



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:12 PM UTC

PDB ID : 4HVB / pdb_00004hvb
Title : Catalytic unit of PI3K γ 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

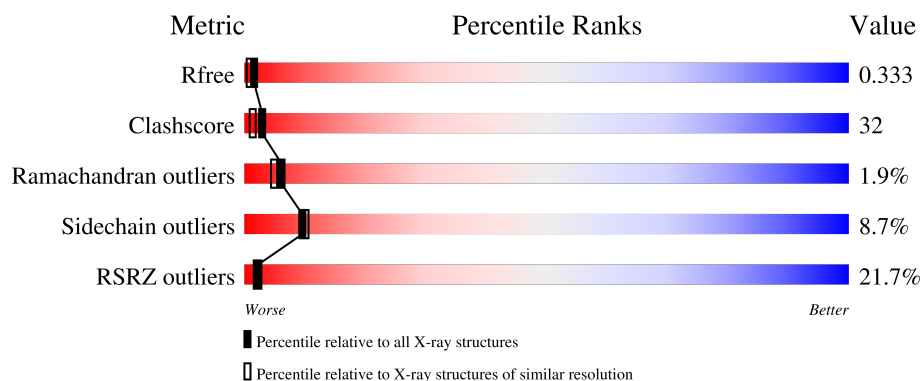
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 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	

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.

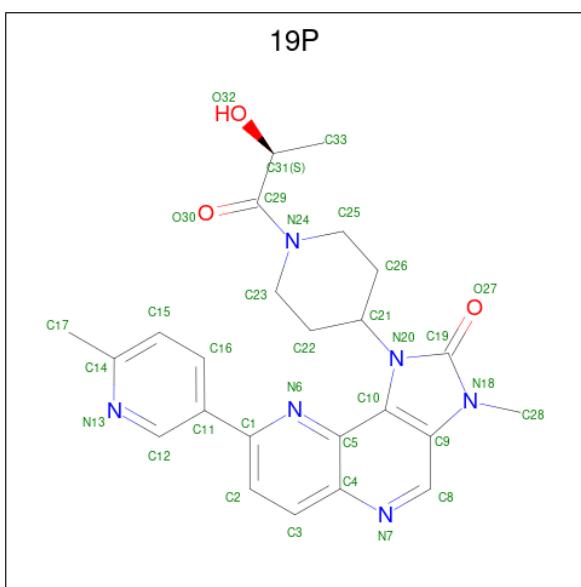
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

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

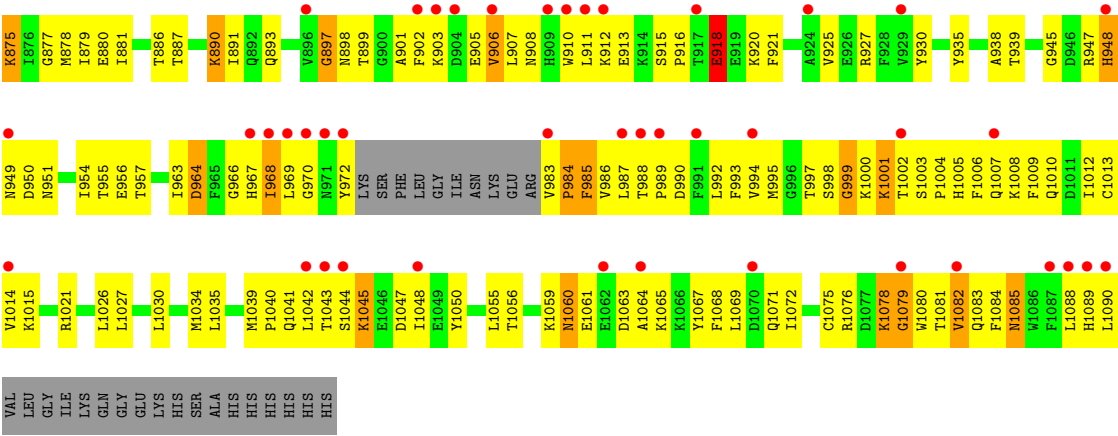
- Molecule 2 is 1-{1-[(2S)-2-hydroxypropanoyl]piperidin-4-yl}-3-methyl-8-(6-methylpyridin-3-yl)-1,3-dihydro-2H-imidazo[4,5-c][1,5]naphthyridin-2-one (CCD ID: 19P) (formula: C₂₄H₂₆N₆O₃).



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		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.80Å 67.58Å 106.90Å 90.00° 95.48° 90.00°	Depositor
Resolution (Å)	50.00 – 2.35 50.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-2.35) 95.3 (50.00-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.34Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.270 , 0.333 0.270 , 0.333	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)	0.32 , 48.7	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	0.92	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 ⓘ

5.1 Standard geometry ⓘ

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	0.46	1/6859 (0.0%)	0.81	8/9274 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	851	MET	SD-CE	-6.51	1.63	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	HIS	CA-C-N	-6.46	113.30	119.89
1	A	199	HIS	C-N-CA	-6.46	113.30	119.89
1	A	819	ASP	CA-C-N	5.73	125.41	119.05
1	A	819	ASP	C-N-CA	5.73	125.41	119.05
1	A	918	GLU	N-CA-C	-5.54	106.68	113.50
1	A	163	THR	N-CA-C	-5.22	107.04	113.41
1	A	906	VAL	N-CA-C	5.10	115.83	110.62
1	A	308	ASP	N-CA-C	5.02	115.15	108.23

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	6717	0	6758	434	0
2	A	33	0	26	6	0
3	A	1	0	0	0	0
All	All	6751	0	6784	437	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 32.

All (437) 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:804:MET:HE2	1:A:812:TRP:HB2	1.26	1.14
1:A:807:LYS:HE3	1:A:807:LYS:H	1.17	1.09
1:A:851:MET:HE1	1:A:938:ALA:HB1	1.39	1.01
1:A:750:LYS:HZ3	1:A:834:HIS:CD2	1.80	0.99
1:A:908:ASN:HD22	1:A:994:VAL:HA	1.29	0.97
1:A:750:LYS:HZ3	1:A:834:HIS:HD2	1.01	0.94
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:839:ARG:HA	1:A:842:MET:HE2	1.52	0.91
1:A:689:LYS:HG2	1:A:728:MET:SD	2.16	0.86
1:A:766:GLN:H	1:A:766:GLN:HE21	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:987:LEU:HD11	1:A:995:MET:HE1	1.62	0.80
1:A:625:GLY:O	1:A:629:GLN:HG3	1.81	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:992:LEU:HD23	1:A:995:MET:HE3	1.68	0.76
1:A:271:VAL:HG21	1:A:282:VAL:HG22	1.69	0.75
1:A:181:VAL:HG12	1:A:185:MET:HE2	1.67	0.75
1:A:291:GLN:HE21	1:A:291:GLN:HA	1.52	0.74
1:A:235:VAL:HG13	1:A:239:ASP:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.69	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:1088:LEU:C	1:A:1090:LEU:H	1.97	0.71
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:964:ASP:HA	2:A:1201:19P:H9	1.73	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
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:1040:PRO:O	1:A:1041:GLN:HB2	1.91	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: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: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:955:THR:C	1:A:957:THR:H	2.03	0.66
1:A:184:ARG:NH1	1:A:722:ARG:HD2	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ASP:HA	1:A:419:LYS:HD3	1.81	0.63
1:A:851:MET:CE	1:A:938:ALA:HB1	2.23	0.63
1:A:162:VAL:HG12	1:A:714:ALA:HB1	1.81	0.63
1:A:320:LYS:H	1:A:320:LYS:CD	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: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
1:A:685:GLY:O	1:A:720:TYR:HE1	1.83	0.61
1:A:614:ARG:O	1:A:614:ARG:HG2	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:992:LEU:HA	1:A:995:MET:HE3	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:910:TRP:CE3	1:A:911:LEU:HD23	2.37	0.60
1:A:168:VAL:HG22	1:A:169:HIS:H	1.66	0.59
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.67	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:HA	1:A:291:GLN:NE2	2.17	0.58
1:A:197:ALA:HA	1:A:689:LYS:HZ1	1.65	0.58
1:A:738:VAL:HG22	1:A:779:LEU:HD11	1.84	0.58
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.34	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:968:ILE:C	1:A:970:GLY:H	2.12	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:1005:HIS:CE1	1:A:1008:LYS:HZ1	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1021:ARG:HE	1:A:1056:THR:CG2	2.17	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:N	1:A:985:PHE:CD2	2.73	0.57
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.23	0.57
1:A:966:GLY:O	1:A:970:GLY:HA3	2.04	0.57
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:1050:TYR:C	1:A:1050:TYR:CD2	2.83	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:908:ASN:ND2	1:A:994:VAL:HA	2.10	0.56
1:A:851:MET:HE1	1:A:938:ALA:CB	2.26	0.56
1:A:241:PRO:HG3	1:A:287:ILE:HG22	1.88	0.56
1:A:210:TYR:HA	1:A:213:LYS:NZ	2.21	0.56
1:A:1043:THR:O	1:A:1045:LYS:N	2.34	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: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:878:MET:C	1:A:879:ILE:HG13	2.29	0.55
1:A:547:MET:HE2	1:A:552:ARG:HA	1.88	0.55
1:A:245:LEU:C	1:A:247:SER:H	2.14	0.55
1:A:1003:SER:O	1:A:1007:GLN:HG3	2.06	0.55
1:A:368:ILE:O	1:A:369:ASP:HB3	2.05	0.55
1:A:1010:GLN:NE2	1:A:1069:LEU:HD22	2.22	0.55
1:A:307:LEU:C	1:A:307:LEU:HD23	2.32	0.54
1:A:955:THR:C	1:A:957:THR:N	2.65	0.54
1:A:165:VAL:HG12	1:A:165:VAL:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1082:VAL:HA	1:A:1085:ASN:HB2	1.90	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:848:LEU:HD12	1:A:851:MET:HE2	1.89	0.53
1:A:863:CYS:SG	1:A:927:ARG:NH1	2.81	0.53
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	1.91	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
1:A:1088:LEU:C	1:A:1090:LEU:N	2.64	0.53
1:A:784:ARG:NH1	1:A:789:PRO:O	2.41	0.53
1:A:811:LEU:N	1:A:811:LEU:HD12	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
2:A:1201:19P:H18	2:A:1201:19P:H6	1.91	0.53
1:A:546:GLU:HA	1:A:546:GLU:OE2	2.09	0.52
1:A:184:ARG:HH21	1:A:321:GLU:CD	2.17	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:1043:THR:C	1:A:1045:LYS:H	2.15	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: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:568:THR:HG22	1:A:571:ASP:CG	2.34	0.51
1:A:370:ILE:HD12	1:A:372:VAL:N	2.26	0.51
1:A:1055:LEU:O	1:A:1056:THR:HG22	2.11	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:199:HIS:O	1:A:200:PRO:C	2.53	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:968:ILE:C	1:A:970:GLY:N	2.70	0.50
1:A:201:TRP:CE2	1:A:291:GLN:HG3	2.46	0.50
1:A:1002:THR:CG2	1:A:1003:SER:N	2.75	0.50
1:A:280:TYR:C	1:A:281:LEU:HD12	2.36	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:731:ASP:OD2	1:A:784:ARG:NE	2.42	0.49
1:A:947:ARG:HH11	1:A:968:ILE:HG23	1.77	0.49
1:A:192:ASP:C	1:A:192:ASP:OD1	2.56	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:214:LYS:HD3	1:A:297:LEU:O	2.11	0.49
1:A:315:LEU:O	1:A:727:ALA:HB2	2.12	0.49
1:A:662:GLN:OE1	1:A:1030:LEU:HD22	2.12	0.49
1:A:734:GLN:O	1:A:738:VAL:HG23	2.12	0.49
1:A:171:ASP:OD1	1:A:472:ARG:NH2	2.45	0.49
1:A:461:LEU:HB3	1:A:462:TYR:CD2	2.47	0.49
1:A:1002:THR:CG2	1:A:1003:SER:H	2.26	0.49
1:A:916:PRO:HG2	1:A:920:LYS:HD3	1.94	0.49
1:A:985:PHE:HZ	1:A:1072:ILE:HG12	1.77	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:861:ASP:OD1	1:A:861:ASP:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:287:ILE:HA	1:A:290:PHE:HD1	1.78	0.48
1:A:998:SER:O	1:A:999:GLY:C	2.54	0.48
1:A:1043:THR:HG22	1:A:1044:SER:N	2.29	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:370:ILE:C	1:A:372:VAL:H	2.21	0.48
1:A:778:GLN:CD	1:A:778:GLN:N	2.72	0.48
1:A:845:LEU:O	1:A:848:LEU:HB2	2.14	0.48
1:A:230:SER:O	1:A:231:GLN:HB3	2.13	0.48
1:A:1035:LEU:HD22	1:A:1039:MET:HG3	1.95	0.48
1:A:601:GLN:HG3	1:A:602:GLU:N	2.28	0.48
1:A:209:GLU:O	1:A:213:LYS:HG2	2.15	0.47
1:A:214:LYS:HZ1	1:A:300:GLY:HA2	1.78	0.47
1:A:707:ARG:HA	1:A:710:GLN:OE1	2.14	0.47
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.97	0.47
1:A:204:SER:HB2	1:A:652:GLU:OE2	2.15	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:1061:GLU:O	1:A:1064:ALA:HB3	2.14	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:804:MET:HE2	1:A:812:TRP:CB	2.19	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:1010:GLN:O	1:A:1014:VAL:HG23	2.14	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: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:1009:PHE:HE2	1:A:1072:ILE:HD13	1.80	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:ASP:OD1	1:A:679:ARG:NE	2.44	0.46
1:A:997:THR:HG21	1:A:1076:ARG:HH22	1.81	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:1008:LYS:O	1:A:1009:PHE:C	2.58	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:373:LEU:C	1:A:373:LEU:HD23	2.41	0.46
1:A:472:ARG:O	1:A:473:PHE:HB2	2.16	0.46
1:A:1083:GLN:NE2	1:A:1083:GLN:HA	2.29	0.46
1:A:144:SER:HB3	1:A:147:SER:OG	2.16	0.46
1:A:470:ASP:OD1	1:A:470:ASP:C	2.59	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:987:LEU:CD1	1:A:995:MET:HE1	2.40	0.45
1:A:163:THR:O	1:A:165:VAL:HG23	2.16	0.45
1:A:245:LEU:C	1:A:247:SER:N	2.74	0.45
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:180:LEU:C	1:A:183:PRO:HD2	2.41	0.45
1:A:198:MET:HE1	1:A:282:VAL:HG11	1.97	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:197:ALA:HA	1:A:689:LYS:HZ2	1.81	0.45
1:A:217:ASN:O	1:A:218:ASN:C	2.60	0.45
1:A:467:LEU:HD13	1:A:672:TYR:CE2	2.51	0.45
1:A:501:LYS:HB3	1:A:501:LYS:HE2	1.74	0.45
1:A:788:ASP:OD1	1:A:788:ASP:C	2.60	0.45
1:A:674:ASP:CG	1:A:679:ARG:HE	2.24	0.45
1:A:857:THR:OG1	1:A:858:GLU:HG3	2.16	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:1027:LEU:HD23	1:A:1027:LEU:HA	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:LYS:O	1:A:1080:TRP:N	2.49	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:408:VAL:C	1:A:409:LEU:HD23	2.43	0.44
1:A:685:GLY:O	1:A:720:TYR:CE1	2.68	0.44
1:A:170:ASP:OD1	1:A:471:HIS:HE1	2.00	0.44
2:A:1201:19P:H25	2:A:1201:19P:C23	2.47	0.44
1:A:1056:THR:O	1:A:1056:THR:CG2	2.61	0.44
1:A:370:ILE:HD13	1:A:370:ILE:C	2.43	0.44
1:A:379:LEU:N	1:A:379:LEU:HD22	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: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:1060:ASN:HD21	1:A:1063:ASP:CG	2.26	0.44
1:A:949:ASN:N	1:A:1083:GLN:HE22	2.15	0.44
1:A:1043:THR:O	1:A:1047:ASP:HB2	2.18	0.44
1:A:381:VAL:HG13	1:A:381:VAL:O	2.18	0.44
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.53	0.44
1:A:640:VAL:O	1:A:641:ARG:C	2.59	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: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:897:GLY:O	1:A:898:ASN:C	2.61	0.43
1:A:964:ASP:OD2	2:A:1201:19P:O32	2.22	0.43
1:A:177:ARG:HE	1:A:177:ARG:HB3	1.53	0.43
1:A:833:LYS:NZ	2:A:1201:19P:O30	2.44	0.43
1:A:862:LEU:N	1:A:862:LEU:HD22	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:848:LEU:HD12	1:A:851:MET:CE	2.48	0.43
1:A:395:CYS:SG	1:A:396:GLN:N	2.92	0.43
1:A:217:ASN:C	1:A:219:CYS:N	2.77	0.42
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:568:THR:CG2	1:A:571:ASP:CG	2.92	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:307:LEU:HD23	1:A:307:LEU:O	2.19	0.42
1:A:489:GLY:HA3	1:A:1041:GLN:NE2	2.34	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:167:ASN:CG	1:A:508:PRO:HA	2.44	0.42
1:A:957:THR:O	1:A:957:THR:OG1	2.37	0.42
1:A:224:ILE:C	1:A:225:HIS:ND1	2.78	0.42
1:A:366:ARG:HB2	1:A:517:SER:HB2	2.01	0.42
1:A:370:ILE:HG23	1:A:372:VAL:H	1.84	0.42
1:A:390:GLY:C	1:A:392:GLN:H	2.27	0.42
1:A:514:MET:HG3	1:A:515:SER:N	2.34	0.42
1:A:915:SER:HA	1:A:916:PRO:HD3	1.84	0.42
1:A:252:MET:SD	1:A:252:MET:C	3.03	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
1:A:497:PHE:HA	1:A:1043:THR:HG21	2.02	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:1069:LEU:O	1:A:1072:ILE:HB	2.19	0.41
1:A:1035:LEU:HA	1:A:1039:MET:HG2	2.02	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: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:833:LYS:HG3	1:A:834:HIS:N	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:LYS:O	1:A:1001:LYS:HB2	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:688:ASN:OD1	1:A:688:ASN:C	2.64	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:1067:TYR:O	1:A:1071:GLN:HG2	2.20	0.41
1:A:998:SER:O	1:A:1000:LYS:N	2.53	0.41
1:A:181:VAL:CG1	1:A:185:MET:HE2	2.43	0.41
1:A:207:LEU:HD13	1:A:208:PRO:HD2	2.02	0.41
1:A:386:ASN:ND2	1:A:386:ASN:N	2.68	0.41
1:A:610:LEU:HD23	1:A:610:LEU:HA	1.86	0.41
1:A:1035:LEU:HA	1:A:1039:MET:CG	2.51	0.41
1:A:244:ILE:O	1:A:244:ILE:HG22	2.21	0.41
1:A:364:LYS:HE2	1:A:411:ASN:HA	2.03	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:799:GLU:H	1:A:799:GLU:HG3	1.31	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:701:SER:OG	1:A:871:SER:HB3	2.21	0.41
1:A:762:GLN:C	1:A:766:GLN:HE22	2.29	0.41
2:A:1201:19P:H25	2:A:1201:19P:H13	2.02	0.41
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:1034:MET:SD	1:A:1039:MET:HE3	2.61	0.40
1:A:1035:LEU:CD2	1:A:1039:MET:HG3	2.50	0.40
1:A:1081:THR:O	1:A:1085:ASN:HB2	2.21	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:199:HIS:O	1:A:199:HIS:CG	2.71	0.40
1:A:734:GLN:HE21	1:A:780:PRO:CB	2.35	0.40
1:A:806:SER:O	1:A:807:LYS:C	2.63	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%)	6 5

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
1	A	227	SER
1	A	956	GLU
1	A	984	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	743/864 (86%)	678 (91%)	65 (9%)	9 10

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	172	GLU
1	A	207	LEU
1	A	213	LYS
1	A	214	LYS
1	A	218	ASN
1	A	246	GLN
1	A	252	MET
1	A	287	ILE
1	A	298	LYS
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	387	ILE
1	A	464	VAL
1	A	472	ARG
1	A	498	ASN
1	A	516	ILE
1	A	546	GLU
1	A	549	ASN
1	A	575	LEU
1	A	601	GLN
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	729	LEU
1	A	740	GLU
1	A	760	SER
1	A	766	GLN
1	A	767	LEU
1	A	792	LYS
1	A	799	GLU
1	A	807	LYS

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Mol	Chain	Res	Type
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	865	LEU
1	A	875	LYS
1	A	886	THR
1	A	890	LYS
1	A	918	GLU
1	A	948	HIS
1	A	964	ASP
1	A	968	ILE
1	A	985	PHE
1	A	1026	LEU
1	A	1059	LYS
1	A	1060	ASN
1	A	1078	LYS
1	A	1082	VAL
1	A	1085	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	291	GLN
1	A	304	HIS
1	A	389	HIS
1	A	392	GLN
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	601	GLN
1	A	639	ASN
1	A	646	GLN
1	A	658	HIS

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Mol	Chain	Res	Type
1	A	734	GLN
1	A	737	GLN
1	A	766	GLN
1	A	769	GLN
1	A	773	ASN
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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	19P	A	1201	-	36,37,37	0.84	2 (5%)	47,55,55	1.84	11 (23%)

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	-	-	0/16/26/26	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	19P	C19-N20	-2.22	1.35	1.38
2	A	1201	19P	C19-N18	-2.22	1.35	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	19P	C8-N7-C4	4.29	121.93	116.96
2	A	1201	19P	C1-N6-C5	4.11	121.34	118.28
2	A	1201	19P	C5-C10-N20	3.82	134.39	129.58
2	A	1201	19P	C26-C21-N20	3.71	121.49	112.27
2	A	1201	19P	C12-N13-C14	3.67	121.86	117.53
2	A	1201	19P	C9-N18-C19	-3.62	108.23	110.10
2	A	1201	19P	N20-C19-N18	3.03	109.45	106.92
2	A	1201	19P	C25-N24-C23	2.97	118.75	112.68
2	A	1201	19P	C28-N18-C19	2.61	125.88	123.59
2	A	1201	19P	C11-C12-N13	-2.31	120.60	124.28
2	A	1201	19P	C15-C16-C11	-2.20	118.29	121.12

There are no chirality outliers.

There are no torsion outliers.

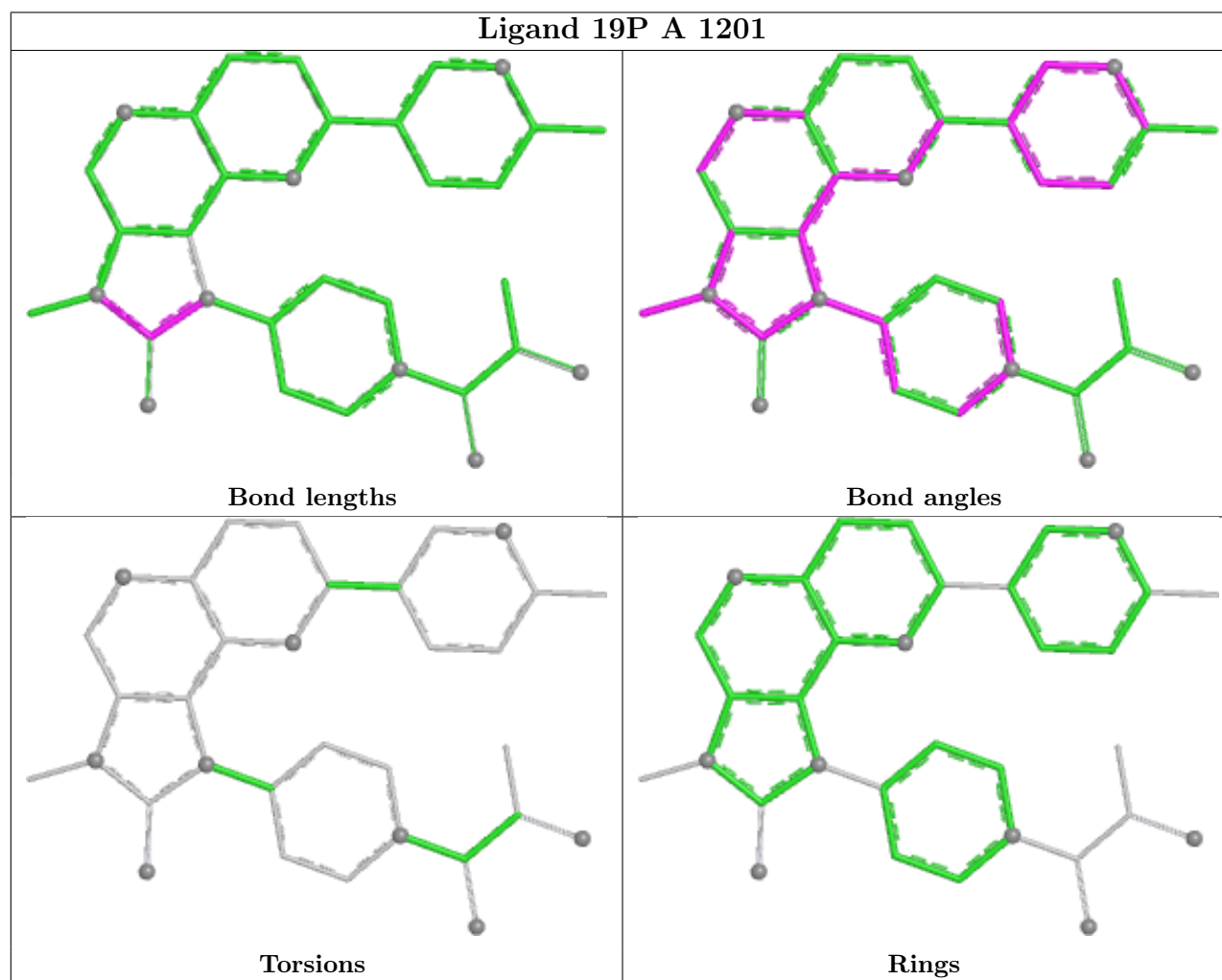
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	19P	6	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	830/966 (85%)	1.27	180 (21%) 2 2	21, 60, 97, 126	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	528	ALA	9.4
1	A	526	PRO	6.5
1	A	245	LEU	6.5
1	A	969	LEU	6.2
1	A	1090	LEU	5.9
1	A	248	PHE	5.6
1	A	527	ILE	5.4
1	A	983	VAL	4.8
1	A	779	LEU	4.7
1	A	220	ILE	4.5
1	A	1089	HIS	4.5
1	A	970	GLY	4.3
1	A	525	HIS	4.3
1	A	1042	LEU	4.3
1	A	151	GLN	4.3
1	A	811	LEU	4.2
1	A	357	CYS	4.1
1	A	253	ALA	3.9
1	A	249	PHE	3.8
1	A	726	THR	3.8
1	A	202	VAL	3.8
1	A	481	VAL	3.8
1	A	1082	VAL	3.8
1	A	771	LEU	3.7
1	A	967	HIS	3.7
1	A	760	SER	3.6
1	A	741	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	207	LEU	3.5
1	A	917	THR	3.4
1	A	366	ARG	3.4
1	A	909	HIS	3.3
1	A	764	ILE	3.3
1	A	318	VAL	3.3
1	A	373	LEU	3.3
1	A	989	PRO	3.3
1	A	972	TYR	3.3
1	A	1044	SER	3.3
1	A	364	LYS	3.2
1	A	296	CYS	3.2
1	A	285	THR	3.2
1	A	380	THR	3.2
1	A	405	THR	3.1
1	A	229	THR	3.1
1	A	244	ILE	3.1
1	A	968	ILE	3.1
1	A	1048	ILE	3.1
1	A	1064	ALA	3.1
1	A	250	THR	3.0
1	A	198	MET	3.0
1	A	497	PHE	3.0
1	A	519	LEU	3.0
1	A	413	TRP	3.0
1	A	522	ASN	3.0
1	A	379	LEU	3.0
1	A	408	VAL	2.9
1	A	489	GLY	2.9
1	A	545	ALA	2.9
1	A	233	ILE	2.9
1	A	761	SER	2.9
1	A	1088	LEU	2.9
1	A	763	VAL	2.9
1	A	232	THR	2.9
1	A	988	THR	2.9
1	A	654	ASP	2.9
1	A	382	PHE	2.8
1	A	271	VAL	2.8
1	A	906	VAL	2.8
1	A	474	LEU	2.8
1	A	860	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	910	TRP	2.8
1	A	409	LEU	2.8
1	A	775	GLN	2.7
1	A	243	ALA	2.7
1	A	168	VAL	2.7
1	A	896	VAL	2.7
1	A	1014	VAL	2.7
1	A	546	GLU	2.7
1	A	991	PHE	2.7
1	A	1007	GLN	2.7
1	A	223	VAL	2.7
1	A	235	VAL	2.7
1	A	770	LYS	2.7
1	A	971	ASN	2.7
1	A	994	VAL	2.7
1	A	1070	ASP	2.7
1	A	212	TRP	2.7
1	A	862	LEU	2.7
1	A	186	ALA	2.6
1	A	144	SER	2.6
1	A	1087	PHE	2.6
1	A	147	SER	2.6
1	A	272	LEU	2.6
1	A	544	ARG	2.5
1	A	416	PHE	2.5
1	A	798	ILE	2.5
1	A	1062	GLU	2.5
1	A	228	THR	2.5
1	A	948	HIS	2.5
1	A	832	PHE	2.5
1	A	460	LEU	2.5
1	A	252	MET	2.5
1	A	288	LYS	2.5
1	A	421	LYS	2.5
1	A	208	PRO	2.5
1	A	162	VAL	2.4
1	A	469	ILE	2.4
1	A	307	LEU	2.4
1	A	911	LEU	2.4
1	A	1079	GLY	2.4
1	A	517	SER	2.4
1	A	367	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	727	ALA	2.4
1	A	303	ILE	2.4
1	A	903	LYS	2.4
1	A	412	VAL	2.4
1	A	300	GLY	2.4
1	A	612	ALA	2.4
1	A	165	VAL	2.4
1	A	275	CYS	2.4
1	A	902	PHE	2.4
1	A	304	HIS	2.4
1	A	280	TYR	2.3
1	A	1043	THR	2.3
1	A	152	ARG	2.3
1	A	216	ALA	2.3
1	A	418	ILE	2.3
1	A	381	VAL	2.3
1	A	404	PHE	2.3
1	A	550	GLN	2.3
1	A	929	VAL	2.3
1	A	241	PRO	2.3
1	A	311	PRO	2.3
1	A	210	TYR	2.3
1	A	224	ILE	2.3
1	A	780	PRO	2.3
1	A	568	THR	2.3
1	A	293	VAL	2.3
1	A	520	LEU	2.2
1	A	987	LEU	2.2
1	A	154	LEU	2.2
1	A	181	VAL	2.2
1	A	394	LEU	2.2
1	A	774	LEU	2.2
1	A	308	ASP	2.2
1	A	146	GLU	2.2
1	A	762	GLN	2.2
1	A	155	THR	2.2
1	A	805	ALA	2.2
1	A	462	TYR	2.2
1	A	365	ILE	2.2
1	A	487	ILE	2.2
1	A	313	PRO	2.2
1	A	1002	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	269	ASP	2.2
1	A	306	VAL	2.2
1	A	363	VAL	2.2
1	A	393	VAL	2.2
1	A	163	THR	2.2
1	A	398	ARG	2.1
1	A	237	PRO	2.1
1	A	924	ALA	2.1
1	A	912	LYS	2.1
1	A	150	PHE	2.1
1	A	396	GLN	2.1
1	A	213	LYS	2.1
1	A	804	MET	2.1
1	A	370	ILE	2.1
1	A	270	PHE	2.1
1	A	240	THR	2.1
1	A	768	LYS	2.1
1	A	800	LYS	2.1
1	A	904	ASP	2.1
1	A	949	ASN	2.1
1	A	283	GLY	2.1
1	A	145	GLU	2.0
1	A	795	ALA	2.0
1	A	498	ASN	2.0
1	A	305	VAL	2.0
1	A	484	MET	2.0
1	A	287	ILE	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.

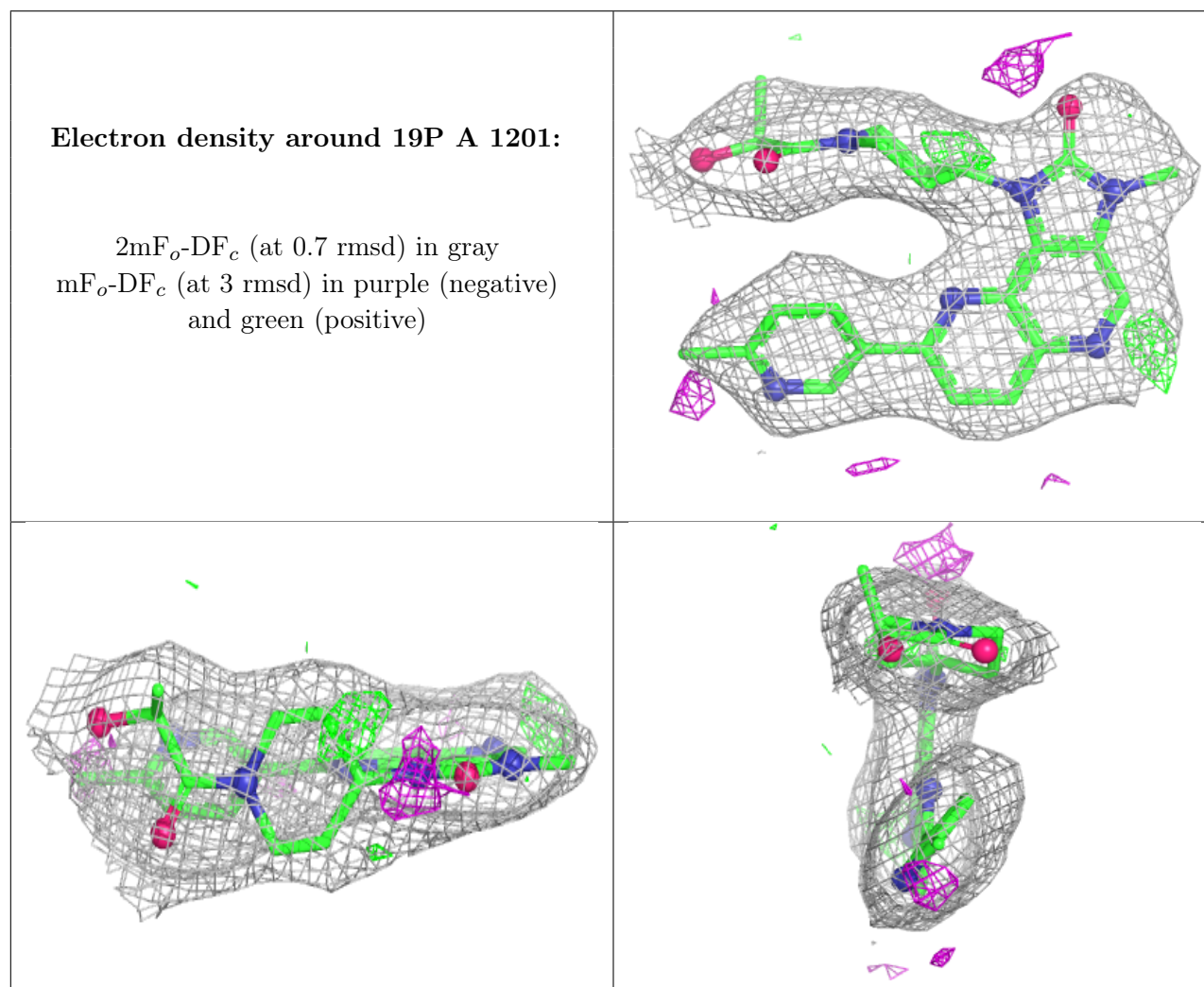
6.4 Ligands [i](#)

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	19P	A	1201	33/33	0.87	0.13	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.