



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:05 pm BST

PDB ID : 4HVB
Title : Catalytic unit of PI3K in complex with PI3K/mTOR dual inhibitor PF-04979064
Authors : Knighton, D.R.; Cheng, H.
Deposited on : 2012-11-05
Resolution : 2.35 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 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

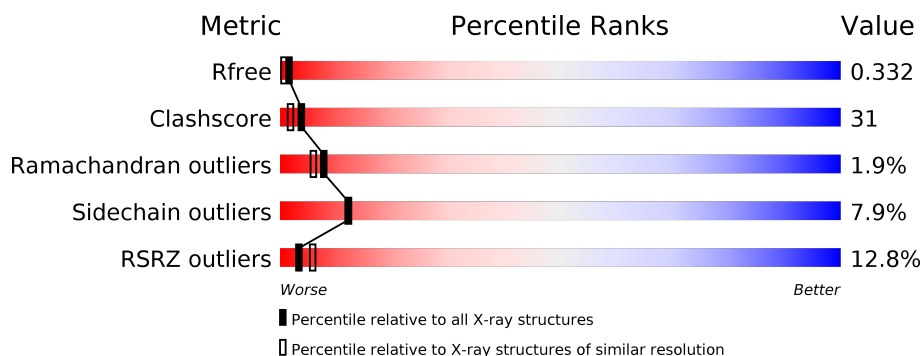
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	966	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6751 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.

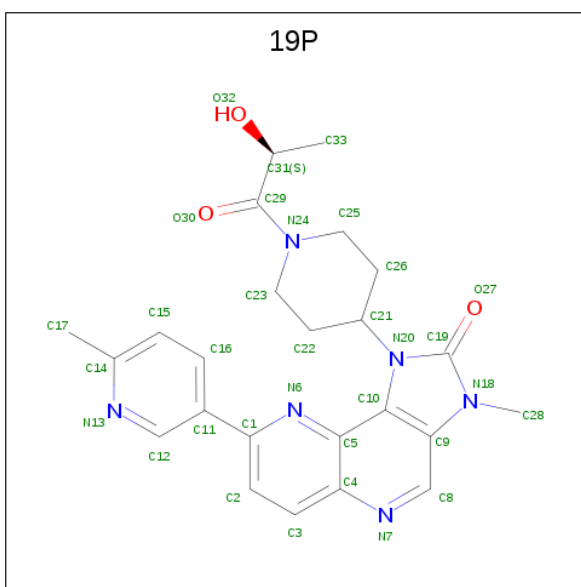
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	830	Total	C	N	O	S	0	0	0
			6717	4317	1144	1221	35			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	EXPRESSION TAG	UNP P48736
A	459	ARG	GLN	CONFLICT	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 1-{1-[(2S)-2-hydroxypropanoyl]piperidin-4-yl}-3-methyl-8-(6-methylpyridin-3-yl)-1,3-dihydro-2H-imidazo[4,5-c][1,5]naphthyridin-2-one (three-letter code: 19P) (formula: C₂₄H₂₆N₆O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	24	6	3		

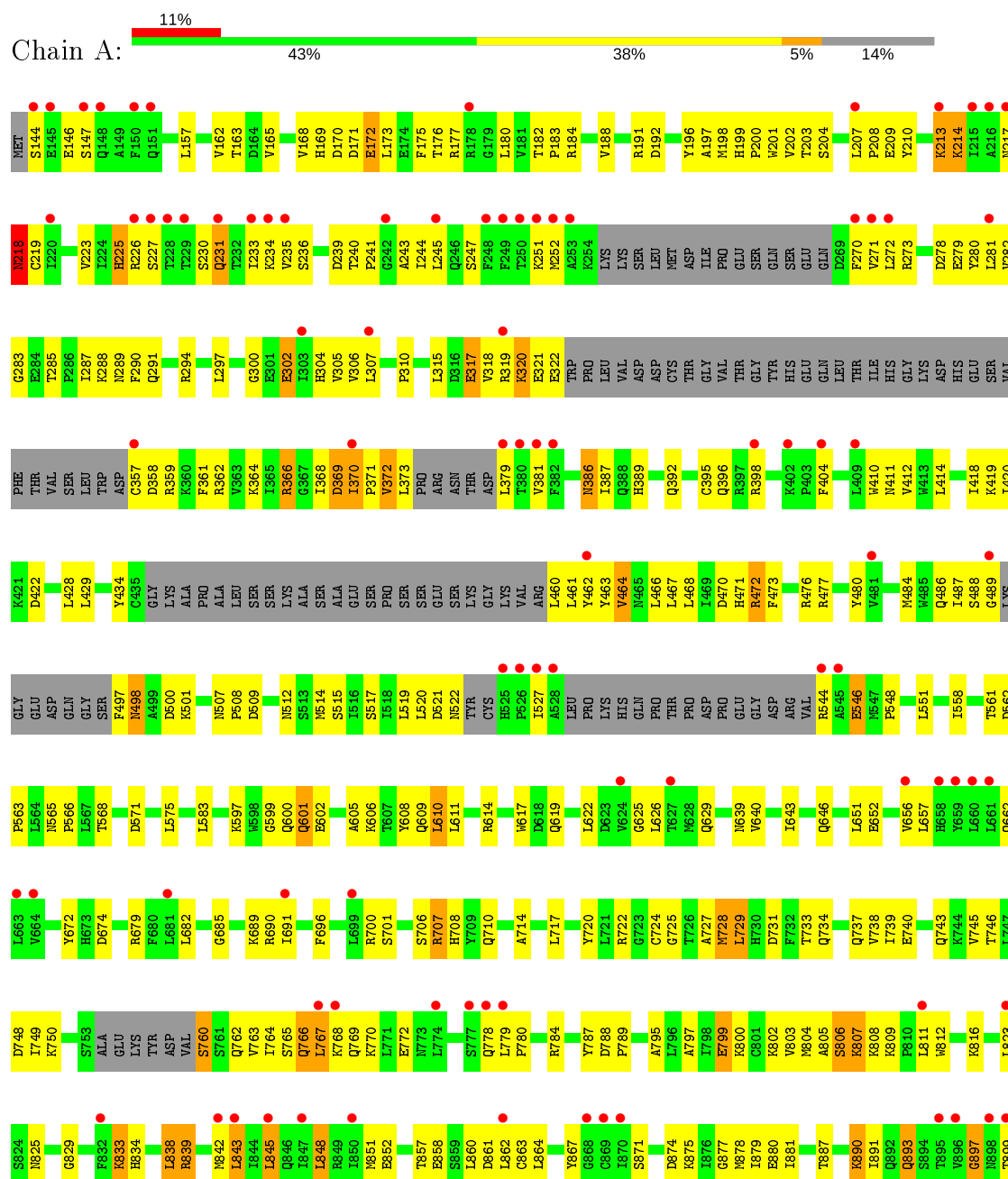
- Molecule 3 is water.

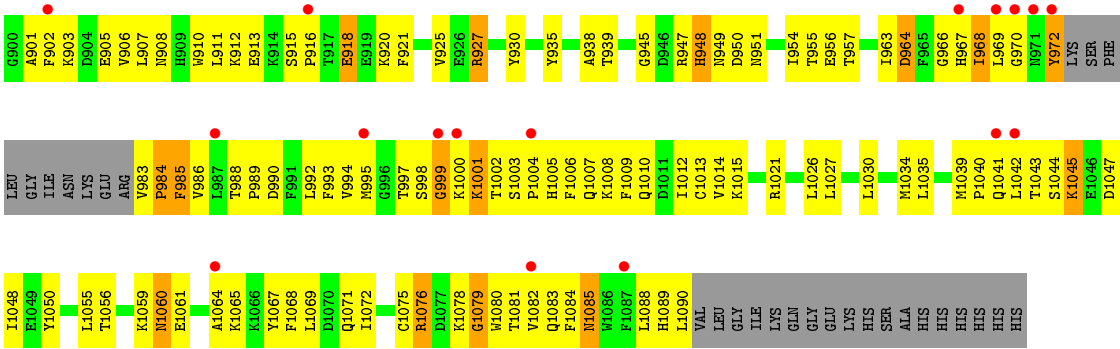
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.80 Å 67.58 Å 106.90 Å 90.00° 95.48° 90.00°	Depositor
Resolution (Å)	50.00 – 2.35 40.98 – 2.34	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-2.35) 94.6 (40.98-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.34 Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.270 , 0.333 0.270 , 0.332	Depositor DCC
R_{free} test set	1302 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.4	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	0.92	EDS
Total number of atoms	6751	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: 19P

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	0.38	0/6859	0.55	0/9274

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	6717	0	6758	417	0
2	A	33	0	26	7	0
3	A	1	0	0	0	0
All	All	6751	0	6784	420	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 31.

All (420) 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:807:LYS:HE3	1:A:807:LYS:H	1.17	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:LYS:HZ3	1:A:834:HIS:CD2	1.81	0.98
1:A:908:ASN:HD22	1:A:994:VAL:HA	1.29	0.97
1:A:750:LYS:HZ3	1:A:834:HIS:HD2	1.00	0.92
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.50	0.91
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.51	0.91
1:A:689:LYS:HG2	1:A:728:MET:SD	2.16	0.86
1:A:766:GLN:HE21	1:A:766:GLN:H	1.23	0.86
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.57	0.86
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.59	0.85
1:A:568:THR:HG23	1:A:571:ASP:H	1.43	0.84
1:A:947:ARG:HD3	1:A:968:ILE:HD12	1.61	0.82
1:A:997:THR:HG21	1:A:1076:ARG:HH12	1.45	0.82
1:A:765:SER:O	1:A:769:GLN:HG3	1.80	0.82
1:A:625:GLY:O	1:A:629:GLN:HG3	1.81	0.80
1:A:851:MET:HE1	1:A:938:ALA:HB1	1.63	0.80
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.64	0.80
1:A:725:GLY:O	1:A:729:LEU:HB2	1.82	0.79
1:A:935:TYR:O	1:A:939:THR:HG22	1.83	0.79
1:A:558:ILE:HG21	1:A:575:LEU:HD21	1.63	0.79
1:A:1001:LYS:HG2	1:A:1002:THR:H	1.49	0.78
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.50	0.77
1:A:198:MET:SD	1:A:282:VAL:HG21	2.26	0.76
1:A:804:MET:HE2	1:A:812:TRP:HE3	1.51	0.75
1:A:271:VAL:HG21	1:A:282:VAL:HG22	1.69	0.75
1:A:291:GLN:HA	1:A:291:GLN:HE21	1.52	0.74
1:A:235:VAL:HG13	1:A:239:ASP:HB2	1.69	0.74
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.69	0.74
1:A:839:ARG:HA	1:A:842:MET:HE2	1.70	0.74
1:A:912:LYS:NZ	1:A:918:GLU:HG2	2.03	0.74
1:A:997:THR:CG2	1:A:1076:ARG:HH12	2.01	0.73
1:A:745:VAL:O	1:A:749:ILE:HD13	1.88	0.73
1:A:172:GLU:HG3	1:A:471:HIS:ND1	2.03	0.73
1:A:843:LEU:HG	1:A:1034:MET:HG3	1.71	0.72
1:A:968:ILE:O	1:A:972:TYR:HB2	1.90	0.72
1:A:614:ARG:NH1	1:A:646:GLN:HE22	1.87	0.72
1:A:1072:ILE:O	1:A:1075:CYS:HB2	1.91	0.71
1:A:486:GLN:HG2	1:A:487:ILE:O	1.91	0.71
1:A:370:ILE:HD13	1:A:371:PRO:N	2.06	0.70
1:A:947:ARG:HD3	1:A:968:ILE:HG21	1.71	0.70
1:A:968:ILE:HG12	1:A:969:LEU:H	1.54	0.70
1:A:197:ALA:HA	1:A:689:LYS:NZ	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1002:THR:HG22	1:A:1003:SER:N	2.06	0.70
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.56	0.70
1:A:477:ARG:HD2	1:A:522:ASN:H	1.57	0.70
1:A:1056:THR:HG23	1:A:1056:THR:O	1.91	0.70
1:A:359:ARG:O	1:A:420:ILE:HG12	1.92	0.69
1:A:370:ILE:HD12	1:A:372:VAL:O	1.93	0.69
1:A:964:ASP:HA	2:A:1201:19P:H9	1.75	0.69
1:A:1040:PRO:O	1:A:1041:GLN:HB2	1.91	0.69
1:A:851:MET:CE	1:A:938:ALA:HB1	2.23	0.69
1:A:1002:THR:HG22	1:A:1003:SER:H	1.58	0.68
1:A:750:LYS:NZ	1:A:834:HIS:HD2	1.86	0.68
1:A:804:MET:CE	1:A:812:TRP:HB2	2.22	0.68
1:A:184:ARG:O	1:A:188:VAL:HG23	1.94	0.67
1:A:236:SER:HB3	1:A:239:ASP:OD1	1.94	0.67
1:A:1088:LEU:C	1:A:1090:LEU:H	1.97	0.67
1:A:371:PRO:O	1:A:372:VAL:HB	1.95	0.67
1:A:1006:PHE:O	1:A:1009:PHE:HB3	1.95	0.66
1:A:184:ARG:NH1	1:A:722:ARG:HD2	2.11	0.66
1:A:992:LEU:HD23	1:A:995:MET:HE3	1.77	0.66
1:A:320:LYS:HD2	1:A:320:LYS:H	1.60	0.65
1:A:910:TRP:HE3	1:A:911:LEU:HD23	1.61	0.65
1:A:272:LEU:CB	1:A:305:VAL:HG11	2.27	0.65
1:A:487:ILE:HG22	1:A:488:SER:N	2.12	0.65
1:A:1060:ASN:ND2	1:A:1060:ASN:H	1.93	0.64
1:A:473:PHE:HD2	1:A:527:ILE:HD13	1.62	0.64
1:A:954:ILE:HG12	1:A:955:THR:N	2.11	0.64
1:A:768:LYS:O	1:A:772:GLU:HG3	1.97	0.64
1:A:202:VAL:HG12	1:A:203:THR:N	2.13	0.64
1:A:887:THR:HG21	1:A:950:ASP:OD1	1.99	0.63
1:A:358:ASP:HA	1:A:419:LYS:HD3	1.81	0.63
1:A:162:VAL:HG12	1:A:714:ALA:HB1	1.81	0.63
1:A:320:LYS:CD	1:A:320:LYS:H	2.11	0.62
1:A:202:VAL:CG1	1:A:203:THR:N	2.63	0.62
1:A:1021:ARG:HH21	1:A:1056:THR:HG23	1.63	0.62
1:A:381:VAL:HB	1:A:404:PHE:CD2	2.33	0.62
1:A:948:HIS:N	1:A:948:HIS:CD2	2.66	0.62
1:A:733:THR:HG22	1:A:737:GLN:HE21	1.65	0.62
1:A:807:LYS:HE3	1:A:807:LYS:N	2.02	0.61
1:A:955:THR:C	1:A:957:THR:H	2.03	0.61
1:A:487:ILE:HG22	1:A:488:SER:H	1.64	0.61
1:A:507:ASN:OD1	1:A:508:PRO:HD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:GLY:O	1:A:720:TYR:HE1	1.83	0.61
1:A:614:ARG:HG2	1:A:614:ARG:O	2.01	0.61
1:A:930:TYR:CD2	1:A:1012:ILE:HD13	2.35	0.61
1:A:361:PHE:HB2	1:A:420:ILE:HD13	1.83	0.60
1:A:389:HIS:O	1:A:392:GLN:HB3	2.01	0.60
1:A:903:LYS:HE2	1:A:905:GLU:HB3	1.84	0.60
1:A:724:CYS:HB2	1:A:728:MET:HE2	1.83	0.60
1:A:910:TRP:CE3	1:A:911:LEU:HD23	2.37	0.60
1:A:804:MET:HE2	1:A:812:TRP:HB2	1.83	0.59
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.67	0.59
1:A:168:VAL:HG22	1:A:169:HIS:H	1.66	0.59
1:A:1014:VAL:HG11	1:A:1065:LYS:HE3	1.83	0.59
1:A:1088:LEU:O	1:A:1090:LEU:N	2.33	0.59
1:A:173:LEU:O	1:A:177:ARG:HG3	2.01	0.59
1:A:597:LYS:HD3	1:A:600:GLN:NE2	2.18	0.59
1:A:746:THR:HA	1:A:811:LEU:HD11	1.85	0.59
1:A:240:THR:HG23	1:A:243:ALA:HB3	1.85	0.58
1:A:947:ARG:HH22	1:A:964:ASP:HB3	1.67	0.58
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.38	0.58
1:A:282:VAL:HG12	1:A:283:GLY:N	2.18	0.58
1:A:291:GLN:NE2	1:A:291:GLN:HA	2.17	0.58
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.34	0.58
1:A:738:VAL:HG22	1:A:779:LEU:HD11	1.84	0.58
1:A:997:THR:HG23	1:A:1001:LYS:HB3	1.85	0.58
1:A:201:TRP:NE1	1:A:291:GLN:HG3	2.18	0.58
1:A:804:MET:HE2	1:A:812:TRP:CE3	2.36	0.57
1:A:230:SER:O	1:A:231:GLN:CB	2.51	0.57
1:A:271:VAL:CG2	1:A:282:VAL:HG22	2.33	0.57
1:A:368:ILE:O	1:A:369:ASP:HB3	2.05	0.57
1:A:240:THR:O	1:A:244:ILE:HG13	2.04	0.57
1:A:473:PHE:HB3	1:A:527:ILE:HG21	1.87	0.57
1:A:912:LYS:HZ3	1:A:918:GLU:HG2	1.66	0.57
1:A:1021:ARG:HE	1:A:1056:THR:CG2	2.17	0.57
1:A:461:LEU:HB3	1:A:462:TYR:CE2	2.39	0.57
1:A:997:THR:HG21	1:A:1076:ARG:NH1	2.19	0.57
1:A:519:LEU:HD12	1:A:520:LEU:N	2.20	0.57
1:A:912:LYS:HZ1	1:A:918:GLU:HG2	1.70	0.57
1:A:760:SER:OG	1:A:763:VAL:HG23	2.04	0.57
1:A:893:GLN:O	1:A:897:GLY:HA2	2.04	0.57
1:A:985:PHE:CD2	1:A:985:PHE:N	2.73	0.57
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:GLY:O	1:A:970:GLY:HA3	2.04	0.57
1:A:1005:HIS:CE1	1:A:1008:LYS:HZ1	2.22	0.56
1:A:201:TRP:HE3	1:A:279:GLU:OE1	1.88	0.56
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.21	0.56
1:A:997:THR:HG22	1:A:998:SER:N	2.20	0.56
1:A:168:VAL:HG22	1:A:170:ASP:H	1.69	0.56
1:A:235:VAL:HG13	1:A:239:ASP:CB	2.35	0.56
1:A:466:LEU:HD11	1:A:476:ARG:HH11	1.69	0.56
1:A:899:THR:HG22	1:A:901:ALA:H	1.69	0.56
1:A:1044:SER:O	1:A:1045:LYS:CB	2.54	0.56
1:A:361:PHE:HA	1:A:420:ILE:HD11	1.87	0.56
1:A:964:ASP:OD2	2:A:1201:19P:O32	2.22	0.56
1:A:908:ASN:ND2	1:A:994:VAL:HA	2.10	0.56
1:A:241:PRO:HG3	1:A:287:ILE:HG22	1.88	0.56
1:A:1043:THR:O	1:A:1045:LYS:N	2.34	0.56
1:A:210:TYR:HA	1:A:213:LYS:NZ	2.21	0.56
1:A:812:TRP:O	1:A:812:TRP:CD1	2.59	0.56
1:A:921:PHE:O	1:A:925:VAL:HG23	2.05	0.56
1:A:197:ALA:HA	1:A:689:LYS:HZ1	1.69	0.55
1:A:203:THR:HG22	1:A:289:ASN:O	2.06	0.55
1:A:750:LYS:HE3	1:A:808:LYS:HA	1.88	0.55
1:A:1003:SER:O	1:A:1007:GLN:HG3	2.06	0.55
1:A:1010:GLN:NE2	1:A:1069:LEU:HD22	2.22	0.55
1:A:1082:VAL:HA	1:A:1085:ASN:HB2	1.90	0.54
1:A:165:VAL:O	1:A:165:VAL:HG12	2.08	0.54
1:A:207:LEU:HB2	1:A:288:LYS:HD2	1.90	0.54
1:A:907:LEU:O	1:A:911:LEU:HG	2.07	0.54
1:A:949:ASN:HB2	1:A:1083:GLN:NE2	2.23	0.54
1:A:477:ARG:CD	1:A:521:ASP:HA	2.38	0.53
1:A:891:ILE:O	1:A:906:VAL:HG11	2.08	0.53
1:A:306:VAL:HG13	1:A:306:VAL:O	2.09	0.53
1:A:223:VAL:HG12	1:A:225:HIS:HE1	1.72	0.53
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	1.91	0.53
1:A:863:CYS:SG	1:A:927:ARG:NH1	2.81	0.53
1:A:606:LYS:O	1:A:609:GLN:HB2	2.09	0.53
1:A:779:LEU:HD12	1:A:780:PRO:HD2	1.89	0.53
2:A:1201:19P:H6	2:A:1201:19P:H18	1.91	0.53
1:A:784:ARG:NH1	1:A:789:PRO:O	2.41	0.53
1:A:811:LEU:HD12	1:A:811:LEU:N	2.23	0.53
1:A:935:TYR:O	1:A:939:THR:CG2	2.56	0.53
1:A:947:ARG:NH2	1:A:951:ASN:HB3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:GLU:OE2	1:A:546:GLU:HA	2.09	0.52
1:A:992:LEU:HA	1:A:995:MET:HE2	1.89	0.52
1:A:476:ARG:HG3	1:A:480:TYR:OH	2.08	0.52
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.77	0.52
1:A:583:LEU:HD22	1:A:610:LEU:CD2	2.36	0.52
1:A:878:MET:C	1:A:879:ILE:HG13	2.29	0.52
1:A:477:ARG:HD2	1:A:521:ASP:HA	1.91	0.52
1:A:602:GLU:O	1:A:605:ALA:HB3	2.09	0.52
1:A:422:ASP:HB3	1:A:599:GLY:O	2.09	0.52
1:A:1050:TYR:C	1:A:1050:TYR:CD2	2.83	0.52
1:A:558:ILE:O	1:A:561:THR:HG22	2.10	0.52
1:A:916:PRO:HG2	1:A:920:LYS:CD	2.39	0.52
1:A:939:THR:OG1	1:A:945:GLY:HA2	2.10	0.52
1:A:983:VAL:HG22	1:A:985:PHE:O	2.08	0.52
1:A:968:ILE:C	1:A:970:GLY:H	2.12	0.51
1:A:1055:LEU:O	1:A:1056:THR:HG22	2.11	0.51
1:A:370:ILE:HD12	1:A:372:VAL:N	2.26	0.51
1:A:947:ARG:NH1	1:A:948:HIS:CE1	2.78	0.51
1:A:381:VAL:HB	1:A:404:PHE:HD2	1.74	0.51
1:A:804:MET:HE3	1:A:812:TRP:HB2	1.91	0.51
1:A:357:CYS:SG	1:A:359:ARG:NH1	2.84	0.51
1:A:800:LYS:O	1:A:802:LYS:HE3	2.10	0.51
1:A:1044:SER:O	1:A:1045:LYS:HB3	2.11	0.51
1:A:240:THR:HG23	1:A:243:ALA:CB	2.41	0.51
1:A:464:VAL:HB	1:A:484:MET:HG2	1.93	0.51
1:A:614:ARG:HH11	1:A:646:GLN:HE22	1.58	0.50
1:A:320:LYS:HD2	1:A:320:LYS:N	2.26	0.50
1:A:466:LEU:HD11	1:A:476:ARG:CD	2.42	0.50
1:A:466:LEU:CD1	1:A:476:ARG:HH11	2.25	0.50
1:A:622:LEU:HD21	1:A:651:LEU:CD2	2.41	0.50
1:A:477:ARG:NH1	1:A:521:ASP:OD1	2.45	0.50
1:A:860:LEU:HD21	1:A:1015:LYS:HD2	1.93	0.50
1:A:984:PRO:HG3	1:A:1071:GLN:O	2.12	0.50
1:A:184:ARG:HH12	1:A:722:ARG:HD2	1.77	0.50
1:A:887:THR:HB	1:A:890:LYS:CD	2.42	0.50
1:A:1002:THR:CG2	1:A:1003:SER:N	2.75	0.50
1:A:201:TRP:CE2	1:A:291:GLN:HG3	2.46	0.50
1:A:428:LEU:HD23	1:A:467:LEU:HD23	1.94	0.50
1:A:968:ILE:HG12	1:A:969:LEU:N	2.26	0.50
1:A:307:LEU:C	1:A:307:LEU:HD23	2.32	0.49
1:A:731:ASP:OD2	1:A:784:ARG:NE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:ARG:HH11	1:A:968:ILE:HG23	1.77	0.49
1:A:955:THR:C	1:A:957:THR:N	2.65	0.49
1:A:245:LEU:C	1:A:247:SER:H	2.14	0.49
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.47	0.49
1:A:182:THR:N	1:A:183:PRO:HD2	2.27	0.49
1:A:197:ALA:HA	1:A:689:LYS:HZ2	1.77	0.49
1:A:214:LYS:HD3	1:A:297:LEU:O	2.11	0.49
1:A:662:GLN:OE1	1:A:1030:LEU:HD22	2.12	0.49
1:A:315:LEU:O	1:A:727:ALA:HB2	2.12	0.49
1:A:734:GLN:O	1:A:738:VAL:HG23	2.12	0.49
1:A:461:LEU:HB3	1:A:462:TYR:CD2	2.47	0.49
1:A:171:ASP:OD1	1:A:472:ARG:NH2	2.45	0.49
1:A:1002:THR:CG2	1:A:1003:SER:H	2.26	0.49
1:A:985:PHE:HZ	1:A:1072:ILE:HG12	1.77	0.49
1:A:916:PRO:HG2	1:A:920:LYS:HD3	1.94	0.49
1:A:223:VAL:HG12	1:A:225:HIS:CE1	2.48	0.49
1:A:913:GLU:O	1:A:913:GLU:HG2	2.13	0.49
1:A:750:LYS:NZ	1:A:834:HIS:O	2.45	0.49
1:A:947:ARG:CD	1:A:968:ILE:HD12	2.39	0.49
1:A:198:MET:CE	1:A:282:VAL:HG11	2.43	0.49
1:A:887:THR:HB	1:A:890:LYS:HD2	1.94	0.49
1:A:168:VAL:HG22	1:A:169:HIS:N	2.28	0.48
1:A:734:GLN:NE2	1:A:780:PRO:HB2	2.27	0.48
1:A:829:GLY:HA3	1:A:881:ILE:HD12	1.94	0.48
1:A:874:ASP:O	1:A:875:LYS:HB2	2.13	0.48
1:A:738:VAL:HG22	1:A:779:LEU:CD1	2.43	0.48
1:A:214:LYS:HZ1	1:A:300:GLY:HA2	1.77	0.48
1:A:287:ILE:HA	1:A:290:PHE:HD1	1.78	0.48
1:A:1043:THR:HG22	1:A:1044:SER:N	2.29	0.48
1:A:1088:LEU:C	1:A:1090:LEU:N	2.64	0.48
1:A:611:LEU:O	1:A:614:ARG:HB2	2.13	0.48
1:A:947:ARG:HH12	1:A:967:HIS:HB3	1.79	0.48
1:A:568:THR:HG22	1:A:571:ASP:CG	2.34	0.48
1:A:845:LEU:O	1:A:848:LEU:HB2	2.14	0.48
1:A:1035:LEU:HD22	1:A:1039:MET:HG3	1.95	0.48
1:A:230:SER:O	1:A:231:GLN:HB3	2.13	0.48
1:A:184:ARG:HH21	1:A:321:GLU:CD	2.17	0.48
1:A:601:GLN:HG3	1:A:602:GLU:N	2.28	0.48
1:A:1043:THR:C	1:A:1045:LYS:H	2.15	0.47
1:A:209:GLU:O	1:A:213:LYS:HG2	2.15	0.47
1:A:707:ARG:HA	1:A:710:GLN:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.97	0.47
1:A:1083:GLN:HA	1:A:1083:GLN:NE2	2.29	0.47
1:A:204:SER:HB2	1:A:652:GLU:OE2	2.15	0.47
1:A:1061:GLU:O	1:A:1064:ALA:HB3	2.14	0.47
1:A:386:ASN:OD1	1:A:396:GLN:HG3	2.15	0.47
1:A:903:LYS:HB3	1:A:906:VAL:HG23	1.97	0.47
1:A:948:HIS:ND1	1:A:951:ASN:OD1	2.48	0.47
1:A:280:TYR:HB3	1:A:282:VAL:HG23	1.97	0.47
1:A:608:TYR:OH	1:A:639:ASN:ND2	2.47	0.47
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.14	0.47
1:A:162:VAL:CG1	1:A:714:ALA:HB1	2.44	0.47
1:A:988:THR:OG1	1:A:990:ASP:OD1	2.24	0.47
1:A:207:LEU:HD23	1:A:288:LYS:O	2.15	0.47
1:A:379:LEU:HB2	1:A:404:PHE:HB3	1.96	0.47
1:A:805:ALA:O	1:A:806:SER:HB2	2.15	0.47
1:A:1009:PHE:HE2	1:A:1072:ILE:HD13	1.80	0.47
1:A:180:LEU:O	1:A:183:PRO:HD2	2.15	0.47
1:A:838:LEU:HD23	1:A:877:GLY:HA3	1.96	0.47
1:A:157:LEU:O	1:A:700:ARG:NE	2.42	0.46
1:A:358:ASP:CA	1:A:419:LYS:HD3	2.45	0.46
1:A:273:ARG:O	1:A:305:VAL:HG13	2.16	0.46
1:A:364:LYS:HG3	1:A:412:VAL:O	2.15	0.46
1:A:997:THR:HG21	1:A:1076:ARG:HH22	1.81	0.46
1:A:370:ILE:HD13	1:A:371:PRO:CD	2.45	0.46
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.98	0.46
1:A:674:ASP:OD1	1:A:679:ARG:NE	2.44	0.46
1:A:470:ASP:HB2	1:A:476:ARG:NH2	2.31	0.46
1:A:706:SER:O	1:A:710:GLN:HB3	2.15	0.46
1:A:472:ARG:HH11	1:A:472:ARG:HB2	1.79	0.46
1:A:807:LYS:H	1:A:807:LYS:CE	2.06	0.46
1:A:199:HIS:O	1:A:199:HIS:CD2	2.69	0.46
1:A:395:CYS:HB3	1:A:418:ILE:HD11	1.98	0.46
1:A:767:LEU:HD12	1:A:803:VAL:HG23	1.98	0.46
1:A:280:TYR:C	1:A:281:LEU:HD12	2.36	0.46
1:A:472:ARG:O	1:A:473:PHE:HB2	2.16	0.46
1:A:144:SER:HB3	1:A:147:SER:OG	2.16	0.46
1:A:806:SER:O	1:A:809:LYS:HG2	2.16	0.46
1:A:812:TRP:O	1:A:812:TRP:HD1	1.97	0.45
1:A:907:LEU:HD22	1:A:994:VAL:HG21	1.99	0.45
1:A:163:THR:O	1:A:165:VAL:HG23	2.16	0.45
1:A:199:HIS:O	1:A:200:PRO:C	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LYS:O	1:A:251:LYS:HD3	2.16	0.45
1:A:803:VAL:HG12	1:A:804:MET:N	2.31	0.45
1:A:233:ILE:HG22	1:A:234:LYS:N	2.31	0.45
1:A:398:ARG:O	1:A:414:LEU:HD21	2.16	0.45
1:A:562:ASP:HB2	1:A:563:PRO:CD	2.47	0.45
1:A:968:ILE:C	1:A:970:GLY:N	2.70	0.45
1:A:501:LYS:HE2	1:A:501:LYS:HB3	1.74	0.45
1:A:467:LEU:HD13	1:A:672:TYR:CE2	2.51	0.45
1:A:857:THR:OG1	1:A:858:GLU:HG3	2.16	0.45
1:A:1027:LEU:HD23	1:A:1027:LEU:HA	1.63	0.45
1:A:171:ASP:O	1:A:175:PHE:HB2	2.16	0.45
1:A:548:PRO:HD2	1:A:551:LEU:HD12	1.98	0.45
1:A:998:SER:O	1:A:999:GLY:C	2.54	0.45
1:A:1078:LYS:O	1:A:1080:TRP:N	2.49	0.45
1:A:192:ASP:C	1:A:192:ASP:OD1	2.56	0.45
1:A:272:LEU:HD22	1:A:305:VAL:HG11	1.99	0.45
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.52	0.45
1:A:509:ASP:OD2	1:A:512:ASN:HB2	2.16	0.45
1:A:955:THR:O	1:A:957:THR:N	2.50	0.45
1:A:364:LYS:NZ	1:A:411:ASN:ND2	2.65	0.45
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.97	0.45
1:A:217:ASN:O	1:A:219:CYS:N	2.50	0.44
1:A:639:ASN:O	1:A:643:ILE:HG23	2.17	0.44
1:A:983:VAL:HB	1:A:1082:VAL:HG21	1.99	0.44
1:A:1034:MET:SD	1:A:1039:MET:HE3	2.57	0.44
1:A:685:GLY:O	1:A:720:TYR:CE1	2.68	0.44
2:A:1201:19P:C23	2:A:1201:19P:H25	2.47	0.44
1:A:170:ASP:OD1	1:A:471:HIS:HE1	2.00	0.44
1:A:1056:THR:CG2	1:A:1056:THR:O	2.61	0.44
1:A:839:ARG:HA	1:A:842:MET:CE	2.44	0.44
1:A:379:LEU:HD22	1:A:379:LEU:N	2.33	0.44
1:A:565:ASN:HA	1:A:566:PRO:HD3	1.88	0.44
1:A:640:VAL:O	1:A:643:ILE:HG12	2.18	0.44
1:A:861:ASP:C	1:A:861:ASP:OD1	2.56	0.44
1:A:270:PHE:CD2	1:A:307:LEU:HD21	2.52	0.44
1:A:317:GLU:HG2	1:A:318:VAL:N	2.32	0.44
1:A:470:ASP:CB	1:A:476:ARG:NH2	2.80	0.44
1:A:947:ARG:HD3	1:A:968:ILE:CG2	2.41	0.44
1:A:1043:THR:O	1:A:1047:ASP:HB2	2.18	0.44
1:A:949:ASN:N	1:A:1083:GLN:HE22	2.15	0.44
1:A:381:VAL:HG13	1:A:381:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.53	0.44
1:A:748:ASP:HB3	1:A:770:LYS:NZ	2.32	0.44
1:A:795:ALA:HB3	1:A:816:LYS:HD2	1.99	0.44
1:A:848:LEU:HD12	1:A:851:MET:CE	2.48	0.44
1:A:969:LEU:O	1:A:1042:LEU:HD12	2.18	0.44
1:A:387:ILE:HD13	1:A:468:LEU:HD11	2.00	0.43
1:A:487:ILE:CG2	1:A:488:SER:N	2.81	0.43
1:A:739:ILE:O	1:A:743:GLN:HG3	2.19	0.43
1:A:833:LYS:HG3	1:A:834:HIS:N	2.33	0.43
1:A:833:LYS:NZ	2:A:1201:19P:O30	2.44	0.43
1:A:177:ARG:HB3	1:A:177:ARG:HE	1.53	0.43
1:A:862:LEU:HD22	1:A:862:LEU:N	2.34	0.43
1:A:370:ILE:C	1:A:372:VAL:H	2.21	0.43
1:A:778:GLN:N	1:A:778:GLN:CD	2.72	0.43
1:A:867:TYR:OH	1:A:963:ILE:HA	2.19	0.43
1:A:226:ARG:HD2	1:A:226:ARG:HA	1.84	0.43
1:A:271:VAL:CG1	1:A:310:PRO:HG3	2.49	0.43
1:A:235:VAL:CG1	1:A:239:ASP:HB2	2.45	0.43
1:A:182:THR:HB	1:A:183:PRO:HD3	2.01	0.43
1:A:519:LEU:HD12	1:A:520:LEU:H	1.84	0.43
1:A:787:TYR:CZ	1:A:880:GLU:HB2	2.54	0.43
1:A:199:HIS:O	1:A:199:HIS:CG	2.71	0.43
1:A:395:CYS:SG	1:A:396:GLN:N	2.92	0.43
1:A:966:GLY:O	1:A:970:GLY:CA	2.67	0.42
1:A:968:ILE:CG1	1:A:969:LEU:H	2.27	0.42
1:A:989:PRO:HD3	1:A:1079:GLY:O	2.19	0.42
1:A:477:ARG:CZ	1:A:521:ASP:OD1	2.67	0.42
1:A:696:PHE:CZ	1:A:700:ARG:HD2	2.54	0.42
1:A:762:GLN:O	1:A:765:SER:HB3	2.20	0.42
1:A:489:GLY:HA3	1:A:1041:GLN:NE2	2.34	0.42
1:A:307:LEU:HD23	1:A:307:LEU:O	2.19	0.42
1:A:802:LYS:HG2	1:A:812:TRP:HB3	2.00	0.42
1:A:964:ASP:OD1	1:A:967:HIS:HB2	2.19	0.42
1:A:985:PHE:HB2	1:A:986:VAL:H	1.68	0.42
1:A:370:ILE:HG23	1:A:372:VAL:H	1.84	0.42
1:A:514:MET:HG3	1:A:515:SER:N	2.34	0.42
1:A:366:ARG:HB2	1:A:517:SER:HB2	2.01	0.42
1:A:915:SER:HA	1:A:916:PRO:HD3	1.84	0.42
1:A:905:GLU:HG3	1:A:993:PHE:CZ	2.55	0.42
1:A:290:PHE:O	1:A:294:ARG:HG3	2.20	0.42
1:A:762:GLN:O	1:A:766:GLN:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:PHE:HA	1:A:1043:THR:HG21	2.02	0.41
1:A:1069:LEU:O	1:A:1072:ILE:HB	2.19	0.41
1:A:371:PRO:O	1:A:372:VAL:CB	2.65	0.41
1:A:749:ILE:HD11	1:A:770:LYS:HD2	2.02	0.41
1:A:1035:LEU:HA	1:A:1039:MET:HG2	2.02	0.41
1:A:373:LEU:C	1:A:373:LEU:HD23	2.41	0.41
1:A:278:ASP:HB2	1:A:784:ARG:HH12	1.85	0.41
1:A:498:ASN:HD22	1:A:500:ASP:H	1.67	0.41
1:A:902:PHE:HE1	1:A:1084:PHE:HA	1.85	0.41
1:A:1000:LYS:O	1:A:1001:LYS:HB2	2.20	0.41
1:A:1008:LYS:O	1:A:1009:PHE:C	2.58	0.41
1:A:657:LEU:HD13	1:A:690:ARG:HE	1.86	0.41
1:A:760:SER:CB	1:A:763:VAL:HG23	2.50	0.41
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.20	0.41
1:A:241:PRO:HD3	1:A:285:THR:O	2.21	0.41
1:A:597:LYS:HD3	1:A:600:GLN:HE21	1.85	0.41
1:A:852:GLU:HG2	1:A:864:LEU:HD12	2.02	0.41
1:A:947:ARG:NH1	1:A:968:ILE:HG23	2.35	0.41
1:A:998:SER:O	1:A:1000:LYS:N	2.53	0.41
1:A:1035:LEU:HA	1:A:1039:MET:CG	2.51	0.41
1:A:207:LEU:HD13	1:A:208:PRO:HD2	2.02	0.41
1:A:386:ASN:N	1:A:386:ASN:ND2	2.68	0.41
1:A:470:ASP:OD1	1:A:470:ASP:C	2.59	0.41
1:A:610:LEU:HA	1:A:610:LEU:HD23	1.86	0.41
1:A:622:LEU:HD21	1:A:651:LEU:HD21	2.02	0.41
1:A:760:SER:HB3	1:A:763:VAL:CG2	2.51	0.41
1:A:954:ILE:HG12	1:A:955:THR:H	1.81	0.41
1:A:966:GLY:O	1:A:970:GLY:N	2.54	0.41
1:A:244:ILE:O	1:A:244:ILE:HG22	2.21	0.41
1:A:245:LEU:C	1:A:247:SER:N	2.74	0.41
1:A:364:LYS:HE2	1:A:411:ASN:HA	2.03	0.41
1:A:799:GLU:HG3	1:A:799:GLU:H	1.31	0.41
2:A:1201:19P:H13	2:A:1201:19P:H25	2.02	0.41
1:A:701:SER:OG	1:A:871:SER:HB3	2.21	0.41
1:A:180:LEU:C	1:A:183:PRO:HD2	2.41	0.40
1:A:656:VAL:HG11	1:A:691:ILE:HD13	2.02	0.40
1:A:829:GLY:CA	1:A:881:ILE:HD12	2.50	0.40
1:A:191:ARG:HD2	1:A:196:TYR:CD1	2.56	0.40
1:A:434:TYR:CE1	1:A:460:LEU:HB2	2.56	0.40
1:A:760:SER:O	1:A:764:ILE:HG13	2.21	0.40
1:A:1035:LEU:CD2	1:A:1039:MET:HG3	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:THR:O	1:A:1085:ASN:HB2	2.21	0.40
1:A:217:ASN:O	1:A:218:ASN:C	2.60	0.40
1:A:674:ASP:CG	1:A:679:ARG:HE	2.24	0.40
1:A:788:ASP:C	1:A:788:ASP:OD1	2.60	0.40
1:A:170:ASP:OD1	1:A:471:HIS:CE1	2.74	0.40
1:A:240:THR:HA	1:A:241:PRO:HD3	1.93	0.40
1:A:812:TRP:CZ3	2:A:1201:19P:H21	2.57	0.40
1:A:734:GLN:HE21	1:A:780:PRO:CB	2.35	0.40
1:A:907:LEU:HD23	1:A:911:LEU:HG	2.02	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	810/966 (84%)	719 (89%)	76 (9%)	15 (2%)	8 6

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	372	VAL
1	A	1045	LYS
1	A	369	ASP
1	A	806	SER
1	A	897	GLY
1	A	999	GLY
1	A	1001	LYS
1	A	1079	GLY
1	A	1089	HIS
1	A	218	ASN
1	A	797	ALA

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Mol	Chain	Res	Type
1	A	227	SER
1	A	956	GLU
1	A	984	PRO

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	743/864 (86%)	684 (92%)	59 (8%)	12	12

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

Mol	Chain	Res	Type
1	A	146	GLU
1	A	172	GLU
1	A	213	LYS
1	A	214	LYS
1	A	218	ASN
1	A	225	HIS
1	A	252	MET
1	A	302	GLU
1	A	317	GLU
1	A	319	ARG
1	A	320	LYS
1	A	322	GLU
1	A	362	ARG
1	A	366	ARG
1	A	370	ILE
1	A	386	ASN
1	A	410	TRP
1	A	464	VAL
1	A	472	ARG
1	A	498	ASN
1	A	544	ARG
1	A	546	GLU
1	A	601	GLN

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Mol	Chain	Res	Type
1	A	610	LEU
1	A	619	GLN
1	A	626	LEU
1	A	682	LEU
1	A	707	ARG
1	A	717	LEU
1	A	728	MET
1	A	729	LEU
1	A	740	GLU
1	A	760	SER
1	A	766	GLN
1	A	767	LEU
1	A	799	GLU
1	A	807	LYS
1	A	823	LEU
1	A	825	ASN
1	A	833	LYS
1	A	838	LEU
1	A	839	ARG
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	890	LYS
1	A	893	GLN
1	A	918	GLU
1	A	927	ARG
1	A	948	HIS
1	A	964	ASP
1	A	968	ILE
1	A	972	TYR
1	A	985	PHE
1	A	1026	LEU
1	A	1059	LYS
1	A	1060	ASN
1	A	1076	ARG
1	A	1085	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	291	GLN

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Mol	Chain	Res	Type
1	A	304	HIS
1	A	411	ASN
1	A	498	ASN
1	A	525	HIS
1	A	554	GLN
1	A	565	ASN
1	A	600	GLN
1	A	639	ASN
1	A	646	GLN
1	A	734	GLN
1	A	737	GLN
1	A	743	GLN
1	A	766	GLN
1	A	773	ASN
1	A	775	GLN
1	A	834	HIS
1	A	893	GLN
1	A	908	ASN
1	A	959	ASN
1	A	967	HIS
1	A	1022	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 carbohydrates 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	19P	A	1201	-	32,37,37	0.73	1 (3%)	39,55,55	1.46	5 (12%)

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	19P	A	1201	-	-	0/12/26/26	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	19P	C10-C9	-2.15	1.39	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	19P	C12-N13-C14	3.81	121.86	117.45
2	A	1201	19P	C25-N24-C23	3.18	118.75	112.62
2	A	1201	19P	C8-N7-C4	3.08	121.93	117.69
2	A	1201	19P	C9-C10-C5	-2.49	118.42	120.80
2	A	1201	19P	C11-C12-N13	-2.25	120.60	124.32

There are no chirality outliers.

There are no torsion outliers.

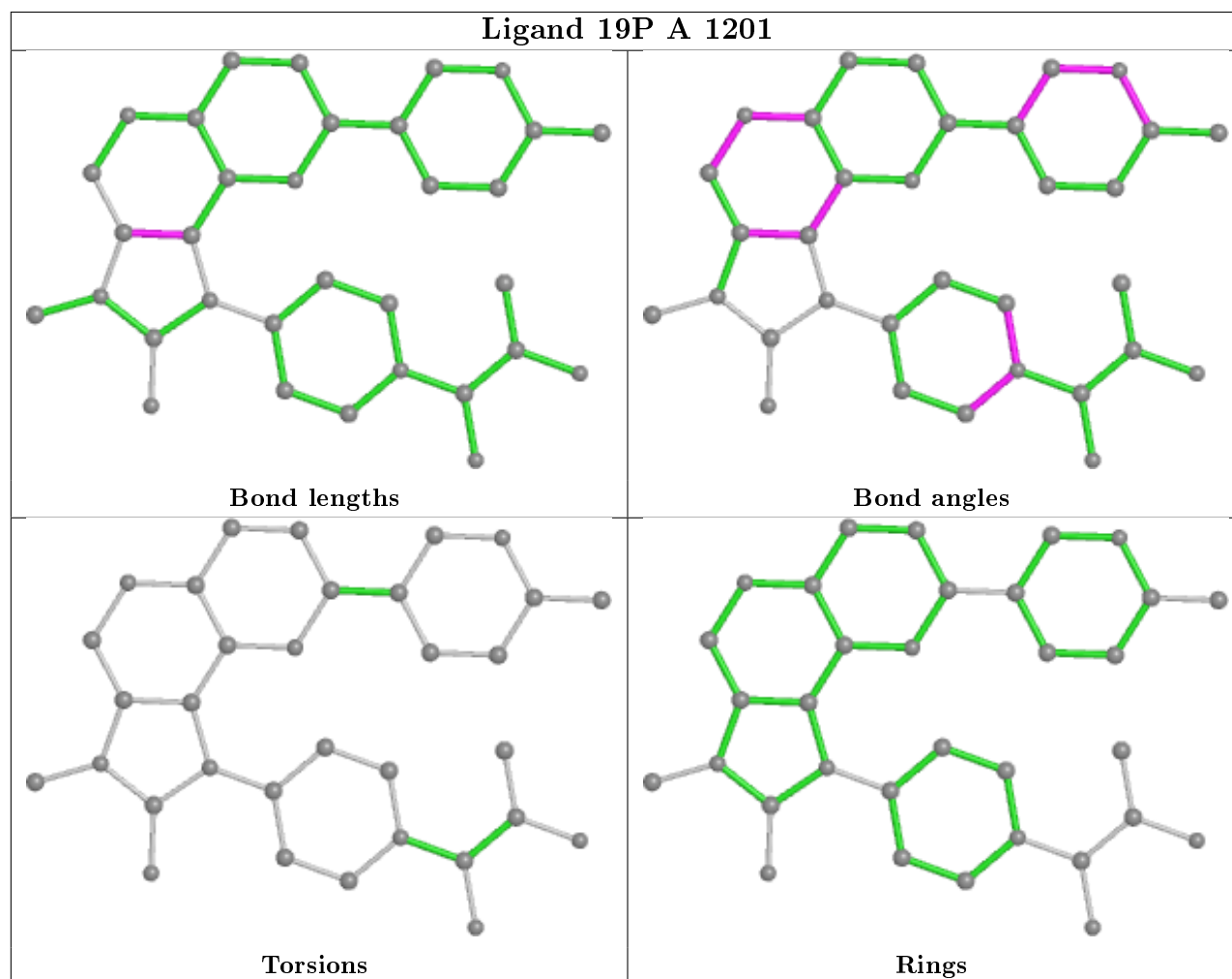
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	19P	7	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 ⓘ

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	830/966 (85%)	0.83	106 (12%) 3 6	21, 60, 97, 126	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	528	ALA	7.2
1	A	379	LEU	6.2
1	A	216	ALA	6.0
1	A	779	LEU	5.4
1	A	972	TYR	5.2
1	A	967	HIS	5.1
1	A	245	LEU	4.8
1	A	526	PRO	4.5
1	A	971	ASN	4.3
1	A	250	THR	4.2
1	A	545	ALA	4.1
1	A	228	THR	4.0
1	A	1082	VAL	4.0
1	A	1041	GLN	4.0
1	A	248	PHE	3.9
1	A	995	MET	3.8
1	A	777	SER	3.8
1	A	234	LYS	3.7
1	A	481	VAL	3.7
1	A	147	SER	3.7
1	A	404	PHE	3.7
1	A	253	ALA	3.6
1	A	319	ARG	3.5
1	A	270	PHE	3.5
1	A	272	LEU	3.5
1	A	249	PHE	3.4
1	A	895	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	987	LEU	3.4
1	A	398	ARG	3.4
1	A	144	SER	3.4
1	A	226	ARG	3.4
1	A	307	LEU	3.4
1	A	231	GLN	3.3
1	A	902	PHE	3.3
1	A	235	VAL	3.3
1	A	489	GLY	3.2
1	A	774	LEU	3.2
1	A	969	LEU	3.1
1	A	660	LEU	3.1
1	A	220	ILE	3.0
1	A	525	HIS	3.0
1	A	1087	PHE	3.0
1	A	242	GLY	3.0
1	A	899	THR	3.0
1	A	1004	PRO	3.0
1	A	178	ARG	3.0
1	A	544	ARG	2.9
1	A	233	ILE	2.9
1	A	409	LEU	2.9
1	A	1042	LEU	2.9
1	A	898	ASN	2.8
1	A	661	LEU	2.8
1	A	215	ILE	2.8
1	A	850	ILE	2.8
1	A	843	LEU	2.8
1	A	207	LEU	2.8
1	A	229	THR	2.8
1	A	370	ILE	2.8
1	A	357	CYS	2.8
1	A	251	LYS	2.8
1	A	823	LEU	2.7
1	A	691	ILE	2.7
1	A	659	TYR	2.7
1	A	847	ILE	2.7
1	A	381	VAL	2.6
1	A	916	PRO	2.6
1	A	869	CYS	2.6
1	A	252	MET	2.6
1	A	382	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	896	VAL	2.6
1	A	227	SER	2.6
1	A	656	VAL	2.6
1	A	380	THR	2.6
1	A	213	LYS	2.5
1	A	1064	ALA	2.5
1	A	271	VAL	2.5
1	A	148	GLN	2.4
1	A	624	VAL	2.4
1	A	999	GLY	2.4
1	A	145	GLU	2.4
1	A	217	ASN	2.4
1	A	842	MET	2.4
1	A	527	ILE	2.3
1	A	811	LEU	2.3
1	A	664	VAL	2.3
1	A	778	GLN	2.3
1	A	868	GLY	2.3
1	A	832	PHE	2.2
1	A	663	LEU	2.2
1	A	768	LYS	2.2
1	A	970	GLY	2.2
1	A	767	LEU	2.2
1	A	658	HIS	2.2
1	A	303	ILE	2.2
1	A	281	LEU	2.1
1	A	151	GLN	2.1
1	A	870	ILE	2.1
1	A	862	LEU	2.1
1	A	845	LEU	2.1
1	A	150	PHE	2.1
1	A	699	LEU	2.0
1	A	627	THR	2.0
1	A	681	LEU	2.0
1	A	462	TYR	2.0
1	A	402	LYS	2.0
1	A	1000	LYS	2.0

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

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](#)

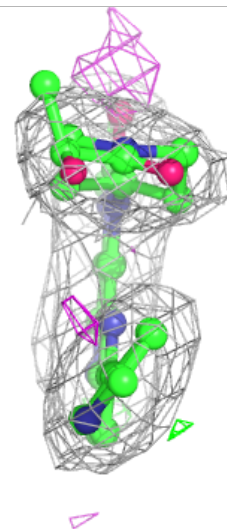
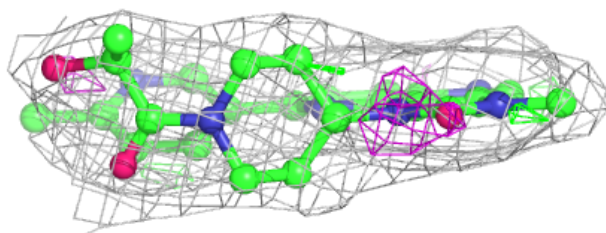
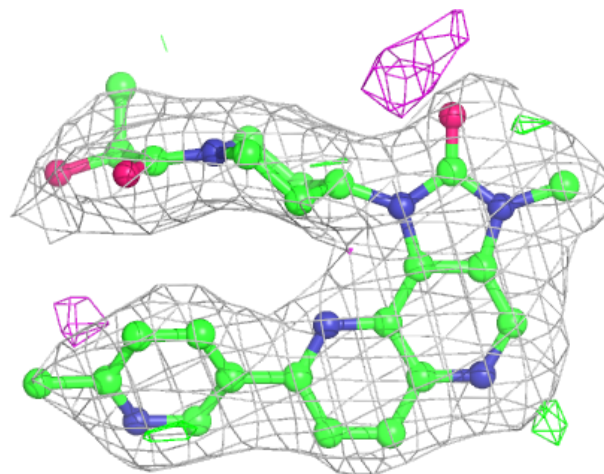
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	19P	A	1201	33/33	0.90	0.19	33,46,55,60	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 19P A 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.