



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:13 PM UTC

PDB ID : 2A5U / pdb_00002a5u
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

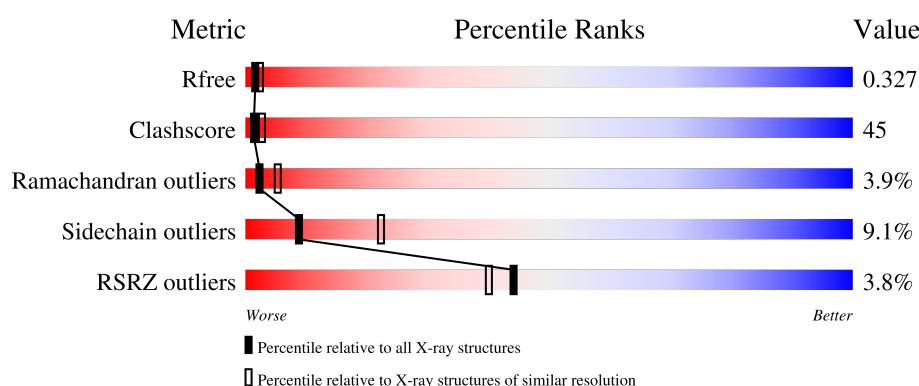
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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.

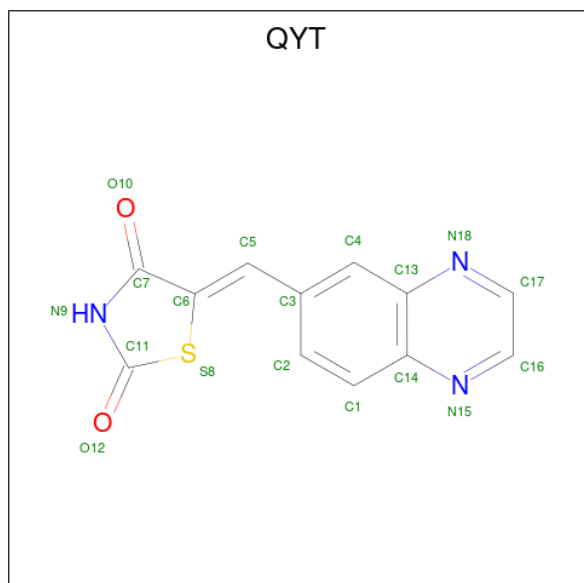
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit, gamma isoform.

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 (CCD ID: QYT) (formula: C₁₂H₇N₃O₂S).



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		

HIS	L1042	GLY	H909	I844
HIS	TI043	ILE	W910	L845
HIS	SI044	ASN	L911	Q846
HIS	K1045	LYS	K912	T847
HIS	E1046	E981	E913	L848
HIS	DI047	R982	K914	R849
	II048	V983	S915	I850
	E1049	P984	P916	M851
	Y1050	F985	T917	E852
	II051	V986	E918	S853
		L987	E919	I854
	AI054	T988	K920	W855
	LI055	P989	F921	F856
	TI056	D990	Q922	T857
	V1057	F991	A923	E858
	G1058	L992	A924	S859
	K1059	F993	V925	L860
	N1060	V994	E926	D861
	E1061	M995	R927	L862
	E1062	G996	F928	
	D1063	T997	V929	L865
	A1064	S998	Y930	P866
	K1065	G999	S931	Y867
	K1066	K1000	C932	
	Y1067		A933	I870
	F1068	SI003	G934	
	L1069	P1004	Y935	K875
	D1070	H1005	C936	I876
	Q1071	F1006	V937	G877
	I1072	Q1007	A938	M878
	E1073	K1008	T939	I879
	V1074	F1009		E880
	C1075	Q1010	G945	I881
	R1076	D1011	D946	V882
	D1077	I1012	R947	K883
	K1078	C1013	H948	D884
	G1079	V1014	N949	A885
	W1080	K1015		T886
	TI081	A1016		T887
	V1082	Y1017	I952	I888
	Q1083	L1018	M953	A889
	F1084	A1019	I954	K890
	N1085	L1020	T957	I891
	H1086	R1021		Q892
	F1087		L960	Q893
	L1088	TI024	F961	S894
	H1089	N1025	H962	T895
	L1090	L1026	I963	V896
	V1091	L1027	D964	G897
	LI092	I1028		M898
	GLY	I1029	H967	T899
	ILE		ILE	G900
	LYS	SI032	LEU	ALA
	GLN		GLY	F902
	GLY	L1035	ASN	K903
	GLU	M1036	TVR	D904
	LYS		LYS	E905
	HIS	M1039	SER	V906
	SER	P1040	PHE	L907
	ALA	Q1041	LEU	N908

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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) 96.4 (19.58-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.87 (at 2.71Å)	Xtriage
Refinement program	CNS, CNX 2002	Depositor
R, R_{free}	0.279 , 0.351 0.258 , 0.327	Depositor DCC
R_{free} test set	2591 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 98.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	0.45	0/6951	0.93	19/9400 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	N-CA-C	-8.00	102.51	111.07
1	A	788	ASP	CA-C-N	7.43	128.08	119.47
1	A	788	ASP	C-N-CA	7.43	128.08	119.47
1	A	484	MET	N-CA-C	7.30	121.73	110.42
1	A	807	LYS	N-CA-C	-7.26	102.40	111.11
1	A	852	GLU	N-CA-C	-6.24	103.19	111.24
1	A	922	GLN	N-CA-C	-5.77	104.91	111.14
1	A	991	PHE	N-CA-C	-5.63	103.97	111.24
1	A	499	ALA	N-CA-C	5.57	119.17	112.38
1	A	1007	GLN	N-CA-C	-5.50	105.36	111.36
1	A	503	THR	N-CA-C	5.45	118.14	110.23
1	A	610	LEU	N-CA-C	-5.33	105.38	111.14
1	A	640	VAL	N-CA-C	-5.30	105.16	110.30
1	A	148	GLN	N-CA-C	-5.24	106.15	112.54
1	A	744	LYS	N-CA-C	-5.09	105.81	111.36
1	A	933	ALA	N-CA-C	-5.09	105.81	111.36
1	A	1028	ILE	CB-CA-C	-5.05	105.40	112.02
1	A	779	LEU	CA-C-N	5.05	125.05	119.90
1	A	779	LEU	C-N-CA	5.05	125.05	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6806	0	6850	612	0
2	A	18	0	7	9	0
3	A	20	0	0	4	0
All	All	6844	0	6857	613	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 45.

All (613) 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	1.17	1.03
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: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:1008:LYS:HZ3	1:A:1011:ASP:HB3	1.43	0.81
1:A:220:ILE:HG13	1:A:287:ILE:HD11	1.60	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:804:MET:HE2	1:A:812:TRP:HB2	1.66	0.77
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:178:ARG:HG2	1:A:178:ARG:HH11	1.52	0.75
1:A:752:LEU:HD13	1:A:766:GLN:NE2	2.01	0.75
1:A:614:ARG:HB2	1:A:618:ASP:OD2	1.86	0.75
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:HG2	1:A:277:ARG:HH11	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:987:LEU:HD11	1:A:995:MET:HE1	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:HH11	1:A:184:ARG:HB2	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:798:ILE:HD12	1:A:798:ILE:H	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	1:A:1042:LEU:H	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:992:LEU:HA	1:A:995:MET:HE3	1.74	0.69
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:1003:SER:O	1:A:1007:GLN:HB2	1.92	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:HD13	1:A:1092:LEU:O	1.94	0.68
1:A:862:LEU:O	1:A:931:SER:HA	1.94	0.67
1:A:272:LEU:HB3	1:A:305:VAL:CG2	2.24	0.67
1:A:741:MET:HE1	1:A:778:GLN:HG2	1.76	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:HB2	1:A:890:LYS:NZ	2.09	0.67
1:A:921:PHE:O	1:A:925:VAL:HG23	1.95	0.66
1:A:180:LEU:C	1:A:183:PRO:HD2	2.20	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:470:ASP:CG	1:A:472:ARG:H	2.03	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:555:LEU:HD23	1:A:555:LEU:C	2.22	0.65
1:A:512:ASN:C	1:A:512:ASN:HD22	2.04	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:547:MET:HE3	1:A:578:PHE:CG	2.33	0.64
1:A:584:LYS:O	1:A:616:VAL:HG11	1.97	0.64
1:A:184:ARG:HH11	1:A:184:ARG:CB	2.11	0.63
1:A:544:ARG:HB3	1:A:544:ARG:NH1	2.10	0.63
1:A:629:GLN:CG	1:A:1029:ILE:HG13	2.22	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: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:1059:LYS:CD	1:A:1059:LYS:H	2.11	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:791:LEU:HD22	1:A:828:ILE:HD11	1.80	0.62
1:A:833:LYS:HZ1	2:A:101:QYT:C11	2.12	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
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:804:MET:HE1	1:A:831:ILE:HG23	1.82	0.61
1:A:576:TRP:O	1:A:579:ARG:HG2	1.99	0.61
1:A:1072:ILE:O	1:A:1075:CYS:HB2	1.99	0.61
1:A:960:LEU:HG	1:A:961:PHE:N	2.15	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:379:LEU:HD12	1:A:435:CYS:HB2	1.83	0.61
1:A:246:GLN:C	1:A:248:PHE:H	2.09	0.61
1:A:390:GLY:C	1:A:392:GLN:H	2.09	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:THR:HG1	1:A:402:LYS:C	2.09	0.60
1:A:625:GLY:O	1:A:629:GLN:HG3	2.01	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:HG2	1:A:277:ARG:NH1	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:HG3	1:A:614:ARG:HH11	1.68	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:1086:TRP:CH2	1:A:1090:LEU:HB3	2.31	0.59
2:A:101:QYT:S8	2:A:101:QYT:H2	2.42	0.59
1:A:198:MET:HE2	1:A:311:PRO:HD2	1.85	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
1:A:878:MET:C	1:A:879:ILE:HD12	2.28	0.59
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: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:1042:LEU:HD22	1:A:1042:LEU:O	2.04	0.58
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.38	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:1018:LEU:HD22	1:A:1061:GLU:OE1	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1090:LEU:HD12	1:A:1091:VAL:N	2.19	0.57
1:A:545:ALA:O	1:A:546:GLU:HB2	2.02	0.57
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.52	0.57
1:A:807:LYS:N	1:A:807:LYS:HD3	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:830:ILE:HG21	1:A:878:MET:HE3	1.87	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
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:992:LEU:HA	1:A:995:MET:CE	2.34	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: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:1021:ARG:HE	1:A:1056:THR:HG23	1.71	0.56
1:A:601:GLN:HG3	1:A:602:GLU:N	2.21	0.55
1:A:796:LEU:C	1:A:796:LEU:HD13	2.30	0.55
1:A:184:ARG:HD3	1:A:719:ALA:O	2.05	0.55
1:A:373:LEU:HD13	1:A:373:LEU:C	2.31	0.55
1:A:653:ASP:OD2	1:A:688:ASN:ND2	2.39	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:231:GLN:HE21	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:982:ARG:C	1:A:983:VAL:HG22	2.32	0.55
1:A:759:VAL:HG22	1:A:809:LYS:NZ	2.21	0.55
1:A:892:GLN:C	1:A:894:SER:H	2.13	0.55
1:A:291:GLN:HA	1:A:291:GLN:NE2	2.21	0.55
1:A:982:ARG:HD2	1:A:982:ARG:N	2.21	0.55
1:A:564:LEU:HD21	1:A:1048:ILE:HG21	1.88	0.54
1:A:1039:MET:SD	1:A:1039:MET:N	2.80	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:584:LYS:C	1:A:616:VAL:HG11	2.32	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:822:ALA:C	1:A:823:LEU:HD12	2.32	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:184:ARG:HD2	1:A:722:ARG:O	2.08	0.54
1:A:905:GLU:HG3	1:A:993:PHE:CZ	2.43	0.54
1:A:947:ARG:HG2	1:A:947:ARG:NH1	2.22	0.54
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:HG3	1:A:614:ARG:NH1	2.23	0.53
1:A:315:LEU:C	1:A:317:GLU:H	2.17	0.53
1:A:375:ARG:O	1:A:376:ASN:C	2.52	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:1042:LEU:HD22	1:A:1042:LEU:C	2.33	0.53
1:A:363:VAL:O	1:A:363:VAL:HG13	2.08	0.53
1:A:1077:ASP:C	1:A:1078:LYS:HD2	2.33	0.53
1:A:233:ILE:HG22	1:A:234:LYS:N	2.24	0.53
1:A:983:VAL:HG21	1:A:1082:VAL:HG21	1.91	0.53
1:A:184:ARG:HD2	1:A:722:ARG:C	2.34	0.53
1:A:741:MET:CE	1:A:778:GLN:HG2	2.39	0.53
1:A:760:SER:O	1:A:764:ILE:HG13	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:758:ASP:CG	1:A:759:VAL:H	2.17	0.52
1:A:806:SER:O	1:A:808:LYS:O	2.27	0.52
1:A:835:GLY:O	1:A:875:LYS:HD2	2.10	0.52
1:A:855:TRP:NE1	1:A:1016:ALA:HB1	2.24	0.52
1:A:913:GLU:HG3	1:A:914:LYS:N	2.24	0.52
1:A:1073:GLU:C	1:A:1075:CYS:N	2.68	0.52
1:A:366:ARG:HH12	1:A:479:GLU:CD	2.17	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:687:ARG:O	1:A:687:ARG:HG2	2.09	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:285:THR:HG22	1:A:289:ASN:HB2	1.91	0.51
1:A:1059:LYS:H	1:A:1059:LYS:HD3	1.74	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:842:MET:HE3	1:A:870:ILE:HD13	1.92	0.51
1:A:287:ILE:C	1:A:287:ILE:HD12	2.36	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:767:LEU:HD21	1:A:811:LEU:HD11	1.92	0.51
1:A:981:GLU:N	1:A:982:ARG:NH1	2.59	0.51
1:A:1024:THR:O	1:A:1028:ILE:HG12	2.11	0.51
1:A:833:LYS:NZ	2:A:101:QYT:C11	2.75	0.50
1:A:146:GLU:O	1:A:149:ALA:HB3	2.11	0.50
1:A:890:LYS:HB2	1:A:890:LYS:HZ2	1.74	0.50
1:A:1043:THR:HG21	1:A:1046:GLU:HG3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:TYR:OH	1:A:728:MET:HE3	2.11	0.50
1:A:164:ASP:OD2	1:A:166:SER:HB3	2.12	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:N	1:A:280:TYR:CD1	2.80	0.49
1:A:808:LYS:HE3	1:A:836:ASP:OD1	2.12	0.49
1:A:865:LEU:H	1:A:935:TYR:HH	1.59	0.49
1:A:773:ASN:HA	1:A:776:ASN:HD21	1.76	0.49
1:A:547:MET:O	1:A:548:PRO:O	2.30	0.49
1:A:756:LYS:O	1:A:757:TYR:C	2.55	0.49
1:A:758:ASP:CG	1:A:759:VAL:N	2.70	0.49
1:A:766:GLN:O	1:A:770:LYS:HG3	2.13	0.49
1:A:1056:THR:HG23	1:A:1056:THR:O	2.12	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:840:GLN:HB3	1:A:1039:MET:HE3	1.94	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:199:HIS:O	1:A:200:PRO:C	2.56	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:148:GLN:O	1:A:152:ARG:HG3	2.13	0.49
1:A:207:LEU:C	1:A:207:LEU:HD13	2.38	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:1078:LYS:O	1:A:1079:GLY:C	2.56	0.49
1:A:170:ASP:OD1	1:A:471:HIS:HE1	1.96	0.49
1:A:804:MET:HE1	1:A:831:ILE:CG2	2.42	0.49
1:A:394:LEU:O	1:A:418:ILE:HD11	2.13	0.48
1:A:292:TRP:O	1:A:295:HIS:HB3	2.13	0.48
1:A:1078:LYS:HD2	1:A:1078:LYS:N	2.28	0.48
1:A:806:SER:O	1:A:807:LYS:C	2.56	0.48
1:A:890:LYS:HA	1:A:893:GLN:CG	2.42	0.48
1:A:905:GLU:N	1:A:905:GLU:CD	2.72	0.48
1:A:929:VAL:HG12	1:A:1012:ILE:CD1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:ILE:HD13	1:A:1051:ILE:HG13	1.94	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:275:CYS:HB3	1:A:821:THR:O	2.13	0.48
1:A:982:ARG:N	1:A:982:ARG:CD	2.75	0.48
1:A:220:ILE:HG13	1:A:287:ILE:CD1	2.37	0.48
1:A:231:GLN:HA	1:A:231:GLN:NE2	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:989:PRO:O	1:A:993:PHE:HB2	2.14	0.48
1:A:1069:LEU:HD23	1:A:1072:ILE:HD12	1.95	0.48
1:A:373:LEU:O	1:A:374:PRO:C	2.56	0.47
1:A:387:ILE:HD13	1:A:423:LEU:HD21	1.96	0.47
1:A:498:ASN:HB3	1:A:1041:GLN:HA	1.96	0.47
1:A:172:GLU:HG2	1:A:673:HIS:HD2	1.78	0.47
1:A:246:GLN:C	1:A:248:PHE:N	2.72	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:860:LEU:HD11	1:A:1015:LYS:HB3	1.96	0.47
1:A:923:ALA:O	1:A:926:GLU:N	2.48	0.47
1:A:1021:ARG:HE	1:A:1056:THR:CG2	2.26	0.47
1:A:193:PRO:HB2	1:A:313:PRO:HB2	1.97	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:912:LYS:HZ1	1:A:918:GLU:HG2	1.79	0.47
1:A:365:ILE:N	1:A:365:ILE:CD1	2.78	0.47
1:A:689:LYS:HE2	1:A:728:MET:SD	2.54	0.47
1:A:750:LYS:HZ2	1:A:834:HIS:CD2	2.33	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:998:SER:O	1:A:999:GLY:C	2.57	0.47
1:A:1078:LYS:O	1:A:1080:TRP:N	2.48	0.47
1:A:207:LEU:HD11	1:A:211:LEU:O	2.14	0.47
1:A:299:ASN:C	1:A:301:GLU:H	2.23	0.47
1:A:933:ALA:O	1:A:936:CYS:HB2	2.13	0.47
1:A:758:ASP:O	1:A:759:VAL:C	2.56	0.47
1:A:1024:THR:HG21	1:A:1057:VAL:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:LEU:O	1:A:842:MET:HG3	2.15	0.47
1:A:989:PRO:HD2	1:A:1080:TRP:CE2	2.50	0.47
1:A:271:VAL:HG13	1:A:282:VAL:HG12	1.96	0.46
1:A:1073:GLU:C	1:A:1075:CYS:H	2.22	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:759:VAL:HG22	1:A:809:LYS:HZ3	1.80	0.46
1:A:1008:LYS:NZ	1:A:1008:LYS:O	2.46	0.46
1:A:214:LYS:HG2	1:A:297:LEU:HD22	1.98	0.46
1:A:641:ARG:HE	1:A:670:GLU:CD	2.23	0.46
1:A:240:THR:C	1:A:242:GLY:N	2.73	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:1028:ILE:HD12	1:A:1051:ILE:HG23	1.97	0.46
1:A:315:LEU:C	1:A:317:GLU:N	2.73	0.46
1:A:365:ILE:HG22	1:A:365:ILE:O	2.14	0.46
1:A:911:LEU:HB2	1:A:921:PHE:HE1	1.80	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:1074:VAL:O	1:A:1074:VAL:HG12	2.15	0.46
1:A:638:GLU:O	1:A:642:ALA:HB2	2.16	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:172:GLU:HG2	1:A:673:HIS:CD2	2.51	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:HG3	1:A:366:ARG:NH1	2.25	0.46
1:A:831:ILE:HG13	1:A:881:ILE:CG1	2.46	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: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:852:GLU:O	1:A:853:SER:C	2.58	0.45
1:A:911:LEU:O	1:A:915:SER:OG	2.32	0.45
1:A:949:ASN:ND2	1:A:1083:GLN:CG	2.79	0.45
1:A:1058:GLY:O	1:A:1059:LYS:C	2.58	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:PHE:HA	1:A:1012:ILE:HD11	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: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:277:ARG:HH11	1:A:277:ARG:CG	2.24	0.45
1:A:808:LYS:O	1:A:809:LYS:HD2	2.17	0.45
1:A:929:VAL:HG12	1:A:1012:ILE:HD11	1.98	0.45
1:A:209:GLU:HB2	1:A:859:SER:HB3	1.98	0.45
1:A:497:PHE:HB2	1:A:1041:GLN:HG3	1.98	0.45
1:A:1014:VAL:O	1:A:1018:LEU:HG	2.17	0.45
1:A:233:ILE:H	1:A:233:ILE:CD1	2.30	0.45
1:A:363:VAL:O	1:A:363:VAL:CG1	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:241:PRO:HB3	1:A:281:LEU:O	2.17	0.44
1:A:512:ASN:C	1:A:512:ASN:ND2	2.75	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:1043:THR:HG21	1:A:1046:GLU:CG	2.47	0.44
1:A:498:ASN:ND2	1:A:500:ASP:H	2.15	0.44
1:A:987:LEU:HD11	1:A:995:MET:CE	2.43	0.44
1:A:1081:THR:HG22	1:A:1082:VAL:N	2.32	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:HD12	1:A:749:ILE:N	2.31	0.44
1:A:768:LYS:HD2	1:A:798:ILE:HG22	1.98	0.44
1:A:964:ASP:HA	2:A:101:QYT:O12	2.18	0.44
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.82	0.44
1:A:773:ASN:HA	1:A:776:ASN:ND2	2.32	0.44
1:A:804:MET:HE1	1:A:831:ILE:HG12	1.98	0.44
1:A:287:ILE:HD12	1:A:287:ILE:O	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:TYR:CE2	1:A:639:ASN:ND2	2.84	0.44
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:245:LEU:HD21	1:A:272:LEU:HG	1.99	0.44
1:A:584:LYS:C	1:A:585:HIS:HD2	2.25	0.44
1:A:689:LYS:HG2	1:A:728:MET:HE2	1.98	0.44
1:A:937:VAL:HG11	1:A:1017:TYR:HA	2.00	0.44
1:A:170:ASP:CG	1:A:171:ASP:N	2.76	0.44
1:A:364:LYS:HE3	1:A:413:TRP:NE1	2.33	0.44
1:A:767:LEU:CD2	1:A:811:LEU:HD11	2.48	0.43
1:A:833:LYS:NZ	2:A:101:QYT:N9	2.65	0.43
1:A:375:ARG:HE	1:A:376:ASN:HB2	1.84	0.43
1:A:624:VAL:O	1:A:628:MET:HG2	2.19	0.43
1:A:779:LEU:HD23	1:A:779:LEU:C	2.43	0.43
1:A:390:GLY:C	1:A:392:GLN:N	2.76	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:1018:LEU:HD12	1:A:1018:LEU:C	2.43	0.43
1:A:1070:ASP:O	1:A:1074:VAL:HG23	2.18	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:181:VAL:HG13	1:A:185:MET:HE2	2.01	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:1008:LYS:O	1:A:1011:ASP:HB3	2.18	0.43
1:A:1028:ILE:HD13	1:A:1051:ILE:CG1	2.49	0.43
1:A:1042:LEU:HD13	1:A:1042:LEU:N	2.27	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: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:734:GLN:O	1:A:738:VAL:HG23	2.19	0.43
1:A:1064:ALA:HA	1:A:1067:TYR:HB3	2.00	0.43
1:A:184:ARG:NH1	1:A:184:ARG:HB3	2.34	0.42
1:A:838:LEU:HD23	1:A:877:GLY:CA	2.49	0.42
1:A:648:LEU:C	1:A:650:SER:N	2.76	0.42
1:A:987:LEU:HG	1:A:992:LEU:HD21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:896:VAL:CG1	1:A:897:GLY:H	2.25	0.42
1:A:1032:SER:O	1:A:1036:MET:HG3	2.20	0.42
1:A:767:LEU:HD21	1:A:811:LEU:HD21	2.02	0.42
1:A:236:SER:C	1:A:238:ASP:H	2.27	0.42
1:A:928:PHE:O	1:A:932:CYS:CB	2.63	0.42
1:A:684:ARG:HD2	1:A:684:ARG:HA	1.76	0.42
1:A:903:LYS:HB2	1:A:906:VAL:CG2	2.37	0.42
1:A:988:THR:OG1	1:A:990:ASP:OD1	2.35	0.42
1:A:185:MET:HE1	1:A:321:GLU:OE1	2.19	0.42
1:A:507:ASN:HA	1:A:508:PRO:HD3	1.87	0.42
1:A:168:VAL:CG1	1:A:170:ASP:O	2.68	0.42
1:A:366:ARG:NH1	1:A:366:ARG:CG	2.82	0.42
1:A:562:ASP:OD1	1:A:562:ASP:C	2.63	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:1090:LEU:HD12	1:A:1090:LEU:C	2.44	0.42
1:A:811:LEU:N	1:A:832:PHE:O	2.39	0.42
1:A:838:LEU:HD12	1:A:838:LEU:HA	1.73	0.42
1:A:916:PRO:HD2	1:A:920:LYS:HD3	2.01	0.42
1:A:1021:ARG:HH21	1:A:1056:THR:HG23	1.85	0.42
1:A:191:ARG:NH2	1:A:723:GLY:O	2.42	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: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:810:PRO:CG	1:A:833:LYS:HG3	2.35	0.41
1:A:946:ASP:CG	1:A:983:VAL:HG23	2.44	0.41
1:A:198:MET:O	1:A:199:HIS:C	2.62	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:HG13	1:A:412:VAL:O	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:H	1:A:799:GLU:HG2	1.57	0.41
1:A:861:ASP:OD1	1:A:861:ASP:C	2.63	0.41
1:A:892:GLN:C	1:A:894:SER:N	2.77	0.41
1:A:907:LEU:HD13	1:A:994:VAL:HG21	2.02	0.41
1:A:1042:LEU:N	1:A:1042:LEU:CD1	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:368:ILE:HG21	1:A:433:ILE:HD11	2.03	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:885:ALA:HB1	1:A:953:MET:HE2	2.02	0.41
1:A:1012:ILE:HG12	1:A:1012:ILE:H	1.66	0.41
1:A:1060:ASN:O	1:A:1061:GLU:C	2.64	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:N	1:A:221:PHE:CD2	2.89	0.41
1:A:210:TYR:CZ	1:A:861:ASP:HB2	2.56	0.41
1:A:240:THR:O	1:A:241:PRO:C	2.63	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:561:THR:HG22	1:A:565:ASN:HB3	2.02	0.41
1:A:603:ILE:HD13	1:A:603:ILE:HA	1.88	0.41
1:A:653:ASP:O	1:A:654:ASP:C	2.64	0.41
1:A:796:LEU:CD1	1:A:801:CYS:SG	3.06	0.41
1:A:896:VAL:CG1	1:A:897:GLY:N	2.83	0.41
1:A:923:ALA:O	1:A:924:ALA:C	2.64	0.41
1:A:1043:THR:HG22	1:A:1046:GLU:H	1.86	0.41
1:A:192:ASP:OD2	1:A:194:LYS:HB3	2.20	0.41
1:A:405:THR:O	1:A:406:GLU:C	2.64	0.41
1:A:840:GLN:HB3	1:A:1039:MET:CE	2.50	0.41
1:A:236:SER:C	1:A:238:ASP:N	2.79	0.40
1:A:373:LEU:HG	1:A:406:GLU:OE2	2.21	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:N	1:A:365:ILE:HD12	2.35	0.40
1:A:555:LEU:HD23	1:A:556:GLU:N	2.35	0.40
1:A:611:LEU:O	1:A:612:ALA:C	2.63	0.40
1:A:643:ILE:HA	1:A:646:GLN:HE21	1.86	0.40
1:A:652:GLU:O	1:A:653:ASP:C	2.64	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:ASP:C	1:A:502:LEU:N	2.79	0.40
1:A:812:TRP:CD1	1:A:812:TRP:C	2.99	0.40
1:A:835:GLY:HA2	1:A:875:LYS:NZ	2.36	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:875:LYS:HE3	1:A:875:LYS:HB3	1.87	0.40
1:A:904:ASP:OD2	1:A:904:ASP:N	2.54	0.40
1:A:1013:CYS:O	1:A:1016:ALA:N	2.54	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
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:1050:TYR:CD2	1:A:1050:TYR:C	2.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	821/966 (85%)	680 (83%)	109 (13%)	32 (4%)	2 5

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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%)	686 (91%)	69 (9%)	9 22

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	163	THR
1	A	168	VAL
1	A	170	ASP
1	A	185	MET
1	A	192	ASP
1	A	233	ILE
1	A	282	VAL
1	A	303	ILE
1	A	306	VAL
1	A	309	THR
1	A	322	GLU
1	A	365	ILE
1	A	374	PRO
1	A	375	ARG
1	A	379	LEU
1	A	387	ILE
1	A	391	GLN
1	A	395	CYS
1	A	410	TRP
1	A	420	ILE
1	A	430	ASN
1	A	466	LEU
1	A	470	ASP
1	A	471	HIS
1	A	475	LEU
1	A	486	GLN
1	A	487	ILE
1	A	498	ASN
1	A	501	LYS
1	A	512	ASN
1	A	519	LEU
1	A	544	ARG
1	A	555	LEU
1	A	570	GLU
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	619	GLN
1	A	626	LEU
1	A	627	THR
1	A	682	LEU
1	A	717	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	757	TYR
1	A	826	GLU
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	883	LYS
1	A	890	LYS
1	A	904	ASP
1	A	907	LEU
1	A	927	ARG
1	A	957	THR
1	A	960	LEU
1	A	964	ASP
1	A	982	ARG
1	A	983	VAL
1	A	1008	LYS
1	A	1012	ILE
1	A	1026	LEU
1	A	1029	ILE
1	A	1039	MET
1	A	1040	PRO
1	A	1042	LEU
1	A	1043	THR
1	A	1090	LEU
1	A	1092	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	231	GLN
1	A	246	GLN
1	A	289	ASN
1	A	291	GLN
1	A	295	HIS
1	A	299	ASN
1	A	304	HIS
1	A	389	HIS
1	A	391	GLN
1	A	392	GLN
1	A	396	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	411	ASN
1	A	483	HIS
1	A	498	ASN
1	A	512	ASN
1	A	550	GLN
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	708	HIS
1	A	710	GLN
1	A	737	GLN
1	A	766	GLN
1	A	773	ASN
1	A	776	ASN
1	A	834	HIS
1	A	892	GLN
1	A	948	HIS
1	A	949	ASN
1	A	951	ASN
1	A	1023	HIS
1	A	1041	GLN
1	A	1083	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	3.15	12 (60%)	28,28,28	3.00	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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	QYT	C4-C3	5.86	1.50	1.38
2	A	101	QYT	C1-C2	5.54	1.48	1.36
2	A	101	QYT	C11-S8	-4.56	1.72	1.78
2	A	101	QYT	C17-C16	4.33	1.50	1.38
2	A	101	QYT	C11-N9	4.15	1.42	1.36
2	A	101	QYT	C4-C13	-4.07	1.35	1.41
2	A	101	QYT	C1-C14	-3.42	1.36	1.41
2	A	101	QYT	C14-C13	3.38	1.49	1.42
2	A	101	QYT	C3-C5	3.09	1.52	1.46
2	A	101	QYT	C13-N18	2.35	1.41	1.37
2	A	101	QYT	C7-N9	2.17	1.43	1.38
2	A	101	QYT	C14-N15	2.05	1.40	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	-10.92	112.20	117.83
2	A	101	QYT	C6-S8-C11	4.68	93.06	91.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	101	QYT	C5-C6-C7	3.85	123.45	120.45
2	A	101	QYT	C6-C7-N9	3.69	113.20	110.21
2	A	101	QYT	S8-C11-N9	3.52	112.45	109.16
2	A	101	QYT	C13-C14-N15	-3.29	118.04	121.00
2	A	101	QYT	C14-C13-N18	-2.82	118.45	121.00
2	A	101	QYT	C17-N18-C13	2.79	121.16	116.93
2	A	101	QYT	C16-N15-C14	2.75	121.10	116.93
2	A	101	QYT	C4-C13-N18	2.63	121.03	118.01
2	A	101	QYT	C3-C5-C6	-2.54	127.50	130.92

There are no chirality outliers.

All (1) torsion outliers are listed below:

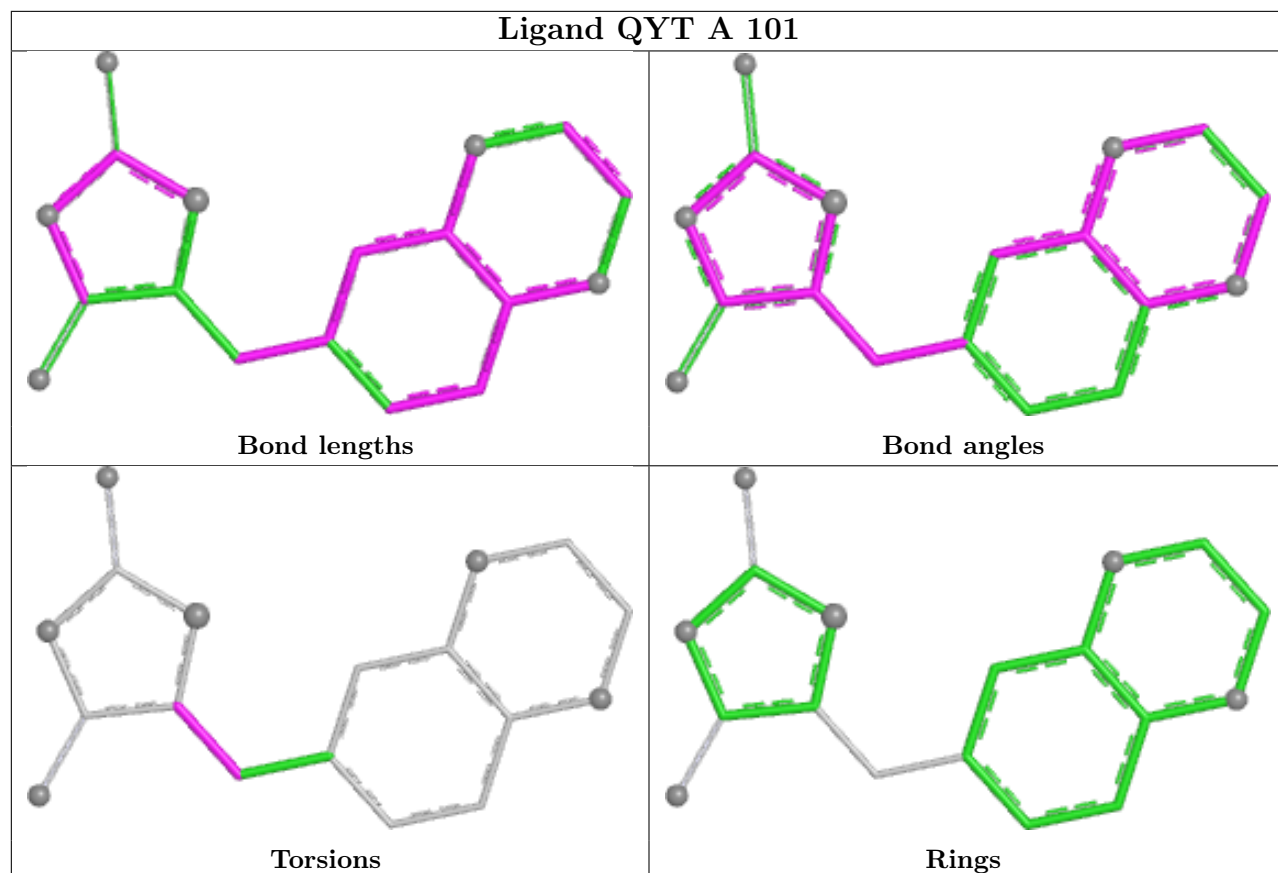
Mol	Chain	Res	Type	Atoms
2	A	101	QYT	C3-C5-C6-S8

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	839/966 (86%)	0.50	32 (3%) 44 40	19, 60, 100, 124	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	ASP	4.2
1	A	1088	LEU	4.0
1	A	900	GLY	3.8
1	A	528	ALA	3.5
1	A	1044	SER	3.3
1	A	373	LEU	3.3
1	A	899	THR	3.2
1	A	773	ASN	3.0
1	A	794	GLY	2.9
1	A	999	GLY	2.9
1	A	377	THR	2.9
1	A	219	CYS	2.9
1	A	1043	THR	2.6
1	A	1054	ALA	2.5
1	A	527	ILE	2.4
1	A	1084	PHE	2.3
1	A	202	VAL	2.3
1	A	1091	VAL	2.3
1	A	912	LYS	2.2
1	A	790	GLY	2.2
1	A	1082	VAL	2.2
1	A	405	THR	2.2
1	A	1011	ASP	2.2
1	A	509	ASP	2.2
1	A	1018	LEU	2.1
1	A	909	HIS	2.1
1	A	1080	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1045	LYS	2.1
1	A	309	THR	2.1
1	A	775	GLN	2.1
1	A	825	ASN	2.0
1	A	1040	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

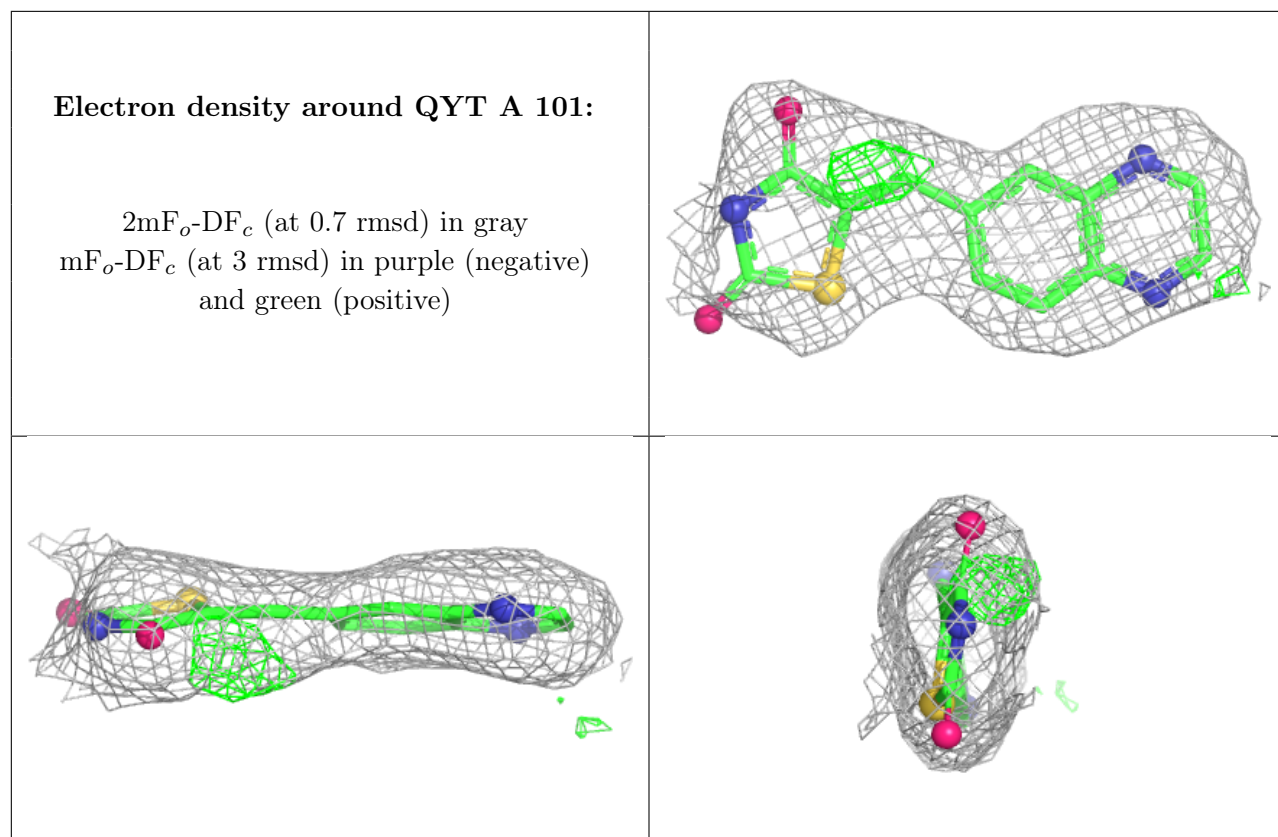
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	QYT	A	101	18/18	0.85	0.11	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.