A:651:LEU:HD22	1:A:655:ASP:CB	2.42	0.49
1:A:999:GLY:O	1:A:1001:LYS:N	2.46	0.49
1:A:629:GLN:HG2	1:A:1029:ILE:HD13	1.95	0.49
1:A:865:LEU:HD23	1:A:961:PHE:CD2	2.48	0.49
1:A:1059:LYS:HE3	1:A:1059:LYS:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:HD13	1:A:373:LEU:HA	1.94	0.48
1:A:379:LEU:CD1	1:A:380:THR:HG22	2.42	0.48
1:A:315:LEU:N	1:A:315:LEU:HD12	2.28	0.48
1:A:363:VAL:HG23	1:A:520:LEU:HD21	1.96	0.48
1:A:370:ILE:HG23	1:A:406:GLU:HA	1.94	0.48
1:A:889:ALA:O	1:A:890:LYS:C	2.52	0.48
1:A:213:LYS:HD3	1:A:213:LYS:O	2.12	0.48
1:A:673:HIS:CD2	1:A:712:ARG:HB2	2.49	0.48
1:A:863:CYS:SG	1:A:927:ARG:HG3	2.54	0.48
1:A:870:ILE:HG22	1:A:871:SER:O	2.13	0.48
1:A:221:PHE:HA	1:A:234:LYS:HA	1.96	0.48
1:A:527:ILE:CD1	1:A:528:ALA:N	2.71	0.48
1:A:233:ILE:N	1:A:233:ILE:HD12	2.28	0.48
1:A:738:VAL:HG12	1:A:742:LEU:CD1	2.43	0.48
1:A:569:ALA:O	1:A:573:GLU:HG3	2.14	0.48
1:A:1083:GLN:HA	1:A:1086:TRP:CD1	2.49	0.48
1:A:960:LEU:HD23	1:A:960:LEU:C	2.34	0.48
1:A:239:ASP:N	1:A:287:ILE:HG22	2.29	0.47
1:A:282:VAL:CG2	1:A:283:GLY:N	2.77	0.47
1:A:568:THR:HG22	1:A:571:ASP:CG	2.34	0.47
1:A:817:CYS:C	1:A:819:ASP:H	2.18	0.47
1:A:745:VAL:O	1:A:749:ILE:HG13	2.14	0.47
1:A:239:ASP:H	1:A:287:ILE:CG2	2.26	0.47
1:A:462:TYR:HA	1:A:485:TRP:O	2.14	0.47
1:A:590:PRO:HG2	1:A:626:LEU:CD1	2.44	0.47
1:A:811:LEU:HA	1:A:811:LEU:HD23	1.61	0.47
1:A:829:GLY:O	1:A:830:ILE:HG13	2.14	0.47
1:A:581:GLU:O	1:A:584:LYS:HG3	2.14	0.47
1:A:370:ILE:HD11	1:A:372:VAL:O	2.14	0.47
1:A:157:LEU:O	1:A:700:ARG:NE	2.46	0.47
1:A:475:LEU:HD23	1:A:475:LEU:C	2.35	0.47
1:A:247:SER:O	1:A:249:PHE:N	2.47	0.47
1:A:268:GLN:C	1:A:270:PHE:H	2.17	0.47
1:A:302:GLU:HG3	1:A:304:HIS:CD2	2.49	0.47
1:A:306:VAL:O	1:A:306:VAL:HG12	2.15	0.47
1:A:840:GLN:HB3	1:A:1039:MET:HE3	1.96	0.47
1:A:889:ALA:O	1:A:891:ILE:N	2.48	0.47
1:A:1008:LYS:HA	1:A:1011:ASP:OD2	2.14	0.47
1:A:271:VAL:HG12	1:A:308:ASP:O	2.15	0.47
1:A:286:PRO:HB2	1:A:289:ASN:ND2	2.30	0.47
1:A:501:LYS:HE2	1:A:501:LYS:HB3	1.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:THR:HG22	1:A:890:LYS:HB3	1.96	0.47
1:A:287:ILE:HD12	1:A:293:VAL:HG21	1.96	0.47
1:A:583:LEU:HD22	1:A:610:LEU:HD11	1.97	0.47
1:A:797:ALA:O	1:A:800:LYS:N	2.48	0.47
1:A:688:ASN:HD22	1:A:688:ASN:C	2.18	0.47
1:A:162:VAL:HG21	1:A:718:GLU:OE1	2.15	0.46
1:A:248:PHE:C	1:A:248:PHE:CD2	2.88	0.46
1:A:764:ILE:HG12	1:A:764:ILE:O	2.16	0.46
1:A:379:LEU:HD13	1:A:380:THR:HG22	1.96	0.46
1:A:363:VAL:HG23	1:A:520:LEU:HD23	1.97	0.46
1:A:628:MET:HE3	1:A:1030:LEU:CD2	2.45	0.46
1:A:798:ILE:C	1:A:800:LYS:H	2.19	0.46
1:A:955:THR:CB	1:A:957:THR:HG22	2.45	0.46
1:A:281:LEU:HA	1:A:290:PHE:CE2	2.51	0.46
1:A:285:THR:HB	1:A:290:PHE:CE1	2.51	0.46
1:A:380:THR:OG1	1:A:401:PRO:HB3	2.16	0.46
1:A:617:TRP:C	1:A:619:GLN:H	2.18	0.46
1:A:830:ILE:H	1:A:881:ILE:HD12	1.81	0.46
1:A:1015:LYS:HD3	1:A:1015:LYS:O	2.14	0.46
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.50	0.46
1:A:1064:ALA:O	1:A:1067:TYR:HB3	2.15	0.46
1:A:212:TRP:HE3	1:A:212:TRP:HA	1.81	0.46
1:A:478:GLY:H	1:A:520:LEU:HB2	1.81	0.46
1:A:706:SER:O	1:A:710:GLN:N	2.48	0.46
1:A:707:ARG:HA	1:A:710:GLN:NE2	2.30	0.46
1:A:1060:ASN:ND2	1:A:1063:ASP:OD1	2.48	0.46
1:A:833:LYS:HZ3	2:A:101:BYM:HN2	1.58	0.46
1:A:860:LEU:CD1	1:A:861:ASP:H	2.28	0.46
1:A:828:ILE:O	1:A:828:ILE:HG22	2.15	0.45
1:A:910:TRP:CH2	1:A:956:GLU:HA	2.51	0.45
1:A:1029:ILE:HD12	1:A:1029:ILE:HA	1.79	0.45
1:A:277:ARG:CD	1:A:292:TRP:CH2	3.00	0.45
1:A:817:CYS:SG	1:A:819:ASP:HB3	2.56	0.45
1:A:862:LEU:HD11	1:A:1012:ILE:CG2	2.46	0.45
1:A:1032:SER:O	1:A:1036:MET:HG3	2.17	0.45
1:A:379:LEU:CG	1:A:380:THR:H	2.29	0.45
1:A:865:LEU:HD12	1:A:865:LEU:HA	1.89	0.45
1:A:245:LEU:O	1:A:249:PHE:HB2	2.17	0.45
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.52	0.45
1:A:660:LEU:O	1:A:664:VAL:HG23	2.17	0.45
1:A:673:HIS:HD2	1:A:712:ARG:NE	2.10	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ARG:C	1:A:474:LEU:H	2.20	0.45
1:A:590:PRO:CD	1:A:626:LEU:HD11	2.46	0.45
1:A:598:TRP:HA	1:A:604:VAL:CG2	2.47	0.45
1:A:986:VAL:HG12	1:A:991:PHE:CE1	2.50	0.45
1:A:157:LEU:O	1:A:700:ARG:NH2	2.48	0.45
1:A:201:TRP:CD2	1:A:291:GLN:HG3	2.52	0.44
1:A:643:ILE:HG13	1:A:644:ALA:N	2.32	0.44
1:A:1042:LEU:HD12	1:A:1043:THR:N	2.32	0.44
1:A:192:ASP:OD2	1:A:194:LYS:HB3	2.17	0.44
1:A:738:VAL:HA	1:A:741:MET:CE	2.47	0.44
1:A:236:SER:C	1:A:238:ASP:N	2.70	0.44
1:A:311:PRO:O	1:A:313:PRO:HD3	2.17	0.44
1:A:382:PHE:CZ	1:A:434:TYR:HB2	2.53	0.44
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.99	0.44
1:A:154:LEU:O	1:A:155:THR:C	2.55	0.44
1:A:277:ARG:HA	1:A:790:GLY:O	2.16	0.44
1:A:286:PRO:CD	1:A:289:ASN:HD22	2.29	0.44
1:A:419:LYS:O	1:A:422:ASP:N	2.49	0.44
1:A:701:SER:O	1:A:705:GLN:HG2	2.17	0.44
1:A:218:ASN:O	1:A:219:CYS:SG	2.76	0.44
1:A:1002:THR:HG22	1:A:1006:PHE:CD2	2.52	0.44
1:A:393:VAL:C	1:A:394:LEU:HD23	2.38	0.44
1:A:702:GLU:HG3	1:A:713:PHE:HE1	1.81	0.44
1:A:741:MET:HB2	1:A:741:MET:HE2	1.79	0.44
1:A:949:ASN:C	1:A:951:ASN:N	2.70	0.44
1:A:220:ILE:O	1:A:235:VAL:N	2.50	0.44
1:A:947:ARG:HG3	1:A:947:ARG:NH1	2.32	0.44
1:A:1060:ASN:C	1:A:1062:GLU:N	2.71	0.44
1:A:1085:ASN:O	1:A:1087:PHE:CD1	2.71	0.44
1:A:306:VAL:HG12	1:A:308:ASP:HB2	1.99	0.44
1:A:464:VAL:HB	1:A:484:MET:HG2	1.98	0.44
1:A:861:ASP:O	1:A:862:LEU:HD22	2.16	0.44
1:A:1035:LEU:HB2	1:A:1042:LEU:CD2	2.48	0.44
1:A:432:GLN:HE22	1:A:501:LYS:HZ3	1.65	0.43
1:A:150:PHE:O	1:A:153:GLN:N	2.51	0.43
1:A:710:GLN:HG2	1:A:711:GLN:N	2.33	0.43
1:A:717:LEU:HD23	1:A:717:LEU:HA	1.90	0.43
1:A:987:LEU:HA	1:A:991:PHE:CD1	2.45	0.43
1:A:1021:ARG:NE	1:A:1055:LEU:O	2.51	0.43
1:A:470:ASP:HB3	1:A:476:ARG:NH2	2.32	0.43
1:A:553:LYS:HA	1:A:556:GLU:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:ASP:O	1:A:750:LYS:N	2.51	0.43
1:A:434:TYR:CE2	1:A:460:LEU:HB2	2.53	0.43
1:A:463:TYR:CD2	1:A:487:ILE:HD11	2.53	0.43
1:A:479:GLU:OE2	1:A:519:LEU:HB2	2.19	0.43
1:A:829:GLY:O	1:A:830:ILE:CG1	2.67	0.43
1:A:1033:MET:HB2	1:A:1033:MET:HE2	1.81	0.43
1:A:203:THR:OG1	1:A:204:SER:N	2.51	0.43
1:A:379:LEU:HD13	1:A:380:THR:O	2.18	0.43
1:A:564:LEU:O	1:A:565:ASN:C	2.56	0.43
1:A:586:PRO:C	1:A:588:ALA:N	2.72	0.43
1:A:310:PRO:HA	1:A:311:PRO:HD3	1.67	0.43
1:A:422:ASP:O	1:A:424:PRO:HD3	2.19	0.43
1:A:583:LEU:HD22	1:A:610:LEU:CD1	2.49	0.43
1:A:831:ILE:HG13	1:A:881:ILE:CG1	2.48	0.43
1:A:161:ASP:OD1	1:A:164:ASP:N	2.52	0.43
1:A:1023:HIS:O	1:A:1024:THR:C	2.55	0.43
1:A:1043:THR:HG22	1:A:1046:GLU:N	2.34	0.43
1:A:384:GLU:HG2	1:A:386:ASN:OD1	2.18	0.43
1:A:432:GLN:NE2	1:A:501:LYS:NZ	2.67	0.43
1:A:889:ALA:C	1:A:891:ILE:N	2.70	0.43
1:A:947:ARG:NH2	1:A:964:ASP:O	2.51	0.43
1:A:148:GLN:CD	1:A:148:GLN:H	2.22	0.42
1:A:860:LEU:HD23	1:A:1016:ALA:HA	2.01	0.42
1:A:173:LEU:HD11	1:A:711:GLN:NE2	2.34	0.42
1:A:271:VAL:HG23	1:A:282:VAL:HB	2.00	0.42
1:A:428:LEU:HD23	1:A:467:LEU:HD23	2.01	0.42
1:A:559:ILE:HD11	1:A:575:LEU:HD11	2.00	0.42
1:A:860:LEU:HD12	1:A:861:ASP:N	2.34	0.42
1:A:752:LEU:N	1:A:752:LEU:CD2	2.74	0.42
1:A:914:LYS:HD2	1:A:956:GLU:HG2	2.00	0.42
1:A:173:LEU:CD1	1:A:711:GLN:HE21	2.33	0.42
1:A:282:VAL:CG2	1:A:283:GLY:H	2.32	0.42
1:A:673:HIS:HD2	1:A:712:ARG:HB2	1.84	0.42
1:A:796:LEU:HA	1:A:815:PHE:HA	2.01	0.42
1:A:248:PHE:O	1:A:249:PHE:CG	2.73	0.42
1:A:585:HIS:O	1:A:588:ALA:HB3	2.20	0.42
1:A:1028:ILE:HG12	1:A:1051:ILE:CG2	2.49	0.42
1:A:217:ASN:OD1	1:A:219:CYS:HB2	2.20	0.42
1:A:233:ILE:HG22	1:A:234:LYS:H	1.84	0.42
1:A:801:CYS:HA	1:A:812:TRP:O	2.19	0.42
1:A:844:ILE:O	1:A:848:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:912:LYS:HA	1:A:921:PHE:CD1	2.55	0.42
1:A:717:LEU:O	1:A:720:TYR:N	2.50	0.42
1:A:273:ARG:O	1:A:305:VAL:HA	2.20	0.42
1:A:622:LEU:HD13	1:A:647:LYS:HD2	2.01	0.41
1:A:1035:LEU:C	1:A:1042:LEU:HD22	2.41	0.41
1:A:215:ILE:C	1:A:217:ASN:H	2.23	0.41
1:A:248:PHE:C	1:A:248:PHE:HD2	2.23	0.41
1:A:775:GLN:O	1:A:776:ASN:C	2.58	0.41
1:A:838:LEU:HD12	1:A:877:GLY:CA	2.50	0.41
1:A:860:LEU:CD2	1:A:1015:LYS:HD3	2.25	0.41
1:A:867:TYR:CE1	2:A:101:BYM:H16	2.55	0.41
1:A:1043:THR:C	1:A:1045:LYS:N	2.74	0.41
1:A:222:ILE:HD11	1:A:287:ILE:HD13	2.01	0.41
1:A:555:LEU:HD23	1:A:559:ILE:HG12	2.03	0.41
1:A:954:ILE:HD11	1:A:955:THR:O	2.20	0.41
1:A:997:THR:HG22	1:A:999:GLY:H	1.85	0.41
1:A:784:ARG:NE	1:A:789:PRO:O	2.54	0.41
1:A:892:GLN:OE1	1:A:902:PHE:HB3	2.20	0.41
1:A:233:ILE:CG2	1:A:234:LYS:H	2.33	0.41
1:A:982:ARG:HB3	1:A:983:VAL:H	1.76	0.41
1:A:1070:ASP:O	1:A:1073:GLU:HB2	2.20	0.41
1:A:467:LEU:HD23	1:A:467:LEU:HA	1.86	0.41
1:A:1043:THR:HB	1:A:1047:ASP:HB2	2.02	0.41
1:A:657:LEU:CD1	1:A:691:ILE:HA	2.51	0.41
1:A:157:LEU:HD13	1:A:721:LEU:HD22	2.02	0.41
1:A:248:PHE:O	1:A:249:PHE:CD2	2.74	0.41
1:A:472:ARG:O	1:A:473:PHE:HB2	2.21	0.41
1:A:482:LEU:HB2	1:A:516:ILE:CG2	2.51	0.41
1:A:648:LEU:C	1:A:650:SER:N	2.74	0.41
1:A:648:LEU:O	1:A:650:SER:N	2.54	0.41
1:A:693:HIS:HE1	1:A:786:PRO:O	2.02	0.41
1:A:861:ASP:C	1:A:861:ASP:OD1	2.60	0.41
1:A:896:VAL:HG12	1:A:897:GLY:H	1.86	0.41
1:A:995:MET:CE	1:A:995:MET:HA	2.50	0.41
1:A:1010:GLN:C	1:A:1012:ILE:N	2.74	0.41
1:A:805:ALA:O	1:A:806:SER:CB	2.69	0.41
1:A:1072:ILE:HG22	1:A:1073:GLU:N	2.35	0.41
1:A:419:LYS:O	1:A:421:LYS:N	2.55	0.40
1:A:858:GLU:O	1:A:860:LEU:N	2.53	0.40
1:A:173:LEU:HD11	1:A:711:GLN:HE21	1.86	0.40
1:A:829:GLY:CA	1:A:881:ILE:HD12	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:THR:O	1:A:1045:LYS:N	2.54	0.40
1:A:1066:LYS:HA	1:A:1069:LEU:HD12	2.03	0.40
1:A:187:GLU:O	1:A:188:VAL:C	2.59	0.40
1:A:225:HIS:CE1	1:A:304:HIS:ND1	2.87	0.40
1:A:361:PHE:HB2	1:A:420:ILE:HD13	2.03	0.40
1:A:597:LYS:HG2	3:A:3:HOH:O	2.22	0.40
1:A:788:ASP:HA	1:A:789:PRO:HD2	1.87	0.40
1:A:954:ILE:CD1	1:A:955:THR:O	2.70	0.40
1:A:584:LYS:O	1:A:586:PRO:HD3	2.20	0.40
1:A:643:ILE:CG1	1:A:644:ALA:N	2.84	0.40
1:A:815:PHE:CD1	1:A:815:PHE:N	2.89	0.40
1:A:888:ILE:HG23	1:A:889:ALA:N	2.36	0.40
1:A:1021:ARG:HE	1:A:1056:THR:HG1	1.69	0.40
1:A:1050:TYR:CD2	1:A:1050:TYR:C	2.94	0.40
1:A:144:SER:C	1:A:146:GLU:H	2.25	0.40
1:A:682:LEU:HA	1:A:682:LEU:HD12	1.73	0.40
1:A:804:MET:HE1	1:A:831:ILE:CG2	2.38	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	792/966 (82%)	633 (80%)	118 (15%)	41 (5%)	<b>2</b> <b>6</b>

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	LYS
1	A	215	ILE
1	A	247	SER
1	A	249	PHE

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Mol	Chain	Res	Type
1	A	406	GLU
1	A	548	PRO
1	A	901	ALA
1	A	948	HIS
1	A	1002	THR
1	A	1040	PRO
1	A	1079	GLY
1	A	1086	TRP
1	A	165	VAL
1	A	197	ALA
1	A	210	TYR
1	A	248	PHE
1	A	749	ILE
1	A	780	PRO
1	A	859	SER
1	A	1000	LYS
1	A	1061	GLU
1	A	237	PRO
1	A	269	ASP
1	A	560	ALA
1	A	776	ASN
1	A	896	VAL
1	A	964	ASP
1	A	1044	SER
1	A	1059	LYS
1	A	471	HIS
1	A	649	GLU
1	A	723	GLY
1	A	818	ALA
1	A	838	LEU
1	A	898	ASN
1	A	196	TYR
1	A	401	PRO
1	A	559	ILE
1	A	799	GLU
1	A	420	ILE
1	A	162	VAL

### 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	643/864 (74%)	592 (92%)	51 (8%)	12	34

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	163	THR
1	A	167	ASN
1	A	192	ASP
1	A	203	THR
1	A	211	LEU
1	A	212	TRP
1	A	248	PHE
1	A	249	PHE
1	A	277	ARG
1	A	280	TYR
1	A	287	ILE
1	A	309	THR
1	A	372	VAL
1	A	379	LEU
1	A	381	VAL
1	A	395	CYS
1	A	396	GLN
1	A	397	ARG
1	A	410	TRP
1	A	512	ASN
1	A	523	TYR
1	A	527	ILE
1	A	619	GLN
1	A	658	HIS
1	A	662	GLN
1	A	688	ASN
1	A	717	LEU
1	A	726	THR
1	A	731	ASP
1	A	752	LEU
1	A	773	ASN
1	A	774	LEU
1	A	784	ARG

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Mol	Chain	Res	Type
1	A	796	LEU
1	A	799	GLU
1	A	821	THR
1	A	841	ASP
1	A	917	THR
1	A	927	ARG
1	A	954	ILE
1	A	983	VAL
1	A	1002	THR
1	A	1011	ASP
1	A	1015	LYS
1	A	1021	ARG
1	A	1026	LEU
1	A	1039	MET
1	A	1061	GLU
1	A	1063	ASP
1	A	1072	ILE

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

Mol	Chain	Res	Type
1	A	167	ASN
1	A	169	HIS
1	A	218	ASN
1	A	225	HIS
1	A	289	ASN
1	A	295	HIS
1	A	392	GLN
1	A	432	GLN
1	A	483	HIS
1	A	498	ASN
1	A	549	ASN
1	A	554	GLN
1	A	585	HIS
1	A	600	GLN
1	A	662	GLN
1	A	673	HIS
1	A	688	ASN
1	A	710	GLN
1	A	711	GLN
1	A	734	GLN
1	A	766	GLN

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Mol	Chain	Res	Type
1	A	773	ASN
1	A	834	HIS
1	A	840	GLN
1	A	949	ASN
1	A	1083	GLN

### 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	BYM	A	101	-	17,21,21	2.60	5 (29%)	28,32,32	2.72	9 (32%)

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	BYM	A	101	-	-	0/4/26/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	BYM	C16-C15	6.21	1.51	1.39
2	A	101	BYM	C11-C8	4.88	1.47	1.38
2	A	101	BYM	C3-N2	3.90	1.41	1.36
2	A	101	BYM	C13-C9	3.76	1.47	1.39
2	A	101	BYM	C9-C8	-2.14	1.33	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	101	BYM	C1-N2-C3	-10.24	112.20	117.79
2	A	101	BYM	C5-C1-N2	4.18	113.71	110.22
2	A	101	BYM	S4-C3-N2	4.07	112.99	109.19
2	A	101	BYM	O12-C9-C8	3.77	112.63	109.72
2	A	101	BYM	O10-C8-C9	3.31	112.27	109.72
2	A	101	BYM	F19-C14-O12	-2.95	107.80	110.07
2	A	101	BYM	O6-C3-N2	-2.89	122.78	125.76
2	A	101	BYM	C18-C5-C1	2.44	122.39	120.47
2	A	101	BYM	F17-C14-O10	-2.03	108.51	110.07

There are no chirality outliers.

There are no torsion outliers.

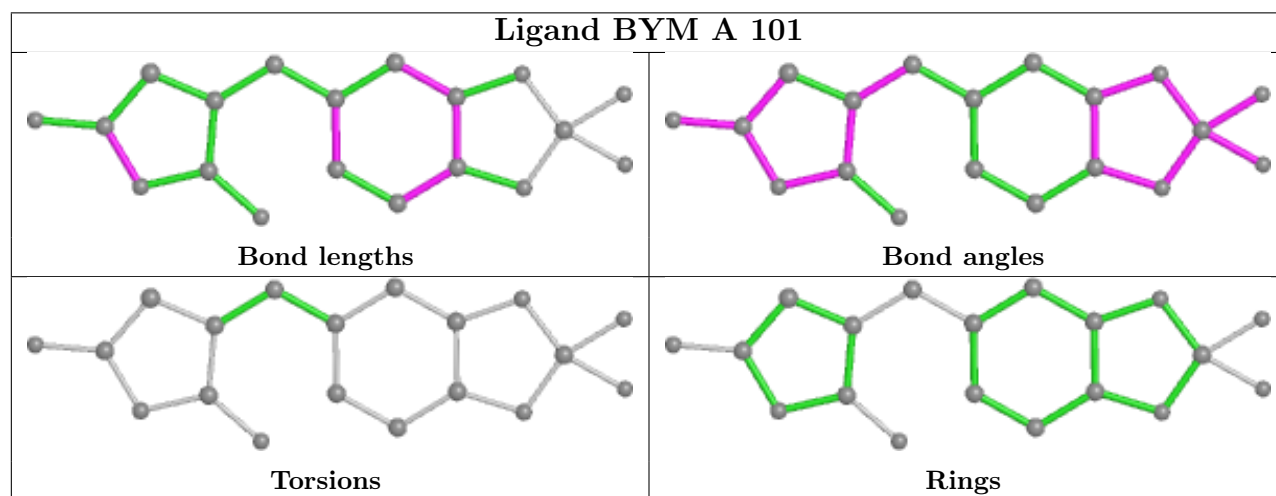
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	101	BYM	5	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, 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	812/966 (84%)	0.14	44 (5%) <span style="border: 1px solid red; padding: 2px;">25</span> <span style="border: 1px solid red; padding: 2px;">22</span>	16, 60, 104, 135	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	524	CYS	9.4
1	A	894	SER	6.1
1	A	523	TYR	5.4
1	A	896	VAL	5.2
1	A	216	ALA	4.9
1	A	1044	SER	4.5
1	A	899	THR	4.4
1	A	1075	CYS	3.9
1	A	148	GLN	3.8
1	A	916	PRO	3.8
1	A	522	ASN	3.7
1	A	1066	LYS	3.6
1	A	380	THR	3.5
1	A	250	THR	3.4
1	A	267	GLU	3.3
1	A	995	MET	3.2
1	A	1086	TRP	3.0
1	A	147	SER	3.0
1	A	776	ASN	2.9
1	A	777	SER	2.9
1	A	999	GLY	2.8
1	A	1064	ALA	2.8
1	A	936	CYS	2.8
1	A	998	SER	2.7
1	A	982	ARG	2.7
1	A	545	ALA	2.6
1	A	422	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1045	LYS	2.5
1	A	527	ILE	2.5
1	A	898	ASN	2.5
1	A	275	CYS	2.4
1	A	1004	PRO	2.4
1	A	230	SER	2.4
1	A	825	ASN	2.2
1	A	243	ALA	2.2
1	A	210	TYR	2.2
1	A	900	GLY	2.1
1	A	270	PHE	2.1
1	A	806	SER	2.1
1	A	544	ARG	2.1
1	A	213	LYS	2.0
1	A	379	LEU	2.0
1	A	217	ASN	2.0
1	A	932	CYS	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](#)

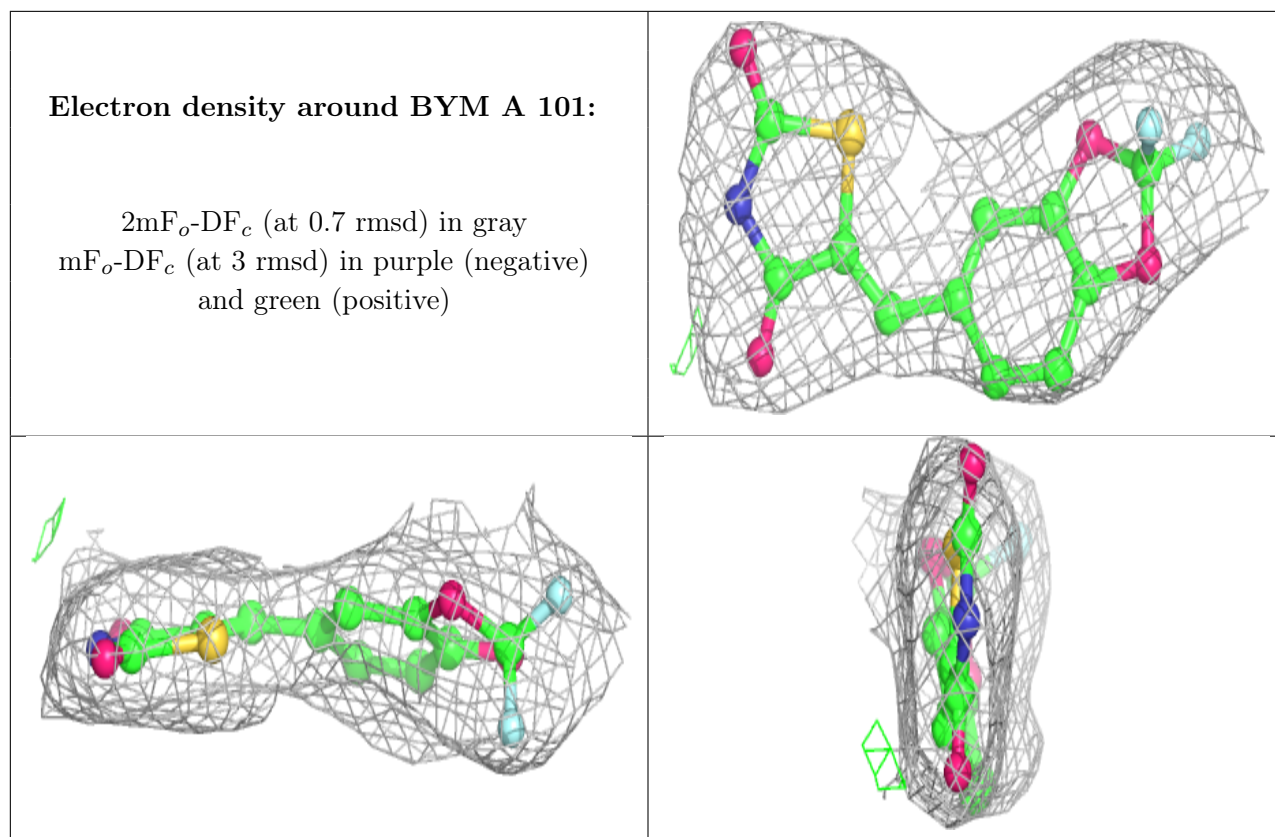
There are no monosaccharides in this entry.

## 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, 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	BYM	A	101	19/19	0.96	0.14	39,43,52,63	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.