



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:44 pm BST

PDB ID : 4OVV
Title : Crystal Structure of PI3Kalpha in complex with diC4-PIP2
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Deposited on : 2014-01-14
Resolution : 3.50 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

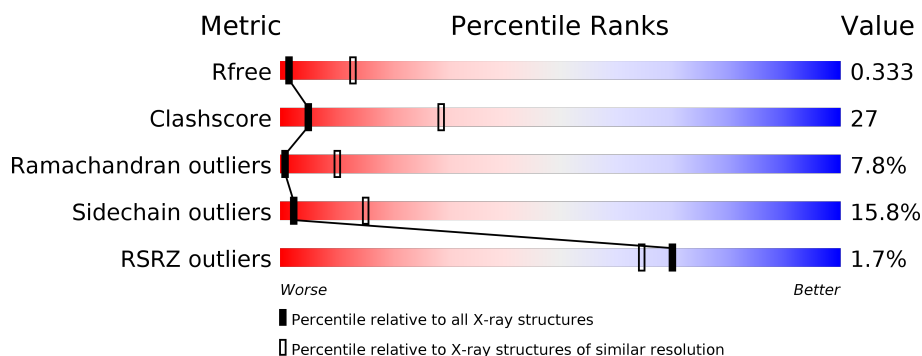
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	1096	<div> <div></div> <div>44%</div> <div>39%</div> <div>11%</div> <div>5%</div> </div>
2	B	279	<div> <div>5%</div> <div>35%</div> <div>39%</div> <div>11%</div> <div>14%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PBU	A	1101	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10671 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 sub-unit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1042	Total	C	N	O	S	0	0	0
			8525	5451	1457	1548	69			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	expression tag	UNP P42336
A	-27	SER	-	expression tag	UNP P42336
A	-26	TYR	-	expression tag	UNP P42336
A	-25	TYR	-	expression tag	UNP P42336
A	-24	HIS	-	expression tag	UNP P42336
A	-23	HIS	-	expression tag	UNP P42336
A	-22	HIS	-	expression tag	UNP P42336
A	-21	HIS	-	expression tag	UNP P42336
A	-20	HIS	-	expression tag	UNP P42336
A	-19	HIS	-	expression tag	UNP P42336
A	-18	ASP	-	expression tag	UNP P42336
A	-17	TYR	-	expression tag	UNP P42336
A	-16	ASP	-	expression tag	UNP P42336
A	-15	ILE	-	expression tag	UNP P42336
A	-14	PRO	-	expression tag	UNP P42336
A	-13	THR	-	expression tag	UNP P42336
A	-12	THR	-	expression tag	UNP P42336
A	-10	GLU	-	expression tag	UNP P42336
A	-9	ASN	-	expression tag	UNP P42336
A	-8	LEU	-	expression tag	UNP P42336
A	-7	TYR	-	expression tag	UNP P42336
A	-6	PHE	-	expression tag	UNP P42336
A	-5	GLN	-	expression tag	UNP P42336
A	-4	GLY	-	expression tag	UNP P42336
A	-3	ALA	-	expression tag	UNP P42336
A	-2	MET	-	expression tag	UNP P42336

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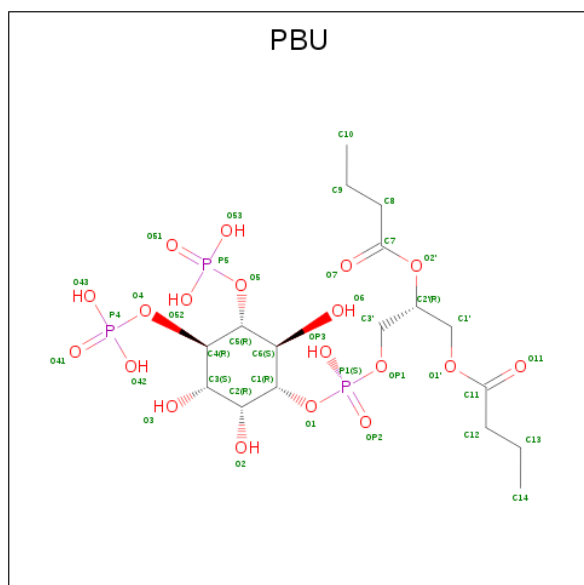
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			2059	1290	363	400	6			

- Molecule 3 is (2R)-3-[[[(R)-HYDROXY{[(1R,2R,3S,4R,5R,6S)-2,3,6-TRIHYDROXY-4,5-BIS(PHOSPHONOOXY)CYCLOHEXYL]OXY}PHOSPHORYL]OXY}PROPANE-1,2-DIYL DIBUTANOATE (three-letter code: PBU) (formula: C₁₇H₃₃O₁₉P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			39	17	19	3		
3	B	1	Total	C	O	P	0	0
			39	17	19	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

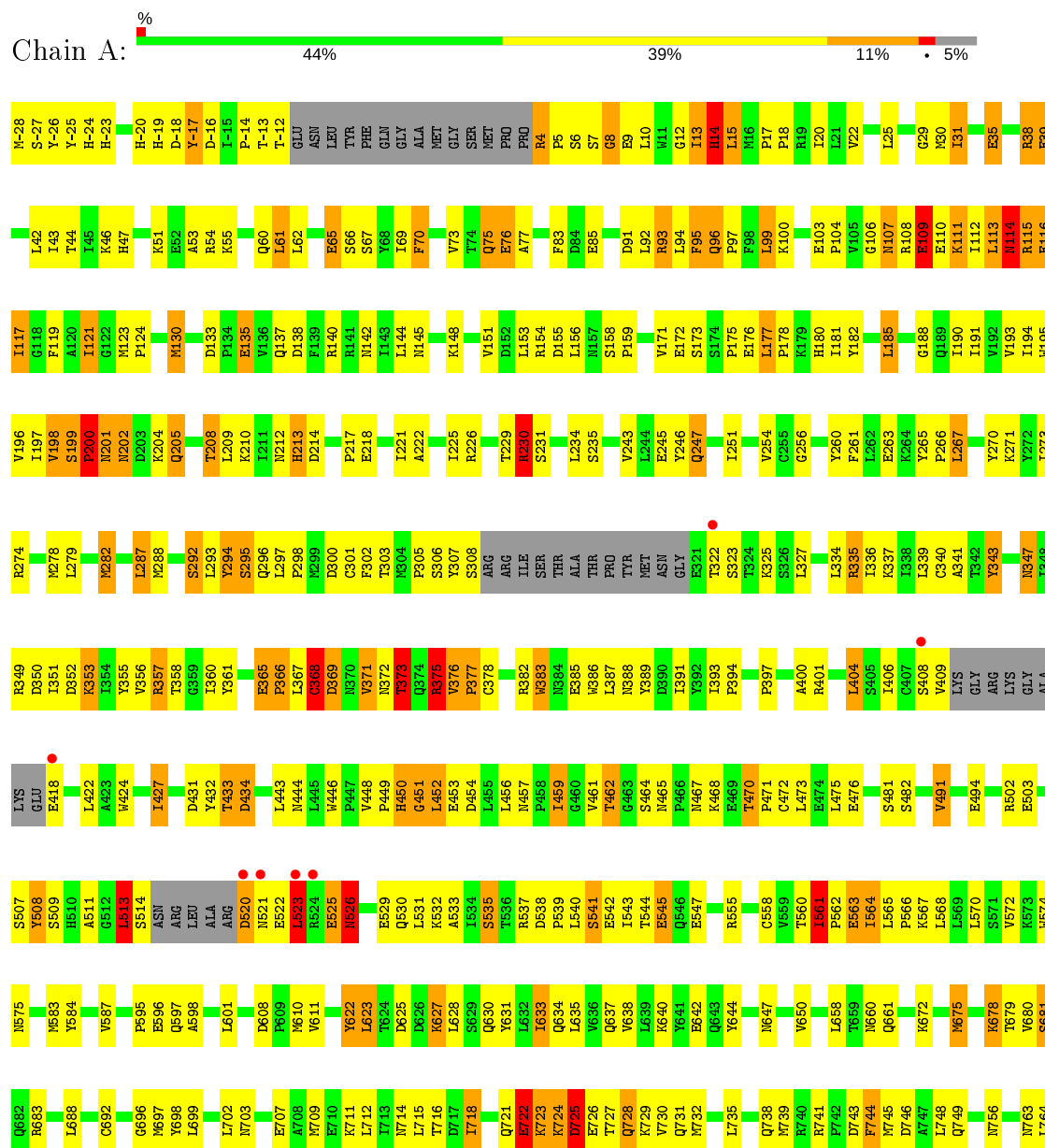
- Molecule 5 is water.

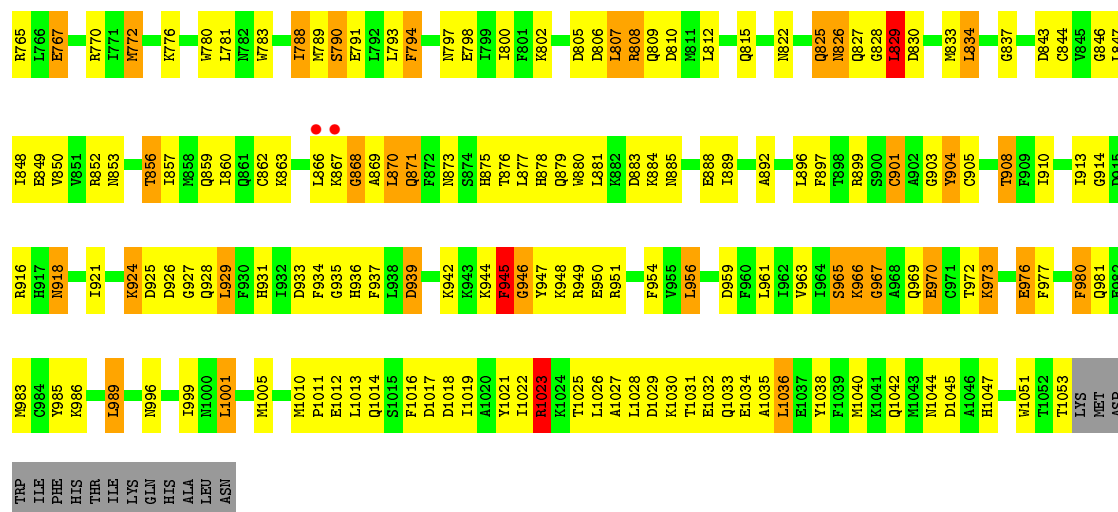
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		

3 Residue-property plots

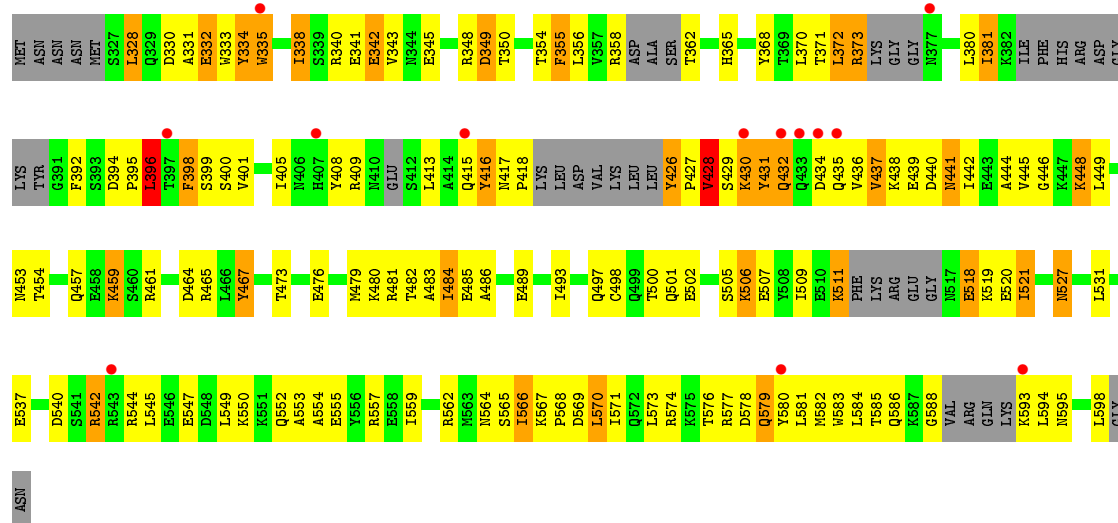
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 alpha isoform





● Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.26Å 116.08Å 148.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.51 – 3.50 39.27 – 3.37	Depositor EDS
% Data completeness (in resolution range)	99.8 (91.51-3.50) 99.7 (39.27-3.37)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.82 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.237 , 0.339 0.230 , 0.333	Depositor DCC
R_{free} test set	1494 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	97.4	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10671	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: PBU, PO4

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	0.85	3/8723 (0.0%)	0.91	12/11792 (0.1%)
2	B	0.68	2/2088 (0.1%)	0.80	2/2792 (0.1%)
All	All	0.82	5/10811 (0.0%)	0.89	14/14584 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	335	TRP	CD2-CE2	5.79	1.48	1.41
2	B	583	TRP	CD2-CE2	5.53	1.48	1.41
1	A	945	PHE	CB-CG	5.40	1.60	1.51
1	A	383	TRP	CD2-CE2	5.05	1.47	1.41
1	A	195	TRP	CD2-CE2	5.02	1.47	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	SER	C-N-CD	-7.12	104.94	120.60
1	A	513	LEU	CA-CB-CG	7.02	131.45	115.30
2	B	396	LEU	CA-CB-CG	5.88	128.82	115.30
1	A	200	PRO	N-CA-C	5.81	127.21	112.10
1	A	199	SER	C-N-CA	5.79	146.34	122.00
1	A	279	LEU	CA-CB-CG	5.71	128.42	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	LEU	CA-CB-CG	5.71	128.42	115.30
1	A	918	ASN	N-CA-C	5.59	126.10	111.00
1	A	623	LEU	CA-CB-CG	5.28	127.43	115.30
2	B	573	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	133	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	A	523	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	1023	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	502	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	LEU	Peptide
1	A	201	ASN	Peptide
1	A	375	ARG	Peptide
1	A	377	PRO	Peptide

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	8525	0	8494	490	0
2	B	2059	0	2020	114	0
3	A	39	0	28	0	0
3	B	39	0	28	1	0
4	A	5	0	0	0	0
5	A	4	0	0	0	0
All	All	10671	0	10570	578	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 27.

All (578) 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:924:LYS:NZ	1:A:928:GLN:HB3	1.59	1.15
1:A:924:LYS:HB2	1:A:924:LYS:HZ2	1.08	1.14
1:A:13:ILE:O	1:A:14:HIS:HB2	1.45	1.09
2:B:355:PHE:HE1	2:B:427:PRO:HA	1.09	1.09
2:B:355:PHE:CE1	2:B:427:PRO:HA	1.92	1.05
1:A:353:LYS:HG3	1:A:377:PRO:HB3	1.39	1.04
1:A:31:ILE:HG12	2:B:531:LEU:HD13	1.37	1.04
1:A:642:GLU:HG2	1:A:647:ASN:CG	1.78	1.04
1:A:924:LYS:CB	1:A:924:LYS:HZ2	1.72	1.02
2:B:461:ARG:O	2:B:465:ARG:HG3	1.58	1.01
1:A:956:LEU:H	1:A:1047:HIS:HE1	1.03	1.00
1:A:177:LEU:HD12	1:A:178:PRO:HD2	1.43	1.00
1:A:508:TYR:O	1:A:508:TYR:HD1	1.42	0.99
1:A:352:ASP:HB2	1:A:409:VAL:O	1.64	0.97
1:A:910:ILE:HA	1:A:1025:THR:HG21	1.47	0.96
1:A:508:TYR:C	1:A:508:TYR:HD1	1.68	0.96
1:A:30:MET:HG2	2:B:527:ASN:HD21	1.31	0.95
1:A:924:LYS:HZ3	1:A:928:GLN:HB3	1.31	0.95
1:A:30:MET:HG2	2:B:527:ASN:ND2	1.83	0.93
1:A:523:LEU:O	1:A:523:LEU:HD23	1.68	0.92
1:A:243:VAL:O	1:A:247:GLN:HB2	1.70	0.90
2:B:398:PHE:HB2	2:B:399:SER:HA	1.54	0.89
2:B:439:GLU:O	2:B:445:VAL:HG23	1.71	0.89
1:A:772:MET:HA	1:A:772:MET:CE	2.04	0.88
1:A:956:LEU:H	1:A:1047:HIS:CE1	1.91	0.87
1:A:924:LYS:CB	1:A:924:LYS:NZ	2.29	0.87
1:A:508:TYR:C	1:A:508:TYR:CD1	2.45	0.86
2:B:398:PHE:CB	2:B:399:SER:HA	2.06	0.85
1:A:735:LEU:O	1:A:739:MET:HG3	1.78	0.84
1:A:35:GLU:O	1:A:35:GLU:HG3	1.77	0.84
2:B:330:ASP:O	2:B:332:GLU:N	2.10	0.84
1:A:358:THR:HG22	1:A:404:LEU:HB3	1.57	0.83
1:A:965:SER:O	1:A:967:GLY:N	2.10	0.83
2:B:441:ASN:HB3	2:B:444:ALA:H	1.43	0.83
1:A:545:GLU:OE2	1:A:545:GLU:HA	1.80	0.81
1:A:508:TYR:O	1:A:508:TYR:CD1	2.31	0.81
1:A:427:ILE:HG13	1:A:443:LEU:HD22	1.62	0.81
1:A:767:GLU:H	1:A:767:GLU:CD	1.84	0.80
1:A:10:LEU:HD21	1:A:97:PRO:HG3	1.63	0.79
1:A:357:ARG:NH1	1:A:371:VAL:HG13	1.97	0.79
1:A:924:LYS:HB2	1:A:924:LYS:NZ	1.83	0.78
1:A:116:GLU:HG2	1:A:703:ASN:ND2	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ILE:CD1	1:A:209:LEU:HG	2.13	0.78
1:A:355:TYR:HE2	1:A:371:VAL:HG12	1.49	0.78
1:A:724:LYS:O	1:A:725:ASP:HB2	1.83	0.77
1:A:343:TYR:O	1:A:343:TYR:CD1	2.38	0.77
1:A:924:LYS:HZ1	1:A:928:GLN:HB3	1.43	0.77
1:A:408:SER:OG	1:A:422:LEU:HD21	1.83	0.77
1:A:443:LEU:HD12	1:A:444:ASN:H	1.50	0.77
1:A:908:THR:HG21	1:A:954:PHE:HB2	1.64	0.77
1:A:772:MET:HA	1:A:772:MET:HE2	1.66	0.76
1:A:942:LYS:CB	1:A:946:GLY:HA3	2.15	0.76
1:A:825:GLN:O	1:A:827:GLN:N	2.18	0.76
1:A:343:TYR:O	1:A:343:TYR:HD1	1.69	0.76
1:A:13:ILE:O	1:A:14:HIS:CB	2.31	0.76
1:A:985:TYR:CE1	1:A:1040:MET:HG2	2.21	0.75
2:B:333:TRP:CZ2	2:B:405:ILE:HG21	2.22	0.75
1:A:200:PRO:CB	1:A:201:ASN:HA	2.16	0.74
1:A:117:ILE:O	1:A:121:ILE:HG13	1.87	0.74
1:A:397:PRO:HG3	1:A:574:TRP:O	1.86	0.74
1:A:-28:MET:C	1:A:-26:TYR:H	1.90	0.73
1:A:278:MET:HA	1:A:278:MET:CE	2.18	0.73
1:A:357:ARG:HH12	1:A:371:VAL:HG13	1.51	0.73
1:A:116:GLU:HG2	1:A:703:ASN:HD21	1.52	0.73
1:A:335:ARG:HB3	1:A:386:TRP:CE3	2.23	0.73
1:A:822:ASN:O	1:A:826:ASN:HB2	1.88	0.73
2:B:578:ASP:O	2:B:582:MET:HG2	1.88	0.72
1:A:608:ASP:HB3	1:A:611:VAL:HG23	1.70	0.72
2:B:398:PHE:CB	2:B:399:SER:CA	2.67	0.72
1:A:8:GLY:HA3	1:A:14:HIS:O	1.89	0.72
2:B:341:GLU:O	2:B:345:GLU:HG2	1.89	0.72
1:A:544:THR:HG23	1:A:547:GLU:OE2	1.90	0.71
1:A:1023:ARG:NH2	1:A:1029:ASP:OD1	2.24	0.71
1:A:194:ILE:HD11	1:A:209:LEU:HG	1.70	0.71
1:A:193:VAL:HG22	1:A:208:THR:HG22	1.73	0.71
1:A:375:ARG:NH2	1:A:385:GLU:HG3	2.06	0.70
1:A:83:PHE:CD1	1:A:109:GLU:OE1	2.45	0.70
1:A:936:HIS:CD2	1:A:1012:GLU:OE2	2.45	0.70
1:A:198:VAL:H	1:A:201:ASN:ND2	1.90	0.70
1:A:806:ASP:OD1	1:A:808:ARG:HG3	1.91	0.69
1:A:300:ASP:HB2	1:A:696:GLY:CA	2.23	0.69
1:A:1038:TYR:O	1:A:1042:GLN:HG2	1.92	0.69
1:A:300:ASP:HB2	1:A:696:GLY:HA3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:GLU:OE2	1:A:523:LEU:HD22	1.93	0.69
1:A:130:MET:HA	1:A:130:MET:CE	2.24	0.68
1:A:980:PHE:O	1:A:983:MET:N	2.25	0.68
1:A:18:ASP:HB3	1:A:889:ILE:HD11	1.75	0.68
1:A:198:VAL:H	1:A:201:ASN:HD22	1.41	0.67
1:A:522:GLU:OE1	1:A:522:GLU:HA	1.94	0.67
1:A:356:VAL:HB	1:A:372:ASN:HD21	1.59	0.67
1:A:942:LYS:HB3	1:A:946:GLY:HA3	1.74	0.67
1:A:38:ARG:HD3	1:A:39:GLU:OE1	1.96	0.66
1:A:542:GLU:CG	2:B:380:LEU:HD22	2.26	0.66
1:A:910:ILE:HA	1:A:1025:THR:CG2	2.24	0.66
2:B:562:ARG:HG2	2:B:566:ILE:HD12	1.78	0.66
1:A:532:LYS:HE3	1:A:561:ILE:HG12	1.77	0.66
1:A:627:LYS:HG3	1:A:631:TYR:CE2	2.31	0.66
1:A:221:ILE:HG23	1:A:287:LEU:HD21	1.78	0.65
1:A:341:ALA:HB2	1:A:473:LEU:HD12	1.79	0.65
1:A:972:THR:HG22	1:A:973:LYS:HD3	1.79	0.65
2:B:398:PHE:HB3	2:B:399:SER:C	2.17	0.65
1:A:945:PHE:H	2:B:577:ARG:HH12	1.45	0.64
1:A:177:LEU:HD12	1:A:178:PRO:CD	2.23	0.64
1:A:159:PRO:HG2	1:A:294:TYR:CD2	2.32	0.64
2:B:562:ARG:HA	2:B:565:SER:HB2	1.79	0.64
1:A:15:LEU:HD21	1:A:738:GLN:NE2	2.13	0.64
1:A:361:TYR:HA	1:A:365:GLU:HA	1.78	0.64
1:A:159:PRO:HG2	1:A:294:TYR:CE2	2.33	0.64
3:B:2001:PBU:H1'2	3:B:2001:PBU:H82	1.78	0.64
1:A:103:GLU:HG3	1:A:104:PRO:CD	2.29	0.63
1:A:767:GLU:N	1:A:767:GLU:CD	2.51	0.63
1:A:901:CYS:HA	1:A:929:LEU:HD21	1.79	0.63
2:B:518:GLU:HA	2:B:521:ILE:HD12	1.81	0.63
1:A:251:ILE:HD12	1:A:288:MET:HB3	1.80	0.63
2:B:542:ARG:O	2:B:542:ARG:HG2	1.98	0.63
1:A:8:GLY:CA	1:A:14:HIS:O	2.47	0.63
1:A:357:ARG:NH1	1:A:371:VAL:CG1	2.61	0.63
1:A:924:LYS:HB3	1:A:924:LYS:NZ	2.10	0.63
1:A:888:GLU:OE1	1:A:892:ALA:HB2	1.99	0.62
1:A:217:PRO:O	1:A:221:ILE:HG13	1.98	0.62
1:A:213:HIS:CE1	1:A:214:ASP:HB3	2.34	0.62
1:A:154:ARG:C	1:A:156:LEU:H	2.03	0.62
1:A:767:GLU:N	1:A:767:GLU:OE2	2.33	0.62
1:A:860:ILE:HG21	1:A:877:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:TYR:CE2	1:A:371:VAL:HG12	2.34	0.62
1:A:360:ILE:HD13	1:A:367:LEU:HD21	1.80	0.62
1:A:375:ARG:NH2	1:A:383:TRP:HB3	2.14	0.62
1:A:608:ASP:HB3	1:A:611:VAL:CG2	2.29	0.61
1:A:254:VAL:HG22	1:A:261:PHE:HE1	1.65	0.61
1:A:35:GLU:CG	1:A:35:GLU:O	2.48	0.61
1:A:542:GLU:HG3	2:B:380:LEU:CD2	2.30	0.61
1:A:977:PHE:HE1	1:A:981:GLN:NE2	1.97	0.61
1:A:229:THR:O	1:A:230:ARG:C	2.39	0.61
1:A:103:GLU:HG3	1:A:104:PRO:HD2	1.83	0.61
1:A:-28:MET:H2	1:A:-25:TYR:H	1.49	0.61
1:A:38:ARG:HD2	1:A:741:ARG:CZ	2.31	0.61
1:A:825:GLN:C	1:A:827:GLN:H	2.03	0.61
1:A:347:ASN:HB3	1:A:350:ASP:HB2	1.83	0.61
2:B:584:LEU:O	2:B:588:GLY:N	2.28	0.61
1:A:805:ASP:O	1:A:807:LEU:HD23	2.01	0.60
2:B:544:ARG:O	2:B:547:GLU:HG2	2.01	0.60
1:A:450:HIS:CE1	2:B:464:ASP:OD1	2.54	0.60
1:A:135:GLU:HB2	1:A:432:TYR:CE1	2.36	0.60
1:A:60:GLN:HG2	1:A:61:LEU:HD12	1.83	0.60
1:A:542:GLU:HG3	2:B:380:LEU:HD22	1.84	0.60
1:A:896:LEU:HD21	1:A:928:GLN:HB2	1.84	0.60
1:A:745:MET:O	1:A:749:GLN:HB2	2.01	0.60
1:A:444:ASN:O	1:A:465:ASN:HB3	2.01	0.59
1:A:375:ARG:HH22	1:A:383:TRP:HB3	1.67	0.59
2:B:350:THR:HG21	2:B:428:VAL:HG11	1.85	0.59
1:A:365:GLU:OE2	1:A:365:GLU:N	2.36	0.59
2:B:398:PHE:HB3	2:B:399:SER:CA	2.33	0.59
1:A:642:GLU:HG2	1:A:647:ASN:CB	2.33	0.59
1:A:727:THR:O	1:A:730:VAL:N	2.32	0.59
1:A:200:PRO:HB2	1:A:201:ASN:HA	1.84	0.58
1:A:367:LEU:CD2	1:A:389:TYR:HB3	2.33	0.58
1:A:336:ILE:HB	1:A:389:TYR:HE2	1.67	0.58
1:A:526:ASN:O	1:A:529:GLU:HB2	2.03	0.58
1:A:903:GLY:C	1:A:905:CYS:H	2.07	0.58
1:A:977:PHE:HE1	1:A:981:GLN:HE21	1.51	0.58
1:A:138:ASP:O	1:A:142:ASN:ND2	2.36	0.58
2:B:445:VAL:HG12	2:B:584:LEU:HD21	1.85	0.58
1:A:637:GLN:OE1	1:A:640:LYS:NZ	2.36	0.58
1:A:948:LYS:O	1:A:950:GLU:N	2.36	0.58
1:A:873:ASN:HD22	1:A:876:THR:HG23	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:THR:HG21	1:A:954:PHE:CB	2.34	0.58
2:B:537:GLU:O	2:B:540:ASP:HB2	2.04	0.58
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.40	0.57
1:A:336:ILE:O	1:A:387:LEU:N	2.29	0.57
2:B:330:ASP:C	2:B:332:GLU:H	2.05	0.57
1:A:870:LEU:O	1:A:871:GLN:HB2	2.04	0.57
1:A:514:SER:O	1:A:522:GLU:HG2	2.05	0.57
1:A:1036:LEU:O	1:A:1040:MET:HG3	2.04	0.57
1:A:198:VAL:N	1:A:201:ASN:HD22	2.02	0.57
1:A:111:LYS:HE2	1:A:306:SER:H	1.70	0.57
1:A:182:TYR:O	1:A:185:LEU:HB2	2.04	0.57
1:A:-28:MET:C	1:A:-26:TYR:N	2.59	0.57
2:B:338:ILE:HB	2:B:342:GLU:HB2	1.86	0.57
1:A:956:LEU:N	1:A:1047:HIS:HE1	1.88	0.56
1:A:642:GLU:HG2	1:A:647:ASN:OD1	2.05	0.56
1:A:800:ILE:CD1	1:A:850:VAL:HG22	2.36	0.56
1:A:404:LEU:HD11	1:A:443:LEU:HD23	1.86	0.56
1:A:977:PHE:O	1:A:980:PHE:HB3	2.05	0.56
1:A:108:ARG:C	1:A:110:GLU:H	2.09	0.56
1:A:461:VAL:HG22	1:A:462:THR:N	2.21	0.56
2:B:566:ILE:O	2:B:566:ILE:CG2	2.53	0.56
1:A:375:ARG:HH21	1:A:385:GLU:HG3	1.69	0.56
1:A:828:GLY:O	1:A:829:LEU:HB2	2.04	0.56
1:A:431:ASP:C	1:A:431:ASP:OD1	2.44	0.56
1:A:929:LEU:O	1:A:929:LEU:HD23	2.06	0.56
1:A:185:LEU:HD13	1:A:188:GLY:HA2	1.88	0.55
1:A:361:TYR:CE2	1:A:365:GLU:HG3	2.42	0.55
1:A:558:CYS:HB3	1:A:564:ILE:HG21	1.88	0.55
1:A:46:LYS:HE3	1:A:65:GLU:HB3	1.89	0.55
1:A:660:ASN:OD1	1:A:660:ASN:C	2.44	0.55
2:B:483:ALA:O	2:B:486:ALA:N	2.39	0.55
1:A:772:MET:HA	1:A:772:MET:HE3	1.86	0.55
1:A:634:GLN:HG2	1:A:1001:LEU:HD22	1.88	0.55
1:A:961:LEU:HD22	1:A:977:PHE:HE2	1.71	0.55
1:A:996:ASN:HD22	1:A:996:ASN:H	1.53	0.55
1:A:357:ARG:HG2	1:A:456:LEU:HD13	1.87	0.55
1:A:83:PHE:HD1	1:A:109:GLU:OE1	1.89	0.55
1:A:25:LEU:CD1	1:A:25:LEU:N	2.70	0.55
1:A:341:ALA:HB2	1:A:473:LEU:CD1	2.37	0.55
1:A:60:GLN:OE1	1:A:60:GLN:N	2.25	0.55
2:B:343:VAL:HG21	2:B:358:ARG:HH11	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:GLU:HG2	2:B:380:LEU:HD22	1.87	0.55
1:A:503:GLU:CD	1:A:555:ARG:HH22	2.08	0.55
2:B:554:ALA:HA	2:B:557:ARG:CZ	2.37	0.55
1:A:945:PHE:H	2:B:577:ARG:NH1	2.04	0.54
1:A:809:GLN:HG2	1:A:1012:GLU:OE2	2.07	0.54
1:A:1027:ALA:HB1	1:A:1030:LYS:HD2	1.88	0.54
1:A:433:THR:O	1:A:434:ASP:HB2	2.07	0.54
1:A:977:PHE:CE1	1:A:981:GLN:NE2	2.74	0.54
2:B:509:ILE:C	2:B:511:LYS:H	2.09	0.54
1:A:897:PHE:O	1:A:901:CYS:HB2	2.07	0.54
1:A:564:ILE:HG13	1:A:564:ILE:O	2.06	0.54
2:B:354:THR:O	2:B:372:LEU:HA	2.07	0.54
1:A:226:ARG:O	1:A:230:ARG:CG	2.56	0.54
1:A:251:ILE:O	1:A:288:MET:HB3	2.07	0.54
1:A:868:GLY:O	1:A:870:LEU:HB2	2.08	0.54
1:A:190:ILE:CD1	1:A:213:HIS:HA	2.38	0.54
1:A:226:ARG:HH21	1:A:243:VAL:HG11	1.73	0.54
1:A:111:LYS:HE2	1:A:306:SER:N	2.23	0.54
1:A:446:TRP:CD2	1:A:465:ASN:HB2	2.42	0.54
1:A:721:GLN:O	1:A:722:GLU:C	2.46	0.53
1:A:745:MET:CE	1:A:745:MET:HA	2.38	0.53
1:A:965:SER:HA	1:A:976:GLU:HG3	1.90	0.53
1:A:1017:ASP:HB2	2:B:345:GLU:OE1	2.07	0.53
1:A:38:ARG:NH2	1:A:743:ASP:OD2	2.28	0.53
1:A:-28:MET:HA	1:A:-23:HIS:CD2	2.44	0.53
1:A:225:ILE:O	1:A:229:THR:HG23	2.08	0.53
2:B:349:ASP:H	2:B:373:ARG:NH2	2.06	0.53
1:A:278:MET:HA	1:A:278:MET:HE2	1.87	0.53
1:A:226:ARG:O	1:A:230:ARG:HG3	2.09	0.53
1:A:630:GLN:O	1:A:815:GLN:NE2	2.40	0.53
1:A:65:GLU:O	1:A:67:SER:N	2.42	0.53
1:A:807:LEU:HG	1:A:846:GLY:HA3	1.89	0.53
1:A:-23:HIS:CD2	1:A:834:LEU:HD13	2.43	0.53
1:A:76:GLU:HG2	1:A:124:PRO:HD3	1.91	0.53
2:B:582:MET:O	2:B:586:GLN:HG3	2.09	0.53
1:A:598:ALA:O	1:A:601:LEU:HB2	2.09	0.52
2:B:448:LYS:HB3	2:B:580:TYR:CE2	2.44	0.52
1:A:422:LEU:HD22	2:B:564:ASN:HB3	1.90	0.52
1:A:451:GLY:HA3	1:A:1014:GLN:HG3	1.89	0.52
1:A:367:LEU:HD12	1:A:367:LEU:C	2.30	0.52
1:A:60:GLN:H	1:A:60:GLN:CD	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:LEU:O	1:A:638:VAL:HG12	2.09	0.52
1:A:470:THR:HB	1:A:471:PRO:CD	2.39	0.52
1:A:43:ILE:HG13	1:A:85:GLU:O	2.09	0.52
1:A:108:ARG:C	1:A:110:GLU:N	2.63	0.52
1:A:397:PRO:HD2	1:A:400:ALA:HB2	1.91	0.52
1:A:529:GLU:HA	1:A:529:GLU:OE1	2.08	0.52
1:A:4:ARG:HG3	1:A:5:PRO:HD2	1.92	0.52
1:A:727:THR:O	1:A:728:GLN:C	2.48	0.52
1:A:42:LEU:HD22	1:A:70:PHE:CD2	2.45	0.52
1:A:193:VAL:HG23	1:A:282:MET:HG2	1.92	0.52
1:A:449:PRO:HA	2:B:467:TYR:HE2	1.75	0.52
1:A:567:LYS:O	1:A:568:LEU:C	2.49	0.52
1:A:883:ASP:OD2	1:A:884:LYS:HD3	2.10	0.51
1:A:829:LEU:HD21	1:A:986:LYS:HB3	1.91	0.51
2:B:355:PHE:HB2	2:B:370:LEU:HD11	1.91	0.51
1:A:878:HIS:HD2	1:A:963:VAL:HA	1.75	0.51
2:B:335:TRP:HB2	2:B:338:ILE:HD11	1.92	0.51
2:B:476:GLU:O	2:B:480:LYS:HG3	2.11	0.51
1:A:181:ILE:HG12	1:A:278:MET:CE	2.41	0.51
1:A:868:GLY:O	1:A:870:LEU:N	2.44	0.51
1:A:293:LEU:C	1:A:295:SER:H	2.13	0.51
2:B:576:THR:HA	2:B:579:GLN:HB2	1.92	0.51
1:A:191:ILE:HG12	1:A:210:LYS:HG3	1.92	0.51
1:A:367:LEU:HD21	1:A:389:TYR:HB3	1.93	0.51
1:A:875:HIS:O	1:A:879:GLN:HG2	2.10	0.51
1:A:111:LYS:HZ1	1:A:305:PRO:HA	1.76	0.51
1:A:903:GLY:O	1:A:905:CYS:N	2.42	0.51
1:A:542:GLU:CG	2:B:380:LEU:CD2	2.88	0.51
1:A:199:SER:HA	1:A:201:ASN:HB2	1.93	0.51
1:A:265:TYR:O	1:A:266:PRO:C	2.49	0.51
1:A:692:CYS:HB3	1:A:699:LEU:HD13	1.92	0.51
2:B:328:LEU:O	2:B:334:TYR:CD2	2.63	0.51
1:A:111:LYS:HD3	1:A:306:SER:HB2	1.92	0.50
1:A:1023:ARG:HB3	1:A:1023:ARG:HH11	1.75	0.50
1:A:538:ASP:OD1	1:A:541:SER:HB3	2.11	0.50
1:A:567:LYS:O	1:A:570:LEU:N	2.43	0.50
1:A:300:ASP:HB2	1:A:696:GLY:HA2	1.93	0.50
1:A:366:PRO:HB2	1:A:575:ASN:HB3	1.93	0.50
1:A:924:LYS:NZ	1:A:928:GLN:CB	2.53	0.50
1:A:956:LEU:N	1:A:956:LEU:HD23	2.27	0.50
2:B:392:PHE:HE2	2:B:413:LEU:HD21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:SER:OG	2:B:401:VAL:N	2.43	0.50
1:A:470:THR:HB	1:A:471:PRO:HD2	1.93	0.50
1:A:749:GLN:HG2	1:A:764:LEU:H	1.76	0.50
1:A:781:LEU:HD13	1:A:783:TRP:CH2	2.47	0.50
1:A:856:THR:O	1:A:857:ILE:C	2.48	0.50
1:A:356:VAL:HG23	1:A:383:TRP:CH2	2.47	0.50
1:A:108:ARG:CZ	1:A:111:LYS:HD2	2.41	0.50
1:A:116:GLU:O	1:A:119:PHE:N	2.45	0.50
1:A:347:ASN:HB3	1:A:350:ASP:CB	2.42	0.50
1:A:945:PHE:O	1:A:947:TYR:HD1	1.95	0.50
1:A:1021:TYR:HE1	1:A:1025:THR:HG1	1.58	0.50
1:A:794:PHE:O	1:A:794:PHE:HD1	1.94	0.50
1:A:833:MET:HA	1:A:904:TYR:HE1	1.76	0.50
1:A:780:TRP:CH2	1:A:850:VAL:HG11	2.47	0.49
1:A:913:ILE:HD12	1:A:914:GLY:O	2.12	0.49
1:A:924:LYS:HZ1	1:A:928:GLN:CB	2.19	0.49
1:A:468:LYS:HB3	2:B:481:ARG:NH2	2.27	0.49
1:A:372:ASN:O	1:A:372:ASN:OD1	2.30	0.49
1:A:61:LEU:N	1:A:61:LEU:HD12	2.27	0.49
1:A:15:LEU:HD21	1:A:738:GLN:HE22	1.77	0.49
1:A:945:PHE:CG	2:B:598:LEU:HB3	2.47	0.49
1:A:467:ASN:HD21	1:A:678:LYS:HE2	1.76	0.49
1:A:542:GLU:HG3	2:B:380:LEU:CD1	2.42	0.49
1:A:372:ASN:O	1:A:373:THR:O	2.29	0.49
1:A:47:HIS:CD2	1:A:51:LYS:HE3	2.47	0.49
1:A:542:GLU:HG3	2:B:380:LEU:HD13	1.94	0.49
1:A:945:PHE:CD2	1:A:946:GLY:N	2.81	0.49
1:A:137:GLN:HE22	1:A:140:ARG:HH11	1.60	0.48
1:A:360:ILE:O	1:A:366:PRO:CD	2.61	0.48
1:A:352:ASP:CB	1:A:409:VAL:O	2.50	0.48
1:A:243:VAL:O	1:A:247:GLN:NE2	2.46	0.48
1:A:572:VAL:HG21	1:A:583:MET:HG2	1.95	0.48
1:A:278:MET:HA	1:A:278:MET:HE3	1.93	0.48
1:A:393:ILE:N	1:A:394:PRO:CD	2.76	0.48
1:A:532:LYS:HG3	1:A:561:ILE:HG21	1.94	0.48
2:B:370:LEU:HD23	2:B:381:ILE:HD12	1.95	0.48
1:A:144:LEU:O	1:A:145:ASN:C	2.51	0.48
1:A:452:LEU:CD1	1:A:454:ASP:HB2	2.43	0.48
1:A:540:LEU:HD11	1:A:999:ILE:HD12	1.96	0.48
1:A:583:MET:O	1:A:587:VAL:HG23	2.12	0.48
2:B:453:ASN:O	2:B:457:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:VAL:HG12	1:A:491:VAL:O	2.13	0.48
1:A:724:LYS:O	1:A:725:ASP:CB	2.59	0.48
1:A:802:LYS:HD2	1:A:805:ASP:HB2	1.96	0.48
1:A:870:LEU:O	1:A:871:GLN:CB	2.61	0.48
1:A:372:ASN:O	1:A:373:THR:C	2.52	0.48
1:A:456:LEU:O	1:A:457:ASN:HB2	2.13	0.48
1:A:218:GLU:HA	1:A:221:ILE:HD12	1.96	0.48
1:A:325:LYS:HE3	1:A:482:SER:HB2	1.95	0.48
2:B:502:GLU:HA	2:B:505:SER:OG	2.14	0.48
1:A:254:VAL:HG22	1:A:261:PHE:CE1	2.46	0.48
1:A:1032:GLU:O	1:A:1033:GLN:C	2.52	0.47
1:A:200:PRO:HB2	1:A:202:ASN:H	1.79	0.47
1:A:881:LEU:HD11	1:A:927:GLY:HA2	1.96	0.47
1:A:172:GLU:HG3	1:A:274:ARG:HD2	1.94	0.47
1:A:8:GLY:HA3	1:A:14:HIS:HA	1.96	0.47
1:A:939:ASP:HB3	1:A:1021:TYR:CE2	2.47	0.47
1:A:404:LEU:HD21	1:A:475:LEU:HD11	1.97	0.47
1:A:1001:LEU:HA	1:A:1001:LEU:HD22	1.75	0.47
1:A:715:LEU:HD21	1:A:735:LEU:HD12	1.97	0.47
1:A:627:LYS:HG3	1:A:631:TYR:HE2	1.76	0.47
1:A:672:LYS:HA	1:A:675:MET:HG2	1.96	0.47
1:A:8:GLY:HA2	1:A:714:ASN:ND2	2.29	0.47
1:A:450:HIS:HD2	1:A:1011:PRO:HB3	1.78	0.47
1:A:8:GLY:HA3	1:A:14:HIS:CA	2.45	0.47
1:A:190:ILE:HD12	1:A:213:HIS:HA	1.97	0.47
1:A:361:TYR:HA	1:A:366:PRO:HD3	1.97	0.47
1:A:94:LEU:O	1:A:95:PHE:HB3	2.14	0.47
1:A:1023:ARG:HH22	1:A:1029:ASP:CG	2.18	0.47
1:A:293:LEU:C	1:A:295:SER:N	2.68	0.47
2:B:567:LYS:N	2:B:568:PRO:HD2	2.30	0.47
1:A:1044:ASN:HA	1:A:1051:TRP:HB2	1.97	0.46
1:A:357:ARG:HH11	1:A:371:VAL:CG1	2.28	0.46
1:A:444:ASN:HB3	1:A:465:ASN:O	2.15	0.46
1:A:511:ALA:C	1:A:513:LEU:H	2.18	0.46
2:B:509:ILE:HD11	2:B:521:ILE:HG23	1.97	0.46
1:A:73:VAL:O	1:A:94:LEU:O	2.32	0.46
2:B:544:ARG:HA	2:B:547:GLU:HG2	1.97	0.46
1:A:355:TYR:HE2	1:A:371:VAL:CG1	2.23	0.46
1:A:4:ARG:HB2	1:A:76:GLU:OE1	2.14	0.46
1:A:623:LEU:HD21	1:A:628:LEU:HB2	1.97	0.46
2:B:358:ARG:HH22	2:B:380:LEU:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:HD3	1:A:148:LYS:O	2.15	0.46
1:A:837:GLY:N	1:A:849:GLU:OE2	2.36	0.46
1:A:96:GLN:OE1	1:A:97:PRO:HD3	2.16	0.46
1:A:229:THR:OG1	1:A:230:ARG:N	2.49	0.46
1:A:565:LEU:HB3	1:A:566:PRO:HD3	1.98	0.46
1:A:15:LEU:HD22	1:A:718:ILE:HD13	1.97	0.46
2:B:446:GLY:O	2:B:449:LEU:HB3	2.16	0.46
1:A:337:LYS:HD2	1:A:476:GLU:OE2	2.15	0.46
1:A:644:TYR:O	1:A:683:ARG:NH2	2.48	0.46
1:A:724:LYS:HA	1:A:731:GLN:NE2	2.31	0.46
2:B:338:ILE:HD12	2:B:343:VAL:HG22	1.98	0.46
1:A:526:ASN:O	1:A:529:GLU:N	2.48	0.46
1:A:540:LEU:HD11	1:A:1019:ILE:HG22	1.97	0.46
1:A:672:LYS:O	1:A:675:MET:HB2	2.15	0.46
1:A:812:LEU:CD2	1:A:1005:MET:HG3	2.45	0.46
1:A:91:ASP:OD1	1:A:711:LYS:NZ	2.45	0.46
1:A:884:LYS:NZ	1:A:925:ASP:OD1	2.40	0.46
2:B:396:LEU:C	2:B:398:PHE:H	2.19	0.46
1:A:1010:MET:HE3	1:A:1013:LEU:HD12	1.98	0.45
1:A:114:ASN:HA	1:A:117:ILE:HG13	1.98	0.45
1:A:154:ARG:C	1:A:156:LEU:N	2.70	0.45
1:A:25:LEU:N	1:A:25:LEU:HD12	2.31	0.45
1:A:622:TYR:N	1:A:622:TYR:CD1	2.84	0.45
1:A:709:MET:HE1	1:A:847:LEU:HD11	1.98	0.45
1:A:530:GLN:O	1:A:533:ALA:HB3	2.17	0.45
1:A:121:ILE:CG2	1:A:688:LEU:HD13	2.47	0.45
2:B:439:GLU:O	2:B:445:VAL:CG2	2.54	0.45
1:A:956:LEU:N	1:A:1047:HIS:CE1	2.71	0.45
1:A:885:ASN:HB3	1:A:889:ILE:HG22	1.98	0.45
1:A:106:GLY:O	1:A:108:ARG:N	2.50	0.45
1:A:200:PRO:CG	1:A:201:ASN:HA	2.46	0.45
1:A:903:GLY:C	1:A:905:CYS:N	2.70	0.45
1:A:939:ASP:O	1:A:942:LYS:HG2	2.16	0.45
1:A:29:GLY:HA2	2:B:497:GLN:CD	2.36	0.45
1:A:267:LEU:HD13	1:A:273:ILE:HG13	1.99	0.45
1:A:595:PRO:C	1:A:597:GLN:H	2.20	0.45
1:A:921:ILE:HG12	1:A:931:HIS:CE1	2.52	0.45
1:A:260:TYR:CD1	1:A:260:TYR:N	2.85	0.45
1:A:509:SER:HB2	1:A:513:LEU:HB3	1.98	0.45
1:A:749:GLN:HG2	1:A:763:ASN:HA	1.97	0.45
1:A:151:VAL:HG11	1:A:302:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:567:LYS:N	2:B:568:PRO:CD	2.80	0.45
1:A:-19:HIS:NE2	1:A:926:ASP:HB2	2.32	0.45
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.52	0.45
1:A:622:TYR:HD1	1:A:622:TYR:N	2.15	0.45
1:A:802:LYS:HD3	1:A:805:ASP:OD2	2.17	0.45
1:A:807:LEU:HD11	1:A:848:ILE:HD11	1.99	0.45
1:A:114:ASN:HD22	1:A:115:ARG:N	2.15	0.44
1:A:172:GLU:HG2	1:A:271:LYS:HG2	2.00	0.44
1:A:300:ASP:C	1:A:301:CYS:SG	2.95	0.44
1:A:735:LEU:O	1:A:735:LEU:HG	2.14	0.44
1:A:114:ASN:C	1:A:114:ASN:ND2	2.71	0.44
1:A:843:ASP:O	1:A:844:CYS:HB2	2.16	0.44
1:A:352:ASP:O	1:A:353:LYS:HD2	2.17	0.44
1:A:457:ASN:OD1	1:A:459:ILE:HG22	2.17	0.44
1:A:797:ASN:OD1	1:A:797:ASN:C	2.56	0.44
2:B:343:VAL:HG21	2:B:358:ARG:HG3	1.99	0.44
1:A:196:VAL:HG22	1:A:287:LEU:HB2	2.00	0.44
1:A:584:TYR:CE1	1:A:610:MET:HG3	2.53	0.44
1:A:12:GLY:O	1:A:13:ILE:C	2.55	0.44
1:A:-28:MET:N	1:A:-25:TYR:H	2.15	0.44
1:A:306:SER:C	1:A:308:SER:H	2.21	0.44
1:A:741:ARG:HB3	1:A:743:ASP:OD1	2.17	0.44
1:A:256:GLY:O	1:A:793:LEU:HD23	2.18	0.44
1:A:916:ARG:HB3	1:A:921:ILE:HD11	1.99	0.44
1:A:939:ASP:HB3	1:A:1021:TYR:HE2	1.82	0.44
1:A:1035:ALA:O	1:A:1036:LEU:C	2.56	0.44
1:A:-17:TYR:CD1	1:A:-17:TYR:C	2.91	0.44
1:A:543:ILE:HD11	1:A:567:LYS:HD3	1.98	0.44
2:B:554:ALA:HA	2:B:557:ARG:NH1	2.33	0.44
1:A:560:THR:O	1:A:562:PRO:HD3	2.18	0.44
1:A:728:GLN:O	1:A:729:LYS:C	2.55	0.44
1:A:843:ASP:OD1	1:A:843:ASP:C	2.56	0.44
2:B:372:LEU:O	2:B:373:ARG:HB2	2.17	0.44
1:A:885:ASN:HB3	1:A:889:ILE:O	2.17	0.44
1:A:970:GLU:OE2	1:A:970:GLU:HA	2.18	0.44
2:B:570:LEU:HG	2:B:570:LEU:O	2.18	0.44
1:A:433:THR:O	1:A:434:ASP:CB	2.66	0.43
1:A:633:ILE:O	1:A:634:GLN:C	2.55	0.43
1:A:724:LYS:C	1:A:724:LYS:HD2	2.37	0.43
1:A:934:PHE:O	1:A:935:GLY:C	2.56	0.43
1:A:961:LEU:HD22	1:A:977:PHE:CE2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:ASN:ND2	1:A:650:VAL:H	2.16	0.43
1:A:-24:HIS:CD2	1:A:852:ARG:HD3	2.53	0.43
1:A:853:ASN:ND2	1:A:925:ASP:OD2	2.51	0.43
1:A:8:GLY:HA3	1:A:14:HIS:C	2.39	0.43
1:A:969:GLN:O	1:A:970:GLU:HB2	2.19	0.43
1:A:961:LEU:CD2	1:A:977:PHE:HE2	2.31	0.43
1:A:77:ALA:HB2	2:B:486:ALA:HB2	2.00	0.43
1:A:800:ILE:HD11	1:A:850:VAL:HG22	2.00	0.43
2:B:426:TYR:O	2:B:428:VAL:HG23	2.18	0.43
1:A:154:ARG:O	1:A:156:LEU:N	2.50	0.43
1:A:-17:TYR:HD1	1:A:-17:TYR:C	2.22	0.43
1:A:453:GLU:HB2	2:B:348:ARG:HH22	1.83	0.43
1:A:520:ASP:HB3	1:A:521:ASN:H	1.46	0.43
1:A:1023:ARG:HA	1:A:1028:LEU:HD12	2.00	0.43
1:A:13:ILE:HG21	1:A:17:PRO:HD3	2.00	0.43
1:A:204:LYS:O	1:A:205:GLN:NE2	2.51	0.43
1:A:788:ILE:H	1:A:788:ILE:HG13	1.61	0.43
1:A:910:ILE:HD13	1:A:1026:LEU:HD21	2.01	0.43
1:A:393:ILE:N	1:A:394:PRO:HD2	2.34	0.43
1:A:859:GLN:O	1:A:863:LYS:N	2.43	0.43
1:A:859:GLN:HA	1:A:862:CYS:HB2	2.01	0.43
1:A:154:ARG:HD2	1:A:658:LEU:O	2.18	0.43
1:A:121:ILE:HG23	1:A:688:LEU:HD13	2.00	0.43
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.84	0.43
1:A:119:PHE:CE2	1:A:707:GLU:HG3	2.54	0.43
1:A:200:PRO:HB2	1:A:202:ASN:N	2.34	0.43
1:A:334:LEU:HD21	1:A:336:ILE:HD11	2.00	0.43
1:A:449:PRO:HA	2:B:467:TYR:CE2	2.54	0.43
1:A:873:ASN:ND2	1:A:876:THR:HG23	2.33	0.42
1:A:18:PRO:HA	1:A:38:ARG:HB2	2.01	0.42
1:A:680:VAL:O	1:A:681:SER:C	2.57	0.42
1:A:702:LEU:HD23	1:A:702:LEU:HA	1.91	0.42
2:B:506:LYS:HA	2:B:509:ILE:HG22	2.00	0.42
1:A:360:ILE:O	1:A:366:PRO:HD2	2.19	0.42
1:A:375:ARG:O	1:A:376:VAL:C	2.56	0.42
1:A:453:GLU:HB2	2:B:348:ARG:NH2	2.34	0.42
1:A:712:LEU:HD11	1:A:781:LEU:HD11	2.01	0.42
1:A:980:PHE:O	1:A:981:GLN:C	2.57	0.42
1:A:540:LEU:HG	1:A:999:ILE:HG21	2.02	0.42
1:A:69:ILE:HD12	1:A:69:ILE:HA	1.70	0.42
1:A:945:PHE:CG	1:A:946:GLY:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:484:ILE:HG13	2:B:545:LEU:HD23	2.00	0.42
2:B:552:GLN:O	2:B:553:ALA:C	2.56	0.42
1:A:53:ALA:O	1:A:55:LYS:N	2.52	0.42
2:B:417:ASN:HA	2:B:418:PRO:HD2	1.91	0.42
2:B:430:LYS:O	2:B:432:GLN:N	2.53	0.42
2:B:473:THR:HG23	2:B:552:GLN:NE2	2.33	0.42
1:A:340:CYS:HB2	1:A:382:ARG:HG3	2.01	0.42
1:A:627:LYS:CG	1:A:631:TYR:HE2	2.33	0.42
2:B:362:THR:OG1	2:B:365:HIS:HD2	2.03	0.42
1:A:448:VAL:HA	1:A:449:PRO:HD3	1.83	0.42
1:A:830:ASP:O	1:A:899:ARG:HD3	2.20	0.42
2:B:459:LYS:HB3	2:B:570:LEU:CD1	2.49	0.42
2:B:362:THR:OG1	2:B:365:HIS:CD2	2.73	0.42
2:B:593:LYS:C	2:B:595:ASN:H	2.23	0.42
1:A:1031:THR:O	1:A:1034:GLU:N	2.53	0.42
1:A:523:LEU:CD2	1:A:523:LEU:O	2.54	0.42
2:B:335:TRP:HB2	2:B:338:ILE:CD1	2.50	0.42
2:B:348:ARG:O	2:B:349:ASP:HB2	2.20	0.42
2:B:501:GLN:OE1	2:B:527:ASN:ND2	2.53	0.42
1:A:293:LEU:O	1:A:295:SER:N	2.53	0.42
1:A:368:CYS:O	1:A:369:ASP:C	2.59	0.42
1:A:5:PRO:HG2	2:B:479:MET:SD	2.59	0.42
1:A:744:PHE:CD2	1:A:748:LEU:HD12	2.55	0.42
2:B:467:TYR:O	2:B:467:TYR:HD1	2.03	0.42
1:A:989:LEU:HD21	1:A:1036:LEU:HG	2.02	0.41
1:A:539:PRO:O	1:A:540:LEU:C	2.58	0.41
1:A:65:GLU:C	1:A:67:SER:N	2.73	0.41
1:A:661:GLN:O	1:A:661:GLN:CG	2.68	0.41
1:A:732:MET:HE3	1:A:732:MET:HB3	1.91	0.41
1:A:945:PHE:HB2	2:B:598:LEU:HD13	2.02	0.41
1:A:22:VAL:HG11	1:A:99:LEU:HD22	2.02	0.41
2:B:544:ARG:O	2:B:547:GLU:CG	2.68	0.41
2:B:567:LYS:H	2:B:568:PRO:HD2	1.85	0.41
1:A:25:LEU:HB2	1:A:100:LYS:HG3	2.01	0.41
1:A:880:TRP:O	1:A:884:LYS:HG2	2.20	0.41
2:B:578:ASP:OD1	2:B:581:LEU:HD23	2.19	0.41
1:A:-23:HIS:CG	1:A:834:LEU:HD13	2.56	0.41
1:A:361:TYR:CD2	1:A:365:GLU:N	2.88	0.41
1:A:367:LEU:HD22	1:A:389:TYR:HB3	2.02	0.41
1:A:446:TRP:CH2	1:A:465:ASN:HA	2.55	0.41
2:B:408:TYR:CD1	2:B:413:LEU:HG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:VAL:CG1	1:A:491:VAL:O	2.68	0.41
1:A:525:GLU:OE2	1:A:525:GLU:N	2.54	0.41
1:A:526:ASN:N	1:A:526:ASN:OD1	2.53	0.41
1:A:942:LYS:HB2	1:A:946:GLY:HA3	2.00	0.41
1:A:190:ILE:HD11	1:A:213:HIS:HA	2.03	0.41
1:A:745:MET:HE2	1:A:745:MET:HA	2.01	0.41
1:A:288:MET:HA	1:A:288:MET:HE3	2.02	0.41
1:A:772:MET:CE	1:A:772:MET:CA	2.88	0.41
1:A:4:ARG:NH1	2:B:482:THR:OG1	2.54	0.41
1:A:1023:ARG:NH2	1:A:1029:ASP:CG	2.74	0.41
1:A:825:GLN:C	1:A:827:GLN:N	2.69	0.41
1:A:7:SER:C	1:A:8:GLY:O	2.59	0.41
1:A:878:HIS:CD2	1:A:963:VAL:HA	2.54	0.41
2:B:566:ILE:HG23	2:B:566:ILE:O	2.21	0.41
1:A:985:TYR:CZ	1:A:1040:MET:HG2	2.56	0.41
1:A:221:ILE:H	1:A:221:ILE:HG13	1.71	0.41
2:B:437:VAL:O	2:B:439:GLU:HG3	2.20	0.41
2:B:480:LYS:HD3	2:B:545:LEU:HD11	2.03	0.41
2:B:505:SER:C	2:B:507:GLU:H	2.24	0.41
2:B:554:ALA:HA	2:B:557:ARG:NH2	2.36	0.41
1:A:355:TYR:CE2	1:A:371:VAL:CG1	3.00	0.41
2:B:555:GLU:O	2:B:559:ILE:HG12	2.21	0.41
1:A:661:GLN:OE1	1:A:698:TYR:HB2	2.20	0.41
1:A:180:HIS:HE1	1:A:825:GLN:HG2	1.85	0.41
1:A:1010:MET:HA	1:A:1011:PRO:HD3	1.87	0.41
1:A:5:PRO:C	1:A:7:SER:H	2.23	0.41
1:A:794:PHE:CD1	1:A:794:PHE:O	2.73	0.41
2:B:518:GLU:O	2:B:521:ILE:HB	2.21	0.41
1:A:5:PRO:C	1:A:7:SER:N	2.74	0.40
1:A:92:LEU:O	1:A:93:ARG:HB2	2.20	0.40
1:A:263:GLU:OE2	1:A:265:TYR:HE2	2.03	0.40
2:B:394:ASP:N	2:B:395:PRO:HD2	2.37	0.40
2:B:489:GLU:O	2:B:493:ILE:HG13	2.22	0.40
2:B:569:ASP:O	2:B:571:ILE:N	2.55	0.40
1:A:537:ARG:HD3	2:B:365:HIS:HE1	1.86	0.40
1:A:722:GLU:O	1:A:723:LYS:HG2	2.21	0.40
1:A:175:PRO:CD	1:A:176:GLU:H	2.34	0.40
1:A:661:GLN:O	1:A:661:GLN:HG2	2.22	0.40
1:A:292:SER:O	1:A:296:GLN:HG3	2.22	0.40
1:A:372:ASN:HB2	1:A:385:GLU:CD	2.42	0.40
1:A:409:VAL:C	1:A:418:GLU:HB2	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:HD12	1:A:456:LEU:HA	1.97	0.40
1:A:789:MET:O	1:A:790:SER:C	2.59	0.40
2:B:435:GLN:C	2:B:437:VAL:N	2.75	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	1032/1096 (94%)	797 (77%)	161 (16%)	74 (7%)	1	11
2	B	225/279 (81%)	168 (75%)	33 (15%)	24 (11%)	0	6
All	All	1257/1375 (91%)	965 (77%)	194 (15%)	98 (8%)	1	10

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	14	HIS
1	A	66	SER
1	A	107	ASN
1	A	114	ASN
1	A	200	PRO
1	A	222	ALA
1	A	298	PRO
1	A	369	ASP
1	A	375	ARG
1	A	450	HIS
1	A	535	SER
1	A	722	GLU
1	A	723	LYS
1	A	808	ARG

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Mol	Chain	Res	Type
1	A	826	ASN
1	A	829	LEU
1	A	866	LEU
1	A	867	LYS
1	A	869	ALA
1	A	871	GLN
1	A	949	ARG
1	A	966	LYS
2	B	331	ALA
2	B	338	ILE
2	B	372	LEU
2	B	430	LYS
2	B	431	TYR
2	B	434	ASP
2	B	438	LYS
2	B	442	ILE
1	A	-27	SER
1	A	13	ILE
1	A	38	ARG
1	A	54	ARG
1	A	235	SER
1	A	373	THR
1	A	434	ASP
1	A	451	GLY
1	A	725	ASP
1	A	791	GLU
1	A	868	GLY
1	A	904	TYR
1	A	939	ASP
1	A	946	GLY
2	B	340	ARG
2	B	428	VAL
2	B	519	LYS
1	A	-14	PRO
1	A	9	GLU
1	A	230	ARG
1	A	247	GLN
1	A	294	TYR
1	A	339	LEU
1	A	378	CYS
1	A	526	ASN
1	A	561	ILE

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Mol	Chain	Res	Type
1	A	563	GLU
1	A	918	ASN
1	A	970	GLU
1	A	1016	PHE
2	B	349	ASP
2	B	398	PHE
2	B	416	TYR
2	B	429	SER
2	B	432	GLN
2	B	484	ILE
2	B	506	LYS
2	B	521	ILE
2	B	594	LEU
1	A	95	PHE
1	A	109	GLU
1	A	307	TYR
1	A	371	VAL
1	A	507	SER
1	A	513	LEU
1	A	596	GLU
1	A	678	LYS
1	A	945	PHE
1	A	980	PHE
1	A	116	GLU
1	A	155	ASP
1	A	245	GLU
1	A	368	CYS
1	A	376	VAL
1	A	728	GLN
1	A	825	GLN
2	B	520	GLU
2	B	570	LEU
1	A	8	GLY
1	A	75	GLN
2	B	437	VAL
1	A	491	VAL
1	A	117	ILE
1	A	366	PRO
1	A	391	ILE
1	A	967	GLY
2	B	436	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	955/999 (96%)	804 (84%)	151 (16%)	2	15
2	B	227/259 (88%)	191 (84%)	36 (16%)	2	14
All	All	1182/1258 (94%)	995 (84%)	187 (16%)	2	15

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-20	HIS
1	A	-17	TYR
1	A	-16	ASP
1	A	-13	THR
1	A	-12	THR
1	A	4	ARG
1	A	14	HIS
1	A	15	LEU
1	A	20	ILE
1	A	31	ILE
1	A	35	GLU
1	A	39	GLU
1	A	44	THR
1	A	61	LEU
1	A	62	LEU
1	A	65	GLU
1	A	70	PHE
1	A	75	GLN
1	A	76	GLU
1	A	93	ARG
1	A	96	GLN
1	A	99	LEU
1	A	107	ASN
1	A	109	GLU
1	A	111	LYS
1	A	112	ILE
1	A	113	LEU

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Mol	Chain	Res	Type
1	A	114	ASN
1	A	115	ARG
1	A	121	ILE
1	A	123	MET
1	A	130	MET
1	A	135	GLU
1	A	153	LEU
1	A	158	SER
1	A	171	VAL
1	A	173	SER
1	A	177	LEU
1	A	197	ILE
1	A	198	VAL
1	A	200	PRO
1	A	202	ASN
1	A	205	GLN
1	A	208	THR
1	A	212	ASN
1	A	213	HIS
1	A	230	ARG
1	A	231	SER
1	A	234	LEU
1	A	246	TYR
1	A	267	LEU
1	A	282	MET
1	A	287	LEU
1	A	292	SER
1	A	295	SER
1	A	297	LEU
1	A	303	THR
1	A	322	THR
1	A	323	SER
1	A	327	LEU
1	A	335	ARG
1	A	343	TYR
1	A	347	ASN
1	A	349	ARG
1	A	351	ILE
1	A	353	LYS
1	A	357	ARG
1	A	365	GLU
1	A	368	CYS

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Mol	Chain	Res	Type
1	A	373	THR
1	A	388	ASN
1	A	401	ARG
1	A	404	LEU
1	A	406	ILE
1	A	427	ILE
1	A	433	THR
1	A	452	LEU
1	A	459	ILE
1	A	462	THR
1	A	464	SER
1	A	470	THR
1	A	472	CYS
1	A	481	SER
1	A	494	GLU
1	A	508	TYR
1	A	520	ASP
1	A	523	LEU
1	A	525	GLU
1	A	526	ASN
1	A	531	LEU
1	A	535	SER
1	A	541	SER
1	A	545	GLU
1	A	561	ILE
1	A	563	GLU
1	A	564	ILE
1	A	622	TYR
1	A	625	ASP
1	A	627	LYS
1	A	633	ILE
1	A	675	MET
1	A	679	THR
1	A	681	SER
1	A	697	MET
1	A	716	THR
1	A	718	ILE
1	A	722	GLU
1	A	724	LYS
1	A	725	ASP
1	A	726	GLU
1	A	744	PHE

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Mol	Chain	Res	Type
1	A	746	ASP
1	A	756	ASN
1	A	765	ARG
1	A	767	GLU
1	A	770	ARG
1	A	772	MET
1	A	776	LYS
1	A	788	ILE
1	A	790	SER
1	A	794	PHE
1	A	798	GLU
1	A	807	LEU
1	A	810	ASP
1	A	829	LEU
1	A	834	LEU
1	A	856	THR
1	A	870	LEU
1	A	901	CYS
1	A	908	THR
1	A	924	LYS
1	A	929	LEU
1	A	933	ASP
1	A	937	PHE
1	A	944	LYS
1	A	945	PHE
1	A	951	ARG
1	A	956	LEU
1	A	959	ASP
1	A	965	SER
1	A	966	LYS
1	A	973	LYS
1	A	976	GLU
1	A	989	LEU
1	A	1001	LEU
1	A	1018	ASP
1	A	1022	ILE
1	A	1023	ARG
1	A	1036	LEU
1	A	1045	ASP
1	A	1053	THR
2	B	328	LEU
2	B	332	GLU

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Mol	Chain	Res	Type
2	B	334	TYR
2	B	342	GLU
2	B	355	PHE
2	B	356	LEU
2	B	368	TYR
2	B	371	THR
2	B	373	ARG
2	B	381	ILE
2	B	396	LEU
2	B	409	ARG
2	B	415	GLN
2	B	416	TYR
2	B	426	TYR
2	B	428	VAL
2	B	431	TYR
2	B	440	ASP
2	B	441	ASN
2	B	448	LYS
2	B	454	THR
2	B	459	LYS
2	B	467	TYR
2	B	485	GLU
2	B	498	CYS
2	B	500	THR
2	B	511	LYS
2	B	518	GLU
2	B	527	ASN
2	B	542	ARG
2	B	549	LEU
2	B	550	LYS
2	B	566	ILE
2	B	574	ARG
2	B	579	GLN
2	B	585	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-23	HIS
1	A	-20	HIS
1	A	75	GLN
1	A	107	ASN

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Mol	Chain	Res	Type
1	A	114	ASN
1	A	137	GLN
1	A	142	ASN
1	A	180	HIS
1	A	205	GLN
1	A	331	ASN
1	A	345	ASN
1	A	372	ASN
1	A	374	GLN
1	A	450	HIS
1	A	467	ASN
1	A	510	HIS
1	A	605	ASN
1	A	647	ASN
1	A	759	HIS
1	A	760	GLN
1	A	795	GLN
1	A	825	GLN
1	A	861	GLN
1	A	873	ASN
1	A	931	HIS
1	A	936	HIS
1	A	940	HIS
1	A	981	GLN
1	A	996	ASN
1	A	1042	GLN
1	A	1047	HIS
2	B	329	GLN
2	B	365	HIS
2	B	415	GLN
2	B	475	GLN
2	B	478	GLN
2	B	501	GLN
2	B	527	ASN
2	B	586	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 ligands are 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$
3	PBU	B	2001	-	39,39,39	1.95	8 (20%)	53,57,57	1.43	9 (16%)
4	PO4	A	1102	-	4,4,4	1.30	1 (25%)	6,6,6	0.48	0
3	PBU	A	1101	-	39,39,39	1.77	6 (15%)	53,57,57	1.67	11 (20%)

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
3	PBU	B	2001	-	-	13/36/60/60	0/1/1/1
3	PBU	A	1101	-	-	10/36/60/60	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	PBU	O1'-C11	6.09	1.51	1.33
3	A	1101	PBU	O1'-C11	5.53	1.49	1.33
3	A	1101	PBU	O2'-C7	4.97	1.48	1.34
3	B	2001	PBU	O2'-C7	4.57	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	PBU	P4-O4	4.15	1.67	1.59
3	B	2001	PBU	P5-O5	3.94	1.66	1.59
3	A	1101	PBU	P5-O5	3.87	1.66	1.59
3	A	1101	PBU	P4-O4	3.35	1.65	1.59
3	B	2001	PBU	P1-O1	2.87	1.68	1.60
3	A	1101	PBU	C1'-C2'	2.85	1.59	1.50
4	A	1102	PO4	P-O1	2.46	1.56	1.50
3	A	1101	PBU	C3'-C2'	2.34	1.57	1.50
3	B	2001	PBU	C5-C4	2.25	1.56	1.52
3	B	2001	PBU	C3-C4	2.25	1.58	1.52
3	B	2001	PBU	C1'-C2'	2.06	1.57	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	PBU	O2'-C7-C8	5.46	123.26	111.50
3	B	2001	PBU	O2'-C7-C8	3.97	120.06	111.50
3	A	1101	PBU	O1'-C11-C12	3.91	124.17	111.91
3	A	1101	PBU	O1-C1-C6	-3.64	100.19	108.66
3	B	2001	PBU	O5-C5-C4	3.43	116.77	108.69
3	A	1101	PBU	O1'-C1'-C2'	3.36	118.21	108.43
3	B	2001	PBU	C2-C3-C4	2.87	116.24	109.68
3	A	1101	PBU	C6-C5-C4	-2.83	105.21	111.66
3	A	1101	PBU	O5-C5-C4	2.79	115.27	108.69
3	A	1101	PBU	O2'-C7-O7	-2.64	117.33	123.70
3	B	2001	PBU	O2'-C7-O7	-2.51	117.65	123.70
3	A	1101	PBU	C3-C2-C1	2.36	115.08	109.68
3	B	2001	PBU	O1'-C1'-C2'	2.36	115.30	108.43
3	A	1101	PBU	O53-P5-O52	2.31	116.47	107.64
3	B	2001	PBU	O53-P5-O52	2.27	116.32	107.64
3	B	2001	PBU	C1'-O1'-C11	2.27	125.53	117.12
3	A	1101	PBU	O1'-C11-O11	-2.20	118.05	123.59
3	B	2001	PBU	O1-C1-C6	2.18	113.74	108.66
3	B	2001	PBU	O1'-C11-C12	2.14	118.63	111.91
3	A	1101	PBU	C6-C1-C2	2.01	113.75	110.85

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2001	PBU	C3'-OP1-P1-OP2
3	B	2001	PBU	C5-O5-P5-O51

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Mol	Chain	Res	Type	Atoms
3	B	2001	PBU	C8-C7-O2'-C2'
3	A	1101	PBU	C2-C1-O1-P1
3	A	1101	PBU	C6-C1-O1-P1
3	B	2001	PBU	O7-C7-O2'-C2'
3	A	1101	PBU	C1-O1-P1-OP1
3	A	1101	PBU	C8-C7-O2'-C2'
3	A	1101	PBU	O7-C7-O2'-C2'
3	B	2001	PBU	C1-O1-P1-OP1
3	B	2001	PBU	C11-C12-C13-C14
3	A	1101	PBU	C1-O1-P1-OP3
3	A	1101	PBU	C4-O4-P4-O41
3	B	2001	PBU	C2'-C3'-OP1-P1
3	A	1101	PBU	C7-C8-C9-C10
3	B	2001	PBU	C3'-OP1-P1-O1
3	B	2001	PBU	C6-C1-O1-P1
3	B	2001	PBU	C4-O4-P4-O41
3	A	1101	PBU	C5-O5-P5-O51
3	B	2001	PBU	O1'-C11-C12-C13
3	B	2001	PBU	C5-O5-P5-O52
3	A	1101	PBU	C5-O5-P5-O53
3	B	2001	PBU	O11-C11-C12-C13

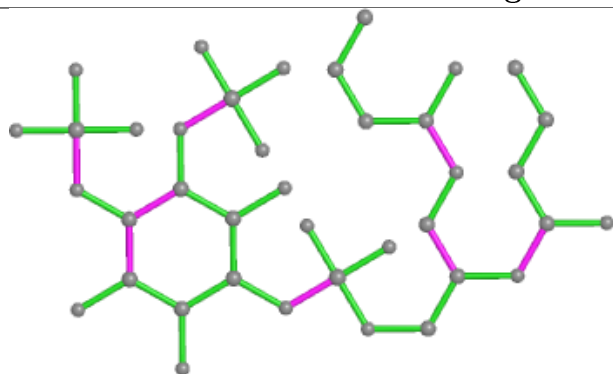
There are no ring outliers.

1 monomer is involved in 1 short contact:

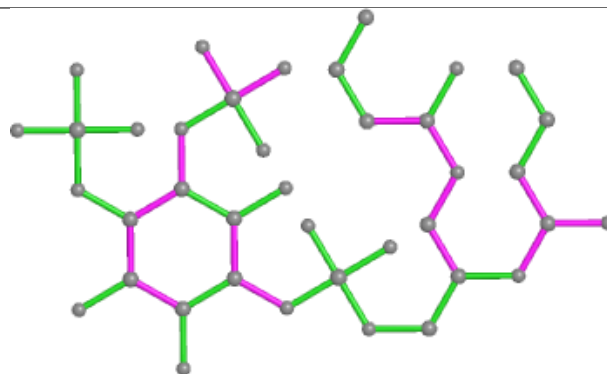
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	PBU	1	0

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.

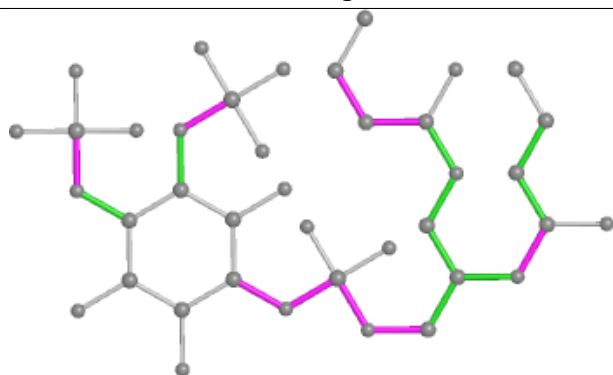
Ligand PBU B 2001



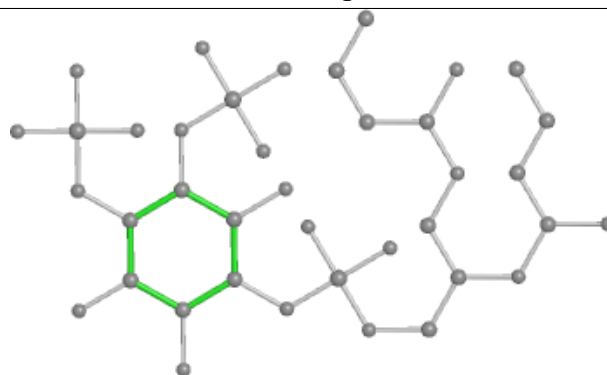
Bond lengths



Bond angles

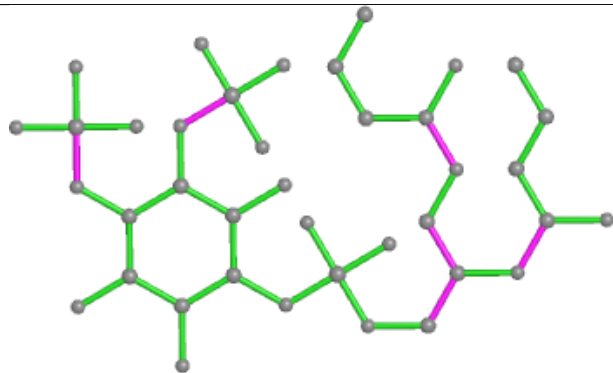


Torsions

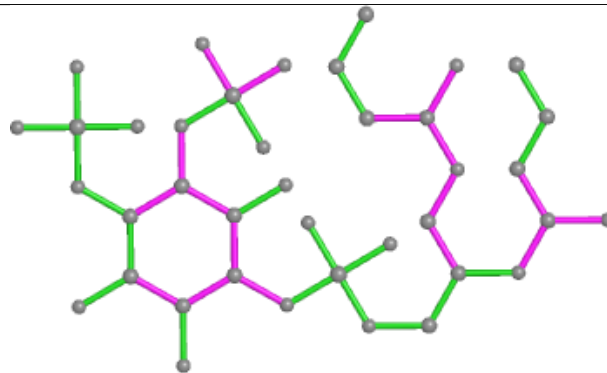


Rings

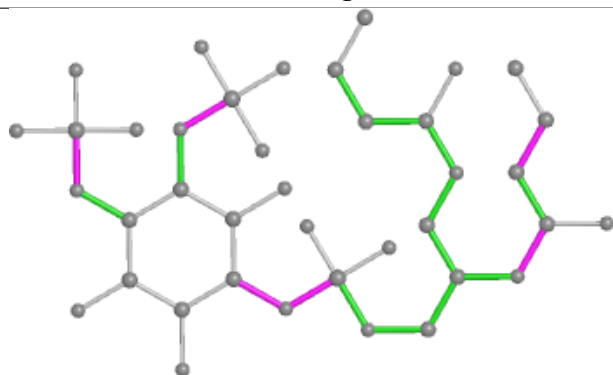
Ligand PBU A 1101



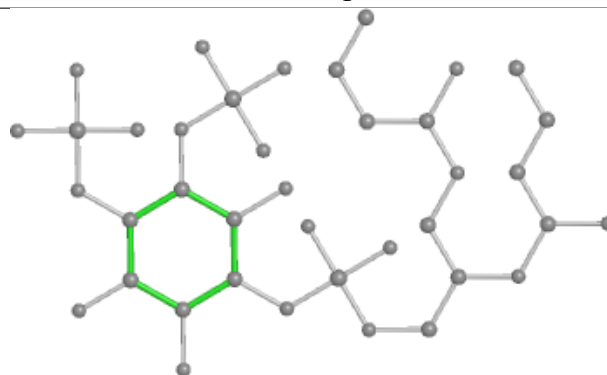
Bond lengths



Bond angles



Torsions



Rings

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	1042/1096 (95%)	-0.25	9 (0%) 84 79	66, 83, 107, 127	0
2	B	241/279 (86%)	0.27	13 (5%) 25 23	108, 130, 154, 163	0
All	All	1283/1375 (93%)	-0.15	22 (1%) 70 64	66, 87, 139, 163	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	520	ASP	6.3
1	A	322	THR	4.8
2	B	434	ASP	4.4
2	B	415	GLN	4.1
2	B	335	TRP	3.3
1	A	521	ASN	3.2
2	B	397	THR	3.0
2	B	377	ASN	2.8
2	B	430	LYS	2.7
1	A	408	SER	2.6
1	A	867	LYS	2.6
2	B	432	GLN	2.4
2	B	407	HIS	2.4
2	B	433	GLN	2.3
1	A	524	ARG	2.3
1	A	523	LEU	2.2
1	A	418	GLU	2.2
2	B	593	LYS	2.1
2	B	543	ARG	2.1
1	A	866	LEU	2.1
2	B	580	TYR	2.1
2	B	435	GLN	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 ⓘ

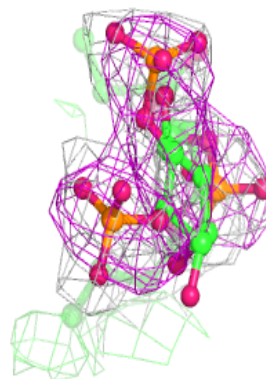
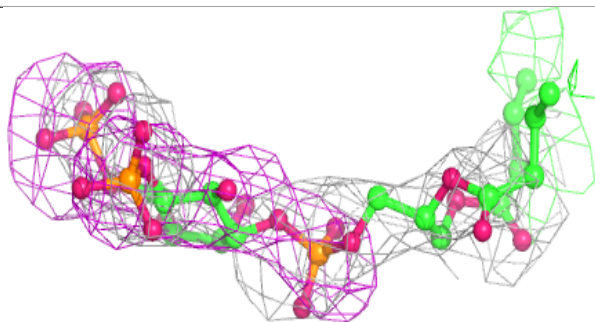
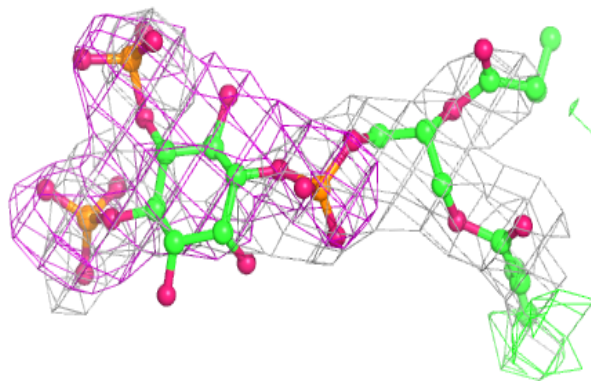
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PBU	A	1101	39/39	0.72	0.50	111,115,121,124	0
3	PBU	B	2001	39/39	0.74	0.38	109,113,117,118	0
4	PO4	A	1102	5/5	0.92	0.28	90,90,90,90	0

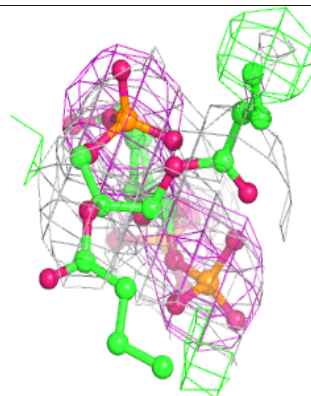
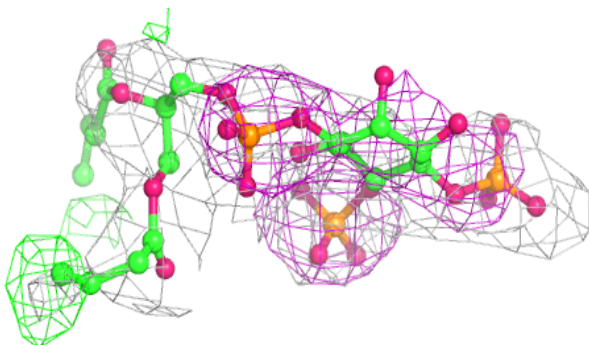
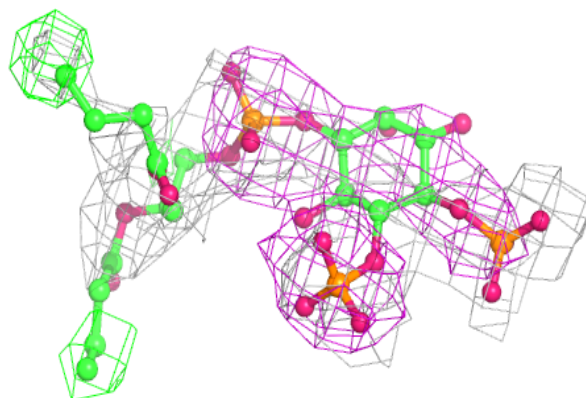
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PBU A 1101:

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

**Electron density around PBU B 2001:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.