



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:43 am BST

PDB ID : 2A5U  
Title : Crystal Structure of human PI3Kgamma complexed with AS605240  
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 : 2005-07-01  
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

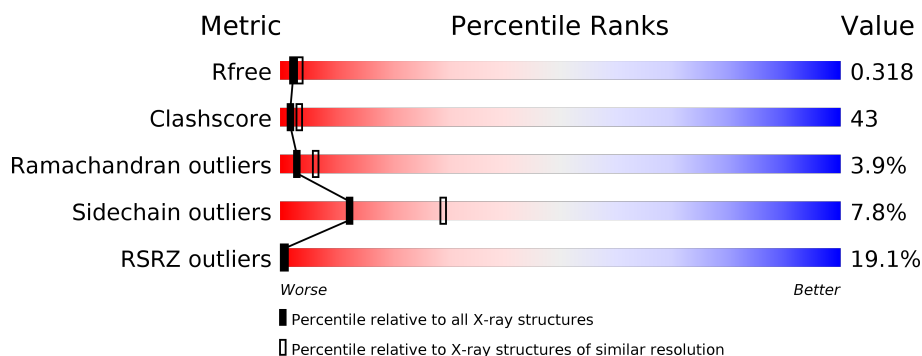
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	QYT	A	101	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6844 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.

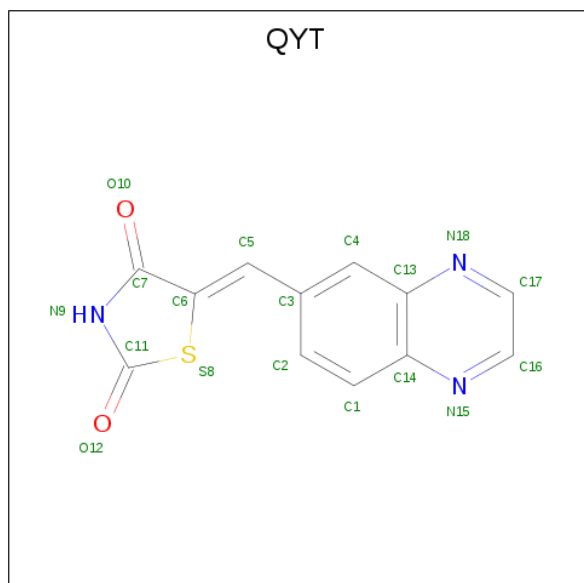
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit, gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	839	Total	C	N	O	S	0	0	0
			6806	4370	1162	1239	35			

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-(QUINOXALIN-6-YLMETHYLENE)-1,3-THIAZOLIDINE-2,4-DIONE (three-letter code: QYT) (formula: C<sub>12</sub>H<sub>7</sub>N<sub>3</sub>O<sub>2</sub>S).

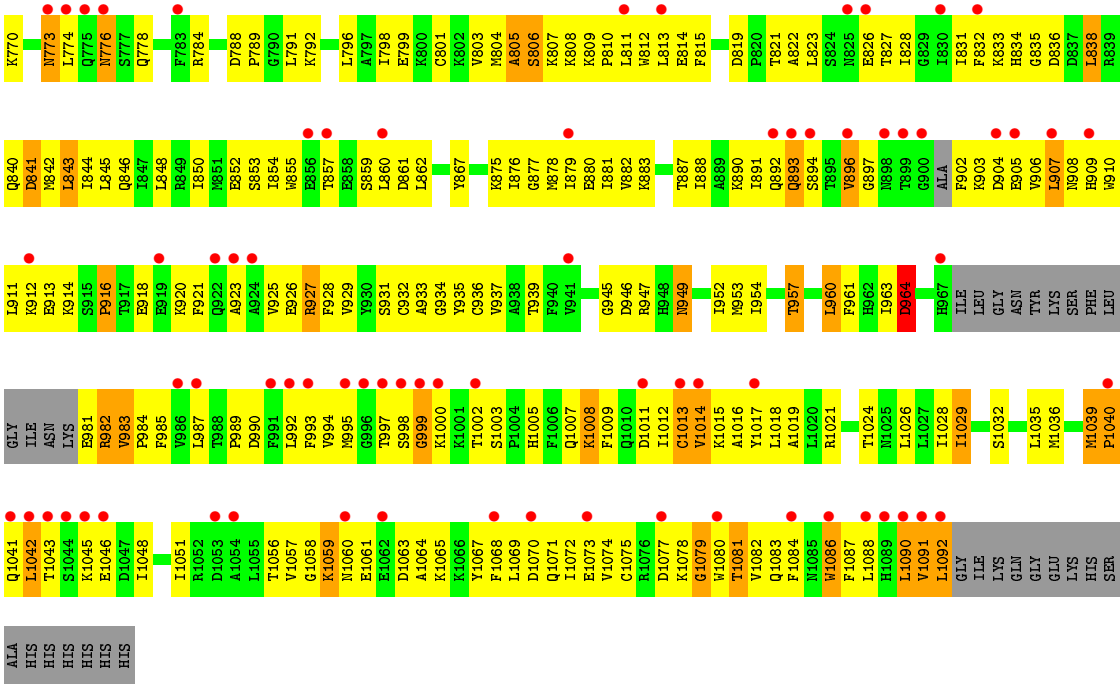


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			18	12	3	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.45Å 67.41Å 105.97Å 90.00° 96.35° 90.00°	Depositor
Resolution (Å)	19.58 – 2.70 19.58 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.58-2.70) 96.7 (19.58-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.87 (at 2.71Å)	Xtriage
Refinement program	CNS, CNX 2002	Depositor
R, $R_{free}$	0.279 , 0.351 0.244 , 0.318	Depositor DCC
$R_{free}$ test set	2591 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.9	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 101.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6844	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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: QYT

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	0.35	0/6951	0.60	0/9400

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	6806	0	6850	581	0
2	A	18	0	7	9	0
3	A	20	0	0	4	0
All	All	6844	0	6857	582	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 43.

All (582) 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:1008:LYS:HZ2	1:A:1012:ILE:HG23	1.11	1.06

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:VAL:HG23	1:A:310:PRO:HG3	1.41	1.02
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.44	0.99
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.41	0.98
1:A:810:PRO:HG3	1:A:833:LYS:HG3	1.47	0.92
1:A:741:MET:HE1	1:A:778:GLN:HG2	1.53	0.90
1:A:749:ILE:HG12	1:A:767:LEU:HD23	1.54	0.90
1:A:903:LYS:HB2	1:A:906:VAL:HG23	1.53	0.88
1:A:379:LEU:HD22	1:A:380:THR:H	1.36	0.88
1:A:544:ARG:HB3	1:A:544:ARG:HH11	1.38	0.87
1:A:286:PRO:HD2	1:A:289:ASN:HD22	1.39	0.86
1:A:410:TRP:HB3	1:A:412:VAL:HG12	1.55	0.86
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.59	0.85
1:A:1008:LYS:NZ	1:A:1012:ILE:HG23	1.92	0.84
1:A:182:THR:HB	1:A:183:PRO:HD3	1.60	0.84
1:A:1086:TRP:HH2	1:A:1090:LEU:HB3	1.42	0.83
1:A:1048:ILE:O	1:A:1051:ILE:HG22	1.78	0.82
1:A:551:LEU:HD23	1:A:554:GLN:NE2	1.95	0.81
1:A:220:ILE:HG13	1:A:287:ILE:HD11	1.60	0.81
1:A:992:LEU:HA	1:A:995:MET:HE3	1.63	0.81
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.63	0.81
1:A:1074:VAL:O	1:A:1078:LYS:HD3	1.81	0.80
1:A:736:VAL:O	1:A:740:GLU:HG2	1.82	0.79
1:A:1018:LEU:HD12	1:A:1019:ALA:N	1.98	0.79
1:A:551:LEU:HD23	1:A:554:GLN:HE22	1.48	0.79
1:A:431:LEU:HD13	1:A:516:ILE:HD13	1.63	0.78
1:A:983:VAL:HG12	1:A:984:PRO:HD2	1.66	0.78
1:A:291:GLN:HE21	1:A:291:GLN:HA	1.49	0.77
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.65	0.77
1:A:147:SER:HA	1:A:319:ARG:HH22	1.50	0.77
1:A:240:THR:HG22	1:A:242:GLY:H	1.50	0.76
1:A:239:ASP:O	1:A:287:ILE:HG23	1.86	0.76
1:A:547:MET:SD	1:A:552:ARG:HA	2.26	0.76
1:A:271:VAL:CG2	1:A:310:PRO:HG3	2.16	0.76
1:A:497:PHE:HB2	1:A:1041:GLN:HE21	1.51	0.76
1:A:312:ASP:OD2	1:A:314:ALA:HB3	1.86	0.75
1:A:752:LEU:HB3	1:A:766:GLN:HE22	1.51	0.75
1:A:804:MET:HE1	1:A:831:ILE:HG23	1.68	0.75
1:A:178:ARG:HH11	1:A:178:ARG:HG2	1.52	0.75
1:A:752:LEU:HD13	1:A:766:GLN:NE2	2.01	0.75
1:A:689:LYS:HG2	1:A:728:MET:HE2	1.68	0.75
1:A:614:ARG:HB2	1:A:618:ASP:OD2	1.86	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:882:VAL:H	2:A:101:QYT:H16	1.49	0.74
1:A:180:LEU:O	1:A:183:PRO:HD2	1.88	0.74
1:A:946:ASP:OD2	1:A:983:VAL:HG23	1.86	0.74
1:A:149:ALA:HA	1:A:152:ARG:HD3	1.70	0.73
1:A:366:ARG:HG3	1:A:366:ARG:HH11	1.53	0.73
1:A:228:THR:HG23	1:A:229:THR:H	1.53	0.73
1:A:147:SER:HA	1:A:319:ARG:NH2	2.04	0.73
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.07	0.73
1:A:213:LYS:HD3	1:A:214:LYS:H	1.54	0.72
1:A:277:ARG:HH11	1:A:277:ARG:HG2	1.54	0.72
1:A:990:ASP:O	1:A:994:VAL:HG23	1.89	0.72
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.72	0.72
1:A:497:PHE:HB2	1:A:1041:GLN:NE2	2.04	0.72
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.25	0.72
1:A:743:GLN:HG2	1:A:876:ILE:HD13	1.69	0.72
1:A:272:LEU:HB3	1:A:305:VAL:HG21	1.70	0.72
1:A:225:HIS:NE2	1:A:823:LEU:HD21	2.04	0.71
1:A:379:LEU:HD13	1:A:380:THR:O	1.90	0.71
1:A:184:ARG:HB2	1:A:184:ARG:HH11	1.54	0.71
1:A:240:THR:O	1:A:244:ILE:HG12	1.90	0.71
1:A:739:ILE:O	1:A:743:GLN:HB2	1.91	0.71
1:A:927:ARG:HH11	1:A:927:ARG:HB2	1.56	0.71
1:A:743:GLN:HG2	1:A:876:ILE:CD1	2.22	0.70
1:A:1008:LYS:HZ3	1:A:1011:ASP:HB3	1.54	0.70
1:A:798:ILE:HD12	1:A:798:ILE:H	1.56	0.70
1:A:579:ARG:HB2	1:A:610:LEU:HD11	1.73	0.70
1:A:217:ASN:ND2	1:A:219:CYS:HB3	2.07	0.70
1:A:434:TYR:CE1	1:A:460:LEU:HB2	2.27	0.70
1:A:796:LEU:HD11	1:A:801:CYS:SG	2.31	0.70
1:A:732:PHE:O	1:A:736:VAL:HG23	1.92	0.70
1:A:928:PHE:O	1:A:932:CYS:HB2	1.92	0.70
1:A:1042:LEU:H	1:A:1042:LEU:HD13	1.57	0.69
1:A:487:ILE:HG23	1:A:488:SER:N	2.07	0.69
1:A:745:VAL:O	1:A:749:ILE:HD13	1.93	0.69
1:A:1003:SER:O	1:A:1007:GLN:HB2	1.92	0.68
1:A:168:VAL:HG13	1:A:170:ASP:H	1.58	0.68
1:A:862:LEU:HD11	1:A:1016:ALA:CB	2.23	0.68
1:A:233:ILE:N	1:A:233:ILE:HD12	2.08	0.68
1:A:627:THR:HG21	1:A:648:LEU:HD21	1.75	0.68
1:A:1092:LEU:O	1:A:1092:LEU:HD13	1.94	0.68
1:A:862:LEU:O	1:A:931:SER:HA	1.94	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:HB3	1:A:305:VAL:CG2	2.24	0.67
1:A:213:LYS:HD3	1:A:214:LYS:N	2.09	0.67
1:A:207:LEU:HD22	1:A:208:PRO:HD2	1.76	0.67
1:A:890:LYS:NZ	1:A:890:LYS:HB2	2.09	0.67
1:A:921:PHE:O	1:A:925:VAL:HG23	1.95	0.66
1:A:995:MET:O	1:A:1005:HIS:HB2	1.95	0.66
1:A:235:VAL:HG11	1:A:244:ILE:HG23	1.78	0.66
1:A:907:LEU:HD12	1:A:990:ASP:OD2	1.95	0.66
1:A:1008:LYS:NZ	1:A:1011:ASP:HB3	2.11	0.65
1:A:215:ILE:HG21	1:A:220:ILE:HD13	1.79	0.65
1:A:359:ARG:HD3	1:A:360:LYS:H	1.62	0.65
1:A:552:ARG:O	1:A:556:GLU:HG3	1.97	0.65
1:A:763:VAL:HA	1:A:766:GLN:NE2	2.12	0.65
1:A:220:ILE:HB	1:A:235:VAL:HG23	1.79	0.65
1:A:184:ARG:O	1:A:188:VAL:HG23	1.97	0.64
1:A:841:ASP:O	1:A:845:LEU:HD22	1.97	0.64
1:A:584:LYS:HA	1:A:616:VAL:HG21	1.77	0.64
1:A:629:GLN:HG2	1:A:1029:ILE:CG1	2.24	0.64
1:A:896:VAL:HG12	1:A:897:GLY:H	1.62	0.64
1:A:910:TRP:HE3	1:A:911:LEU:HD23	1.63	0.64
1:A:1078:LYS:O	1:A:1081:THR:N	2.24	0.64
1:A:373:LEU:HB3	1:A:374:PRO:HD3	1.79	0.64
1:A:584:LYS:O	1:A:616:VAL:HG11	1.97	0.64
1:A:629:GLN:CG	1:A:1029:ILE:HG13	2.22	0.63
1:A:184:ARG:CB	1:A:184:ARG:HH11	2.11	0.63
1:A:544:ARG:HB3	1:A:544:ARG:NH1	2.10	0.63
1:A:559:ILE:HG12	1:A:588:ALA:HB2	1.80	0.63
1:A:947:ARG:HG2	1:A:947:ARG:HH11	1.63	0.63
1:A:1059:LYS:CD	1:A:1059:LYS:H	2.11	0.63
1:A:278:ASP:HB2	1:A:792:LYS:NZ	2.14	0.63
1:A:425:LYS:HE2	1:A:672:TYR:CZ	2.32	0.63
1:A:201:TRP:CE2	1:A:291:GLN:HG3	2.34	0.63
1:A:483:HIS:CD2	1:A:510:LYS:HG2	2.34	0.63
1:A:583:LEU:HD22	1:A:610:LEU:CD2	2.28	0.63
1:A:240:THR:HG23	1:A:241:PRO:HD2	1.80	0.62
1:A:740:GLU:O	1:A:744:LYS:HG3	1.98	0.62
1:A:635:PHE:O	1:A:641:ARG:HD2	1.98	0.62
1:A:833:LYS:HZ1	2:A:101:QYT:C11	2.12	0.62
1:A:791:LEU:HD22	1:A:828:ILE:HD11	1.80	0.62
1:A:737:GLN:O	1:A:741:MET:HG2	2.00	0.62
1:A:223:VAL:HG22	1:A:232:THR:HG23	1.82	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ALA:O	1:A:246:GLN:HB2	2.00	0.62
1:A:380:THR:HG23	1:A:381:VAL:N	2.14	0.61
1:A:888:ILE:HG12	1:A:952:ILE:O	2.00	0.61
1:A:1072:ILE:O	1:A:1075:CYS:HB2	1.99	0.61
1:A:180:LEU:C	1:A:183:PRO:HD2	2.20	0.61
1:A:576:TRP:O	1:A:579:ARG:HG2	1.99	0.61
1:A:1008:LYS:O	1:A:1012:ILE:HG12	2.00	0.61
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.35	0.61
1:A:960:LEU:HG	1:A:961:PHE:N	2.15	0.61
1:A:379:LEU:HD12	1:A:435:CYS:HB2	1.83	0.61
1:A:759:VAL:HG12	1:A:764:ILE:HD11	1.82	0.61
1:A:303:ILE:HD12	1:A:303:ILE:N	2.15	0.61
1:A:381:VAL:HG23	1:A:434:TYR:O	2.00	0.60
1:A:470:ASP:CG	1:A:472:ARG:H	2.03	0.60
1:A:208:PRO:HG2	1:A:211:LEU:HB2	1.82	0.60
1:A:833:LYS:HG2	1:A:834:HIS:N	2.16	0.60
1:A:183:PRO:HG2	1:A:679:ARG:HD2	1.82	0.60
1:A:625:GLY:O	1:A:629:GLN:HG3	2.01	0.60
1:A:555:LEU:C	1:A:555:LEU:HD23	2.22	0.60
1:A:512:ASN:C	1:A:512:ASN:HD22	2.04	0.60
1:A:759:VAL:O	1:A:764:ILE:HD11	2.01	0.60
1:A:997:THR:HG22	1:A:998:SER:N	2.17	0.60
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.84	0.60
1:A:277:ARG:NH1	1:A:277:ARG:HG2	2.12	0.60
1:A:904:ASP:O	1:A:990:ASP:HA	2.02	0.60
1:A:196:TYR:O	1:A:689:LYS:HD2	2.01	0.60
1:A:749:ILE:CG1	1:A:767:LEU:HD23	2.30	0.59
1:A:614:ARG:HH11	1:A:614:ARG:HG3	1.68	0.59
2:A:101:QYT:S8	2:A:101:QYT:H2	2.42	0.59
1:A:1086:TRP:CH2	1:A:1090:LEU:HB3	2.31	0.59
1:A:545:ALA:O	1:A:546:GLU:HB2	2.02	0.59
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.83	0.59
1:A:730:HIS:O	1:A:734:GLN:HG2	2.01	0.59
1:A:202:VAL:HG12	1:A:290:PHE:HA	1.84	0.59
1:A:228:THR:HG23	1:A:229:THR:N	2.16	0.59
1:A:697:TRP:HZ3	3:A:2:HOH:O	1.85	0.59
1:A:833:LYS:O	1:A:876:ILE:HG13	2.02	0.59
1:A:925:VAL:O	1:A:929:VAL:HG23	2.02	0.59
1:A:220:ILE:HB	1:A:235:VAL:CG2	2.32	0.59
1:A:178:ARG:HG2	1:A:178:ARG:NH1	2.17	0.59
1:A:882:VAL:H	2:A:101:QYT:C16	2.15	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.38	0.59
1:A:627:THR:HG21	1:A:648:LEU:CD2	2.33	0.59
1:A:908:ASN:ND2	1:A:994:VAL:HA	2.17	0.59
1:A:949:ASN:H	1:A:1083:GLN:NE2	1.99	0.58
1:A:483:HIS:O	1:A:506:THR:HG23	2.02	0.58
1:A:909:HIS:O	1:A:913:GLU:HG2	2.04	0.58
1:A:150:PHE:HB2	1:A:319:ARG:NH1	2.19	0.58
1:A:293:VAL:O	1:A:297:LEU:HG	2.03	0.58
1:A:1042:LEU:HD22	1:A:1042:LEU:O	2.04	0.58
1:A:144:SER:HB3	1:A:147:SER:CB	2.34	0.58
1:A:368:ILE:HG22	1:A:516:ILE:HB	1.85	0.58
1:A:960:LEU:HG	1:A:961:PHE:H	1.69	0.58
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.38	0.58
1:A:198:MET:HE2	1:A:311:PRO:HD2	1.85	0.58
1:A:1018:LEU:HD22	1:A:1061:GLU:OE1	2.04	0.58
1:A:210:TYR:CE2	1:A:861:ASP:HB2	2.39	0.58
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.86	0.58
1:A:752:LEU:O	1:A:753:SER:HB2	2.03	0.58
1:A:987:LEU:HD11	1:A:995:MET:HE1	1.85	0.58
1:A:233:ILE:HD11	1:A:248:PHE:HD1	1.68	0.58
1:A:501:LYS:NZ	1:A:501:LYS:HB3	2.18	0.58
1:A:224:ILE:HA	1:A:305:VAL:HG12	1.85	0.57
1:A:561:THR:HG21	1:A:565:ASN:ND2	2.19	0.57
1:A:927:ARG:HB2	1:A:927:ARG:NH1	2.19	0.57
1:A:359:ARG:HD3	1:A:360:LYS:N	2.19	0.57
1:A:1008:LYS:HE2	1:A:1008:LYS:HA	1.85	0.57
1:A:1090:LEU:HD12	1:A:1091:VAL:N	2.19	0.57
1:A:460:LEU:O	1:A:461:LEU:HD23	2.05	0.57
1:A:796:LEU:O	1:A:798:ILE:HD12	2.04	0.57
1:A:815:PHE:O	1:A:827:THR:HB	2.04	0.57
1:A:952:ILE:CG2	1:A:960:LEU:HD11	2.35	0.57
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.52	0.57
1:A:807:LYS:HD3	1:A:807:LYS:N	2.19	0.57
1:A:912:LYS:NZ	1:A:918:GLU:HG2	2.20	0.57
1:A:641:ARG:O	1:A:644:ALA:HB3	2.05	0.57
1:A:244:ILE:HD11	1:A:287:ILE:HG21	1.86	0.57
1:A:207:LEU:HD12	1:A:212:TRP:CD1	2.40	0.57
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.87	0.57
1:A:184:ARG:CB	1:A:184:ARG:NH1	2.68	0.56
1:A:674:ASP:OD1	1:A:679:ARG:NE	2.38	0.56
1:A:360:LYS:HB3	1:A:416:PHE:O	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:GLN:CA	1:A:391:GLN:HE21	2.18	0.56
1:A:741:MET:HB2	1:A:774:LEU:HD13	1.88	0.56
1:A:246:GLN:C	1:A:248:PHE:H	2.09	0.56
1:A:564:LEU:HG	1:A:1028:ILE:HG21	1.87	0.56
1:A:896:VAL:HG12	1:A:897:GLY:N	2.21	0.56
1:A:273:ARG:HA	1:A:280:TYR:HA	1.88	0.56
1:A:390:GLY:C	1:A:392:GLN:H	2.09	0.56
1:A:1021:ARG:HE	1:A:1056:THR:HG23	1.71	0.56
1:A:181:VAL:HG22	1:A:184:ARG:HH22	1.70	0.56
1:A:890:LYS:HA	1:A:893:GLN:HG2	1.88	0.56
1:A:945:GLY:O	1:A:985:PHE:HA	2.06	0.56
1:A:601:GLN:HG3	1:A:602:GLU:N	2.21	0.55
1:A:653:ASP:OD2	1:A:688:ASN:ND2	2.39	0.55
1:A:184:ARG:HD3	1:A:719:ALA:O	2.05	0.55
1:A:724:CYS:HB2	1:A:728:MET:HG3	1.88	0.55
1:A:984:PRO:HG2	1:A:985:PHE:H	1.71	0.55
1:A:379:LEU:HD13	1:A:380:THR:N	2.21	0.55
1:A:963:ILE:O	1:A:964:ASP:O	2.25	0.55
1:A:231:GLN:HE21	1:A:231:GLN:HA	1.70	0.55
1:A:617:TRP:CZ3	1:A:626:LEU:HD12	2.41	0.55
1:A:198:MET:SD	1:A:282:VAL:HG11	2.47	0.55
1:A:752:LEU:HD22	1:A:766:GLN:OE1	2.06	0.55
1:A:992:LEU:HA	1:A:995:MET:CE	2.34	0.55
1:A:759:VAL:HG22	1:A:809:LYS:NZ	2.21	0.55
1:A:291:GLN:NE2	1:A:291:GLN:HA	2.21	0.55
1:A:982:ARG:HD2	1:A:982:ARG:N	2.21	0.55
1:A:1039:MET:N	1:A:1039:MET:SD	2.80	0.54
1:A:564:LEU:HD21	1:A:1048:ILE:HG21	1.88	0.54
1:A:935:TYR:O	1:A:939:THR:HG22	2.07	0.54
1:A:750:LYS:NZ	1:A:834:HIS:HD2	2.05	0.54
1:A:197:ALA:HB2	1:A:316:ASP:OD2	2.07	0.54
1:A:878:MET:C	1:A:879:ILE:HD12	2.28	0.54
1:A:796:LEU:HD23	1:A:815:PHE:CE2	2.42	0.54
1:A:803:VAL:CG1	1:A:809:LYS:HE3	2.37	0.54
1:A:1060:ASN:OD1	1:A:1063:ASP:N	2.39	0.54
1:A:201:TRP:NE1	1:A:291:GLN:HG3	2.23	0.54
1:A:481:VAL:HG12	1:A:481:VAL:O	2.08	0.54
1:A:380:THR:HG1	1:A:402:LYS:C	2.11	0.54
1:A:184:ARG:HD2	1:A:722:ARG:O	2.08	0.54
1:A:947:ARG:NH1	1:A:947:ARG:HG2	2.22	0.54
1:A:905:GLU:HG3	1:A:993:PHE:CZ	2.43	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:CYS:HB2	1:A:418:ILE:HD11	1.89	0.53
1:A:506:THR:HG22	1:A:507:ASN:N	2.24	0.53
1:A:614:ARG:NH1	1:A:614:ARG:HG3	2.23	0.53
1:A:379:LEU:HD22	1:A:380:THR:N	2.14	0.53
1:A:910:TRP:CE3	1:A:911:LEU:HD23	2.43	0.53
1:A:363:VAL:O	1:A:363:VAL:HG13	2.08	0.53
1:A:487:ILE:CG2	1:A:488:SER:N	2.72	0.53
1:A:983:VAL:HG21	1:A:1082:VAL:HG21	1.91	0.53
1:A:233:ILE:HG22	1:A:234:LYS:N	2.24	0.53
1:A:760:SER:O	1:A:764:ILE:HG13	2.09	0.53
1:A:235:VAL:HG11	1:A:244:ILE:HD12	1.89	0.52
1:A:270:PHE:HD2	1:A:307:LEU:HG	1.74	0.52
1:A:214:LYS:HE2	1:A:300:GLY:HA2	1.90	0.52
1:A:562:ASP:OD1	1:A:565:ASN:N	2.43	0.52
1:A:796:LEU:HD22	1:A:814:GLU:O	2.08	0.52
1:A:984:PRO:HB2	1:A:985:PHE:CD2	2.44	0.52
1:A:576:TRP:CZ3	1:A:579:ARG:HD3	2.44	0.52
1:A:796:LEU:HD21	1:A:813:LEU:HB3	1.92	0.52
1:A:807:LYS:HD3	1:A:807:LYS:H	1.74	0.52
1:A:643:ILE:O	1:A:646:GLN:HB3	2.10	0.52
1:A:806:SER:O	1:A:808:LYS:O	2.27	0.52
1:A:855:TRP:NE1	1:A:1016:ALA:HB1	2.24	0.52
1:A:835:GLY:O	1:A:875:LYS:HD2	2.10	0.52
1:A:913:GLU:HG3	1:A:914:LYS:N	2.24	0.52
1:A:687:ARG:HG2	1:A:687:ARG:O	2.09	0.52
1:A:923:ALA:O	1:A:926:GLU:HB3	2.10	0.52
1:A:952:ILE:HG22	1:A:960:LEU:HD11	1.92	0.52
1:A:997:THR:HG22	1:A:998:SER:H	1.73	0.52
1:A:882:VAL:N	2:A:101:QYT:H16	2.23	0.51
1:A:233:ILE:HD12	1:A:233:ILE:H	1.72	0.51
1:A:317:GLU:O	1:A:726:THR:HG23	2.10	0.51
1:A:954:ILE:HA	1:A:960:LEU:HA	1.91	0.51
1:A:1059:LYS:H	1:A:1059:LYS:HD3	1.74	0.51
1:A:285:THR:HG22	1:A:289:ASN:HB2	1.91	0.51
1:A:752:LEU:CB	1:A:766:GLN:HE22	2.20	0.51
1:A:286:PRO:HD2	1:A:289:ASN:ND2	2.17	0.51
1:A:788:ASP:OD2	1:A:791:LEU:HD12	2.11	0.51
1:A:303:ILE:HD12	1:A:303:ILE:H	1.75	0.51
1:A:814:GLU:HA	1:A:828:ILE:O	2.10	0.51
1:A:1024:THR:O	1:A:1028:ILE:HG12	2.11	0.51
1:A:373:LEU:HD13	1:A:373:LEU:C	2.31	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:LEU:HD13	1:A:796:LEU:C	2.30	0.51
1:A:767:LEU:HD21	1:A:811:LEU:HD11	1.92	0.51
1:A:892:GLN:C	1:A:894:SER:H	2.13	0.51
1:A:981:GLU:N	1:A:982:ARG:NH1	2.59	0.51
1:A:833:LYS:NZ	2:A:101:QYT:C11	2.75	0.50
1:A:1043:THR:HG21	1:A:1046:GLU:HG3	1.93	0.50
1:A:146:GLU:O	1:A:149:ALA:HB3	2.11	0.50
1:A:890:LYS:HZ2	1:A:890:LYS:HB2	1.74	0.50
1:A:164:ASP:OD2	1:A:166:SER:HB3	2.12	0.50
1:A:982:ARG:C	1:A:983:VAL:HG22	2.32	0.50
1:A:569:ALA:O	1:A:573:GLU:HG3	2.12	0.50
1:A:617:TRP:HZ3	1:A:626:LEU:HD12	1.75	0.50
1:A:564:LEU:HG	1:A:1028:ILE:CG2	2.42	0.50
1:A:892:GLN:HE22	1:A:906:VAL:HB	1.77	0.50
1:A:359:ARG:HG3	1:A:360:LYS:O	2.10	0.50
1:A:280:TYR:CD1	1:A:280:TYR:N	2.80	0.49
1:A:808:LYS:HE3	1:A:836:ASP:OD1	2.12	0.49
1:A:584:LYS:C	1:A:616:VAL:HG11	2.32	0.49
1:A:773:ASN:HA	1:A:776:ASN:HD21	1.76	0.49
1:A:1056:THR:O	1:A:1056:THR:HG23	2.12	0.49
1:A:547:MET:O	1:A:548:PRO:O	2.30	0.49
1:A:766:GLN:O	1:A:770:LYS:HG3	2.13	0.49
1:A:215:ILE:HG13	1:A:215:ILE:O	2.12	0.49
1:A:287:ILE:O	1:A:293:VAL:HG21	2.12	0.49
1:A:702:GLU:O	1:A:706:SER:HB3	2.13	0.49
1:A:843:LEU:O	1:A:846:GLN:HB3	2.12	0.49
1:A:144:SER:HB3	1:A:147:SER:HB2	1.94	0.49
1:A:282:VAL:HG23	1:A:283:GLY:N	2.26	0.49
1:A:225:HIS:CE1	1:A:304:HIS:CD2	2.94	0.49
1:A:615:GLU:O	1:A:619:GLN:HB2	2.12	0.49
1:A:822:ALA:C	1:A:823:LEU:HD12	2.32	0.49
1:A:987:LEU:HD11	1:A:995:MET:CE	2.43	0.49
1:A:1077:ASP:C	1:A:1078:LYS:HD2	2.33	0.49
1:A:148:GLN:O	1:A:152:ARG:HG3	2.13	0.49
1:A:214:LYS:HG2	1:A:297:LEU:CD2	2.43	0.49
1:A:302:GLU:HB2	1:A:304:HIS:HE1	1.78	0.49
1:A:358:ASP:OD1	1:A:419:LYS:HD3	2.12	0.49
1:A:1042:LEU:HD22	1:A:1042:LEU:C	2.33	0.49
1:A:170:ASP:OD1	1:A:471:HIS:HE1	1.96	0.49
1:A:315:LEU:C	1:A:317:GLU:H	2.17	0.48
1:A:375:ARG:O	1:A:376:ASN:C	2.52	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LEU:O	1:A:418:ILE:HD11	2.13	0.48
1:A:1078:LYS:N	1:A:1078:LYS:HD2	2.28	0.48
1:A:292:TRP:O	1:A:295:HIS:HB3	2.13	0.48
1:A:890:LYS:HA	1:A:893:GLN:CG	2.42	0.48
1:A:1028:ILE:HD13	1:A:1051:ILE:HG13	1.94	0.48
1:A:929:VAL:HG12	1:A:1012:ILE:CD1	2.44	0.48
1:A:191:ARG:HD2	1:A:196:TYR:CG	2.49	0.48
1:A:219:CYS:SG	1:A:234:LYS:HD3	2.53	0.48
1:A:233:ILE:N	1:A:233:ILE:CD1	2.76	0.48
1:A:660:LEU:O	1:A:664:VAL:HG23	2.14	0.48
1:A:700:ARG:HD3	3:A:2:HOH:O	2.12	0.48
1:A:833:LYS:HG2	1:A:834:HIS:H	1.76	0.48
1:A:184:ARG:HD2	1:A:722:ARG:C	2.34	0.48
1:A:275:CYS:HB3	1:A:821:THR:O	2.13	0.48
1:A:982:ARG:CD	1:A:982:ARG:N	2.75	0.48
1:A:220:ILE:HG13	1:A:287:ILE:CD1	2.37	0.48
1:A:231:GLN:NE2	1:A:231:GLN:HA	2.29	0.48
1:A:762:GLN:O	1:A:766:GLN:HG3	2.14	0.48
1:A:888:ILE:O	1:A:891:ILE:HB	2.13	0.48
1:A:1069:LEU:HD23	1:A:1072:ILE:HD12	1.95	0.48
1:A:989:PRO:O	1:A:993:PHE:HB2	2.14	0.48
1:A:498:ASN:HB3	1:A:1041:GLN:HA	1.96	0.47
1:A:387:ILE:HD13	1:A:423:LEU:HD21	1.96	0.47
1:A:172:GLU:HG2	1:A:673:HIS:HD2	1.78	0.47
1:A:304:HIS:O	1:A:305:VAL:HB	2.14	0.47
1:A:796:LEU:HD23	1:A:815:PHE:CZ	2.49	0.47
1:A:758:ASP:CG	1:A:759:VAL:H	2.17	0.47
1:A:860:LEU:HD11	1:A:1015:LYS:HB3	1.96	0.47
1:A:1021:ARG:HE	1:A:1056:THR:CG2	2.26	0.47
1:A:1073:GLU:C	1:A:1075:CYS:N	2.68	0.47
1:A:923:ALA:O	1:A:926:GLU:N	2.48	0.47
1:A:193:PRO:HB2	1:A:313:PRO:HB2	1.97	0.47
1:A:366:ARG:HH12	1:A:479:GLU:CD	2.17	0.47
1:A:805:ALA:O	1:A:806:SER:O	2.32	0.47
1:A:867:TYR:OH	1:A:963:ILE:HA	2.14	0.47
1:A:1078:LYS:O	1:A:1080:TRP:N	2.48	0.47
1:A:365:ILE:CD1	1:A:365:ILE:N	2.78	0.47
1:A:689:LYS:HE2	1:A:728:MET:SD	2.54	0.47
1:A:757:TYR:CD1	1:A:757:TYR:N	2.83	0.47
1:A:862:LEU:N	1:A:862:LEU:HD23	2.28	0.47
1:A:207:LEU:HD11	1:A:211:LEU:O	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:ALA:O	1:A:936:CYS:HB2	2.13	0.47
1:A:1024:THR:HG21	1:A:1057:VAL:HG22	1.96	0.47
1:A:989:PRO:HD2	1:A:1080:TRP:CE2	2.50	0.47
1:A:838:LEU:O	1:A:842:MET:HG3	2.15	0.47
1:A:271:VAL:HG13	1:A:282:VAL:HG12	1.96	0.46
1:A:226:ARG:HB3	1:A:227:SER:H	1.54	0.46
1:A:653:ASP:O	1:A:656:VAL:N	2.48	0.46
1:A:214:LYS:HG2	1:A:297:LEU:HD22	1.98	0.46
1:A:1028:ILE:HD12	1:A:1051:ILE:HG23	1.97	0.46
1:A:497:PHE:HB3	1:A:1042:LEU:O	2.15	0.46
1:A:682:LEU:O	1:A:682:LEU:HD22	2.14	0.46
1:A:957:THR:HG23	1:A:957:THR:O	2.15	0.46
1:A:287:ILE:C	1:A:287:ILE:HD12	2.36	0.46
1:A:365:ILE:O	1:A:365:ILE:HG22	2.14	0.46
1:A:911:LEU:HB2	1:A:921:PHE:HE1	1.80	0.46
1:A:1074:VAL:O	1:A:1074:VAL:HG12	2.15	0.46
1:A:144:SER:HB3	1:A:147:SER:HB3	1.97	0.46
1:A:364:LYS:HB2	1:A:413:TRP:CD2	2.51	0.46
1:A:369:ASP:OD1	1:A:407:GLU:HB2	2.15	0.46
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.41	0.46
1:A:1069:LEU:O	1:A:1072:ILE:HB	2.15	0.46
1:A:638:GLU:O	1:A:642:ALA:HB2	2.16	0.46
1:A:181:VAL:HG22	1:A:184:ARG:NH2	2.31	0.46
1:A:357:CYS:SG	1:A:359:ARG:HB3	2.56	0.46
1:A:366:ARG:NH1	1:A:366:ARG:HG3	2.25	0.46
1:A:172:GLU:HG2	1:A:673:HIS:CD2	2.51	0.46
1:A:1005:HIS:O	1:A:1008:LYS:HB3	2.16	0.46
1:A:1080:TRP:O	1:A:1084:PHE:HB3	2.16	0.46
1:A:831:ILE:HG13	1:A:881:ILE:CG1	2.46	0.46
1:A:527:ILE:HG13	1:A:528:ALA:N	2.31	0.45
1:A:768:LYS:HE2	1:A:798:ILE:O	2.16	0.45
1:A:803:VAL:HG11	1:A:809:LYS:HE3	1.97	0.45
1:A:949:ASN:ND2	1:A:1083:GLN:CG	2.79	0.45
1:A:1009:PHE:HA	1:A:1012:ILE:HD11	1.99	0.45
1:A:379:LEU:CD2	1:A:380:THR:H	2.19	0.45
1:A:887:THR:HA	1:A:953:MET:HG2	1.99	0.45
1:A:233:ILE:HD11	1:A:248:PHE:CD1	2.50	0.45
1:A:910:TRP:O	1:A:914:LYS:HB2	2.16	0.45
1:A:953:MET:O	1:A:960:LEU:HG	2.16	0.45
1:A:435:CYS:O	1:A:435:CYS:SG	2.74	0.45
1:A:750:LYS:HZ3	1:A:834:HIS:HD2	1.62	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PHE:O	1:A:153:GLN:HB3	2.17	0.45
1:A:178:ARG:HH11	1:A:178:ARG:CG	2.26	0.45
1:A:838:LEU:HD23	1:A:877:GLY:HA3	1.99	0.45
1:A:929:VAL:HG12	1:A:1012:ILE:HD11	1.98	0.45
1:A:277:ARG:HH11	1:A:277:ARG:CG	2.24	0.45
1:A:758:ASP:CG	1:A:759:VAL:N	2.70	0.45
1:A:808:LYS:O	1:A:809:LYS:HD2	2.17	0.45
1:A:1014:VAL:O	1:A:1018:LEU:HG	2.17	0.45
1:A:497:PHE:HB2	1:A:1041:GLN:HG3	1.98	0.45
1:A:756:LYS:O	1:A:757:TYR:C	2.55	0.45
1:A:209:GLU:HB2	1:A:859:SER:HB3	1.98	0.45
1:A:233:ILE:CD1	1:A:233:ILE:H	2.30	0.45
1:A:363:VAL:CG1	1:A:363:VAL:O	2.64	0.45
1:A:555:LEU:O	1:A:558:ILE:HB	2.17	0.45
1:A:697:TRP:CH2	1:A:739:ILE:HD13	2.52	0.45
1:A:773:ASN:O	1:A:776:ASN:ND2	2.51	0.45
1:A:989:PRO:HA	1:A:992:LEU:HB2	1.98	0.45
1:A:1043:THR:HG21	1:A:1046:GLU:CG	2.47	0.44
1:A:241:PRO:HB3	1:A:281:LEU:O	2.17	0.44
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.98	0.44
1:A:807:LYS:H	1:A:807:LYS:CD	2.26	0.44
1:A:853:SER:O	1:A:857:THR:HG23	2.17	0.44
1:A:1081:THR:HG22	1:A:1082:VAL:N	2.32	0.44
1:A:199:HIS:O	1:A:200:PRO:C	2.56	0.44
1:A:498:ASN:ND2	1:A:500:ASP:H	2.15	0.44
1:A:964:ASP:HA	2:A:101:QYT:O12	2.18	0.44
1:A:200:PRO:HG3	1:A:282:VAL:HG22	2.00	0.44
1:A:240:THR:O	1:A:242:GLY:N	2.50	0.44
1:A:640:VAL:O	1:A:643:ILE:HG12	2.17	0.44
1:A:749:ILE:N	1:A:749:ILE:HD12	2.31	0.44
1:A:768:LYS:HD2	1:A:798:ILE:HG22	1.98	0.44
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.82	0.44
1:A:759:VAL:HG22	1:A:809:LYS:HZ3	1.83	0.44
1:A:773:ASN:HA	1:A:776:ASN:ND2	2.32	0.44
1:A:1078:LYS:O	1:A:1079:GLY:C	2.56	0.44
1:A:207:LEU:HD13	1:A:207:LEU:C	2.38	0.44
1:A:287:ILE:O	1:A:287:ILE:HD12	2.18	0.44
1:A:850:ILE:O	1:A:854:ILE:HG13	2.17	0.44
1:A:989:PRO:HG2	1:A:1080:TRP:NE1	2.33	0.44
1:A:390:GLY:O	1:A:391:GLN:CB	2.66	0.44
1:A:608:TYR:CE2	1:A:639:ASN:ND2	2.84	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:ILE:HB	1:A:879:ILE:HB	1.99	0.44
1:A:935:TYR:O	1:A:939:THR:CG2	2.65	0.44
1:A:862:LEU:HB3	1:A:934:GLY:CA	2.48	0.44
1:A:937:VAL:HG11	1:A:1017:TYR:HA	2.00	0.44
1:A:245:LEU:HD21	1:A:272:LEU:HG	1.99	0.44
1:A:364:LYS:HE3	1:A:413:TRP:NE1	2.33	0.44
1:A:1002:THR:O	1:A:1003:SER:OG	2.31	0.43
1:A:833:LYS:NZ	2:A:101:QYT:N9	2.65	0.43
1:A:806:SER:O	1:A:807:LYS:C	2.56	0.43
1:A:767:LEU:CD2	1:A:811:LEU:HD11	2.48	0.43
1:A:375:ARG:HE	1:A:376:ASN:HB2	1.84	0.43
1:A:905:GLU:N	1:A:905:GLU:CD	2.72	0.43
1:A:624:VAL:O	1:A:628:MET:HG2	2.19	0.43
1:A:1070:ASP:O	1:A:1074:VAL:HG23	2.18	0.43
1:A:527:ILE:HG13	1:A:528:ALA:H	1.83	0.43
1:A:833:LYS:HE2	2:A:101:QYT:N9	2.33	0.43
1:A:902:PHE:HD1	1:A:1080:TRP:CE3	2.36	0.43
1:A:321:GLU:O	1:A:322:GLU:HB3	2.18	0.43
1:A:890:LYS:HB2	1:A:890:LYS:HZ3	1.83	0.43
1:A:1008:LYS:O	1:A:1011:ASP:HB3	2.18	0.43
1:A:1042:LEU:N	1:A:1042:LEU:HD13	2.27	0.43
1:A:1028:ILE:HD13	1:A:1051:ILE:CG1	2.49	0.43
1:A:277:ARG:HD2	1:A:292:TRP:CH2	2.53	0.43
1:A:572:LYS:HB3	1:A:595:SER:HB2	2.01	0.43
1:A:695:LEU:HD11	1:A:699:LEU:HD11	2.00	0.43
1:A:373:LEU:O	1:A:374:PRO:C	2.56	0.43
1:A:1058:GLY:O	1:A:1059:LYS:O	2.37	0.43
1:A:1068:PHE:O	1:A:1071:GLN:HB2	2.18	0.43
1:A:1081:THR:O	1:A:1084:PHE:HB3	2.19	0.43
1:A:315:LEU:O	1:A:317:GLU:N	2.44	0.43
1:A:933:ALA:HB1	1:A:1013:CYS:SG	2.59	0.43
1:A:1064:ALA:HA	1:A:1067:TYR:HB3	2.00	0.43
1:A:734:GLN:O	1:A:738:VAL:HG23	2.19	0.43
1:A:912:LYS:HZ3	1:A:918:GLU:HG2	1.83	0.43
1:A:184:ARG:HB3	1:A:184:ARG:NH1	2.34	0.42
1:A:838:LEU:HD23	1:A:877:GLY:CA	2.49	0.42
1:A:987:LEU:HG	1:A:992:LEU:HD21	2.01	0.42
1:A:1032:SER:O	1:A:1036:MET:HG3	2.20	0.42
1:A:389:HIS:O	1:A:392:GLN:HB3	2.19	0.42
1:A:611:LEU:O	1:A:614:ARG:HG3	2.19	0.42
1:A:788:ASP:HA	1:A:789:PRO:HD2	1.78	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:VAL:CG1	1:A:897:GLY:H	2.25	0.42
1:A:767:LEU:HD21	1:A:811:LEU:HD21	2.02	0.42
1:A:998:SER:O	1:A:999:GLY:C	2.57	0.42
1:A:928:PHE:O	1:A:932:CYS:CB	2.63	0.42
1:A:299:ASN:C	1:A:301:GLU:H	2.23	0.42
1:A:684:ARG:HA	1:A:684:ARG:HD2	1.76	0.42
1:A:903:LYS:HB2	1:A:906:VAL:CG2	2.37	0.42
1:A:912:LYS:HZ1	1:A:918:GLU:HG2	1.85	0.42
1:A:507:ASN:HA	1:A:508:PRO:HD3	1.87	0.42
1:A:758:ASP:O	1:A:759:VAL:C	2.56	0.42
1:A:1073:GLU:C	1:A:1075:CYS:H	2.22	0.42
1:A:168:VAL:CG1	1:A:170:ASP:O	2.68	0.42
1:A:315:LEU:C	1:A:317:GLU:N	2.73	0.42
1:A:366:ARG:NH1	1:A:366:ARG:CG	2.82	0.42
1:A:743:GLN:HG2	1:A:876:ILE:HD11	2.00	0.42
1:A:879:ILE:HG22	1:A:880:GLU:O	2.19	0.42
1:A:1021:ARG:HH21	1:A:1056:THR:HG23	1.85	0.42
1:A:811:LEU:N	1:A:832:PHE:O	2.39	0.42
1:A:838:LEU:HA	1:A:838:LEU:HD12	1.73	0.42
1:A:916:PRO:HD2	1:A:920:LYS:HD3	2.01	0.42
1:A:273:ARG:HH22	1:A:821:THR:HG21	1.85	0.42
1:A:393:VAL:HG12	1:A:395:CYS:H	1.85	0.42
1:A:191:ARG:NH2	1:A:723:GLY:O	2.42	0.42
1:A:276:GLY:HA2	1:A:819:ASP:OD2	2.20	0.41
1:A:913:GLU:HG3	1:A:914:LYS:H	1.85	0.41
1:A:240:THR:C	1:A:242:GLY:N	2.73	0.41
1:A:641:ARG:HE	1:A:670:GLU:CD	2.23	0.41
1:A:810:PRO:CG	1:A:833:LYS:HG3	2.35	0.41
1:A:1042:LEU:CD1	1:A:1042:LEU:N	2.83	0.41
1:A:233:ILE:CG2	1:A:234:LYS:N	2.83	0.41
1:A:246:GLN:O	1:A:248:PHE:N	2.53	0.41
1:A:412:VAL:O	1:A:412:VAL:HG13	2.19	0.41
1:A:506:THR:CG2	1:A:507:ASN:N	2.84	0.41
1:A:749:ILE:HD11	1:A:770:LYS:HD2	2.03	0.41
1:A:799:GLU:HG2	1:A:799:GLU:H	1.57	0.41
1:A:907:LEU:HD13	1:A:994:VAL:HG21	2.02	0.41
1:A:627:THR:HG22	1:A:628:MET:N	2.35	0.41
1:A:773:ASN:HD22	1:A:776:ASN:ND2	2.19	0.41
1:A:784:ARG:NH2	1:A:792:LYS:HE3	2.35	0.41
1:A:838:LEU:HD21	1:A:879:ILE:HD11	2.03	0.41
1:A:198:MET:HG2	1:A:280:TYR:CG	2.56	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ILE:HG21	1:A:433:ILE:HD11	2.03	0.41
1:A:1012:ILE:H	1:A:1012:ILE:HG12	1.66	0.41
1:A:224:ILE:HA	1:A:305:VAL:CG1	2.47	0.41
1:A:364:LYS:HA	1:A:413:TRP:HA	2.03	0.41
1:A:561:THR:CG2	1:A:565:ASN:HB3	2.50	0.41
1:A:812:TRP:O	1:A:812:TRP:CD1	2.73	0.41
1:A:175:PHE:O	1:A:179:GLY:N	2.49	0.41
1:A:835:GLY:HA2	1:A:875:LYS:HE3	2.03	0.41
1:A:221:PHE:CD2	1:A:221:PHE:N	2.89	0.41
1:A:601:GLN:CG	1:A:602:GLU:N	2.83	0.41
1:A:1043:THR:HG22	1:A:1046:GLU:H	1.86	0.41
1:A:430:ASN:OD1	1:A:430:ASN:O	2.39	0.41
1:A:477:ARG:HG3	1:A:521:ASP:HA	2.03	0.41
1:A:603:ILE:HD13	1:A:603:ILE:HA	1.88	0.41
1:A:796:LEU:CD1	1:A:801:CYS:SG	3.06	0.41
1:A:1058:GLY:O	1:A:1059:LYS:C	2.58	0.41
1:A:561:THR:HG22	1:A:565:ASN:HB3	2.02	0.41
1:A:210:TYR:CZ	1:A:861:ASP:HB2	2.56	0.41
1:A:896:VAL:CG1	1:A:897:GLY:N	2.83	0.41
1:A:192:ASP:OD2	1:A:194:LYS:HB3	2.20	0.41
1:A:750:LYS:NZ	1:A:834:HIS:CD2	2.87	0.41
1:A:804:MET:HE1	1:A:831:ILE:CG2	2.42	0.41
1:A:840:GLN:HB3	1:A:1039:MET:CE	2.50	0.41
1:A:852:GLU:O	1:A:853:SER:C	2.58	0.41
1:A:953:MET:HE2	1:A:953:MET:HB3	1.92	0.41
1:A:373:LEU:HG	1:A:406:GLU:OE2	2.21	0.40
1:A:804:MET:CE	1:A:812:TRP:HB2	2.51	0.40
1:A:840:GLN:O	1:A:844:ILE:HG12	2.20	0.40
1:A:361:PHE:HA	1:A:420:ILE:CD1	2.51	0.40
1:A:365:ILE:HD12	1:A:365:ILE:N	2.35	0.40
1:A:555:LEU:HD23	1:A:556:GLU:N	2.35	0.40
1:A:643:ILE:HA	1:A:646:GLN:HE21	1.86	0.40
1:A:177:ARG:HG2	3:A:8:HOH:O	2.21	0.40
1:A:464:VAL:HG21	1:A:482:LEU:HB3	2.02	0.40
1:A:710:GLN:CG	1:A:711:GLN:N	2.85	0.40
1:A:835:GLY:HA2	1:A:875:LYS:NZ	2.36	0.40
1:A:1013:CYS:O	1:A:1016:ALA:N	2.54	0.40
1:A:390:GLY:HA3	3:A:12:HOH:O	2.22	0.40
1:A:425:LYS:HD2	1:A:672:TYR:OH	2.21	0.40
1:A:759:VAL:HG22	1:A:809:LYS:HZ1	1.86	0.40
1:A:875:LYS:HE3	1:A:875:LYS:HB3	1.87	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:ASP:N	1:A:904:ASP:OD2	2.54	0.40
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.84	0.40
1:A:1042:LEU:HD21	1:A:1048:ILE:HD11	2.02	0.40
1:A:170:ASP:OD1	1:A:471:HIS:CE1	2.75	0.40
1:A:381:VAL:CG2	1:A:433:ILE:HG23	2.51	0.40
1:A:593:PHE:CZ	1:A:611:LEU:HD21	2.57	0.40
1:A:626:LEU:HD22	1:A:626:LEU:HA	1.95	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	821/966 (85%)	680 (83%)	109 (13%)	32 (4%)	<b>3</b> <b>6</b>

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	PRO
1	A	376	ASN
1	A	548	PRO
1	A	805	ALA
1	A	806	SER
1	A	916	PRO
1	A	1040	PRO
1	A	1059	LYS
1	A	1081	THR
1	A	1088	LEU
1	A	226	ARG
1	A	546	GLU
1	A	753	SER
1	A	776	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	896	VAL
1	A	964	ASP
1	A	1000	LYS
1	A	1045	LYS
1	A	1079	GLY
1	A	1086	TRP
1	A	247	SER
1	A	377	THR
1	A	470	ASP
1	A	999	GLY
1	A	1013	CYS
1	A	305	VAL
1	A	373	LEU
1	A	893	GLN
1	A	949	ASN
1	A	1087	PHE
1	A	1091	VAL
1	A	1014	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	755/864 (87%)	696 (92%)	59 (8%)	12	29

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	168	VAL
1	A	170	ASP
1	A	185	MET
1	A	192	ASP
1	A	213	LYS
1	A	226	ARG
1	A	291	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	306	VAL
1	A	309	THR
1	A	322	GLU
1	A	374	PRO
1	A	375	ARG
1	A	379	LEU
1	A	391	GLN
1	A	395	CYS
1	A	410	TRP
1	A	430	ASN
1	A	466	LEU
1	A	470	ASP
1	A	486	GLN
1	A	487	ILE
1	A	498	ASN
1	A	512	ASN
1	A	519	LEU
1	A	544	ARG
1	A	570	GLU
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	613	ARG
1	A	626	LEU
1	A	653	ASP
1	A	717	LEU
1	A	731	ASP
1	A	743	GLN
1	A	757	TYR
1	A	773	ASN
1	A	826	GLU
1	A	838	LEU
1	A	841	ASP
1	A	843	LEU
1	A	848	LEU
1	A	883	LYS
1	A	907	LEU
1	A	927	ARG
1	A	957	THR
1	A	960	LEU
1	A	964	ASP
1	A	982	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	983	VAL
1	A	1008	LYS
1	A	1026	LEU
1	A	1029	ILE
1	A	1039	MET
1	A	1040	PRO
1	A	1042	LEU
1	A	1090	LEU
1	A	1092	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	218	ASN
1	A	231	GLN
1	A	246	GLN
1	A	289	ASN
1	A	291	GLN
1	A	304	HIS
1	A	389	HIS
1	A	391	GLN
1	A	483	HIS
1	A	498	ASN
1	A	512	ASN
1	A	554	GLN
1	A	565	ASN
1	A	585	HIS
1	A	601	GLN
1	A	646	GLN
1	A	705	GLN
1	A	710	GLN
1	A	737	GLN
1	A	766	GLN
1	A	773	ASN
1	A	775	GLN
1	A	776	ASN
1	A	834	HIS
1	A	892	GLN
1	A	948	HIS
1	A	949	ASN
1	A	951	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1023	HIS
1	A	1041	GLN
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 carbohydrates 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	QYT	A	101	-	20,20,20	3.08	11 (55%)	28,28,28	2.88	11 (39%)

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	QYT	A	101	-	-	1/4/16/16	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	QYT	C1-C2	5.71	1.48	1.36
2	A	101	QYT	C4-C3	5.23	1.50	1.38
2	A	101	QYT	C11-S8	-4.51	1.72	1.78
2	A	101	QYT	C11-N9	4.28	1.42	1.36
2	A	101	QYT	C17-C16	4.25	1.50	1.38
2	A	101	QYT	C4-C13	-3.97	1.35	1.41
2	A	101	QYT	C14-C13	3.29	1.49	1.42
2	A	101	QYT	C1-C14	-3.28	1.36	1.41
2	A	101	QYT	C3-C5	2.96	1.52	1.46
2	A	101	QYT	C7-N9	2.44	1.43	1.38
2	A	101	QYT	C13-N18	2.22	1.41	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	101	QYT	C7-N9-C11	-10.24	112.20	117.79
2	A	101	QYT	C6-S8-C11	4.72	93.06	91.69
2	A	101	QYT	C5-C6-C7	3.77	123.45	120.47
2	A	101	QYT	C6-C7-N9	3.57	113.20	110.22
2	A	101	QYT	S8-C11-N9	3.50	112.45	109.19
2	A	101	QYT	C13-C14-N15	-3.10	118.04	121.00
2	A	101	QYT	C17-N18-C13	2.73	121.16	116.93
2	A	101	QYT	C16-N15-C14	2.69	121.10	116.93
2	A	101	QYT	C4-C13-N18	2.69	121.03	117.97
2	A	101	QYT	C14-C13-N18	-2.67	118.45	121.00
2	A	101	QYT	C3-C5-C6	-2.51	127.50	130.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	101	QYT	C3-C5-C6-S8

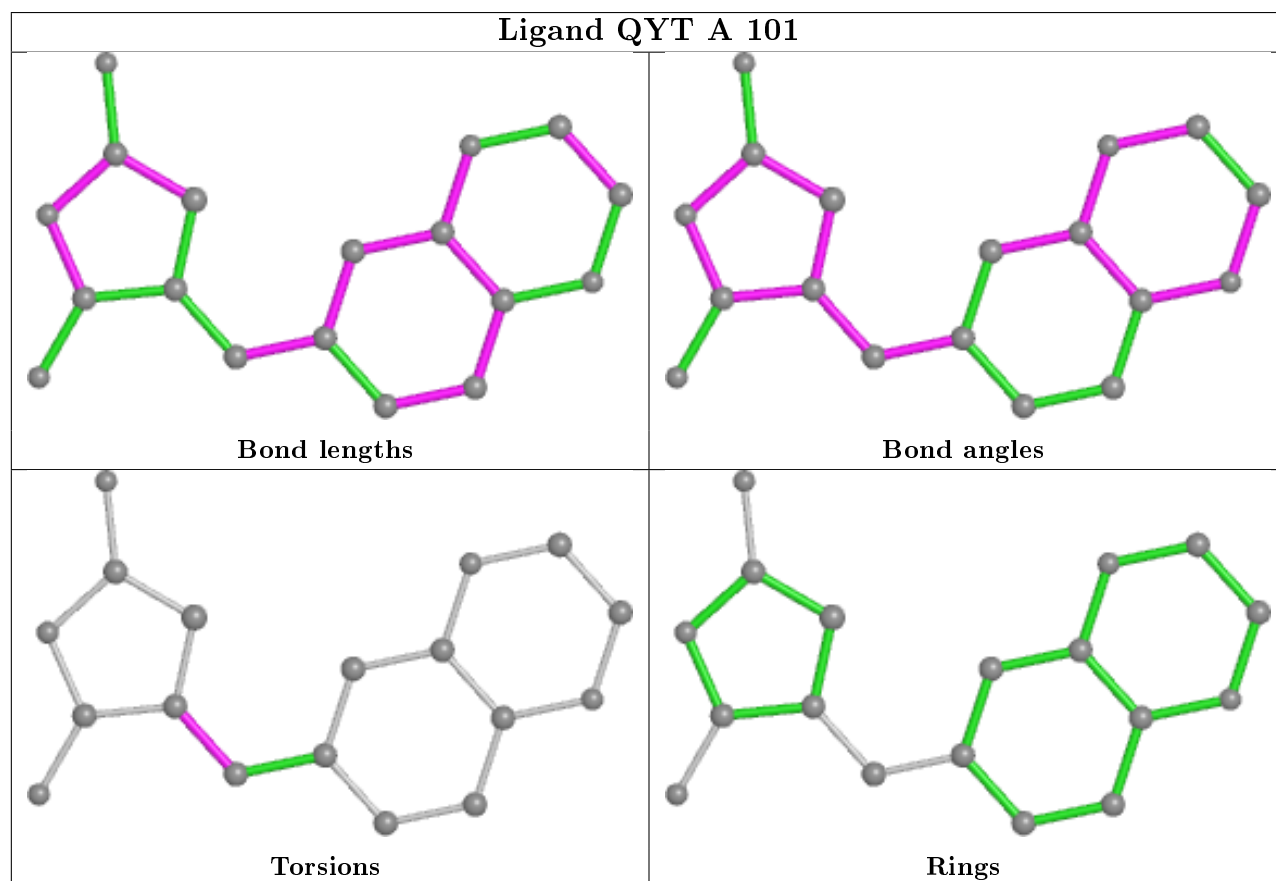
There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	101	QYT	9	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	839/966 (86%)	1.12	160 (19%) <b>1</b> <b>0</b>	19, 60, 100, 124	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	528	ALA	9.4
1	A	1044	SER	8.5
1	A	373	LEU	8.2
1	A	1091	VAL	7.6
1	A	374	PRO	6.7
1	A	1090	LEU	6.3
1	A	376	ASN	5.9
1	A	757	TYR	5.7
1	A	377	THR	5.7
1	A	894	SER	5.6
1	A	209	GLU	5.5
1	A	250	THR	5.5
1	A	899	THR	5.5
1	A	1092	LEU	5.4
1	A	900	GLY	5.4
1	A	1089	HIS	5.1
1	A	229	THR	5.0
1	A	526	PRO	4.8
1	A	216	ALA	4.6
1	A	219	CYS	4.5
1	A	149	ALA	4.4
1	A	776	ASN	4.3
1	A	148	GLN	4.2
1	A	431	LEU	4.2
1	A	222	ILE	4.2
1	A	375	ARG	4.0
1	A	907	LEU	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	544	ARG	4.0
1	A	1043	THR	3.9
1	A	489	GLY	3.9
1	A	1045	LYS	3.8
1	A	998	SER	3.7
1	A	1088	LEU	3.6
1	A	898	ASN	3.5
1	A	210	TYR	3.5
1	A	832	PHE	3.5
1	A	1062	GLU	3.5
1	A	996	GLY	3.4
1	A	1000	LYS	3.4
1	A	987	LEU	3.4
1	A	716	ILE	3.4
1	A	379	LEU	3.4
1	A	1013	CYS	3.3
1	A	825	ASN	3.3
1	A	1046	GLU	3.3
1	A	246	GLN	3.3
1	A	896	VAL	3.3
1	A	773	ASN	3.3
1	A	301	GLU	3.3
1	A	681	LEU	3.3
1	A	742	LEU	3.3
1	A	253	ALA	3.3
1	A	272	LEU	3.2
1	A	593	PHE	3.2
1	A	249	PHE	3.2
1	A	305	VAL	3.2
1	A	993	PHE	3.2
1	A	322	GLU	3.2
1	A	243	ALA	3.1
1	A	145	GLU	3.1
1	A	378	ASP	3.1
1	A	309	THR	3.0
1	A	247	SER	3.0
1	A	967	HIS	2.9
1	A	1042	LEU	2.9
1	A	924	ALA	2.9
1	A	1086	TRP	2.9
1	A	1060	ASN	2.9
1	A	892	GLN	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	774	LEU	2.9
1	A	361	PHE	2.9
1	A	488	SER	2.9
1	A	721	LEU	2.8
1	A	527	ILE	2.8
1	A	385	ALA	2.8
1	A	605	ALA	2.8
1	A	423	LEU	2.8
1	A	551	LEU	2.7
1	A	1011	ASP	2.7
1	A	999	GLY	2.7
1	A	1084	PHE	2.7
1	A	775	GLN	2.7
1	A	192	ASP	2.7
1	A	1041	GLN	2.7
1	A	1017	TYR	2.7
1	A	1080	TRP	2.7
1	A	614	ARG	2.7
1	A	811	LEU	2.7
1	A	1068	PHE	2.6
1	A	429	LEU	2.6
1	A	560	ALA	2.6
1	A	615	GLU	2.6
1	A	592	LEU	2.6
1	A	287	ILE	2.5
1	A	904	ASP	2.5
1	A	477	ARG	2.5
1	A	856	GLU	2.5
1	A	218	ASN	2.5
1	A	215	ILE	2.5
1	A	244	ILE	2.5
1	A	300	GLY	2.4
1	A	228	THR	2.4
1	A	468	LEU	2.4
1	A	383	VAL	2.4
1	A	293	VAL	2.4
1	A	986	VAL	2.4
1	A	1002	THR	2.4
1	A	321	GLU	2.4
1	A	546	GLU	2.4
1	A	613	ARG	2.4
1	A	146	GLU	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	923	ALA	2.4
1	A	922	GLN	2.4
1	A	1073	GLU	2.4
1	A	616	VAL	2.4
1	A	1077	ASP	2.3
1	A	912	LYS	2.3
1	A	549	ASN	2.3
1	A	221	PHE	2.3
1	A	284	GLU	2.3
1	A	857	THR	2.3
1	A	213	LYS	2.3
1	A	320	LYS	2.3
1	A	652	GLU	2.3
1	A	826	GLU	2.3
1	A	589	TYR	2.3
1	A	783	PHE	2.3
1	A	235	VAL	2.3
1	A	992	LEU	2.2
1	A	611	LEU	2.2
1	A	909	HIS	2.2
1	A	144	SER	2.2
1	A	387	ILE	2.2
1	A	830	ILE	2.2
1	A	254	LYS	2.2
1	A	406	GLU	2.2
1	A	905	GLU	2.2
1	A	575	LEU	2.2
1	A	813	LEU	2.2
1	A	1070	ASP	2.2
1	A	860	LEU	2.2
1	A	1040	PRO	2.2
1	A	566	PRO	2.1
1	A	217	ASN	2.1
1	A	997	THR	2.1
1	A	919	GLU	2.1
1	A	879	ILE	2.1
1	A	1014	VAL	2.1
1	A	178	ARG	2.1
1	A	941	VAL	2.1
1	A	269	ASP	2.1
1	A	991	PHE	2.1
1	A	392	GLN	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	893	GLN	2.1
1	A	640	VAL	2.0
1	A	1053	ASP	2.0
1	A	1054	ALA	2.0
1	A	995	MET	2.0
1	A	682	LEU	2.0
1	A	281	LEU	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](#)

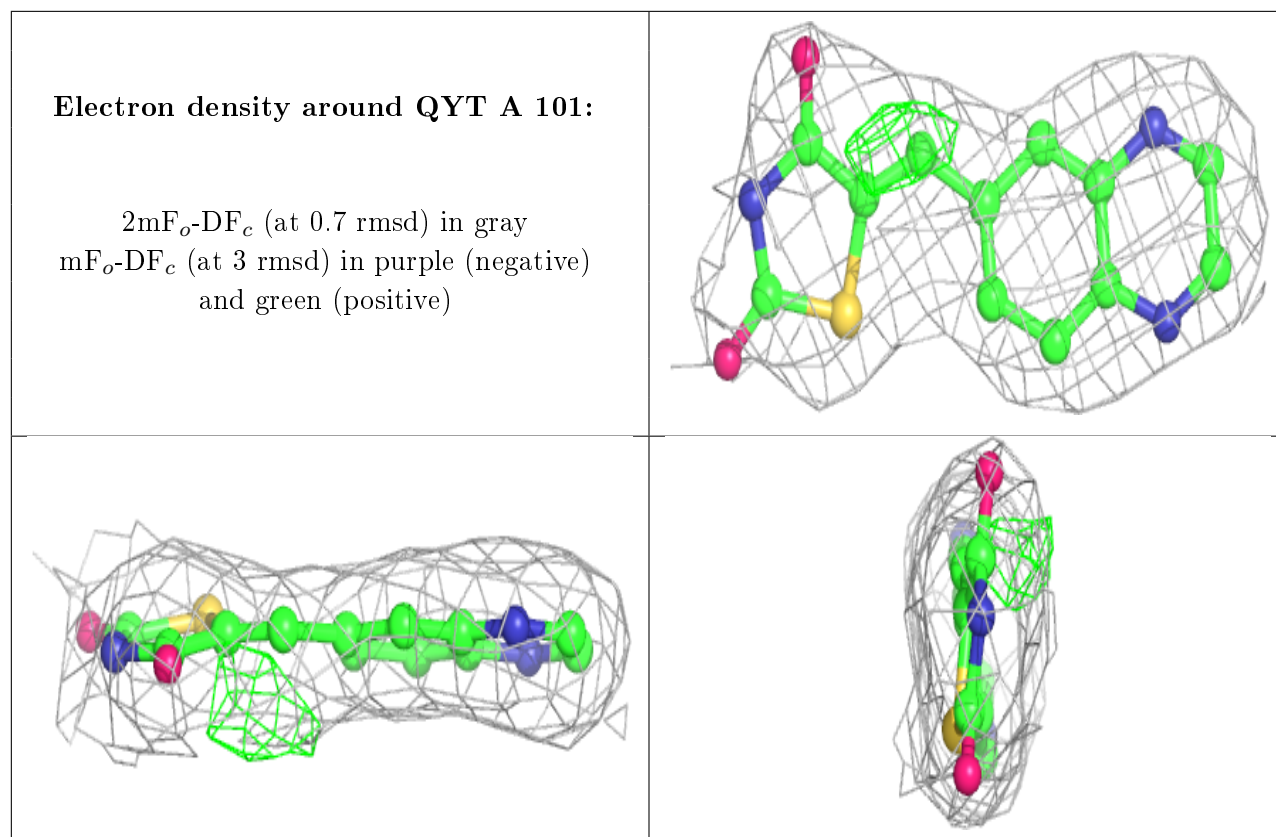
There are no carbohydrates in this entry.

## 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( $\text{\AA}^2$ )	Q<0.9
2	QYT	A	101	18/18	0.90	0.23	28,38,70,71	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.