Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2021 – 03:01 PM EDT

PDB ID	:	3EJL
Title	:	Replacement of Val3 in Human Thymidylate Synthase Affects Its Kinetic Properties and Intracellular Stability
Authors	:	Huang, X.; Gibson, L.M.; Bell, B.J.; Lovelace, L.L.; Pena, M.M.; Berger, F.G.; Berger, S.H.
Deposited on	:	2008-09-18
Resolution	:	3.20 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 (i) symbol.

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

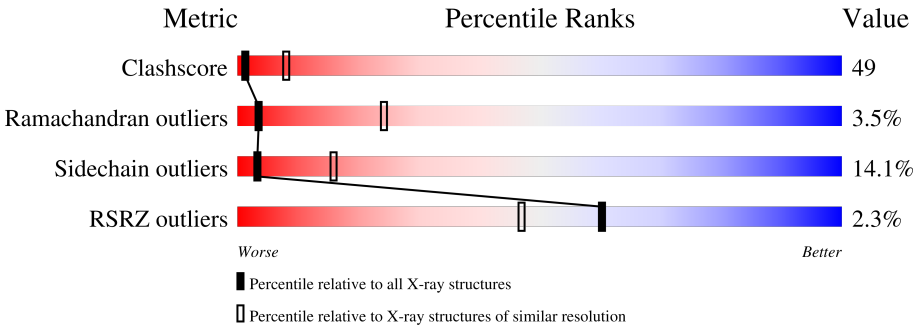
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	313	2% 33% 53% • 10%
1	B	313	2% 27% 53% 10% 10%
1	C	313	2% 28% 53% 9% 10%
1	D	313	3% 26% 51% 11% • 10%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	D	616	-	-	X	-
3	UFP	D	314	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9217 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.

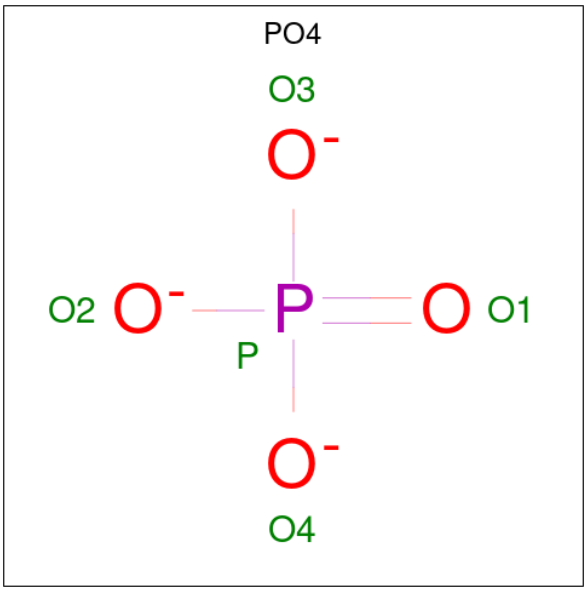
- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2287	1463	400	413	11			
1	B	283	Total	C	N	O	S	0	0	0
			2287	1463	400	413	11			
1	C	283	Total	C	N	O	S	0	0	0
			2287	1463	400	413	11			
1	D	283	Total	C	N	O	S	0	0	0
			2287	1463	400	413	11			

There are 4 discrepancies between the modelled and reference sequences:

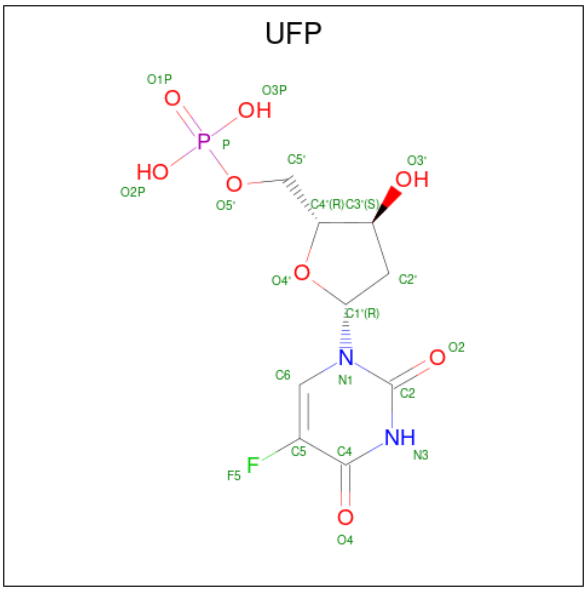
Chain	Residue	Modelled	Actual	Comment	Reference
A	3	PHE	VAL	engineered mutation	UNP P04818
B	3	PHE	VAL	engineered mutation	UNP P04818
C	3	PHE	VAL	engineered mutation	UNP P04818
D	3	PHE	VAL	engineered mutation	UNP P04818

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

- Molecule 3 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: UFP) (formula: $C_9H_{12}FN_2O_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	F	N	O	P	0	0
			21	9	1	2	8	1		

- Molecule 4 is water.

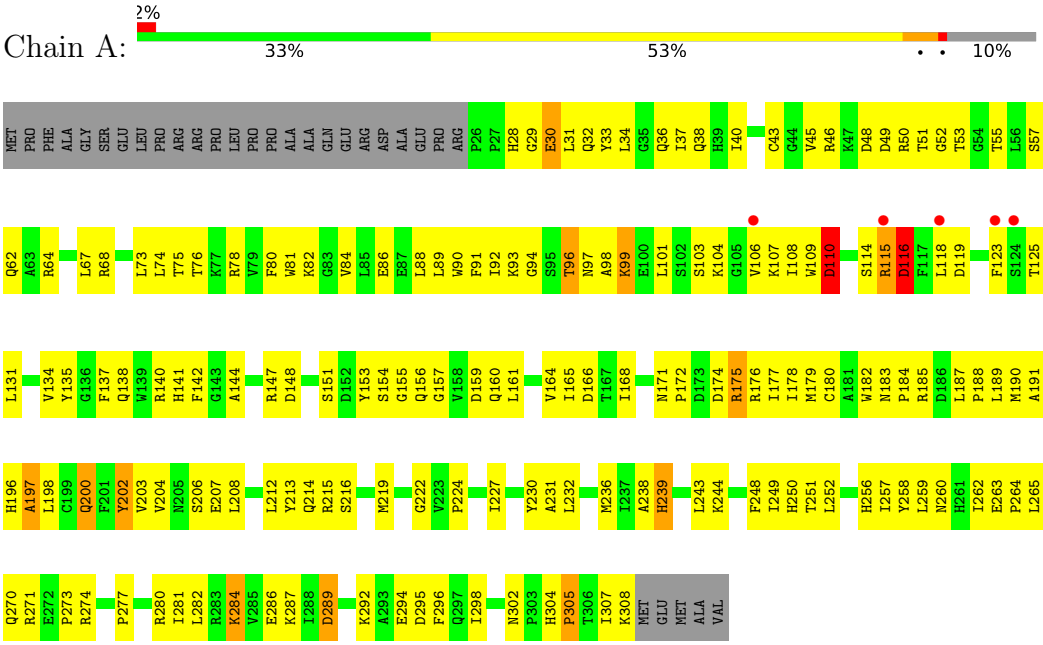
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	11	Total	O	0	0
			11	11		
4	C	8	Total	O	0	0
			8	8		
4	D	6	Total	O	0	0
			6	6		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

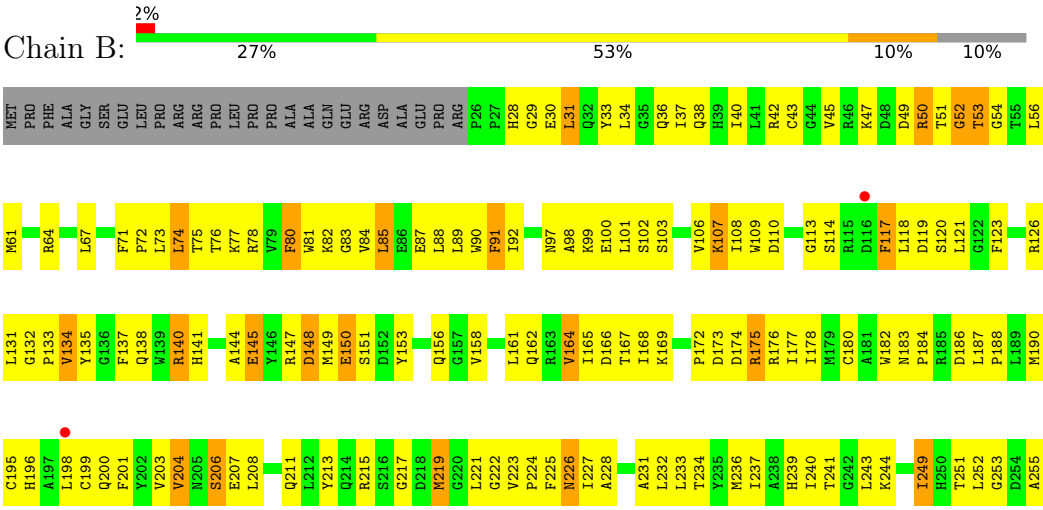
• Molecule 1: Thymidylate synthase

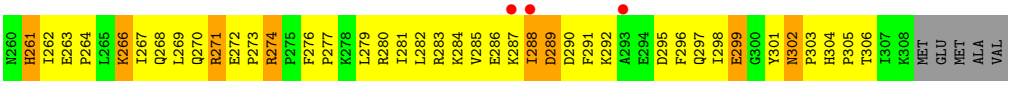
Chain A:



• Molecule 1: Thymidylate synthase

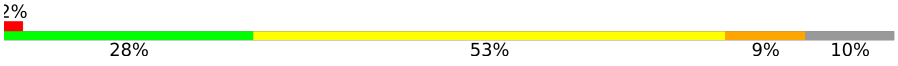
Chain B:

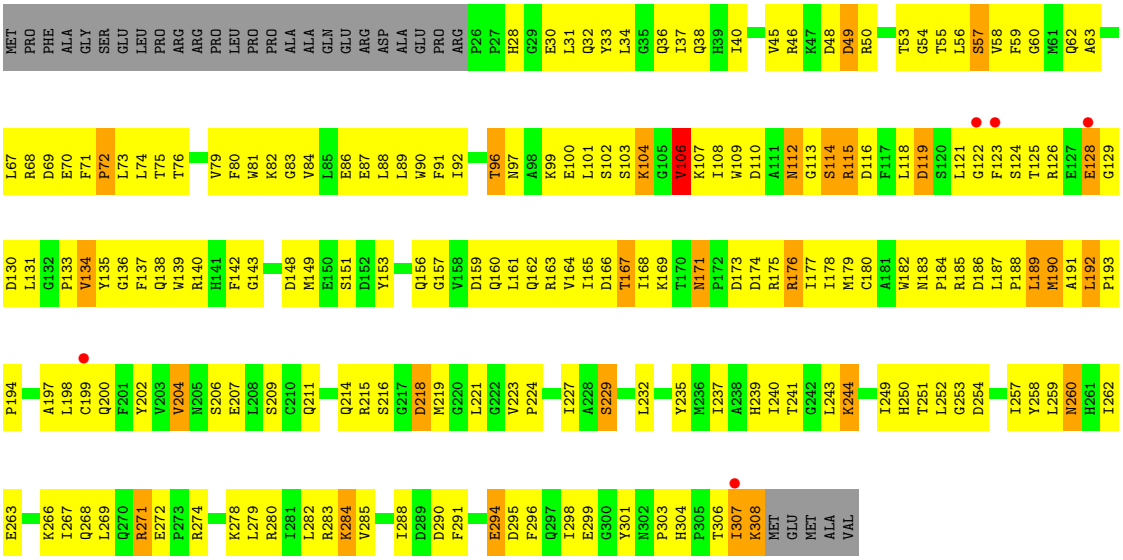




• Molecule 1: Thymidylate synthase

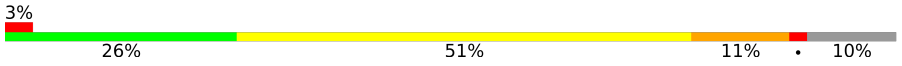
Chain C:

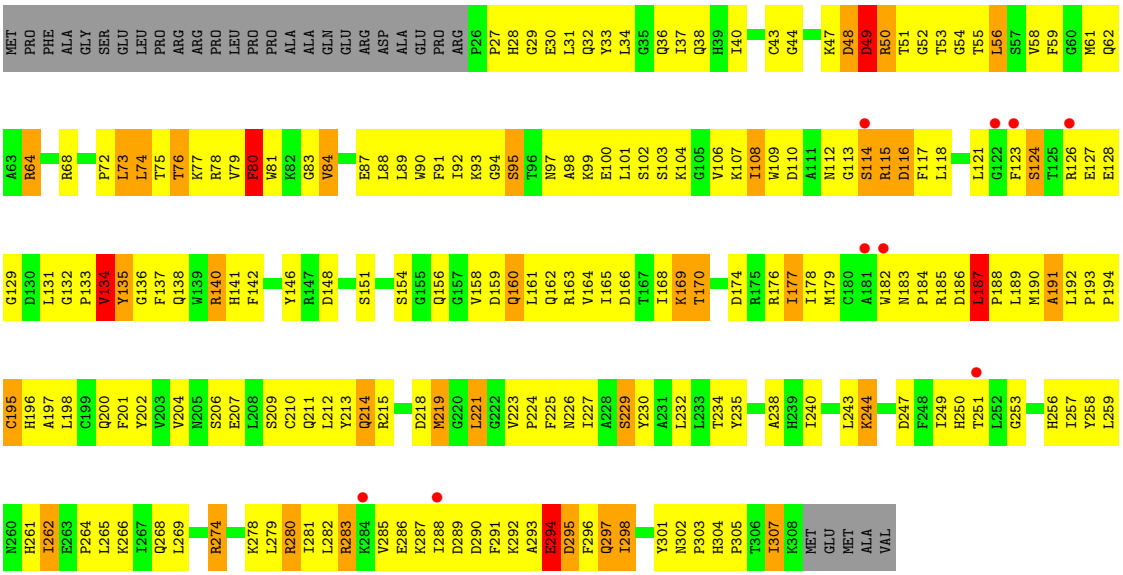




• Molecule 1: Thymidylate synthase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.44Å 94.64Å 131.99Å 90.00° 122.35° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 43.56 – 2.78	Depositor EDS
% Data completeness (in resolution range)	72.0 (50.00-3.20) 62.1 (43.56-2.78)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.257 0.237 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	70.6	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 109.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9217	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: UFP, 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	0.48	0/2347	0.65	0/3175
1	B	0.46	0/2347	0.70	3/3175 (0.1%)
1	C	0.47	0/2347	0.64	0/3175
1	D	0.48	0/2347	0.75	5/3175 (0.2%)
All	All	0.47	0/9388	0.69	8/12700 (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	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	49	ASP	N-CA-CB	-8.55	95.21	110.60
1	D	56	LEU	N-CA-C	-7.47	90.83	111.00
1	B	52	GLY	N-CA-C	6.85	130.23	113.10
1	D	294	GLU	N-CA-C	6.46	128.45	111.00
1	D	295	ASP	N-CA-C	6.13	127.55	111.00
1	B	150	GLU	N-CA-C	5.36	125.47	111.00
1	D	48	ASP	CA-C-N	-5.16	105.85	117.20
1	B	274	ARG	NE-CZ-NH1	-5.11	117.75	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2287	0	2258	179	1
1	B	2287	0	2259	258	1
1	C	2287	0	2259	242	0
1	D	2287	0	2257	290	0
2	B	10	0	0	1	0
2	D	5	0	0	3	0
3	D	21	0	10	14	0
4	A	8	0	0	0	0
4	B	11	0	0	1	0
4	C	8	0	0	1	0
4	D	6	0	0	0	0
All	All	9217	0	9043	902	1

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 49.

All (902) 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:C:143:GLY:HA3	1:D:185:ARG:HD3	1.31	1.12
1:A:153:TYR:O	1:A:156:GLN:HB3	1.48	1.11
1:D:97:ASN:HD22	1:D:100:GLU:HG2	1.12	1.10
1:D:49:ASP:OD2	1:D:54:GLY:HA2	1.53	1.06
1:A:153:TYR:O	1:A:156:GLN:CB	2.05	1.04
1:C:267:ILE:HD12	1:C:307:ILE:HD11	1.39	1.04
1:C:176:ARG:HD3	3:D:314:UFP:H2'1	1.35	1.03
1:D:193:PRO:HG2	3:D:314:UFP:H2'2	1.39	1.02
1:B:92:ILE:CD1	1:B:288:ILE:HD11	1.89	1.01
1:B:50:ARG:C	1:B:52:GLY:H	1.62	1.00
1:D:282:LEU:HD11	1:D:297:GLN:HB2	1.42	0.99
1:B:274:ARG:NH2	1:B:304:HIS:HA	1.77	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ASP:OD1	1:D:151:SER:HB2	1.63	0.99
1:D:138:GLN:HE22	1:D:183:ASN:HB2	1.25	0.98
1:C:50:ARG:HD2	1:D:176:ARG:HH21	1.28	0.98
1:D:164:VAL:HG13	1:D:177:ILE:HG22	1.47	0.96
1:B:92:ILE:CD1	1:B:288:ILE:CD1	2.42	0.96
1:C:38:GLN:HE21	1:C:269:LEU:HD13	1.28	0.94
1:B:92:ILE:HD12	1:B:288:ILE:HD13	1.50	0.93
1:C:282:LEU:HG	1:C:295:ASP:O	1.67	0.93
1:B:73:LEU:HB2	1:B:277:PRO:HG2	1.51	0.93
1:A:174:ASP:OD2	1:A:176:ARG:HG2	1.69	0.93
1:D:50:ARG:HD3	1:D:50:ARG:H	1.34	0.92
1:A:176:ARG:NH1	1:B:193:PRO:HG2	1.84	0.92
1:D:292:LYS:C	1:D:294:GLU:H	1.71	0.91
1:C:176:ARG:CZ	1:D:193:PRO:HB3	2.01	0.91
1:B:97:ASN:HD22	1:B:100:GLU:HB2	1.37	0.90
1:C:97:ASN:HA	1:C:129:GLY:O	1.71	0.90
1:D:193:PRO:HG2	3:D:314:UFP:C2'	2.02	0.89
1:B:118:LEU:HD13	1:B:126:ARG:HG2	1.55	0.89
1:D:50:ARG:NH1	1:D:258:TYR:OH	2.05	0.89
1:D:126:ARG:NH2	1:D:131:LEU:O	2.04	0.89
1:C:40:ILE:HD13	1:C:219:MET:HG3	1.55	0.89
1:A:118:LEU:HD21	1:A:126:ARG:HB3	1.52	0.89
1:A:214:GLN:HB3	1:A:252:LEU:HD23	1.54	0.89
1:D:50:ARG:HG2	3:D:314:UFP:O5'	1.74	0.88
1:D:133:PRO:HG3	1:D:146:TYR:CG	2.08	0.88
1:A:98:ALA:HB2	1:A:131:LEU:HD11	1.56	0.87
1:C:282:LEU:HD12	1:C:294:GLU:O	1.74	0.87
1:B:75:THR:HG21	1:B:274:ARG:O	1.75	0.87
1:B:92:ILE:CG1	1:B:288:ILE:HD11	2.05	0.86
1:B:92:ILE:HD12	1:B:288:ILE:CD1	2.06	0.85
1:D:97:ASN:ND2	1:D:100:GLU:HG2	1.91	0.85
1:B:169:LYS:HE3	1:B:241:THR:HG22	1.59	0.85
1:C:99:LYS:HE2	1:C:128:GLU:OE2	1.76	0.84
1:D:48:ASP:HA	1:D:49:ASP:OD2	1.76	0.84
1:A:148:ASP:OD2	1:A:151:SER:HB2	1.77	0.84
1:C:165:ILE:HG12	1:C:237:ILE:HD12	1.60	0.84
1:B:49:ASP:O	1:B:52:GLY:HA2	1.79	0.83
1:B:240:ILE:HG23	1:B:286:GLU:O	1.79	0.83
1:D:161:LEU:HD21	1:D:288:ILE:HD13	1.58	0.83
1:C:112:ASN:HB3	1:C:192:LEU:HD11	1.61	0.82
1:B:92:ILE:HG13	1:B:288:ILE:HD11	1.58	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LYS:HG2	1:B:289:ASP:OD2	1.81	0.81
1:D:140:ARG:NH2	1:D:161:LEU:HB3	1.95	0.81
1:B:288:ILE:HA	1:B:291:PHE:CD2	2.16	0.81
1:C:40:ILE:CD1	1:C:219:MET:HG3	2.10	0.80
1:D:83:GLY:HA2	1:D:106:VAL:HG21	1.61	0.80
1:D:91:PHE:CE1	1:D:135:TYR:HB2	2.17	0.80
1:D:97:ASN:HD21	1:D:99:LYS:HB2	1.47	0.79
1:C:267:ILE:CD1	1:C:307:ILE:HD11	2.11	0.78
1:B:174:ASP:O	1:B:177:ILE:HD11	1.83	0.78
1:C:143:GLY:CA	1:D:185:ARG:HD3	2.12	0.78
1:D:274:ARG:HB2	1:D:274:ARG:HH11	1.48	0.78
1:A:91:PHE:CE1	1:A:135:TYR:HB2	2.18	0.77
1:A:187:LEU:HA	1:A:190:MET:HE3	1.65	0.77
1:B:285:VAL:HG13	1:B:290:ASP:HB2	1.66	0.77
1:A:257:ILE:O	1:A:257:ILE:HG13	1.83	0.76
1:B:73:LEU:CB	1:B:277:PRO:HG2	2.16	0.76
1:C:214:GLN:HB3	1:C:252:LEU:HD23	1.67	0.76
1:C:200:GLN:NE2	1:D:215:ARG:HB2	2.00	0.76
1:B:267:ILE:HD13	1:B:270:GLN:HE21	1.51	0.76
1:B:92:ILE:HD11	1:B:288:ILE:HD11	1.67	0.76
1:C:219:MET:HB2	1:C:257:ILE:HG23	1.67	0.76
1:D:133:PRO:HD3	1:D:146:TYR:CD2	2.19	0.76
1:D:148:ASP:OD1	1:D:151:SER:CB	2.34	0.75
1:A:206:SER:O	1:A:244:LYS:HG2	1.85	0.75
1:B:92:ILE:HG21	1:B:288:ILE:HG12	1.68	0.75
1:B:240:ILE:HD11	1:B:291:PHE:HE2	1.49	0.75
1:B:102:SER:HA	1:B:106:VAL:O	1.86	0.75
1:B:177:ILE:HD12	1:B:177:ILE:H	1.52	0.75
1:B:192:LEU:HD22	4:B:316:HOH:O	1.86	0.75
1:A:204:VAL:HG21	1:B:45:VAL:HG21	1.67	0.74
1:B:274:ARG:NH1	1:B:303:PRO:C	2.39	0.74
1:A:161:LEU:O	1:A:165:ILE:HG12	1.87	0.74
1:A:274:ARG:HD2	1:A:302:ASN:O	1.87	0.74
1:A:265:LEU:O	1:A:269:LEU:HB2	1.87	0.74
1:B:279:LEU:HD11	1:B:296:PHE:HB3	1.69	0.74
1:D:115:ARG:NH2	1:D:124:SER:HA	2.03	0.74
1:D:138:GLN:NE2	1:D:183:ASN:HB2	2.00	0.74
1:D:292:LYS:O	1:D:294:GLU:N	2.21	0.74
1:D:133:PRO:HG3	1:D:146:TYR:CB	2.17	0.73
1:A:292:LYS:HD2	1:A:294:GLU:OE2	1.88	0.73
1:C:193:PRO:HD2	1:D:176:ARG:NH1	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ILE:HG21	1:C:307:ILE:HG13	1.71	0.73
1:D:112:ASN:ND2	1:D:192:LEU:HB2	2.03	0.73
1:B:161:LEU:O	1:B:165:ILE:HD12	1.87	0.73
1:C:153:TYR:HA	1:C:156:GLN:OE1	1.89	0.73
1:D:279:LEU:HD11	1:D:296:PHE:HB3	1.69	0.73
1:B:97:ASN:HB2	1:B:149:MET:SD	2.29	0.73
1:C:271:ARG:HH12	1:C:307:ILE:HB	1.53	0.73
1:B:240:ILE:CD1	1:B:288:ILE:N	2.52	0.72
1:B:274:ARG:NH1	1:B:303:PRO:O	2.21	0.72
1:D:133:PRO:HD3	1:D:146:TYR:CE2	2.24	0.72
1:B:280:ARG:HD2	1:B:299:GLU:OE1	1.89	0.72
1:D:50:ARG:CD	3:D:314:UFP:O2P	2.37	0.72
1:B:83:GLY:O	1:B:87:GLU:HB2	1.90	0.72
1:C:279:LEU:HD13	1:C:298:ILE:HD13	1.72	0.71
1:B:274:ARG:HD3	1:B:302:ASN:O	1.90	0.71
1:B:231:ALA:O	1:B:234:THR:HB	1.90	0.71
1:D:50:ARG:NE	3:D:314:UFP:O2P	2.24	0.70
1:A:147:ARG:NE	1:A:151:SER:OG	2.15	0.70
1:B:74:LEU:HG	1:B:224:PRO:HB3	1.72	0.70
1:B:211:GLN:HA	1:B:249:ILE:O	1.92	0.70
1:B:90:TRP:CE3	1:B:101:LEU:HD22	2.27	0.70
1:B:240:ILE:HD13	1:B:288:ILE:H	1.56	0.70
1:C:268:GLN:HA	1:C:271:ARG:HD3	1.73	0.70
1:A:64:ARG:CZ	1:A:249:ILE:HD11	2.22	0.70
1:C:140:ARG:O	1:C:159:ASP:HA	1.91	0.70
1:D:88:LEU:HD23	1:D:232:LEU:HD23	1.73	0.70
1:D:196:HIS:HD2	1:D:230:TYR:CE2	2.09	0.70
1:A:88:LEU:HD23	1:A:232:LEU:HD23	1.73	0.70
1:A:267:ILE:HG21	1:A:307:ILE:HD11	1.74	0.69
1:C:88:LEU:HD23	1:C:232:LEU:HD23	1.72	0.69
1:A:154:SER:C	1:A:156:GLN:H	1.94	0.69
1:D:292:LYS:C	1:D:294:GLU:N	2.45	0.69
1:A:90:TRP:HA	1:A:93:LYS:HE2	1.75	0.69
1:D:294:GLU:HB3	1:D:295:ASP:OD2	1.92	0.69
1:B:37:ILE:HD11	1:B:219:MET:HB3	1.73	0.69
1:C:97:ASN:HD22	1:C:100:GLU:HB2	1.58	0.69
1:C:102:SER:HB2	1:C:107:LYS:CD	2.21	0.69
1:B:288:ILE:HA	1:B:291:PHE:HD2	1.57	0.68
1:C:307:ILE:HD13	1:C:308:LYS:N	2.08	0.68
1:D:36:GLN:OE1	1:D:61:MET:HB3	1.94	0.68
1:A:32:GLN:NE2	1:A:64:ARG:H	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:GLU:HG2	1:C:104:LYS:HG3	1.74	0.68
1:C:142:PHE:CE2	1:D:184:PRO:HD2	2.29	0.68
1:D:166:ASP:O	1:D:169:LYS:HG3	1.94	0.68
1:B:97:ASN:HB2	1:B:149:MET:CG	2.23	0.68
1:A:176:ARG:CZ	1:B:193:PRO:HG2	2.22	0.68
1:D:37:ILE:HD13	1:D:219:MET:HG3	1.73	0.68
1:D:285:VAL:HG13	1:D:290:ASP:HB2	1.75	0.67
1:A:99:LYS:HG3	1:A:129:GLY:HA3	1.74	0.67
1:C:241:THR:OG1	1:C:243:LEU:HD12	1.94	0.67
1:A:81:TRP:CH2	1:A:298:ILE:HD11	2.29	0.67
1:C:76:THR:HA	1:C:304:HIS:HD2	1.59	0.67
1:D:106:VAL:HG12	1:D:108:ILE:HD12	1.76	0.67
1:B:50:ARG:C	1:B:52:GLY:N	2.38	0.67
1:C:130:ASP:HB2	1:C:149:MET:HG2	1.74	0.67
1:C:153:TYR:O	1:C:156:GLN:HB2	1.95	0.67
1:D:249:ILE:N	1:D:249:ILE:HD12	2.10	0.67
1:A:89:LEU:O	1:A:93:LYS:HG3	1.95	0.67
1:B:177:ILE:HD13	1:B:201:PHE:O	1.95	0.67
1:C:200:GLN:HE22	1:D:215:ARG:HB2	1.60	0.66
1:A:107:LYS:HB3	1:A:110:ASP:OD2	1.96	0.66
1:B:274:ARG:CD	1:B:302:ASN:O	2.43	0.66
1:D:101:LEU:CD2	1:D:108:ILE:HD11	2.26	0.66
1:C:133:PRO:HG2	1:C:186:ASP:HB3	1.78	0.66
1:C:263:GLU:HA	1:C:266:LYS:HD3	1.77	0.66
1:D:259:LEU:HA	1:D:262:ILE:CD1	2.26	0.66
1:B:73:LEU:HD23	1:B:301:TYR:CD1	2.31	0.66
1:A:263:GLU:HB3	1:A:264:PRO:HD3	1.77	0.66
1:C:182:TRP:O	1:C:184:PRO:HD3	1.96	0.66
1:B:183:ASN:O	1:B:187:LEU:HG	1.95	0.65
1:C:176:ARG:HH21	1:D:187:LEU:HD11	1.61	0.65
1:C:218:ASP:OD2	1:C:221:LEU:HD23	1.96	0.65
1:D:184:PRO:O	1:D:187:LEU:HB2	1.96	0.65
1:A:36:GLN:O	1:A:40:ILE:HD13	1.96	0.65
1:B:97:ASN:HB2	1:B:149:MET:HG3	1.77	0.65
1:D:80:PHE:CE2	1:D:106:VAL:HG13	2.32	0.65
1:C:207:GLU:HG3	1:C:244:LYS:HZ3	1.61	0.65
1:D:118:LEU:HA	1:D:121:LEU:HD12	1.79	0.65
1:A:154:SER:C	1:A:156:GLN:N	2.49	0.65
1:D:33:TYR:HD1	1:D:34:LEU:HD23	1.61	0.65
1:B:34:LEU:HD11	1:B:76:THR:HG21	1.77	0.65
1:A:164:VAL:O	1:A:168:ILE:HG12	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:GLN:NE2	1:D:269:LEU:HD23	2.11	0.64
1:D:97:ASN:HA	1:D:129:GLY:O	1.97	0.64
1:B:36:GLN:O	1:B:40:ILE:HG12	1.97	0.64
1:C:223:VAL:HB	1:C:224:PRO:HD3	1.79	0.64
1:B:177:ILE:CG2	1:B:201:PHE:HB2	2.27	0.64
1:B:259:LEU:O	1:B:262:ILE:HG12	1.98	0.64
1:C:176:ARG:HH22	1:D:194:PRO:HD2	1.62	0.64
1:C:186:ASP:O	1:C:190:MET:HG2	1.96	0.64
1:D:40:ILE:HD12	1:D:219:MET:HG2	1.80	0.64
1:C:176:ARG:HE	1:D:187:LEU:HD11	1.62	0.64
1:D:97:ASN:ND2	1:D:99:LYS:HB2	2.12	0.64
1:D:287:LYS:HB3	1:D:290:ASP:OD1	1.97	0.64
1:A:64:ARG:HB2	1:A:249:ILE:HD13	1.79	0.64
1:D:142:PHE:HB3	1:D:158:VAL:HB	1.79	0.64
1:C:86:GLU:CG	1:C:104:LYS:HG3	2.28	0.64
1:C:176:ARG:CZ	1:D:193:PRO:CB	2.73	0.64
1:D:193:PRO:HG2	3:D:314:UFP:O3'	1.98	0.63
1:C:88:LEU:HD23	1:C:232:LEU:CD2	2.28	0.63
1:C:115:ARG:HE	1:C:115:ARG:HA	1.63	0.63
1:C:240:ILE:HD11	1:C:288:ILE:HA	1.79	0.63
1:D:50:ARG:HD2	3:D:314:UFP:O2P	1.98	0.63
1:A:271:ARG:NH2	1:A:307:ILE:HB	2.13	0.63
1:B:240:ILE:HD13	1:B:288:ILE:N	2.12	0.63
1:C:32:GLN:HB3	1:C:63:ALA:HB1	1.80	0.63
1:C:176:ARG:HD3	3:D:314:UFP:C2'	2.21	0.63
1:A:37:ILE:HD13	1:A:265:LEU:CD2	2.29	0.63
1:C:123:PHE:CZ	1:C:189:LEU:HA	2.33	0.63
1:D:196:HIS:CD2	1:D:230:TYR:CE2	2.87	0.63
1:D:75:THR:HG21	1:D:274:ARG:O	1.98	0.63
1:C:139:TRP:C	1:C:140:ARG:HD2	2.19	0.63
1:C:168:ILE:HD13	1:C:177:ILE:HD13	1.81	0.63
1:B:267:ILE:HA	1:B:270:GLN:HG3	1.81	0.63
1:B:50:ARG:O	1:B:52:GLY:N	2.31	0.62
1:A:30:GLU:OE2	1:A:76:THR:HG23	1.98	0.62
1:C:71:PHE:HE1	1:C:73:LEU:HD13	1.64	0.62
1:C:142:PHE:CZ	1:D:184:PRO:HD2	2.34	0.62
1:D:282:LEU:O	1:D:283:ARG:HB2	2.00	0.62
1:D:196:HIS:CE1	1:D:226:ASN:CG	2.73	0.62
1:A:151:SER:O	1:A:153:TYR:CE1	2.53	0.62
1:B:91:PHE:CE1	1:B:135:TYR:HB2	2.34	0.62
1:C:30:GLU:OE1	1:C:75:THR:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ASN:H	1:C:112:ASN:ND2	1.98	0.62
1:D:108:ILE:HD13	1:D:108:ILE:H	1.64	0.62
1:B:117:PHE:O	1:B:120:SER:HB3	2.00	0.62
1:B:240:ILE:HD11	1:B:288:ILE:N	2.13	0.62
1:D:195:CYS:O	1:D:214:GLN:HA	1.98	0.62
1:D:298:ILE:HD13	1:D:298:ILE:N	2.14	0.62
1:C:134:VAL:O	1:C:138:GLN:HG2	2.00	0.62
1:C:60:GLY:O	1:D:64:ARG:NH1	2.33	0.61
1:C:76:THR:HA	1:C:304:HIS:CD2	2.35	0.61
1:C:307:ILE:HD13	1:C:307:ILE:C	2.20	0.61
1:D:49:ASP:CG	1:D:53:THR:O	2.37	0.61
1:D:178:ILE:HD13	1:D:200:GLN:HB2	1.80	0.61
1:D:229:SER:HG	1:D:230:TYR:HD2	1.46	0.61
1:B:140:ARG:CZ	1:B:161:LEU:HD23	2.30	0.61
1:B:241:THR:OG1	1:B:243:LEU:HD12	2.01	0.61
1:D:196:HIS:HE1	1:D:226:ASN:CG	2.03	0.61
1:B:92:ILE:HD11	1:B:288:ILE:CD1	2.27	0.61
1:B:233:LEU:HD11	1:B:237:ILE:HD11	1.81	0.61
1:D:154:SER:O	1:D:156:GLN:HG3	1.99	0.61
1:D:211:GLN:HG3	1:D:249:ILE:HB	1.83	0.61
1:D:94:GLY:HA2	1:D:136:GLY:O	2.00	0.61
1:D:114:SER:O	1:D:118:LEU:HG	2.00	0.61
1:D:261:HIS:C	1:D:264:PRO:HD2	2.20	0.61
1:A:175:ARG:NH1	1:B:47:LYS:NZ	2.49	0.61
1:B:92:ILE:CD1	1:B:288:ILE:HD13	2.17	0.61
1:B:102:SER:HB3	1:B:110:ASP:OD1	2.01	0.61
1:A:98:ALA:HB2	1:A:131:LEU:HD21	1.83	0.61
1:B:85:LEU:HD12	1:B:89:LEU:HD11	1.81	0.61
1:A:37:ILE:HD13	1:A:265:LEU:HD21	1.83	0.61
1:B:240:ILE:CD1	1:B:288:ILE:H	2.14	0.61
1:C:107:LYS:HD2	1:C:110:ASP:OD2	2.00	0.61
1:B:201:PHE:CZ	1:B:237:ILE:HD12	2.35	0.60
1:C:283:ARG:NH2	1:C:285:VAL:HG22	2.16	0.60
1:D:212:LEU:HD13	1:D:230:TYR:CE1	2.36	0.60
1:D:135:TYR:CE1	1:D:194:PRO:HB3	2.36	0.60
1:B:262:ILE:O	1:B:266:LYS:HG2	2.00	0.60
1:C:283:ARG:HH22	1:C:285:VAL:HG22	1.66	0.60
1:D:117:PHE:CE2	1:D:121:LEU:HD11	2.36	0.60
1:B:126:ARG:HG3	1:B:130:ASP:HB3	1.83	0.60
1:C:130:ASP:HB2	1:C:149:MET:CG	2.31	0.60
1:B:92:ILE:HG13	1:B:288:ILE:CD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:LEU:HD12	1:D:198:LEU:C	2.21	0.60
1:B:182:TRP:HZ3	1:B:215:ARG:HE	1.50	0.60
1:B:34:LEU:HD21	1:B:268:GLN:HE21	1.66	0.60
1:B:233:LEU:O	1:B:237:ILE:HG13	2.01	0.60
1:A:126:ARG:HD3	1:A:130:ASP:O	2.02	0.59
1:D:102:SER:HA	1:D:106:VAL:O	2.01	0.59
1:D:59:PHE:HA	1:D:253:GLY:O	2.02	0.59
1:D:76:THR:HB	1:D:268:GLN:HG3	1.84	0.59
1:D:81:TRP:O	1:D:84:VAL:HB	2.02	0.59
1:A:135:TYR:HE1	1:A:196:HIS:HB2	1.67	0.59
1:C:271:ARG:HH21	1:C:304:HIS:HB3	1.66	0.59
1:B:118:LEU:HD22	1:B:126:ARG:HG2	1.84	0.59
1:B:118:LEU:CD1	1:B:126:ARG:HG2	2.31	0.59
1:D:261:HIS:O	1:D:264:PRO:HD2	2.03	0.59
1:C:214:GLN:HB3	1:C:252:LEU:CD2	2.31	0.59
1:D:80:PHE:O	1:D:84:VAL:HG23	2.03	0.59
1:A:98:ALA:H	1:A:131:LEU:HG	1.67	0.59
1:A:198:LEU:HD11	1:B:213:TYR:CE2	2.38	0.59
1:A:126:ARG:HG2	1:A:130:ASP:HB3	1.84	0.58
1:A:148:ASP:OD1	1:A:151:SER:N	2.36	0.58
1:A:219:MET:HB2	1:A:257:ILE:HG22	1.83	0.58
1:C:168:ILE:CD1	1:C:177:ILE:HD13	2.33	0.58
1:D:282:LEU:CD1	1:D:297:GLN:HB2	2.26	0.58
1:A:48:ASP:HB3	1:A:52:GLY:O	2.03	0.58
1:A:271:ARG:HH21	1:A:307:ILE:HD13	1.69	0.58
1:B:233:LEU:O	1:B:233:LEU:HD12	2.03	0.58
1:C:143:GLY:CA	1:D:185:ARG:HH11	2.16	0.58
1:D:87:GLU:HG2	1:D:91:PHE:CE2	2.38	0.58
1:C:102:SER:HB2	1:C:107:LYS:HD2	1.84	0.58
1:B:272:GLU:OE2	1:B:273:PRO:HG2	2.04	0.58
1:C:68:ARG:NE	1:C:207:GLU:OE2	2.36	0.58
1:A:236:MET:O	1:A:239:HIS:HB3	2.03	0.58
1:B:118:LEU:HD11	1:B:128:GLU:HA	1.85	0.58
1:B:281:ILE:HD12	1:B:281:ILE:H	1.68	0.58
1:A:142:PHE:CE2	1:B:184:PRO:HD2	2.38	0.58
1:C:50:ARG:NH1	1:D:174:ASP:OD1	2.36	0.58
1:C:99:LYS:HA	1:C:102:SER:OG	2.03	0.58
1:D:193:PRO:HG2	3:D:314:UFP:C3'	2.32	0.58
1:A:204:VAL:HG21	1:B:45:VAL:CG2	2.34	0.58
1:B:279:LEU:CD1	1:B:296:PHE:HB3	2.34	0.58
1:C:55:THR:HG22	1:C:258:TYR:CD1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:SER:O	1:C:244:LYS:HG3	2.03	0.58
1:D:259:LEU:HA	1:D:262:ILE:HD13	1.84	0.58
1:B:34:LEU:HD22	1:B:269:LEU:HD23	1.86	0.58
1:B:118:LEU:HD22	1:B:126:ARG:CD	2.34	0.58
1:C:79:VAL:HG23	1:C:301:TYR:OH	2.04	0.58
1:C:282:LEU:HG	1:C:295:ASP:C	2.24	0.58
1:D:140:ARG:O	1:D:159:ASP:HA	2.04	0.57
1:B:203:VAL:HA	1:B:207:GLU:O	2.03	0.57
1:B:207:GLU:OE1	1:B:244:LYS:HG3	2.04	0.57
1:D:135:TYR:CZ	1:D:194:PRO:HB3	2.39	0.57
1:A:287:LYS:HE3	1:A:289:ASP:OD1	2.05	0.57
1:C:168:ILE:HD11	1:C:177:ILE:HG21	1.86	0.57
1:C:192:LEU:HD22	1:C:192:LEU:H	1.69	0.57
1:B:71:PHE:N	1:B:277:PRO:O	2.32	0.57
1:C:176:ARG:HH21	1:D:187:LEU:CD1	2.17	0.57
1:D:135:TYR:HD1	1:D:135:TYR:H	1.51	0.57
1:D:198:LEU:HD12	1:D:198:LEU:O	2.05	0.57
1:B:153:TYR:O	1:B:156:GLN:HB2	2.05	0.57
1:B:90:TRP:CD2	1:B:101:LEU:HB2	2.39	0.57
1:A:32:GLN:HE21	1:A:64:ARG:H	1.53	0.57
1:B:102:SER:HB3	1:B:110:ASP:OD2	2.05	0.57
1:B:272:GLU:HG2	1:B:273:PRO:HD2	1.86	0.57
1:C:97:ASN:ND2	1:C:100:GLU:H	2.03	0.57
1:D:177:ILE:N	1:D:177:ILE:HD13	2.18	0.57
1:B:187:LEU:N	1:B:188:PRO:HD2	2.20	0.57
1:C:28:HIS:O	1:C:31:LEU:HG	2.05	0.57
1:D:49:ASP:OD2	1:D:49:ASP:N	2.32	0.57
1:A:32:GLN:O	1:A:36:GLN:HG3	2.04	0.57
1:B:71:PHE:O	1:B:277:PRO:HD2	2.05	0.57
1:C:115:ARG:HH12	1:C:124:SER:HA	1.70	0.57
1:D:132:GLY:O	1:D:134:VAL:N	2.37	0.57
1:A:97:ASN:HD21	1:A:99:LYS:HB2	1.70	0.56
1:A:214:GLN:HG2	1:A:216:SER:O	2.04	0.56
1:C:92:ILE:HD13	1:C:161:LEU:HD21	1.87	0.56
1:C:137:PHE:HD2	1:C:138:GLN:NE2	2.01	0.56
1:D:240:ILE:HD11	1:D:291:PHE:HE2	1.68	0.56
1:D:108:ILE:HG12	1:D:109:TRP:CD1	2.39	0.56
1:A:88:LEU:O	1:A:92:ILE:HG12	2.04	0.56
1:C:62:GLN:HA	1:C:250:HIS:O	2.04	0.56
1:C:128:GLU:HG2	1:C:129:GLY:N	2.19	0.56
1:C:140:ARG:HE	1:C:140:ARG:HA	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ILE:HD11	1:C:250:HIS:ND1	2.20	0.56
1:A:80:PHE:O	1:A:84:VAL:HG23	2.05	0.56
1:B:73:LEU:HD23	1:B:301:TYR:CE1	2.40	0.56
1:D:37:ILE:HG21	1:D:269:LEU:HD11	1.88	0.56
1:C:50:ARG:HH12	1:D:174:ASP:CG	2.08	0.56
1:D:140:ARG:CZ	1:D:161:LEU:HB3	2.35	0.56
1:C:187:LEU:HB2	1:C:188:PRO:HD3	1.88	0.56
1:D:30:GLU:OE2	1:D:74:LEU:HA	2.05	0.56
1:D:74:LEU:HD12	1:D:224:PRO:HB3	1.88	0.56
1:D:80:PHE:HE2	1:D:106:VAL:HG13	1.70	0.56
1:D:206:SER:HB3	1:D:244:LYS:HE3	1.88	0.56
1:C:161:LEU:O	1:C:164:VAL:HB	2.05	0.56
1:A:62:GLN:HA	1:A:250:HIS:O	2.05	0.56
1:D:178:ILE:CD1	1:D:200:GLN:HB2	2.36	0.56
1:B:73:LEU:CB	1:B:277:PRO:CG	2.84	0.55
1:C:48:ASP:HA	1:C:53:THR:O	2.07	0.55
1:D:240:ILE:HD11	1:D:291:PHE:CE2	2.41	0.55
1:B:107:LYS:HA	1:B:110:ASP:OD2	2.06	0.55
1:D:166:ASP:O	1:D:170:THR:HG23	2.05	0.55
1:D:108:ILE:HG12	1:D:109:TRP:HD1	1.71	0.55
1:A:108:ILE:HG13	1:A:108:ILE:O	2.05	0.55
1:C:280:ARG:O	1:C:282:LEU:CD2	2.55	0.55
1:B:161:LEU:O	1:B:164:VAL:HB	2.06	0.55
1:C:100:GLU:O	1:C:104:LYS:HE2	2.06	0.55
1:D:61:MET:HE2	1:D:61:MET:HA	1.89	0.55
1:D:109:TRP:O	1:D:131:LEU:HD21	2.07	0.55
1:A:214:GLN:HB3	1:A:252:LEU:CD2	2.32	0.55
1:B:74:LEU:HG	1:B:224:PRO:CB	2.37	0.55
1:B:109:TRP:CE3	1:B:131:LEU:HD13	2.41	0.55
1:B:203:VAL:HG23	1:B:208:LEU:HD12	1.87	0.55
1:B:227:ILE:HG22	1:B:228:ALA:N	2.20	0.55
1:D:193:PRO:CG	3:D:314:UFP:H2'2	2.26	0.55
1:A:134:VAL:O	1:A:138:GLN:HG2	2.06	0.55
1:C:69:ASP:O	1:C:70:GLU:HG3	2.06	0.55
1:D:30:GLU:OE1	1:D:74:LEU:HB3	2.07	0.55
1:D:93:LYS:HG3	1:D:95:SER:HB3	1.88	0.55
1:D:280:ARG:HD2	1:D:297:GLN:O	2.07	0.55
1:B:30:GLU:OE1	1:B:76:THR:HG23	2.08	0.54
1:C:126:ARG:NH2	1:C:189:LEU:O	2.40	0.54
1:A:207:GLU:HG2	1:A:244:LYS:HG3	1.88	0.54
1:B:38:GLN:O	1:B:42:ARG:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:VAL:O	1:B:138:GLN:HG2	2.07	0.54
1:C:50:ARG:HD2	1:D:176:ARG:NH2	2.11	0.54
1:C:164:VAL:O	1:C:168:ILE:HG12	2.07	0.54
1:A:98:ALA:CB	1:A:131:LEU:HD21	2.37	0.54
1:C:240:ILE:HD13	1:C:288:ILE:HB	1.88	0.54
1:C:178:ILE:HD12	1:C:178:ILE:N	2.23	0.54
1:B:187:LEU:H	1:B:188:PRO:HD2	1.73	0.54
1:B:274:ARG:HH11	1:B:302:ASN:C	2.11	0.54
1:C:88:LEU:CD2	1:C:232:LEU:HD23	2.38	0.54
1:B:77:LYS:HG3	1:B:306:THR:HG22	1.89	0.54
1:C:38:GLN:NE2	1:C:269:LEU:HD13	2.10	0.54
1:C:109:TRP:CE3	1:C:131:LEU:HD13	2.43	0.54
1:D:49:ASP:OD1	1:D:53:THR:O	2.25	0.54
1:D:87:GLU:OE2	1:D:225:PHE:CE2	2.61	0.54
1:D:44:GLY:HA2	1:D:58:VAL:HG22	1.89	0.54
1:D:73:LEU:HD23	1:D:301:TYR:CZ	2.43	0.54
1:A:82:LYS:O	1:A:86:GLU:HB2	2.08	0.54
1:A:88:LEU:HD23	1:A:232:LEU:CD2	2.36	0.54
1:C:249:ILE:HD12	1:C:249:ILE:H	1.72	0.54
1:A:40:ILE:HG13	1:A:58:VAL:HG23	1.90	0.53
1:D:33:TYR:CD1	1:D:34:LEU:HD23	2.43	0.53
1:D:88:LEU:HD23	1:D:232:LEU:CD2	2.39	0.53
1:B:274:ARG:NH2	1:B:304:HIS:ND1	2.49	0.53
1:D:187:LEU:O	1:D:190:MET:HB2	2.08	0.53
1:A:189:LEU:HD23	1:A:189:LEU:O	2.08	0.53
1:B:101:LEU:HD23	1:B:109:TRP:HB2	1.89	0.53
1:B:281:ILE:HD12	1:B:281:ILE:N	2.22	0.53
1:C:239:HIS:NE2	1:C:284:LYS:HA	2.23	0.53
1:C:75:THR:HG21	1:C:274:ARG:O	2.09	0.53
1:C:176:ARG:NH2	1:D:187:LEU:HD21	2.24	0.53
1:A:176:ARG:HH12	1:B:193:PRO:HG2	1.70	0.53
1:A:215:ARG:HG3	1:A:216:SER:N	2.23	0.53
1:C:108:ILE:HG13	1:C:109:TRP:N	2.23	0.53
1:C:190:MET:SD	1:C:194:PRO:HD3	2.49	0.53
1:A:178:ILE:HD11	1:B:215:ARG:HB2	1.91	0.53
1:B:162:GLN:NE2	1:B:166:ASP:OD2	2.42	0.53
1:D:281:ILE:O	1:D:295:ASP:HB3	2.09	0.53
1:D:79:VAL:HG11	1:D:225:PHE:HA	1.91	0.53
1:D:187:LEU:HA	1:D:190:MET:HE2	1.91	0.53
1:A:200:GLN:HG2	1:B:213:TYR:OH	2.09	0.53
1:B:75:THR:O	1:B:303:PRO:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:SER:OG	1:C:254:ASP:OD2	2.27	0.53
1:C:229:SER:O	1:C:232:LEU:HB3	2.09	0.53
1:D:106:VAL:HG12	1:D:108:ILE:HG23	1.91	0.53
1:A:153:TYR:O	1:A:156:GLN:HB2	2.05	0.52
1:A:284:LYS:HE2	1:A:286:GLU:HG2	1.91	0.52
1:C:87:GLU:O	1:C:90:TRP:HB3	2.10	0.52
1:D:92:ILE:O	1:D:140:ARG:HD2	2.10	0.52
1:A:198:LEU:C	1:A:198:LEU:HD12	2.29	0.52
1:D:224:PRO:HA	1:D:227:ILE:HD12	1.90	0.52
1:C:69:ASP:O	1:C:69:ASP:OD1	2.27	0.52
1:C:109:TRP:CZ3	1:C:192:LEU:HD21	2.44	0.52
1:D:285:VAL:CG1	1:D:290:ASP:HB2	2.38	0.52
1:A:57:SER:HB2	1:A:256:HIS:HB3	1.91	0.52
1:B:92:ILE:CG2	1:B:288:ILE:HG12	2.37	0.52
1:B:102:SER:HB3	1:B:110:ASP:CG	2.30	0.52
1:B:108:ILE:HG13	1:B:109:TRP:N	2.25	0.52
1:C:71:PHE:CE1	1:C:73:LEU:HD13	2.45	0.52
1:C:74:LEU:HD12	1:C:224:PRO:HB3	1.90	0.52
1:D:108:ILE:HG12	1:D:109:TRP:N	2.24	0.52
1:D:211:GLN:HG3	1:D:249:ILE:CG2	2.40	0.52
1:C:136:GLY:O	1:C:140:ARG:HG2	2.10	0.52
1:D:50:ARG:HG2	3:D:314:UFP:P	2.50	0.52
1:D:192:LEU:HD12	1:D:193:PRO:HD2	1.90	0.52
1:A:262:ILE:O	1:A:266:LYS:HG3	2.09	0.52
1:B:118:LEU:HD22	1:B:126:ARG:HD3	1.91	0.52
1:C:249:ILE:HD12	1:C:249:ILE:N	2.25	0.52
1:D:133:PRO:HG3	1:D:146:TYR:HB2	1.90	0.52
1:B:40:ILE:HD12	1:B:255:ALA:O	2.10	0.52
1:D:37:ILE:CD1	1:D:219:MET:HG3	2.40	0.52
1:D:109:TRP:CE3	1:D:131:LEU:HD13	2.44	0.52
1:B:165:ILE:HA	1:B:168:ILE:HD12	1.90	0.51
1:B:184:PRO:HA	1:B:187:LEU:HD12	1.92	0.51
1:C:283:ARG:HH21	1:C:283:ARG:HG3	1.76	0.51
1:D:32:GLN:HE22	1:D:64:ARG:H	1.57	0.51
1:A:292:LYS:N	1:A:295:ASP:OD1	2.41	0.51
1:B:206:SER:O	1:B:244:LYS:HG2	2.10	0.51
1:D:196:HIS:CE1	1:D:226:ASN:ND2	2.79	0.51
1:A:34:LEU:HD11	1:A:76:THR:HG21	1.92	0.51
1:A:55:THR:HG22	1:A:258:TYR:CD1	2.45	0.51
1:A:86:GLU:HB3	1:A:106:VAL:HG21	1.93	0.51
1:C:121:LEU:HD12	1:C:121:LEU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LEU:C	1:C:198:LEU:HD12	2.30	0.51
1:D:218:ASP:OD2	1:D:221:LEU:N	2.44	0.51
1:A:178:ILE:HG12	1:A:200:GLN:HB3	1.93	0.51
1:B:258:TYR:HB2	1:B:261:HIS:CD2	2.46	0.51
1:B:87:GLU:O	1:B:90:TRP:HB3	2.10	0.51
1:B:121:LEU:HD12	1:B:123:PHE:HE2	1.76	0.51
1:D:108:ILE:HD13	1:D:108:ILE:N	2.25	0.51
1:D:110:ASP:O	1:D:113:GLY:N	2.32	0.51
1:A:183:ASN:O	1:A:187:LEU:HG	2.10	0.51
1:B:145:GLU:HB3	1:B:147:ARG:CZ	2.41	0.51
1:B:165:ILE:HD12	1:B:165:ILE:H	1.75	0.51
1:D:89:LEU:HA	1:D:92:ILE:HG12	1.93	0.51
1:D:117:PHE:CD2	1:D:121:LEU:HD11	2.45	0.51
1:D:165:ILE:HA	1:D:168:ILE:HD12	1.92	0.51
1:B:288:ILE:HA	1:B:291:PHE:CE2	2.45	0.51
1:D:160:GLN:NE2	1:D:179:MET:HA	2.25	0.51
1:D:238:ALA:HB1	1:D:243:LEU:O	2.11	0.51
1:B:274:ARG:CZ	1:B:304:HIS:HA	2.38	0.51
1:C:148:ASP:N	1:C:148:ASP:OD2	2.44	0.51
1:C:262:ILE:O	1:C:266:LYS:HG3	2.11	0.51
1:A:59:PHE:HE2	1:B:200:GLN:HE21	1.58	0.50
1:D:88:LEU:O	1:D:91:PHE:HB2	2.11	0.50
1:A:89:LEU:HA	1:A:92:ILE:HG12	1.92	0.50
1:A:294:GLU:CD	1:A:294:GLU:H	2.15	0.50
1:B:97:ASN:ND2	1:B:100:GLU:HB2	2.18	0.50
1:C:103:SER:HB2	1:C:104:LYS:HD3	1.92	0.50
1:A:91:PHE:CD1	1:A:135:TYR:HB2	2.46	0.50
1:A:284:LYS:HG3	1:A:284:LYS:O	2.09	0.50
1:D:32:GLN:NE2	1:D:64:ARG:H	2.10	0.50
1:D:94:GLY:HA2	1:D:136:GLY:C	2.32	0.50
1:C:223:VAL:O	1:C:227:ILE:HG12	2.11	0.50
1:B:211:GLN:HG3	1:B:249:ILE:HB	1.93	0.50
1:D:38:GLN:HE22	1:D:269:LEU:HD23	1.77	0.50
1:D:93:LYS:HG3	1:D:95:SER:H	1.77	0.50
1:A:98:ALA:HB2	1:A:131:LEU:CD1	2.34	0.50
1:C:202:TYR:HB3	1:C:209:SER:HB2	1.94	0.50
1:B:282:LEU:HD11	1:B:297:GLN:CG	2.42	0.50
1:D:90:TRP:O	1:D:93:LYS:HG2	2.12	0.50
1:D:206:SER:O	1:D:244:LYS:HG2	2.11	0.50
1:B:45:VAL:O	1:B:56:LEU:HA	2.12	0.50
1:B:240:ILE:HD13	1:B:287:LYS:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:ARG:HD3	1:D:301:TYR:CE2	2.47	0.50
1:A:90:TRP:CD2	1:A:101:LEU:HD22	2.47	0.49
1:B:186:ASP:O	1:B:190:MET:HB2	2.12	0.49
1:C:259:LEU:HA	1:C:262:ILE:HG12	1.93	0.49
1:D:262:ILE:CD1	1:D:262:ILE:N	2.75	0.49
1:B:31:LEU:CD2	1:B:273:PRO:HG3	2.42	0.49
1:B:274:ARG:HE	1:B:304:HIS:CE1	2.29	0.49
1:D:32:GLN:O	1:D:36:GLN:HG3	2.13	0.49
1:B:53:THR:CG2	1:B:54:GLY:N	2.75	0.49
1:C:133:PRO:CG	1:C:186:ASP:HB3	2.41	0.49
1:D:106:VAL:CG1	1:D:108:ILE:HD12	2.42	0.49
1:D:280:ARG:CZ	1:D:280:ARG:HB3	2.42	0.49
1:B:92:ILE:O	1:B:140:ARG:HD2	2.13	0.49
1:C:176:ARG:NH2	1:D:194:PRO:HD2	2.26	0.49
1:B:268:GLN:O	1:B:268:GLN:HG2	2.13	0.49
1:C:96:THR:O	1:C:130:ASP:HA	2.13	0.49
1:C:278:LYS:HB2	1:C:299:GLU:HG3	1.95	0.49
1:D:109:TRP:HB3	1:D:131:LEU:HD11	1.95	0.49
1:D:135:TYR:CD1	1:D:135:TYR:N	2.81	0.49
1:A:200:GLN:O	1:A:200:GLN:HG3	2.12	0.49
1:B:240:ILE:HD11	1:B:291:PHE:CE2	2.39	0.49
1:C:62:GLN:HG3	1:C:251:THR:OG1	2.12	0.49
1:C:102:SER:HB2	1:C:107:LYS:HD3	1.94	0.49
1:C:271:ARG:HH12	1:C:307:ILE:CB	2.24	0.49
1:A:263:GLU:HA	1:A:266:LYS:HD3	1.95	0.49
1:B:172:PRO:HB2	1:B:203:VAL:HG11	1.94	0.49
1:B:285:VAL:CG1	1:B:290:ASP:HB2	2.39	0.49
1:D:133:PRO:CG	1:D:146:TYR:CG	2.90	0.49
1:B:88:LEU:HD22	1:B:232:LEU:HD23	1.94	0.49
1:C:219:MET:SD	1:C:223:VAL:HG21	2.53	0.49
1:D:193:PRO:CG	3:D:314:UFP:O3'	2.61	0.49
1:A:115:ARG:O	1:A:119:ASP:OD1	2.30	0.48
1:A:281:ILE:N	1:A:281:ILE:HD12	2.28	0.48
1:B:40:ILE:HG21	1:B:257:ILE:HG13	1.93	0.48
1:B:97:ASN:ND2	1:B:100:GLU:H	2.11	0.48
1:B:144:ALA:HB2	1:B:156:GLN:O	2.13	0.48
1:C:200:GLN:OE1	1:D:253:GLY:HA3	2.13	0.48
1:B:130:ASP:OD1	1:B:148:ASP:HB2	2.13	0.48
1:C:36:GLN:O	1:C:40:ILE:HG13	2.13	0.48
1:C:162:GLN:NE2	1:C:166:ASP:OD2	2.45	0.48
1:A:74:LEU:HG	1:A:224:PRO:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TYR:CE1	1:A:196:HIS:HB2	2.47	0.48
1:A:196:HIS:HD1	1:A:230:TYR:HH	1.52	0.48
1:B:90:TRP:CE2	1:B:101:LEU:HB2	2.48	0.48
1:B:274:ARG:HD2	1:B:302:ASN:O	2.13	0.48
1:C:176:ARG:NE	1:D:193:PRO:HB3	2.27	0.48
1:A:168:ILE:HD11	1:A:177:ILE:HG21	1.95	0.48
1:B:37:ILE:CD1	1:B:219:MET:HB3	2.43	0.48
1:C:163:ARG:O	1:C:167:THR:OG1	2.30	0.48
1:C:187:LEU:CB	1:C:188:PRO:HD3	2.42	0.48
1:C:301:TYR:CD2	1:C:303:PRO:HD3	2.48	0.48
1:D:292:LYS:HG3	1:D:294:GLU:HB2	1.94	0.48
1:D:265:LEU:O	1:D:269:LEU:HD13	2.12	0.48
1:D:282:LEU:HD12	1:D:295:ASP:O	2.14	0.48
1:D:187:LEU:HB3	1:D:188:PRO:HD3	1.94	0.48
1:A:259:LEU:HD23	1:A:262:ILE:HD11	1.95	0.48
1:C:142:PHE:CD2	1:C:143:GLY:N	2.81	0.48
1:D:132:GLY:O	1:D:134:VAL:HG22	2.13	0.48
1:A:106:VAL:HG12	1:A:108:ILE:HG23	1.96	0.48
1:A:140:ARG:HH11	1:A:161:LEU:HD23	1.79	0.48
1:B:40:ILE:HD13	1:B:58:VAL:HB	1.96	0.48
1:B:132:GLY:O	1:B:134:VAL:HG22	2.14	0.48
1:C:130:ASP:HB2	1:C:149:MET:SD	2.53	0.48
1:D:101:LEU:HD21	1:D:108:ILE:HD11	1.96	0.48
1:D:116:ASP:OD1	1:D:116:ASP:N	2.45	0.48
1:A:251:THR:HG21	1:B:251:THR:HG21	1.96	0.47
1:B:71:PHE:O	1:B:276:PHE:HB3	2.14	0.47
1:B:84:VAL:HG22	1:B:225:PHE:CE1	2.49	0.47
1:B:184:PRO:HA	1:B:187:LEU:CD1	2.43	0.47
1:C:176:ARG:HH21	1:D:187:LEU:HD21	1.78	0.47
1:D:98:ALA:HB1	1:D:110:ASP:OD1	2.14	0.47
1:D:262:ILE:HD13	1:D:262:ILE:H	1.79	0.47
1:A:76:THR:OG1	1:A:268:GLN:NE2	2.45	0.47
1:B:40:ILE:CD1	1:B:58:VAL:HB	2.44	0.47
1:C:260:ASN:N	1:C:260:ASN:OD1	2.47	0.47
1:D:176:ARG:NH2	2:D:616:PO4:O2	2.47	0.47
1:A:33:TYR:CE2	1:A:224:PRO:HG3	2.49	0.47
1:C:160:GLN:HB3	1:C:179:MET:HG3	1.96	0.47
1:C:283:ARG:NH2	1:C:284:LYS:O	2.47	0.47
1:A:49:ASP:OD2	1:A:51:THR:HG23	2.14	0.47
1:A:178:ILE:HG22	1:A:179:MET:N	2.29	0.47
1:B:272:GLU:CG	1:B:273:PRO:HD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:GLN:O	1:C:36:GLN:HG3	2.15	0.47
1:C:271:ARG:HH21	1:C:304:HIS:CB	2.26	0.47
1:D:274:ARG:HH11	1:D:274:ARG:CB	2.23	0.47
1:B:64:ARG:NH2	1:B:249:ILE:HD12	2.30	0.47
1:C:267:ILE:HD12	1:C:307:ILE:CD1	2.28	0.47
1:D:223:VAL:O	1:D:227:ILE:HG13	2.14	0.47
1:A:64:ARG:HB2	1:A:249:ILE:CD1	2.44	0.47
1:A:137:PHE:CZ	1:A:144:ALA:HB3	2.49	0.47
1:A:175:ARG:HH12	1:B:47:LYS:NZ	2.11	0.47
1:B:42:ARG:O	1:B:42:ARG:HD2	2.14	0.47
1:A:213:TYR:HE2	1:B:211:GLN:OE1	1.96	0.47
1:B:263:GLU:N	1:B:264:PRO:HD2	2.30	0.47
1:C:69:ASP:C	1:C:70:GLU:HG3	2.36	0.47
1:C:92:ILE:CD1	1:C:161:LEU:HD21	2.45	0.47
1:B:36:GLN:HE21	1:B:61:MET:HB3	1.80	0.47
1:C:102:SER:HB3	1:C:110:ASP:OD1	2.15	0.47
1:C:143:GLY:HA2	1:D:185:ARG:HH11	1.80	0.47
1:C:143:GLY:O	1:D:185:ARG:NH1	2.47	0.47
1:C:206:SER:HB2	1:C:244:LYS:HZ2	1.80	0.47
1:D:160:GLN:O	1:D:164:VAL:HG23	2.15	0.47
1:B:236:MET:HE3	1:B:291:PHE:CG	2.49	0.47
1:B:283:ARG:NH1	1:B:285:VAL:HG22	2.30	0.47
1:D:281:ILE:O	1:D:295:ASP:O	2.33	0.47
1:A:144:ALA:HB2	1:A:157:GLY:HA3	1.97	0.46
1:B:177:ILE:HG21	1:B:201:PHE:HB2	1.95	0.46
1:A:140:ARG:HB2	1:A:141:HIS:CD2	2.50	0.46
1:B:80:PHE:CE1	1:B:82:LYS:HB3	2.50	0.46
1:B:83:GLY:HA2	1:B:106:VAL:HG11	1.97	0.46
1:B:282:LEU:HD11	1:B:297:GLN:HG2	1.96	0.46
1:C:283:ARG:NH2	1:C:283:ARG:HG3	2.29	0.46
1:A:187:LEU:HB2	1:A:188:PRO:HD3	1.96	0.46
1:A:281:ILE:HG13	1:A:296:PHE:CD2	2.50	0.46
1:D:123:PHE:HB3	1:D:126:ARG:HG3	1.98	0.46
1:A:140:ARG:HA	1:A:159:ASP:HA	1.98	0.46
1:B:241:THR:O	1:B:243:LEU:HG	2.16	0.46
1:A:60:GLY:O	1:B:64:ARG:NH1	2.49	0.46
1:C:211:GLN:HE22	1:D:253:GLY:HA2	1.80	0.46
1:B:92:ILE:CG1	1:B:288:ILE:CD1	2.81	0.46
1:C:202:TYR:HB2	1:D:59:PHE:CZ	2.50	0.46
1:D:49:ASP:CG	1:D:54:GLY:HA2	2.30	0.46
1:D:258:TYR:HB2	1:D:261:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD23	1:A:273:PRO:HG2	1.97	0.46
1:B:193:PRO:HB2	1:B:215:ARG:NH2	2.31	0.46
1:C:53:THR:HG22	1:C:54:GLY:N	2.31	0.46
1:C:81:TRP:O	1:C:84:VAL:N	2.49	0.46
1:D:59:PHE:CD2	1:D:253:GLY:O	2.68	0.46
1:D:282:LEU:HD11	1:D:297:GLN:CB	2.30	0.46
1:A:37:ILE:HD13	1:A:265:LEU:HD22	1.98	0.46
1:A:168:ILE:HD13	1:A:177:ILE:HD13	1.98	0.46
1:A:224:PRO:HA	1:A:227:ILE:HD12	1.96	0.46
1:C:215:ARG:HB2	1:D:200:GLN:NE2	2.30	0.46
1:D:115:ARG:HH21	1:D:124:SER:HA	1.80	0.46
1:A:178:ILE:HG12	1:A:200:GLN:CB	2.46	0.46
1:C:86:GLU:HB3	1:C:106:VAL:HG21	1.98	0.46
1:B:162:GLN:HE21	1:B:166:ASP:CG	2.20	0.46
1:B:172:PRO:HB2	1:B:203:VAL:CG1	2.46	0.46
1:D:177:ILE:HB	1:D:201:PHE:HB2	1.98	0.46
1:D:206:SER:CB	1:D:244:LYS:HE3	2.45	0.46
1:A:97:ASN:ND2	1:A:99:LYS:HB2	2.30	0.45
1:B:118:LEU:HD22	1:B:126:ARG:CG	2.45	0.45
1:C:112:ASN:H	1:C:112:ASN:HD22	1.60	0.45
1:A:184:PRO:HA	1:A:187:LEU:HD12	1.97	0.45
1:B:73:LEU:HB3	1:B:277:PRO:CG	2.45	0.45
1:B:195:CYS:O	1:B:196:HIS:ND1	2.50	0.45
1:A:171:ASN:HA	1:A:172:PRO:HD2	1.84	0.45
1:A:263:GLU:O	1:A:266:LYS:HB2	2.16	0.45
1:B:101:LEU:HD12	1:B:101:LEU:O	2.17	0.45
1:B:266:LYS:O	1:B:269:LEU:HB2	2.16	0.45
1:D:193:PRO:HA	1:D:194:PRO:HD3	1.72	0.45
1:B:223:VAL:HA	1:B:226:ASN:OD1	2.16	0.45
1:B:288:ILE:CA	1:B:291:PHE:HD2	2.26	0.45
1:B:98:ALA:HB2	1:B:131:LEU:HD21	1.98	0.45
1:C:171:ASN:ND2	1:C:173:ASP:OD2	2.50	0.45
1:D:81:TRP:HE1	1:D:298:ILE:HD11	1.81	0.45
1:D:195:CYS:HA	1:D:215:ARG:HG2	1.98	0.45
1:D:307:ILE:H	1:D:307:ILE:HG13	1.47	0.45
1:A:153:TYR:O	1:A:156:GLN:N	2.49	0.45
1:A:212:LEU:HD22	1:A:230:TYR:CD2	2.52	0.45
1:B:30:GLU:CG	1:B:273:PRO:HB3	2.47	0.45
1:C:176:ARG:HG3	1:D:182:TRP:HH2	1.80	0.45
1:D:140:ARG:NH2	1:D:162:GLN:H	2.14	0.45
1:D:183:ASN:CG	1:D:186:ASP:HB3	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ASP:OD1	1:A:53:THR:HB	2.17	0.45
1:A:62:GLN:HG3	1:A:251:THR:OG1	2.16	0.45
1:B:78:ARG:CZ	1:B:303:PRO:HG3	2.47	0.45
1:B:114:SER:O	1:B:118:LEU:HG	2.17	0.45
1:C:193:PRO:HD3	4:C:315:HOH:O	2.17	0.45
1:A:48:ASP:HA	1:A:53:THR:O	2.17	0.45
1:A:292:LYS:O	1:A:295:ASP:HB2	2.17	0.45
1:B:145:GLU:OE2	1:B:145:GLU:HA	2.12	0.45
1:C:113:GLY:O	1:C:114:SER:O	2.34	0.45
1:C:135:TYR:CZ	1:C:194:PRO:HB3	2.52	0.45
1:C:280:ARG:O	1:C:282:LEU:HD23	2.17	0.45
1:D:301:TYR:CE1	1:D:303:PRO:HD3	2.51	0.45
1:A:28:HIS:ND1	1:A:29:GLY:N	2.65	0.45
1:B:53:THR:HG23	1:B:54:GLY:N	2.32	0.45
1:C:142:PHE:CG	1:C:143:GLY:N	2.85	0.45
1:C:198:LEU:HD12	1:C:199:CYS:N	2.32	0.45
1:D:206:SER:HA	1:D:243:LEU:CD2	2.45	0.45
1:A:193:PRO:HG2	1:B:176:ARG:NE	2.32	0.45
1:A:207:GLU:HA	1:A:244:LYS:O	2.17	0.45
1:B:127:GLU:OE2	1:B:150:GLU:OE2	2.35	0.44
1:C:68:ARG:HG3	1:C:68:ARG:HH11	1.82	0.44
1:C:91:PHE:HB3	1:C:139:TRP:CE3	2.52	0.44
1:C:142:PHE:CD2	1:D:184:PRO:HB2	2.52	0.44
1:D:135:TYR:OH	1:D:194:PRO:HA	2.16	0.44
1:D:244:LYS:HG2	1:D:244:LYS:H	1.58	0.44
1:A:238:ALA:O	1:A:243:LEU:N	2.50	0.44
1:C:176:ARG:NH2	1:D:193:PRO:HB3	2.29	0.44
1:D:301:TYR:CD1	1:D:303:PRO:HD3	2.53	0.44
1:A:108:ILE:HG13	1:A:109:TRP:CD1	2.52	0.44
1:A:153:TYR:HA	1:A:156:GLN:OE1	2.17	0.44
1:C:282:LEU:CG	1:C:295:ASP:O	2.53	0.44
1:D:50:ARG:CG	3:D:314:UFP:O5'	2.55	0.44
1:D:140:ARG:HH21	1:D:162:GLN:H	1.65	0.44
1:C:176:ARG:HH21	1:D:187:LEU:CD2	2.30	0.44
1:D:190:MET:HG2	1:D:193:PRO:HA	1.99	0.44
1:C:251:THR:HG21	1:D:251:THR:HG21	2.00	0.44
1:C:271:ARG:NH2	1:C:304:HIS:HB3	2.33	0.44
1:D:137:PHE:CE1	1:D:141:HIS:HB2	2.53	0.44
1:D:138:GLN:HE22	1:D:183:ASN:CB	2.13	0.44
1:B:59:PHE:HA	1:B:253:GLY:O	2.17	0.44
1:B:67:LEU:HD23	1:B:72:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:TYR:O	1:C:37:ILE:HG12	2.18	0.44
1:C:83:GLY:HA2	1:C:106:VAL:HG13	1.98	0.44
1:B:28:HIS:ND1	1:B:29:GLY:N	2.66	0.44
1:B:126:ARG:HD3	1:B:130:ASP:O	2.17	0.44
1:B:145:GLU:HB3	1:B:147:ARG:NH2	2.33	0.44
1:B:148:ASP:C	1:B:148:ASP:OD1	2.56	0.44
1:B:240:ILE:HG12	1:B:286:GLU:O	2.16	0.44
1:C:87:GLU:HA	1:C:101:LEU:CD1	2.48	0.44
1:D:33:TYR:CZ	1:D:224:PRO:HG3	2.53	0.44
1:A:101:LEU:HD12	1:A:104:LYS:HB2	2.00	0.44
1:B:67:LEU:CD2	1:B:72:PRO:HD3	2.48	0.44
1:B:176:ARG:C	1:B:178:ILE:HD12	2.38	0.44
1:C:50:ARG:CD	1:D:176:ARG:HH21	2.14	0.44
1:A:67:LEU:HD11	1:A:248:PHE:HB2	2.00	0.44
1:A:115:ARG:NH2	1:A:126:ARG:O	2.51	0.44
1:A:153:TYR:O	1:A:156:GLN:CA	2.62	0.44
1:B:99:LYS:HA	1:B:102:SER:OG	2.17	0.44
1:C:115:ARG:HH21	1:C:118:LEU:HB3	1.81	0.44
1:C:193:PRO:HA	1:C:194:PRO:HD3	1.86	0.44
1:D:56:LEU:HB3	1:D:257:ILE:HB	1.99	0.44
1:A:203:VAL:HG22	1:A:208:LEU:HD13	2.00	0.43
1:C:174:ASP:HB3	1:C:177:ILE:HD11	1.99	0.43
1:C:176:ARG:NH2	1:D:187:LEU:HD11	2.30	0.43
1:C:240:ILE:HG22	1:C:241:THR:N	2.31	0.43
1:A:182:TRP:CE3	1:A:194:PRO:HD2	2.52	0.43
1:D:256:HIS:CD2	1:D:258:TYR:CE2	3.06	0.43
1:A:67:LEU:HD21	1:A:231:ALA:HB1	1.99	0.43
1:B:121:LEU:HD12	1:B:123:PHE:CE2	2.53	0.43
1:B:137:PHE:O	1:B:141:HIS:HB2	2.19	0.43
1:B:217:GLY:HA3	1:B:252:LEU:HD21	2.00	0.43
1:B:267:ILE:HA	1:B:270:GLN:CG	2.46	0.43
1:D:62:GLN:HA	1:D:250:HIS:O	2.18	0.43
1:D:77:LYS:O	1:D:77:LYS:HG2	2.17	0.43
1:A:48:ASP:O	1:B:173:ASP:OD2	2.36	0.43
1:A:304:HIS:O	1:A:305:PRO:O	2.36	0.43
1:B:182:TRP:HE3	1:B:194:PRO:HB2	1.84	0.43
1:B:267:ILE:CD1	1:B:270:GLN:HE21	2.27	0.43
1:C:279:LEU:HD11	1:C:296:PHE:HB3	2.00	0.43
1:A:28:HIS:CE1	1:A:30:GLU:H	2.36	0.43
1:A:45:VAL:HG21	1:B:204:VAL:HG11	2.01	0.43
1:A:191:ALA:O	1:A:192:LEU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:VAL:HB	1:D:135:TYR:H	1.61	0.43
1:A:195:CYS:O	1:A:214:GLN:HA	2.19	0.43
1:A:284:LYS:CE	1:A:286:GLU:HG2	2.49	0.43
1:B:107:LYS:O	1:B:110:ASP:HB2	2.19	0.43
1:B:269:LEU:HD23	1:B:269:LEU:HA	1.86	0.43
1:C:99:LYS:HE2	1:C:128:GLU:CD	2.37	0.43
1:C:200:GLN:HE22	1:D:215:ARG:CB	2.27	0.43
1:D:75:THR:O	1:D:304:HIS:HD2	2.01	0.43
1:A:197:ALA:HB1	1:B:198:LEU:HD21	2.01	0.43
1:B:236:MET:CE	1:B:288:ILE:HG13	2.48	0.43
1:C:49:ASP:OD1	1:C:53:THR:HB	2.18	0.43
1:C:97:ASN:HB2	1:C:149:MET:CE	2.48	0.43
1:C:183:ASN:ND2	1:C:186:ASP:OD1	2.52	0.43
1:D:109:TRP:HE3	1:D:131:LEU:HD13	1.84	0.43
1:D:291:PHE:CD1	1:D:296:PHE:CZ	3.06	0.43
1:B:33:TYR:HE1	1:B:268:GLN:HE22	1.67	0.43
1:C:30:GLU:CD	1:C:75:THR:H	2.22	0.43
1:D:78:ARG:HD3	1:D:301:TYR:HE2	1.84	0.43
1:D:87:GLU:OE2	1:D:225:PHE:CZ	2.72	0.43
1:A:192:LEU:HD13	1:A:192:LEU:O	2.19	0.43
1:B:38:GLN:O	1:B:38:GLN:HG3	2.18	0.43
1:B:85:LEU:O	1:B:89:LEU:HG	2.19	0.43
1:D:109:TRP:CZ3	1:D:134:VAL:HG11	2.54	0.42
1:D:176:ARG:CZ	2:D:616:PO4:O4	2.67	0.42
1:B:274:ARG:HH22	1:B:304:HIS:HA	1.73	0.42
1:C:59:PHE:HD2	1:C:253:GLY:O	2.01	0.42
1:D:29:GLY:O	1:D:32:GLN:HB2	2.20	0.42
1:B:28:HIS:HB3	1:B:31:LEU:HD23	2.02	0.42
1:C:185:ARG:O	1:C:188:PRO:HD2	2.20	0.42
1:C:237:ILE:HG22	1:C:237:ILE:O	2.19	0.42
1:D:68:ARG:HG3	1:D:68:ARG:HH11	1.84	0.42
1:D:148:ASP:OD1	1:D:151:SER:N	2.52	0.42
1:A:307:ILE:O	1:A:308:LYS:HB2	2.19	0.42
1:C:34:LEU:HD22	1:C:269:LEU:HD23	2.00	0.42
1:C:88:LEU:HD23	1:C:232:LEU:CG	2.50	0.42
1:D:204:VAL:O	1:D:207:GLU:HB2	2.19	0.42
1:D:278:LYS:O	1:D:298:ILE:HA	2.19	0.42
1:A:140:ARG:NE	1:A:159:ASP:OD2	2.51	0.42
1:B:239:HIS:CE1	1:B:281:ILE:HG21	2.54	0.42
1:B:271:ARG:NH2	1:B:305:PRO:O	2.52	0.42
1:A:64:ARG:CB	1:A:249:ILE:HD13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:NH2	1:A:207:GLU:OE1	2.51	0.42
1:B:176:ARG:HH11	1:B:176:ARG:CG	2.32	0.42
1:C:178:ILE:HD13	1:D:182:TRP:CH2	2.54	0.42
1:C:200:GLN:HE22	1:D:215:ARG:CA	2.32	0.42
1:C:211:GLN:NE2	1:D:253:GLY:HA2	2.35	0.42
1:D:259:LEU:HA	1:D:262:ILE:HD11	2.02	0.42
1:B:118:LEU:HB3	1:B:123:PHE:HB2	2.02	0.42
1:B:177:ILE:HD12	1:B:177:ILE:N	2.29	0.42
1:D:135:TYR:OH	1:D:195:CYS:N	2.53	0.42
1:D:197:ALA:HB3	1:D:213:TYR:HD2	1.84	0.42
1:C:73:LEU:HD23	1:C:301:TYR:CE1	2.55	0.42
1:C:89:LEU:O	1:C:92:ILE:HB	2.19	0.42
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.87	0.42
1:C:279:LEU:HD13	1:C:298:ILE:CD1	2.43	0.42
1:D:88:LEU:CD1	1:D:92:ILE:HD11	2.50	0.42
1:A:166:ASP:OD2	1:A:166:ASP:N	2.53	0.42
1:B:119:ASP:OD2	1:B:123:PHE:O	2.38	0.42
1:C:45:VAL:CG2	1:D:204:VAL:HG21	2.50	0.42
1:C:68:ARG:CZ	1:C:207:GLU:OE2	2.68	0.42
1:D:229:SER:OG	1:D:230:TYR:HD2	2.02	0.42
1:B:186:ASP:O	1:B:190:MET:CE	2.68	0.42
1:C:176:ARG:NH1	1:D:182:TRP:CZ3	2.88	0.42
1:D:100:GLU:O	1:D:104:LYS:HG2	2.20	0.42
1:D:117:PHE:O	1:D:121:LEU:HG	2.20	0.42
1:D:190:MET:O	1:D:191:ALA:O	2.38	0.42
1:A:280:ARG:HA	1:A:280:ARG:HD3	1.53	0.41
1:B:178:ILE:HG23	1:B:198:LEU:HD13	2.02	0.41
1:B:193:PRO:HA	1:B:194:PRO:HD3	1.76	0.41
1:C:71:PHE:HA	1:C:72:PRO:HD2	1.84	0.41
1:C:163:ARG:HH11	1:C:163:ARG:HG2	1.85	0.41
1:C:207:GLU:HA	1:C:244:LYS:O	2.20	0.41
1:D:56:LEU:HA	1:D:56:LEU:HD12	1.75	0.41
1:D:87:GLU:OE2	1:D:225:PHE:HE2	2.01	0.41
1:A:73:LEU:HD12	1:A:73:LEU:HA	1.89	0.41
1:A:74:LEU:N	1:A:74:LEU:HD23	2.33	0.41
1:A:202:TYR:HB2	1:B:59:PHE:CE2	2.55	0.41
1:B:140:ARG:HB2	1:B:141:HIS:CD2	2.55	0.41
1:C:140:ARG:HA	1:C:140:ARG:NE	2.33	0.41
1:D:176:ARG:NH2	2:D:616:PO4:O4	2.53	0.41
1:A:198:LEU:HD12	1:A:198:LEU:O	2.20	0.41
1:B:239:HIS:NE2	1:B:284:LYS:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:VAL:HG12	1:C:80:PHE:H	1.85	0.41
1:C:88:LEU:HD23	1:C:232:LEU:HG	2.02	0.41
1:D:161:LEU:HD21	1:D:288:ILE:CD1	2.40	0.41
1:A:89:LEU:HA	1:A:92:ILE:CG1	2.50	0.41
1:C:115:ARG:O	1:C:119:ASP:OD1	2.37	0.41
1:C:280:ARG:HG3	1:C:299:GLU:OE1	2.19	0.41
1:D:230:TYR:N	1:D:230:TYR:CD2	2.88	0.41
1:A:59:PHE:HE2	1:B:200:GLN:NE2	2.18	0.41
1:A:67:LEU:CD2	1:A:231:ALA:HB1	2.51	0.41
1:A:81:TRP:CZ3	1:A:298:ILE:HD11	2.55	0.41
1:A:193:PRO:HA	1:A:194:PRO:HD3	1.81	0.41
1:D:31:LEU:HD23	1:D:31:LEU:HA	1.87	0.41
1:D:206:SER:HA	1:D:243:LEU:HD23	2.01	0.41
1:D:259:LEU:C	1:D:261:HIS:H	2.23	0.41
1:A:28:HIS:CE1	1:A:30:GLU:HB2	2.55	0.41
1:A:184:PRO:HB3	1:B:158:VAL:HG11	2.02	0.41
1:B:73:LEU:HB2	1:B:277:PRO:CG	2.35	0.41
1:B:102:SER:CB	1:B:110:ASP:OD2	2.68	0.41
1:C:59:PHE:CZ	1:D:202:TYR:HB2	2.56	0.41
1:C:97:ASN:ND2	1:C:100:GLU:N	2.67	0.41
1:C:115:ARG:NH2	1:C:118:LEU:HB3	2.35	0.41
1:D:38:GLN:HE21	1:D:38:GLN:HB2	1.68	0.41
1:D:249:ILE:N	1:D:249:ILE:CD1	2.79	0.41
1:B:30:GLU:CD	1:B:273:PRO:HB3	2.41	0.41
1:B:204:VAL:O	1:B:207:GLU:HB2	2.20	0.41
1:C:97:ASN:ND2	1:C:100:GLU:HB2	2.29	0.41
1:C:140:ARG:HD2	1:C:140:ARG:N	2.36	0.41
1:D:30:GLU:OE1	1:D:76:THR:OG1	2.38	0.41
1:D:40:ILE:HA	1:D:58:VAL:HG21	2.03	0.41
1:D:140:ARG:HA	1:D:159:ASP:OD2	2.19	0.41
1:D:201:PHE:CE1	1:D:210:CYS:SG	3.14	0.41
1:A:94:GLY:O	1:A:96:THR:HG22	2.20	0.41
1:A:116:ASP:OD1	1:A:116:ASP:N	2.47	0.41
1:B:292:LYS:O	1:B:295:ASP:HB2	2.21	0.41
1:C:30:GLU:HG3	1:C:74:LEU:HD22	2.02	0.41
1:C:122:GLY:O	1:C:124:SER:N	2.54	0.41
1:C:278:LYS:O	1:C:299:GLU:HG2	2.20	0.41
1:D:280:ARG:HG2	1:D:297:GLN:HB3	2.02	0.41
1:A:75:THR:HB	1:A:274:ARG:HB2	2.03	0.41
1:A:182:TRP:HZ3	1:A:215:ARG:HE	1.69	0.41
1:B:113:GLY:HA2	1:B:129:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HD13	1:B:126:ARG:CG	2.39	0.41
1:B:292:LYS:N	1:B:295:ASP:OD1	2.41	0.41
1:C:135:TYR:O	1:C:136:GLY:C	2.58	0.41
1:D:28:HIS:O	1:D:31:LEU:HB2	2.20	0.41
1:D:102:SER:HB2	1:D:107:LYS:HE3	2.02	0.41
1:D:274:ARG:NH1	1:D:302:ASN:O	2.50	0.41
1:B:92:ILE:HG13	1:B:288:ILE:CG1	2.51	0.41
1:B:127:GLU:H	1:B:127:GLU:HG3	1.68	0.41
1:C:58:VAL:HG12	1:C:59:PHE:N	2.36	0.41
1:D:197:ALA:HB3	1:D:213:TYR:O	2.21	0.41
1:B:30:GLU:HB3	1:B:273:PRO:CB	2.52	0.40
1:B:277:PRO:HG3	1:B:301:TYR:CD1	2.56	0.40
1:B:298:ILE:HG21	1:B:301:TYR:HB2	2.04	0.40
1:C:148:ASP:OD2	1:C:151:SER:HB2	2.20	0.40
1:A:260:ASN:ND2	1:A:260:ASN:H	2.20	0.40
1:C:92:ILE:HD12	1:C:288:ILE:HG13	2.03	0.40
1:C:97:ASN:HB2	1:C:149:MET:SD	2.60	0.40
1:C:204:VAL:HG23	1:D:47:LYS:HE3	2.03	0.40
1:D:133:PRO:HB3	1:D:137:PHE:CD2	2.56	0.40
1:A:126:ARG:NH2	1:A:189:LEU:O	2.55	0.40
1:B:137:PHE:O	1:B:141:HIS:N	2.54	0.40
1:B:175:ARG:HG2	2:B:616:PO4:O4	2.21	0.40
1:C:142:PHE:O	1:C:157:GLY:HA3	2.21	0.40
1:A:304:HIS:HB3	1:A:305:PRO:HD2	2.03	0.40
1:B:203:VAL:HG22	1:B:207:GLU:O	2.22	0.40
1:C:103:SER:C	1:C:104:LYS:HD3	2.42	0.40
1:C:175:ARG:HH21	1:D:50:ARG:HD2	1.87	0.40
1:D:79:VAL:O	1:D:81:TRP:N	2.54	0.40
1:D:91:PHE:CD1	1:D:135:TYR:HB2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLY:O	1:B:120:SER:O[2_555]	2.05	0.15

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	281/313 (90%)	233 (83%)	41 (15%)	7 (2%)	5	32
1	B	281/313 (90%)	224 (80%)	47 (17%)	10 (4%)	3	23
1	C	281/313 (90%)	232 (83%)	43 (15%)	6 (2%)	7	37
1	D	281/313 (90%)	230 (82%)	35 (12%)	16 (6%)	1	14
All	All	1124/1252 (90%)	919 (82%)	166 (15%)	39 (4%)	3	24

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	PRO
1	B	50	ARG
1	B	134	VAL
1	C	114	SER
1	C	197	ALA
1	D	51	THR
1	D	191	ALA
1	D	283	ARG
1	D	293	ALA
1	A	116	ASP
1	A	222	GLY
1	B	51	THR
1	B	128	GLU
1	B	222	GLY
1	D	74	LEU
1	D	80	PHE
1	D	307	ILE
1	A	110	ASP
1	A	277	PRO
1	B	219	MET
1	D	52	GLY
1	D	114	SER

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Mol	Chain	Res	Type
1	B	81	TRP
1	B	261	HIS
1	C	72	PRO
1	C	191	ALA
1	D	27	PRO
1	A	197	ALA
1	D	134	VAL
1	D	187	LEU
1	D	229	SER
1	A	239	HIS
1	B	288	ILE
1	C	134	VAL
1	C	106	VAL
1	D	84	VAL
1	B	133	PRO
1	D	305	PRO
1	D	72	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	247/271 (91%)	222 (90%)	25 (10%)	7 29
1	B	247/271 (91%)	216 (87%)	31 (13%)	4 21
1	C	247/271 (91%)	208 (84%)	39 (16%)	2 12
1	D	247/271 (91%)	203 (82%)	44 (18%)	2 9
All	All	988/1084 (91%)	849 (86%)	139 (14%)	3 16

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	38	GLN
1	A	43	CYS
1	A	46	ARG

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Mol	Chain	Res	Type
1	A	50	ARG
1	A	78	ARG
1	A	96	THR
1	A	99	LYS
1	A	103	SER
1	A	110	ASP
1	A	114	SER
1	A	115	ARG
1	A	116	ASP
1	A	123	PHE
1	A	125	THR
1	A	160	GLN
1	A	175	ARG
1	A	180	CYS
1	A	185	ARG
1	A	192	LEU
1	A	200	GLN
1	A	270	GLN
1	A	282	LEU
1	A	284	LYS
1	A	289	ASP
1	B	31	LEU
1	B	43	CYS
1	B	53	THR
1	B	74	LEU
1	B	80	PHE
1	B	85	LEU
1	B	91	PHE
1	B	103	SER
1	B	107	LYS
1	B	117	PHE
1	B	128	GLU
1	B	140	ARG
1	B	145	GLU
1	B	148	ASP
1	B	151	SER
1	B	164	VAL
1	B	167	THR
1	B	175	ARG
1	B	180	CYS
1	B	193	PRO
1	B	199	CYS

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Mol	Chain	Res	Type
1	B	204	VAL
1	B	206	SER
1	B	221	LEU
1	B	226	ASN
1	B	249	ILE
1	B	266	LYS
1	B	271	ARG
1	B	289	ASP
1	B	299	GLU
1	B	302	ASN
1	C	46	ARG
1	C	49	ASP
1	C	56	LEU
1	C	57	SER
1	C	67	LEU
1	C	82	LYS
1	C	96	THR
1	C	104	LYS
1	C	106	VAL
1	C	112	ASN
1	C	115	ARG
1	C	116	ASP
1	C	119	ASP
1	C	125	THR
1	C	128	GLU
1	C	167	THR
1	C	169	LYS
1	C	171	ASN
1	C	176	ARG
1	C	180	CYS
1	C	189	LEU
1	C	190	MET
1	C	192	LEU
1	C	204	VAL
1	C	216	SER
1	C	218	ASP
1	C	229	SER
1	C	235	TYR
1	C	244	LYS
1	C	260	ASN
1	C	271	ARG
1	C	272	GLU

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Mol	Chain	Res	Type
1	C	284	LYS
1	C	290	ASP
1	C	291	PHE
1	C	294	GLU
1	C	306	THR
1	C	307	ILE
1	C	308	LYS
1	D	43	CYS
1	D	49	ASP
1	D	50	ARG
1	D	55	THR
1	D	64	ARG
1	D	73	LEU
1	D	76	THR
1	D	80	PHE
1	D	95	SER
1	D	103	SER
1	D	108	ILE
1	D	115	ARG
1	D	116	ASP
1	D	124	SER
1	D	127	GLU
1	D	128	GLU
1	D	134	VAL
1	D	135	TYR
1	D	140	ARG
1	D	160	GLN
1	D	163	ARG
1	D	169	LYS
1	D	170	THR
1	D	177	ILE
1	D	187	LEU
1	D	189	LEU
1	D	195	CYS
1	D	209	SER
1	D	214	GLN
1	D	219	MET
1	D	221	LEU
1	D	234	THR
1	D	235	TYR
1	D	244	LYS
1	D	247	ASP

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Mol	Chain	Res	Type
1	D	262	ILE
1	D	266	LYS
1	D	274	ARG
1	D	280	ARG
1	D	286	GLU
1	D	289	ASP
1	D	294	GLU
1	D	297	GLN
1	D	298	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	200	GLN
1	A	226	ASN
1	A	256	HIS
1	A	260	ASN
1	A	268	GLN
1	A	270	GLN
1	B	36	GLN
1	B	97	ASN
1	B	141	HIS
1	B	156	GLN
1	B	160	GLN
1	B	250	HIS
1	B	261	HIS
1	B	268	GLN
1	B	270	GLN
1	C	32	GLN
1	C	38	GLN
1	C	62	GLN
1	C	97	ASN
1	C	112	ASN
1	C	138	GLN
1	C	171	ASN
1	C	183	ASN
1	C	200	GLN
1	C	211	GLN
1	C	214	GLN
1	C	226	ASN
1	C	302	ASN

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Mol	Chain	Res	Type
1	C	304	HIS
1	D	38	GLN
1	D	39	HIS
1	D	97	ASN
1	D	112	ASN
1	D	138	GLN
1	D	160	GLN
1	D	162	GLN
1	D	196	HIS
1	D	214	GLN
1	D	226	ASN
1	D	297	GLN
1	D	304	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 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	$\#\|Z\| > 2$
2	PO4	B	314	-	4,4,4	1.55	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	UFP	D	314	-	19,22,22	2.04	5 (26%)	24,33,33	3.55	11 (45%)
2	PO4	B	616	-	4,4,4	1.48	0	6,6,6	0.44	0
2	PO4	D	616	-	4,4,4	1.97	3 (75%)	6,6,6	0.48	0

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	UFP	D	314	-	-	0/7/22/22	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	314	UFP	C4-C5	4.78	1.44	1.38
3	D	314	UFP	O4'-C1'	4.30	1.52	1.42
3	D	314	UFP	P-O1P	3.39	1.61	1.50
3	D	314	UFP	C4-N3	3.24	1.38	1.33
2	D	616	PO4	P-O4	-2.30	1.47	1.54
3	D	314	UFP	P-O3P	2.13	1.63	1.54
2	D	616	PO4	P-O3	-2.06	1.48	1.54
2	D	616	PO4	P-O2	-2.01	1.48	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	314	UFP	P-O5'-C5'	-7.77	96.90	118.30
3	D	314	UFP	C4-N3-C2	7.02	121.06	115.14
3	D	314	UFP	C2'-C1'-N1	-6.25	99.85	114.27
3	D	314	UFP	C4'-O4'-C1'	-5.89	95.23	109.45
3	D	314	UFP	O4'-C4'-C5'	5.76	128.34	109.37
3	D	314	UFP	O5'-C5'-C4'	4.73	125.27	108.99
3	D	314	UFP	C5'-C4'-C3'	-3.87	92.00	114.74
3	D	314	UFP	O4'-C1'-C2'	-3.76	99.15	106.25
3	D	314	UFP	O2P-P-O5'	3.13	115.07	106.73
3	D	314	UFP	O4'-C4'-C3'	-3.11	98.42	105.67
3	D	314	UFP	C5-C4-N3	-2.65	119.60	122.39

There are no chirality outliers.

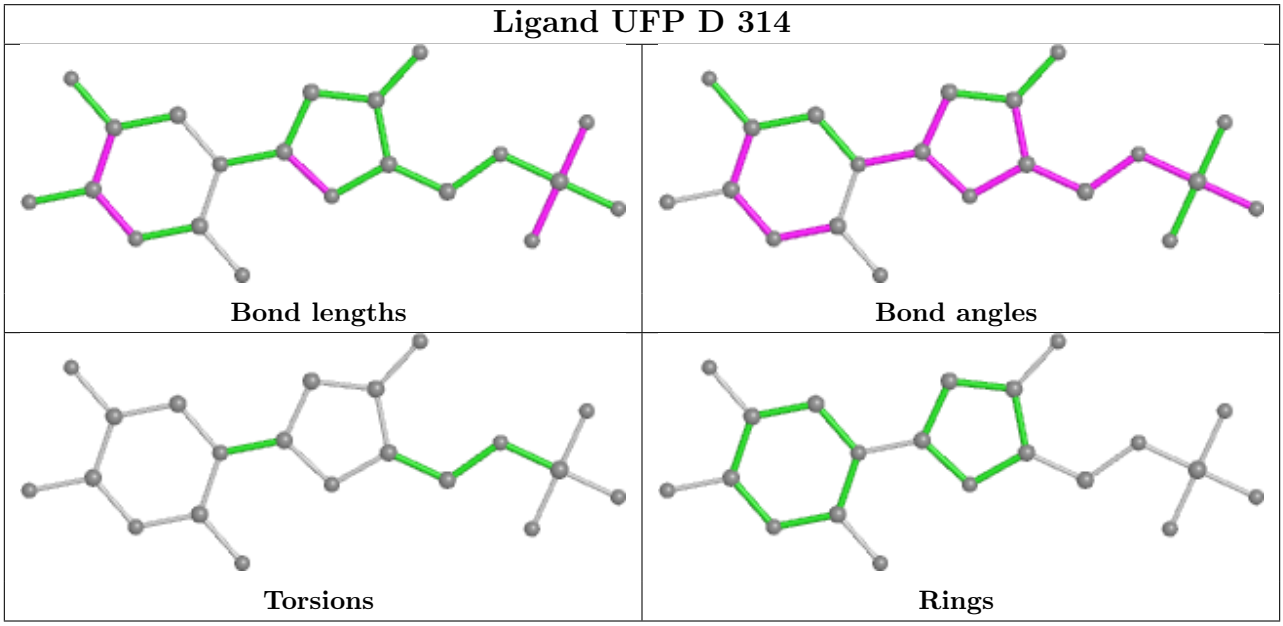
There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	314	UFP	14	0
2	B	616	PO4	1	0
2	D	616	PO4	3	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 then 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, 95^{th} 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	283/313 (90%)	-0.45	6 (2%)	63	49	21, 78, 142, 160	0
1	B	283/313 (90%)	-0.29	6 (2%)	63	49	21, 96, 153, 161	0
1	C	283/313 (90%)	-0.34	5 (1%)	68	55	21, 86, 136, 161	0
1	D	283/313 (90%)	-0.18	9 (3%)	47	31	21, 97, 145, 161	0
All	All	1132/1252 (90%)	-0.32	26 (2%)	60	47	21, 90, 146, 161	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	126	ARG	3.5
1	A	195	CYS	3.4
1	C	307	ILE	3.3
1	C	122	GLY	3.3
1	B	288	ILE	3.1
1	D	284	LYS	2.8
1	B	128	GLU	2.6
1	A	123	PHE	2.6
1	C	128	GLU	2.6
1	C	123	PHE	2.5
1	B	293	ALA	2.5
1	D	288	ILE	2.4
1	B	116	ASP	2.4
1	B	287	LYS	2.4
1	A	118	LEU	2.4
1	D	114	SER	2.2
1	D	122	GLY	2.2
1	D	182	TRP	2.2
1	D	251	THR	2.2
1	C	199	CYS	2.1
1	A	124	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	181	ALA	2.1
1	D	123	PHE	2.0
1	A	115	ARG	2.0
1	B	198	LEU	2.0
1	A	106	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

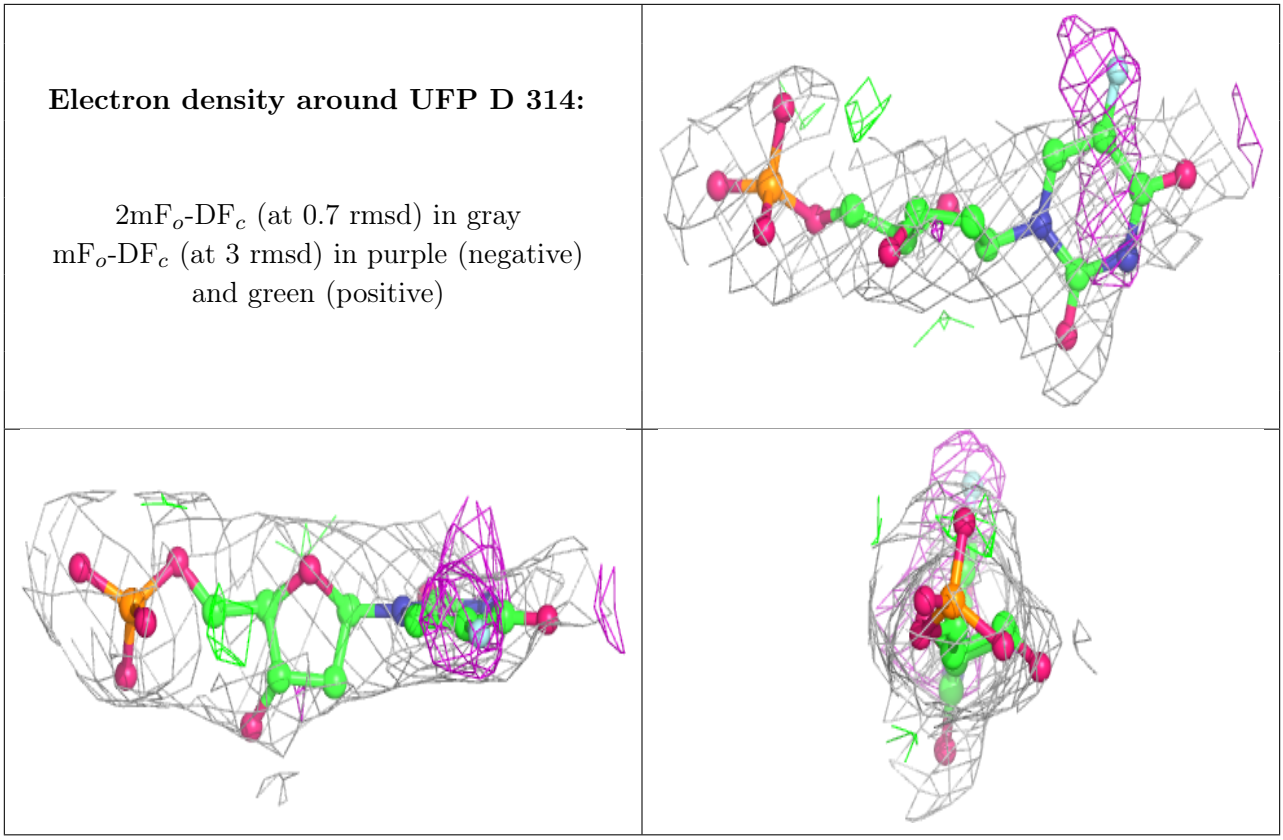
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	UFP	D	314	21/21	0.89	0.18	63,86,95,97	0
2	PO4	B	616	5/5	0.92	0.17	110,111,113,114	0
2	PO4	B	314	5/5	0.95	0.13	107,107,109,110	0
2	PO4	D	616	5/5	0.97	0.20	90,96,98,98	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 UFP D 314:

$2mF_o$-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.