



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2014 – 01:45 PM EDT

PDB ID : 4HVB
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

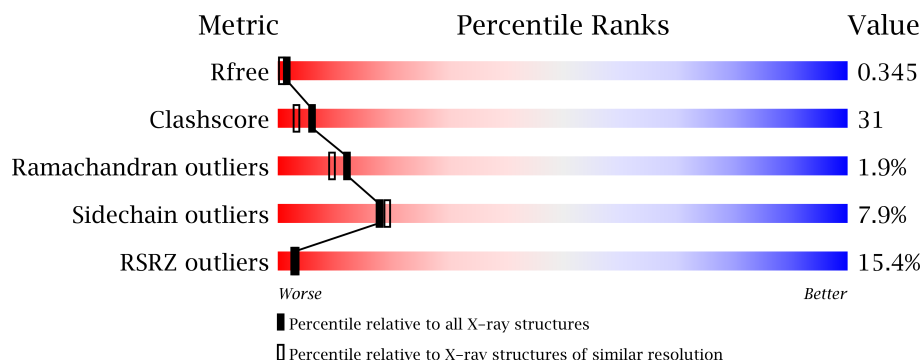
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

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}	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	966	

2 Entry composition i

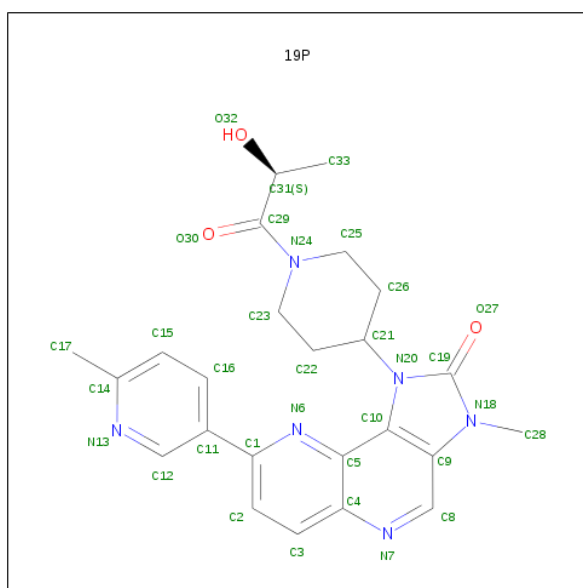
There are 3 unique types of molecules in this entry. The entry contains 6751 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

- 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		

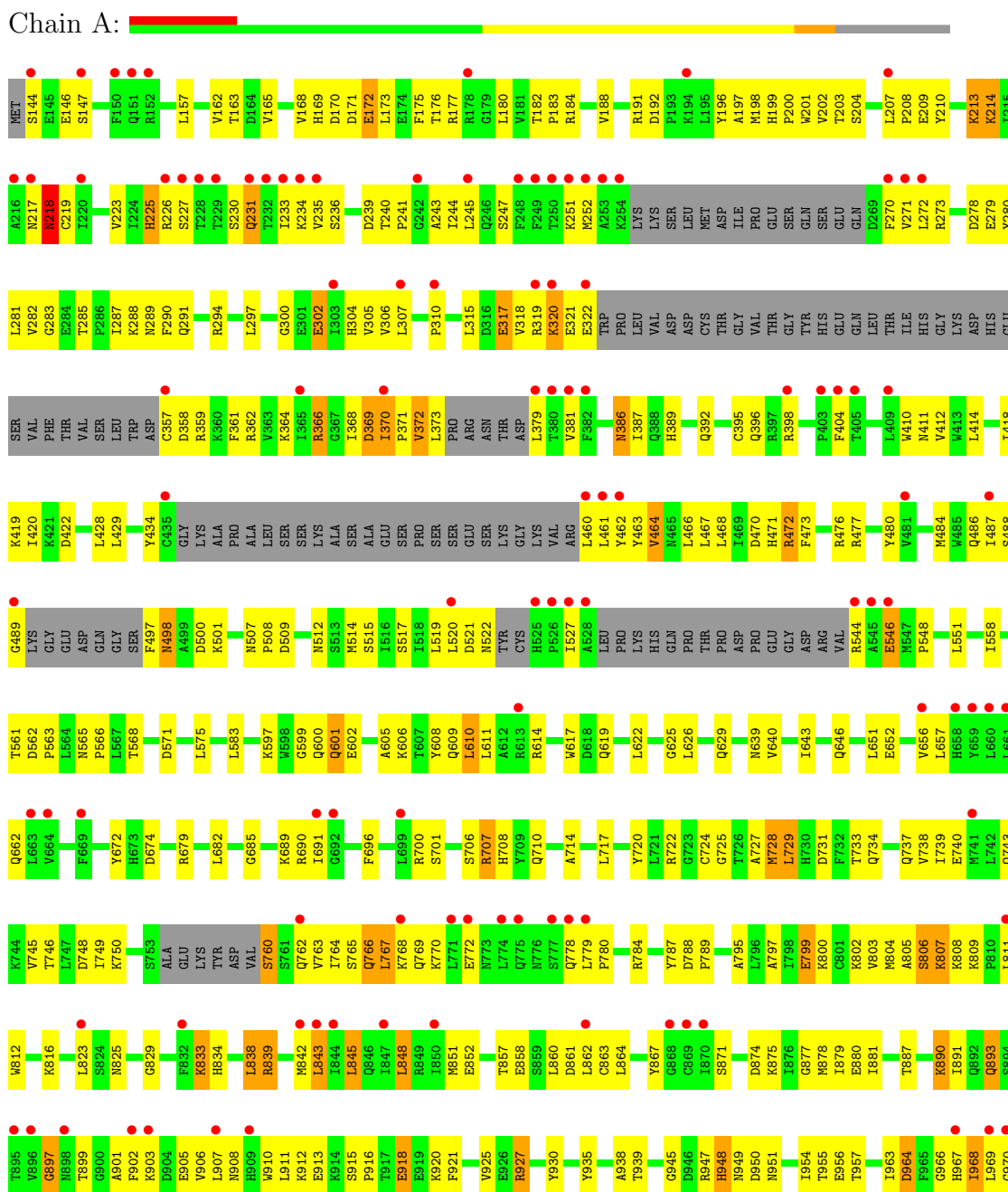
- Molecule 3 is water.

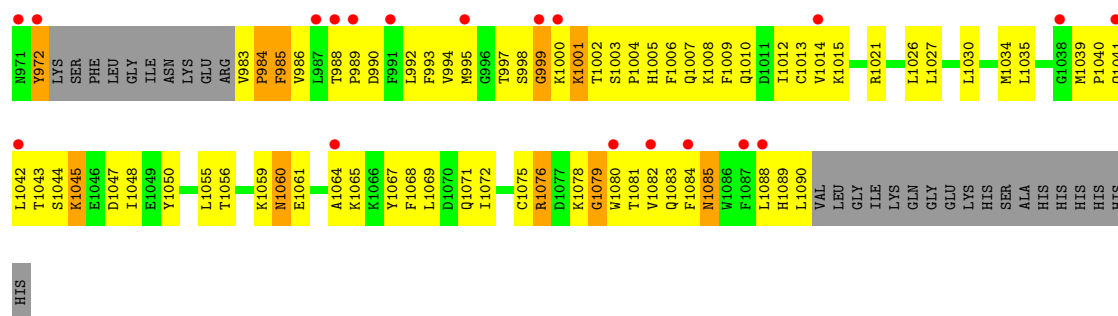
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		

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 errors 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	144.80Å 67.58Å 106.90Å 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) 94.7 (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 2.34Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.270 , 0.333 0.277 , 0.345	Depositor DCC
R_{free} test set	1246 reflections (3.11%)	DCC
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 , 41.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 43131 reflections	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.

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	0.38	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

All (420) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:807:LYS:HE3	1:A:807:LYS:H	1.17	1.09

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Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:1002:THR:HG22	1:A:1003:SER:N	2.06	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:203:THR:HG22	1:A:289:ASN:O	2.06	0.55
1:A:197:ALA:HA	1:A:689:LYS:HZ1	1.69	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:860:LEU:HD21	1:A:1015:LYS:HD2	1.93	0.50
1:A:477:ARG:NH1	1:A:521:ASP:OD1	2.45	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
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:662:GLN:OE1	1:A:1030:LEU:HD22	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:197:ALA:HA	1:A:689:LYS:HZ2	1.77	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: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: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:287:ILE:HA	1:A:290:PHE:HD1	1.78	0.48
1:A:214:LYS:HZ1	1:A:300:GLY:HA2	1.77	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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:467:LEU:HD13	1:A:672:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:501:LYS:HE2	1:A:501:LYS:HB3	1.74	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:983:VAL:HB	1:A:1082:VAL:HG21	1.99	0.44
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: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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:989:PRO:HD3	1:A:1079:GLY:O	2.19	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: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: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: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: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: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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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	810/966 (84%)	719 (89%)	76 (9%)	15 (2%)	12 9

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 ⓘ

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%)	18 19

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	A	1022	HIS
1	A	1041	GLN
1	A	1083	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	-	37,37,37	0.68	0	53,55,55	1.32	7 (13%)

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	19P	C12-N13-C14	3.38	121.86	117.44
2	A	1201	19P	C25-N24-C23	3.26	118.75	112.57
2	A	1201	19P	C8-N7-C4	2.69	121.93	117.87
2	A	1201	19P	C26-C21-N20	2.42	121.49	112.53
2	A	1201	19P	C9-C10-C5	-2.40	118.42	120.93
2	A	1201	19P	C11-C12-N13	-2.21	120.60	124.34
2	A	1201	19P	C2-C3-C4	-2.09	118.53	120.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

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%)	1.01	128 (15%) 3 3	21, 60, 97, 126	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	LEU	9.1
1	A	528	ALA	7.9
1	A	245	LEU	7.1
1	A	779	LEU	7.1
1	A	216	ALA	6.0
1	A	404	PHE	5.4
1	A	526	PRO	5.3
1	A	253	ALA	5.2
1	A	248	PHE	5.2
1	A	972	TYR	5.1
1	A	249	PHE	4.8
1	A	228	THR	4.5
1	A	270	PHE	4.4
1	A	234	LYS	4.3
1	A	250	THR	4.3
1	A	220	ILE	4.3
1	A	987	LEU	4.2
1	A	545	ALA	4.1
1	A	971	ASN	4.1
1	A	319	ARG	4.1
1	A	235	VAL	4.0
1	A	233	ILE	4.0
1	A	481	VAL	4.0
1	A	147	SER	3.9
1	A	380	THR	3.9
1	A	902	PHE	3.9
1	A	229	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	774	LEU	3.8
1	A	995	MET	3.8
1	A	307	LEU	3.8
1	A	381	VAL	3.8
1	A	398	ARG	3.7
1	A	967	HIS	3.6
1	A	207	LEU	3.6
1	A	272	LEU	3.6
1	A	489	GLY	3.6
1	A	969	LEU	3.6
1	A	409	LEU	3.6
1	A	231	GLN	3.5
1	A	252	MET	3.5
1	A	1082	VAL	3.5
1	A	999	GLY	3.5
1	A	991	PHE	3.4
1	A	144	SER	3.4
1	A	777	SER	3.4
1	A	771	LEU	3.4
1	A	525	HIS	3.3
1	A	382	PHE	3.3
1	A	226	ARG	3.3
1	A	227	SER	3.2
1	A	896	VAL	3.2
1	A	1041	GLN	3.2
1	A	691	ILE	3.2
1	A	811	LEU	3.1
1	A	254	LYS	3.1
1	A	907	LEU	3.1
1	A	242	GLY	3.1
1	A	178	ARG	3.1
1	A	895	THR	3.1
1	A	661	LEU	3.0
1	A	405	THR	2.9
1	A	151	GLN	2.9
1	A	869	CYS	2.9
1	A	322	GLU	2.9
1	A	357	CYS	2.9
1	A	435	CYS	2.9
1	A	850	ILE	2.8
1	A	989	PRO	2.8
1	A	194	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	303	ILE	2.8
1	A	232	THR	2.8
1	A	370	ILE	2.7
1	A	656	VAL	2.7
1	A	271	VAL	2.7
1	A	1000	LYS	2.6
1	A	898	ASN	2.6
1	A	460	LEU	2.6
1	A	775	GLN	2.6
1	A	843	LEU	2.6
1	A	544	ARG	2.6
1	A	741	MET	2.5
1	A	842	MET	2.5
1	A	251	LYS	2.5
1	A	970	GLY	2.5
1	A	664	VAL	2.5
1	A	847	ILE	2.5
1	A	462	TYR	2.5
1	A	1042	LEU	2.5
1	A	659	TYR	2.4
1	A	320	LYS	2.4
1	A	546	GLU	2.4
1	A	1087	PHE	2.4
1	A	909	HIS	2.4
1	A	870	ILE	2.4
1	A	403	PRO	2.4
1	A	1064	ALA	2.4
1	A	217	ASN	2.4
1	A	868	GLY	2.3
1	A	699	LEU	2.3
1	A	832	PHE	2.3
1	A	862	LEU	2.3
1	A	365	ILE	2.3
1	A	762	GLN	2.3
1	A	1038	GLY	2.3
1	A	768	LYS	2.3
1	A	772	GLU	2.2
1	A	778	GLN	2.2
1	A	669	PHE	2.2
1	A	663	LEU	2.2
1	A	310	PRO	2.2
1	A	692	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	520	LEU	2.2
1	A	658	HIS	2.2
1	A	527	ILE	2.2
1	A	150	PHE	2.2
1	A	487	ILE	2.1
1	A	461	LEU	2.1
1	A	823	LEU	2.1
1	A	1084	PHE	2.1
1	A	1080	TRP	2.1
1	A	152	ARG	2.1
1	A	1014	VAL	2.1
1	A	1088	LEU	2.1
1	A	988	THR	2.1
1	A	660	LEU	2.1
1	A	613	ARG	2.1
1	A	844	ILE	2.0
1	A	903	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	19P	A	1201	33/33	0.19	0.16	33,46,55,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.