



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:10 pm BST

PDB ID : 3QQU  
Title : Cocrystal structure of unphosphorylated igf with pyrimidine 8  
Authors : Huang, X.  
Deposited on : 2011-02-16  
Resolution : 2.90 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

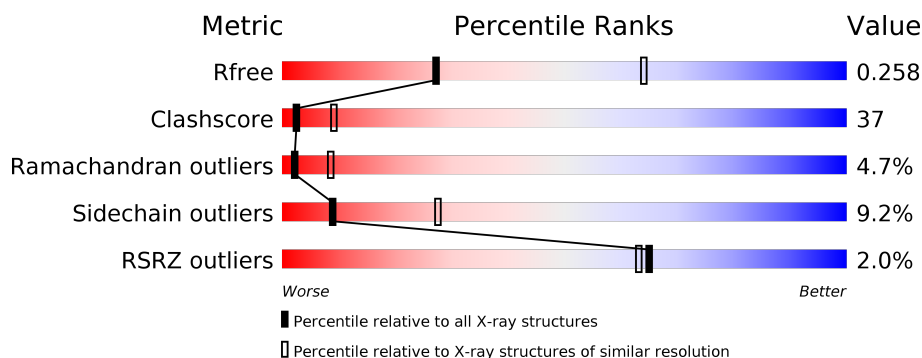
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	301	<div> <div style="width: 40%; background-color: green;"></div> <div style="width: 48%; background-color: yellow;"></div> <div style="width: 7%; background-color: orange;"></div> <div style="width: 5%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div>
1	B	301	<div> <div style="width: 42%; background-color: green;"></div> <div style="width: 44%; background-color: yellow;"></div> <div style="width: 9%; background-color: orange;"></div> <div style="width: 3%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div>
1	C	301	<div> <div style="width: 42%; background-color: green;"></div> <div style="width: 48%; background-color: yellow;"></div> <div style="width: 8%; background-color: orange;"></div> <div style="width: 3%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div>
1	D	301	<div> <div style="width: 43%; background-color: green;"></div> <div style="width: 46%; background-color: yellow;"></div> <div style="width: 7%; background-color: orange;"></div> <div style="width: 3%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	01P	B	1	-	X	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9305 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.

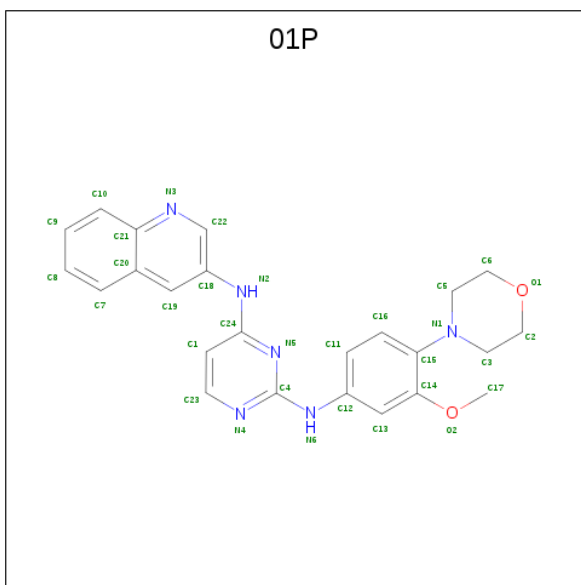
- Molecule 1 is a protein called Insulin-like growth factor 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2227	1418	372	415	22			
1	B	288	Total	C	N	O	S	0	0	0
			2258	1436	376	424	22			
1	C	293	Total	C	N	O	S	0	0	0
			2263	1442	376	422	23			
1	D	292	Total	C	N	O	S	0	0	0
			2266	1441	378	426	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	983	GLY	-	EXPRESSION TAG	UNP P08069
A	984	SER	-	EXPRESSION TAG	UNP P08069
B	983	GLY	-	EXPRESSION TAG	UNP P08069
B	984	SER	-	EXPRESSION TAG	UNP P08069
C	983	GLY	-	EXPRESSION TAG	UNP P08069
C	984	SER	-	EXPRESSION TAG	UNP P08069
D	983	GLY	-	EXPRESSION TAG	UNP P08069
D	984	SER	-	EXPRESSION TAG	UNP P08069

- Molecule 2 is N 2 -[3-methoxy-4-(morpholin-4-yl)phenyl]-N 4 -(quinolin-3-yl)pyrimidine-2,4-diamine (three-letter code: 01P) (formula: C<sub>24</sub>H<sub>24</sub>N<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	24	6	2		
2	B	1	Total	C	N	O	0	0
			32	24	6	2		
2	C	1	Total	C	N	O	0	0
			32	24	6	2		
2	D	1	Total	C	N	O	0	0
			32	24	6	2		

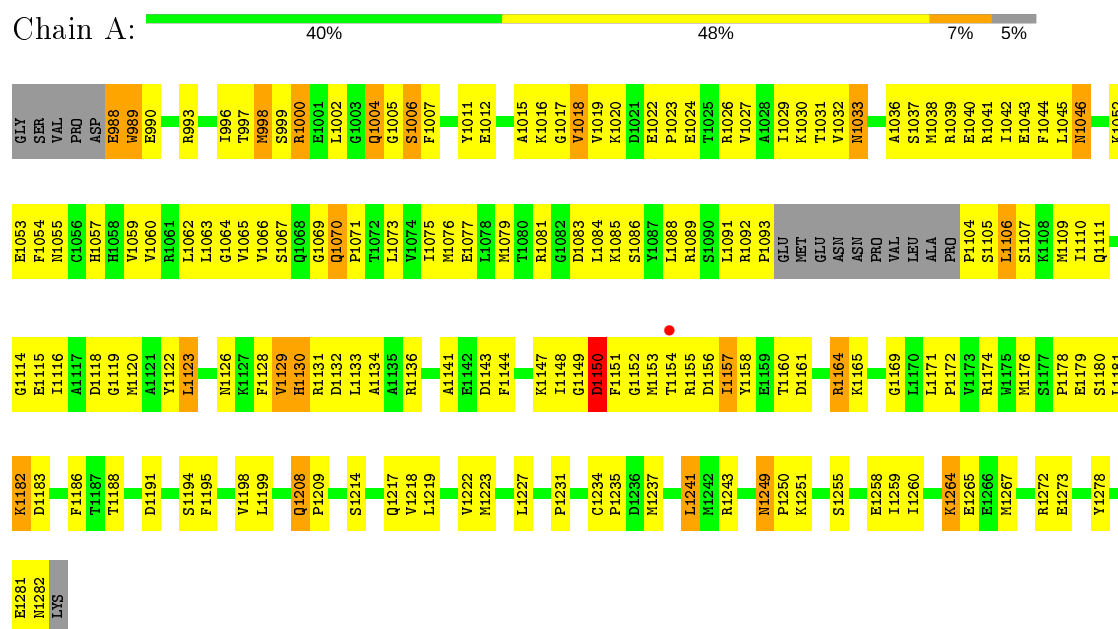
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	46	Total	O	0	0
			46	46		
3	C	33	Total	O	0	0
			33	33		
3	D	38	Total	O	0	0
			38	38		

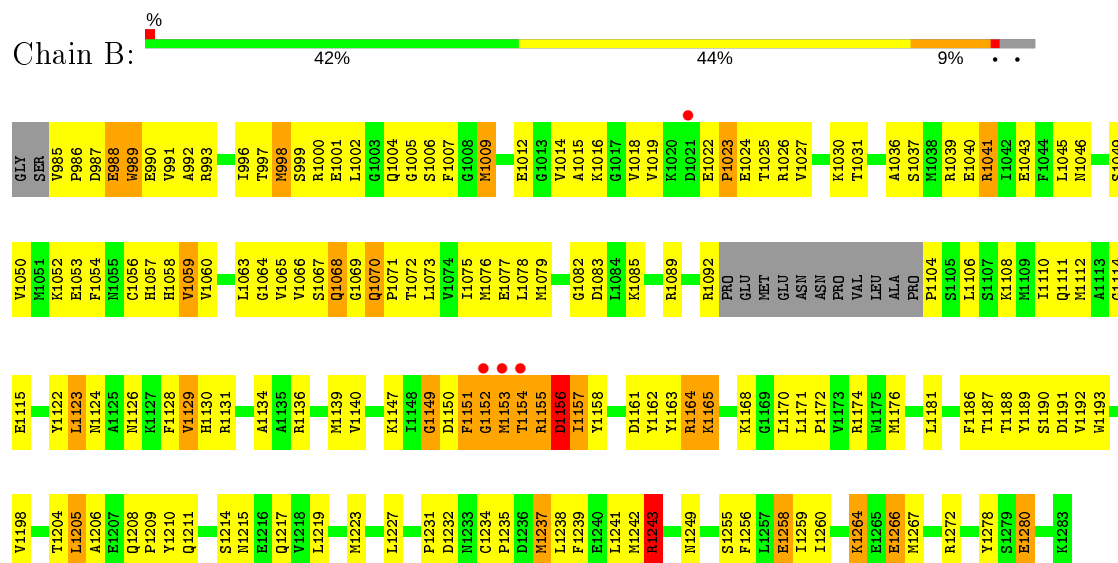
### 3 Residue-property plots

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.

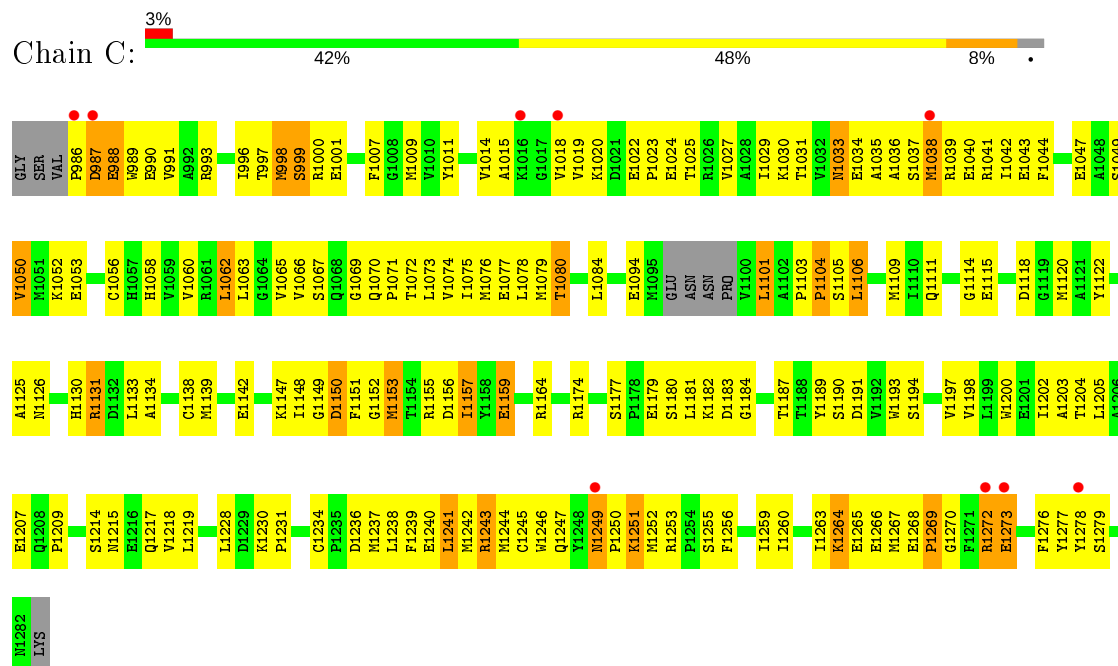
#### • Molecule 1: Insulin-like growth factor 1 receptor



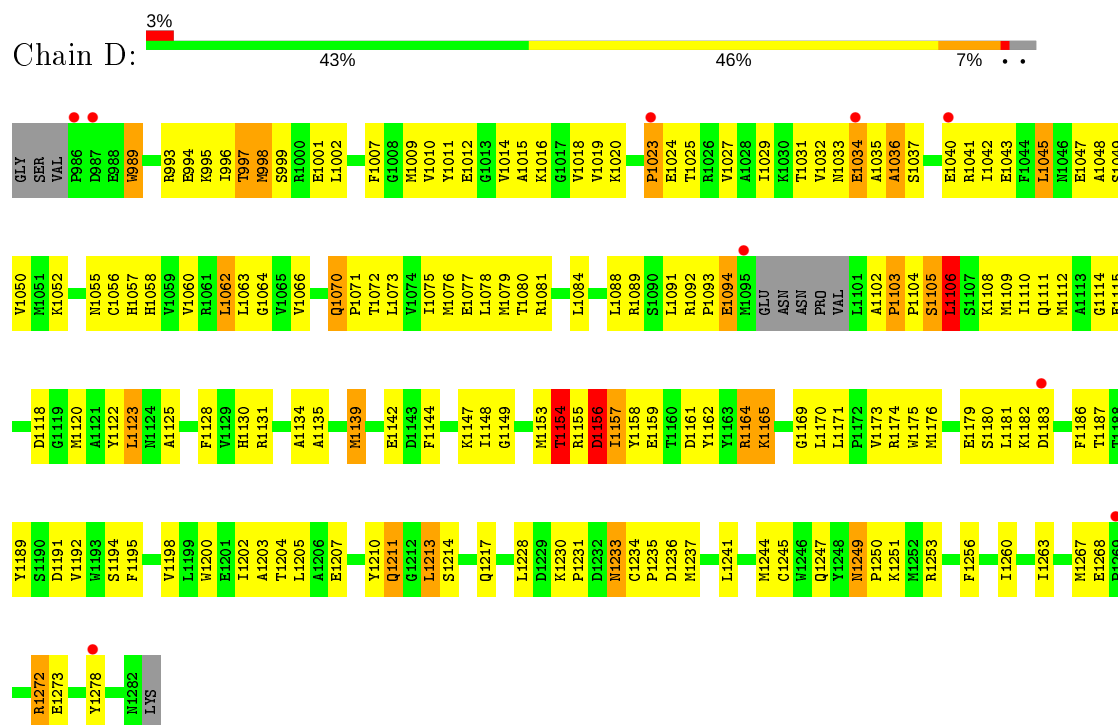
#### • Molecule 1: Insulin-like growth factor 1 receptor



- Molecule 1: Insulin-like growth factor 1 receptor



- Molecule 1: Insulin-like growth factor 1 receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.79Å 90.93Å 96.97Å 65.37° 89.42° 84.67°	Depositor
Resolution (Å)	30.00 – 2.90 29.98 – 2.91	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-2.90) 93.6 (29.98-2.91)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.273 , 0.302 0.226 , 0.258	Depositor DCC
$R_{free}$ test set	2035 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.7	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9305	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 01P

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	0.55	0/2273	0.81	2/3067 (0.1%)
1	B	0.54	0/2305	0.81	2/3111 (0.1%)
1	C	0.53	0/2312	0.86	2/3128 (0.1%)
1	D	0.52	0/2315	0.83	3/3132 (0.1%)
All	All	0.54	0/9205	0.83	9/12438 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1243	ARG	NE-CZ-NH2	-14.29	113.15	120.30
1	C	1243	ARG	NE-CZ-NH1	13.20	126.90	120.30
1	D	1164	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	D	1164	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	B	1243	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	B	1243	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	D	1106	LEU	N-CA-C	-5.50	96.15	111.00
1	A	1093	PRO	N-CA-CB	5.37	109.74	103.30
1	A	1130	HIS	N-CA-C	-5.23	96.89	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2227	0	2143	144	0
1	B	2258	0	2177	164	0
1	C	2263	0	2161	178	0
1	D	2266	0	2160	184	0
2	A	32	0	24	3	0
2	B	32	0	24	4	0
2	C	32	0	24	5	0
2	D	32	0	24	3	0
3	A	46	0	0	5	0
3	B	46	0	0	2	0
3	C	33	0	0	0	0
3	D	38	0	0	1	0
All	All	9305	0	8737	662	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 37.

All (662) 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:B:1110:ILE:HD11	1:B:1237:MET:SD	1.90	1.10
1:C:1019:VAL:HG12	1:C:1020:LYS:H	1.13	1.05
1:D:1155:ARG:HH12	1:D:1170:LEU:HD21	1.22	1.03
1:D:1272:ARG:HA	1:D:1278:TYR:HD2	1.23	1.02
1:C:1231:PRO:HG2	1:C:1234:CYS:HB2	1.44	0.99
1:B:1018:VAL:HG11	1:B:1063:LEU:HD13	1.45	0.99
1:C:1018:VAL:CG1	1:C:1063:LEU:HB3	1.94	0.97
1:B:1155:ARG:O	1:B:1156:ASP:HB2	1.61	0.97
1:C:1018:VAL:HG11	1:C:1063:LEU:HB3	1.50	0.93
1:C:1231:PRO:HG2	1:C:1234:CYS:CB	2.01	0.90
1:D:1155:ARG:NH1	1:D:1170:LEU:HD21	1.85	0.90
1:D:1164:ARG:HA	1:D:1170:LEU:H	1.36	0.90
1:D:1272:ARG:HA	1:D:1278:TYR:CD2	2.07	0.90
1:C:1139:MET:HG3	1:C:1149:GLY:HA3	1.54	0.89
1:D:1018:VAL:HG11	1:D:1063:LEU:HB3	1.54	0.89
1:D:1070:GLN:HG2	1:D:1071:PRO:HA	1.53	0.89
1:B:1018:VAL:HG12	1:B:1019:VAL:HG23	1.56	0.87
1:D:1018:VAL:CG1	1:D:1063:LEU:HB3	2.03	0.87
1:B:1231:PRO:HG2	1:B:1234:CYS:HB2	1.58	0.85
1:D:1231:PRO:HG2	1:D:1234:CYS:CB	2.05	0.85
1:B:1004:GLN:NE2	1:B:1009:MET:HG2	1.93	0.84
1:C:1019:VAL:HG12	1:C:1020:LYS:N	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1231:PRO:HG2	1:A:1234:CYS:HB2	1.60	0.84
1:A:1062:LEU:HA	1:A:1076:MET:HG2	1.60	0.83
1:D:1249:ASN:C	1:D:1249:ASN:HD22	1.80	0.83
1:B:1111:GLN:O	1:B:1115:GLU:HG3	1.78	0.82
1:B:986:PRO:HD2	1:C:987:ASP:HB3	1.60	0.82
1:C:1022:GLU:HG2	1:C:1024:GLU:O	1.79	0.82
1:C:1155:ARG:HD2	1:C:1159:GLU:HG2	1.62	0.82
1:C:986:PRO:O	1:C:987:ASP:HB2	1.80	0.82
1:C:1111:GLN:O	1:C:1115:GLU:HG3	1.79	0.81
1:D:1214:SER:OG	1:D:1217:GLN:HG3	1.80	0.81
1:C:996:ILE:HD13	1:C:1075:ILE:HD11	1.62	0.81
1:A:1241:LEU:HD21	1:A:1259:ILE:HG23	1.63	0.81
1:D:1034:GLU:HA	1:D:1070:GLN:OE1	1.81	0.81
1:C:998:MET:HE2	1:C:1029:ILE:HD13	1.61	0.80
1:D:1118:ASP:HA	1:D:1260:ILE:HD11	1.64	0.80
1:A:1111:GLN:O	1:A:1115:GLU:HG3	1.82	0.79
1:B:999:SER:HB3	1:D:1233:ASN:OD1	1.83	0.79
1:C:1214:SER:OG	1:C:1217:GLN:HG3	1.82	0.79
1:D:1058:HIS:ND1	1:D:1118:ASP:HB3	1.97	0.78
1:D:1062:LEU:HA	1:D:1076:MET:HG2	1.64	0.77
1:C:1019:VAL:CG1	1:C:1020:LYS:H	1.97	0.77
1:A:1130:HIS:HD2	1:A:1132:ASP:H	1.33	0.76
1:B:1214:SER:OG	1:B:1217:GLN:HG3	1.84	0.76
1:C:1272:ARG:HA	1:C:1278:TYR:CD2	2.20	0.76
1:B:996:ILE:HD13	1:B:1075:ILE:HD11	1.66	0.76
1:C:1101:LEU:H	1:C:1101:LEU:HD23	1.51	0.76
1:D:1052:LYS:HG2	1:D:1062:LEU:HD22	1.66	0.76
1:B:1001:GLU:HG3	1:D:1103:PRO:O	1.86	0.76
1:D:1042:ILE:HG22	1:D:1042:ILE:O	1.84	0.75
1:A:1018:VAL:HG13	1:A:1018:VAL:O	1.88	0.74
2:C:1:01P:H3	2:C:1:01P:O2	1.87	0.74
1:D:1089:ARG:O	1:D:1092:ARG:HG3	1.87	0.74
1:D:1249:ASN:ND2	1:D:1251:LYS:H	1.85	0.74
1:C:1001:GLU:HG2	1:C:1011:TYR:CE2	2.23	0.74
1:D:1194:SER:O	1:D:1198:VAL:HG23	1.88	0.74
1:B:1089:ARG:HD3	1:B:1092:ARG:NH1	2.02	0.74
1:B:1046:ASN:HD21	1:C:1043:GLU:HG3	1.52	0.74
1:A:1111:GLN:HA	1:A:1267:MET:HE3	1.70	0.74
1:D:1249:ASN:HD21	1:D:1251:LYS:HB2	1.52	0.74
1:A:1264:LYS:HE2	3:A:3:HOH:O	1.88	0.74
1:C:1101:LEU:N	1:C:1101:LEU:HD23	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1089:ARG:O	1:A:1092:ARG:HG3	1.89	0.73
1:B:1157:ILE:O	1:B:1157:ILE:CG1	2.36	0.73
1:C:1072:THR:O	1:C:1073:LEU:HD23	1.89	0.73
1:A:1002:LEU:HD21	1:A:1012:GLU:HB2	1.70	0.73
1:D:1231:PRO:HG2	1:D:1234:CYS:SG	2.28	0.72
1:A:1081:ARG:HD2	1:A:1141:ALA:O	1.87	0.72
1:C:1033:ASN:ND2	1:C:1035:ALA:H	1.86	0.72
1:C:1066:VAL:HB	1:C:1073:LEU:HB2	1.70	0.72
1:C:1033:ASN:HD22	1:C:1034:GLU:N	1.88	0.71
1:D:1139:MET:HG3	1:D:1149:GLY:HA3	1.73	0.71
1:D:1052:LYS:HG2	1:D:1062:LEU:CD2	2.21	0.71
1:D:1092:ARG:HG2	1:D:1205:LEU:HD13	1.70	0.71
1:D:1048:ALA:O	1:D:1052:LYS:HG3	1.91	0.70
1:D:1231:PRO:HG2	1:D:1234:CYS:HB2	1.73	0.70
1:A:1019:VAL:HG12	1:A:1020:LYS:N	2.07	0.70
1:D:1109:MET:HE1	1:D:1203:ALA:HA	1.73	0.69
1:C:1272:ARG:HA	1:C:1278:TYR:HD2	1.57	0.69
1:C:1164:ARG:HG2	1:C:1164:ARG:HH11	1.58	0.69
1:B:993:ARG:HH22	1:B:1071:PRO:C	1.97	0.68
1:C:1118:ASP:HA	1:C:1260:ILE:HD11	1.76	0.68
1:D:1111:GLN:O	1:D:1115:GLU:HG3	1.94	0.68
1:C:1204:THR:HB	1:C:1207:GLU:CD	2.14	0.68
1:A:1105:SER:O	1:A:1106:LEU:HB2	1.91	0.68
1:D:1122:TYR:O	1:D:1125:ALA:HB3	1.94	0.68
1:D:1093:PRO:O	1:D:1094:GLU:CB	2.42	0.68
1:C:1105:SER:O	1:C:1106:LEU:HB2	1.94	0.67
1:D:1164:ARG:HA	1:D:1170:LEU:N	2.10	0.67
1:B:1077:GLU:OE1	1:B:1147:LYS:NZ	2.22	0.67
1:D:1156:ASP:HB3	1:D:1157:ILE:HG23	1.76	0.67
1:B:1181:LEU:HD22	1:B:1219:LEU:HD22	1.77	0.67
1:B:1208:GLN:HG2	3:B:13:HOH:O	1.93	0.67
1:B:989:TRP:CZ3	1:B:1052:LYS:HB3	2.30	0.67
1:A:1249:ASN:ND2	1:A:1251:LYS:H	1.91	0.66
1:A:1249:ASN:HD22	1:A:1250:PRO:N	1.92	0.66
1:B:1174:ARG:HB3	1:B:1209:PRO:HB2	1.77	0.66
1:C:1179:GLU:CD	1:C:1253:ARG:HH22	1.98	0.66
1:D:1066:VAL:HB	1:D:1073:LEU:HB2	1.77	0.66
1:C:1230:LYS:NZ	1:C:1236:ASP:OD1	2.29	0.66
1:C:1255:SER:O	1:C:1259:ILE:HG13	1.96	0.66
1:A:1178:PRO:HB3	1:A:1222:VAL:O	1.95	0.66
1:B:1037:SER:HB3	1:C:1131:ARG:NE	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:SER:OG	1:A:1040:GLU:HG3	1.97	0.65
1:A:1130:HIS:CD2	1:A:1132:ASP:H	2.13	0.65
1:D:1060:VAL:HG23	1:D:1149:GLY:HA2	1.78	0.65
1:B:1157:ILE:HG13	1:B:1157:ILE:O	1.95	0.65
1:C:1156:ASP:OD2	1:C:1157:ILE:HG22	1.96	0.65
1:D:1001:GLU:OE2	1:D:1009:MET:HG2	1.96	0.65
1:C:1276:PHE:HA	1:C:1279:SER:HB3	1.78	0.65
1:A:1018:VAL:O	1:A:1018:VAL:CG1	2.43	0.65
1:B:1004:GLN:HE22	1:B:1009:MET:HG2	1.61	0.64
1:A:993:ARG:HH22	1:A:1071:PRO:C	2.01	0.64
1:B:1255:SER:OG	1:B:1258:GLU:HB2	1.97	0.64
1:C:1182:LYS:HE2	1:C:1183:ASP:OD1	1.98	0.64
1:D:1084:LEU:O	1:D:1088:LEU:HG	1.97	0.64
1:A:1249:ASN:HD22	1:A:1249:ASN:C	2.01	0.64
1:D:1256:PHE:O	1:D:1260:ILE:HG13	1.97	0.64
2:A:1:01P:O2	2:A:1:01P:H3	1.96	0.64
1:A:1155:ARG:O	1:A:1156:ASP:HB2	1.97	0.64
1:B:1165:LYS:HG2	1:B:1165:LYS:O	1.97	0.64
1:D:1037:SER:OG	1:D:1040:GLU:HG3	1.97	0.64
1:D:1249:ASN:ND2	1:D:1249:ASN:C	2.51	0.64
1:A:1119:GLY:HA3	1:A:1148:ILE:HD12	1.80	0.64
1:A:1154:THR:O	1:A:1156:ASP:OD1	2.16	0.63
2:D:1:01P:H3A	2:D:1:01P:O2	1.98	0.63
1:A:1181:LEU:HD22	1:A:1219:LEU:HD22	1.80	0.63
1:A:1272:ARG:HA	1:A:1278:TYR:CD2	2.34	0.63
1:D:1091:LEU:HD13	1:D:1104:PRO:HG3	1.80	0.63
1:D:1192:VAL:O	1:D:1195:PHE:HB3	1.98	0.63
1:A:1255:SER:O	1:A:1259:ILE:HG13	1.98	0.63
1:B:1016:LYS:O	1:B:1023:PRO:O	2.16	0.63
1:B:1037:SER:OG	1:B:1040:GLU:HG3	1.99	0.62
1:C:1018:VAL:HG13	1:C:1063:LEU:HB3	1.79	0.62
1:C:1056:CYS:HB2	1:C:1122:TYR:CD2	2.34	0.62
1:B:1108:LYS:O	1:B:1112:MET:HG3	1.98	0.62
1:D:1072:THR:O	1:D:1073:LEU:HD23	1.99	0.62
1:B:1131:ARG:HG2	1:B:1186:PHE:CB	2.30	0.62
1:B:1054:PHE:CE1	1:B:1123:LEU:HD11	2.34	0.62
1:B:1114:GLY:HA3	1:B:1267:MET:SD	2.40	0.62
1:B:1134:ALA:HA	1:B:1198:VAL:HG22	1.80	0.62
1:C:1134:ALA:HA	1:C:1198:VAL:HG22	1.82	0.62
1:B:999:SER:CB	1:D:1233:ASN:OD1	2.48	0.61
1:B:1280:GLU:HG3	1:B:1280:GLU:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1165:LYS:NZ	1:B:1219:LEU:HD13	2.15	0.61
1:B:1231:PRO:HG2	1:B:1234:CYS:CB	2.31	0.61
1:B:1272:ARG:HA	1:B:1278:TYR:CD2	2.35	0.61
1:C:1000:ARG:O	1:C:1011:TYR:HB3	2.01	0.61
1:A:1018:VAL:HG11	1:A:1063:LEU:HD13	1.81	0.61
1:B:1131:ARG:HG2	1:B:1186:PHE:HB2	1.83	0.61
1:B:989:TRP:HD1	1:B:1064:GLY:HA2	1.66	0.61
1:D:1070:GLN:CG	1:D:1071:PRO:HA	2.29	0.60
1:D:1106:LEU:HD23	1:D:1106:LEU:O	2.01	0.60
1:B:1012:GLU:OE1	1:B:1026:ARG:NH2	2.33	0.60
1:B:1155:ARG:O	1:B:1156:ASP:CB	2.41	0.60
1:B:1227:LEU:CD1	1:B:1243:ARG:HE	2.14	0.60
1:B:996:ILE:HD13	1:B:1075:ILE:CD1	2.31	0.60
1:C:1240:GLU:HG3	1:C:1244:MET:CE	2.31	0.60
1:D:1002:LEU:O	2:D:1:01P:H8	2.01	0.60
1:B:986:PRO:HD2	1:C:987:ASP:CB	2.29	0.60
1:C:990:GLU:OE2	1:C:1067:SER:N	2.29	0.60
1:C:1062:LEU:HA	1:C:1076:MET:HG2	1.83	0.60
1:C:1122:TYR:O	1:C:1125:ALA:HB3	2.02	0.60
1:B:1139:MET:HE1	1:B:1150:ASP:HB2	1.83	0.60
1:B:1037:SER:HB3	1:C:1131:ARG:CZ	2.32	0.60
1:D:1249:ASN:ND2	1:D:1251:LYS:N	2.50	0.60
1:A:1077:GLU:O	2:A:1:01P:H23	2.00	0.60
1:A:996:ILE:CD1	1:A:1075:ILE:HG13	2.32	0.60
1:D:1231:PRO:O	1:D:1234:CYS:HB3	2.02	0.60
1:D:1230:LYS:NZ	1:D:1236:ASP:OD1	2.35	0.60
1:C:1079:MET:CE	1:C:1147:LYS:HD2	2.32	0.59
1:D:995:LYS:O	1:D:1015:ALA:HA	2.01	0.59
1:D:1014:VAL:HG11	1:D:1024:GLU:CD	2.22	0.59
1:D:1108:LYS:O	1:D:1112:MET:HG3	2.03	0.59
1:B:993:ARG:HH21	1:B:1069:GLY:C	2.05	0.59
1:C:1018:VAL:HG11	1:C:1063:LEU:HD13	1.85	0.59
1:C:1015:ALA:HB1	1:C:1018:VAL:CG2	2.33	0.59
1:A:1053:GLU:OE1	1:A:1053:GLU:HA	2.03	0.58
1:A:1165:LYS:NZ	1:A:1171:LEU:HD12	2.19	0.58
1:C:993:ARG:HH12	1:C:1071:PRO:HD2	1.68	0.58
1:B:1243:ARG:HG3	1:B:1243:ARG:HH11	1.69	0.58
1:B:1165:LYS:HE2	1:B:1181:LEU:O	2.04	0.58
1:D:1130:HIS:O	1:D:1191:ASP:OD1	2.22	0.58
1:A:1019:VAL:HG12	1:A:1020:LYS:H	1.69	0.58
1:A:989:TRP:CZ3	1:A:1052:LYS:HB3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1255:SER:OG	1:A:1258:GLU:HG3	2.03	0.58
1:B:1085:LYS:NZ	1:B:1161:ASP:OD1	2.37	0.58
1:C:1241:LEU:HD21	1:C:1259:ILE:HG23	1.86	0.57
1:D:1007:PHE:O	1:D:1032:VAL:HA	2.04	0.57
1:B:1056:CYS:HB2	1:B:1122:TYR:CD2	2.39	0.57
1:A:1018:VAL:HG12	1:A:1019:VAL:HG23	1.86	0.57
1:C:1034:GLU:HG2	1:C:1070:GLN:NE2	2.19	0.57
1:C:1240:GLU:HG3	1:C:1244:MET:HE2	1.85	0.57
1:B:1041:ARG:HB2	1:C:1050:VAL:HG11	1.86	0.57
1:B:1018:VAL:CG1	1:B:1063:LEU:HD13	2.29	0.57
1:C:1111:GLN:HA	1:C:1267:MET:HE3	1.85	0.57
1:C:1250:PRO:HG2	1:C:1251:LYS:H	1.69	0.57
1:B:1165:LYS:NZ	1:B:1219:LEU:HD22	2.19	0.57
1:C:1041:ARG:HD3	1:C:1072:THR:OG1	2.04	0.57
1:C:1150:ASP:C	1:C:1152:GLY:H	2.08	0.57
1:A:1249:ASN:ND2	1:A:1249:ASN:C	2.59	0.56
1:A:1114:GLY:HA3	1:A:1267:MET:SD	2.45	0.56
1:C:1242:MET:HB3	1:C:1246:TRP:CZ3	2.40	0.56
1:D:1012:GLU:HG3	1:D:1078:LEU:CD2	2.35	0.56
1:D:1139:MET:HG3	1:D:1149:GLY:CA	2.35	0.56
1:B:1072:THR:O	1:B:1073:LEU:HD23	2.06	0.56
1:A:1041:ARG:HH11	1:A:1041:ARG:HG3	1.70	0.56
1:B:1139:MET:HG3	1:B:1149:GLY:HA3	1.87	0.56
1:B:1219:LEU:HB3	1:B:1223:MET:CE	2.36	0.56
1:C:1044:PHE:CE2	1:C:1074:VAL:HG23	2.41	0.56
1:D:1057:HIS:O	1:D:1147:LYS:HE2	2.05	0.56
1:D:1092:ARG:HD3	1:D:1205:LEU:HB3	1.88	0.56
1:B:1255:SER:O	1:B:1259:ILE:HG13	2.05	0.56
1:D:1200:TRP:CG	1:D:1228:LEU:HD13	2.40	0.56
1:D:1018:VAL:CG1	1:D:1063:LEU:HD13	2.36	0.56
1:A:1243:ARG:HB2	3:A:8:HOH:O	2.05	0.55
1:A:999:SER:O	1:A:1000:ARG:HB2	2.06	0.55
1:B:1068:GLN:HA	1:C:1053:GLU:OE2	2.06	0.55
1:D:1109:MET:CE	1:D:1203:ALA:HA	2.36	0.55
1:B:997:THR:O	1:B:998:MET:CB	2.55	0.55
1:C:1249:ASN:HD22	1:C:1249:ASN:C	2.10	0.55
1:C:996:ILE:HD12	1:C:1066:VAL:HG21	1.89	0.55
1:D:989:TRP:CE3	1:D:1052:LYS:HD3	2.42	0.55
1:C:997:THR:O	1:C:998:MET:HB3	2.06	0.55
1:A:1038:MET:SD	1:A:1038:MET:O	2.65	0.55
1:D:1134:ALA:HA	1:D:1198:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:993:ARG:HG3	1:C:1066:VAL:HG11	1.89	0.55
1:A:1007:PHE:O	1:A:1032:VAL:HA	2.07	0.55
1:C:1038:MET:O	1:C:1042:ILE:HG13	2.07	0.55
1:C:1109:MET:HE3	1:C:1202:ILE:HG22	1.89	0.55
1:C:1109:MET:CE	1:C:1203:ALA:HA	2.36	0.55
1:C:1130:HIS:O	1:C:1191:ASP:OD1	2.25	0.55
1:B:990:GLU:OE2	1:B:1067:SER:N	2.40	0.54
1:D:1187:THR:HG1	1:D:1189:TYR:HD2	1.51	0.54
1:A:1249:ASN:HD22	1:A:1250:PRO:CD	2.20	0.54
1:C:1231:PRO:CG	1:C:1234:CYS:HB2	2.28	0.54
1:D:1249:ASN:HD22	1:D:1251:LYS:H	1.53	0.54
1:D:1120:MET:HB3	1:D:1256:PHE:CD2	2.42	0.54
1:A:1012:GLU:OE2	1:A:1026:ARG:NH2	2.41	0.54
1:A:1179:GLU:HG2	1:A:1180:SER:N	2.23	0.54
1:D:1033:ASN:OD1	1:D:1035:ALA:HB3	2.07	0.54
1:B:1256:PHE:O	1:B:1260:ILE:HG13	2.07	0.54
1:B:1031:THR:HG22	1:B:1073:LEU:CD2	2.38	0.54
1:C:1105:SER:O	1:C:1106:LEU:CB	2.56	0.54
1:D:1018:VAL:HG11	1:D:1063:LEU:HD13	1.90	0.54
1:C:1156:ASP:CG	1:C:1157:ILE:HG22	2.29	0.53
1:C:1157:ILE:O	1:C:1157:ILE:CG1	2.56	0.53
1:C:1109:MET:HE1	1:C:1203:ALA:HA	1.89	0.53
1:D:1118:ASP:HA	1:D:1260:ILE:CD1	2.37	0.53
1:D:1210:TYR:O	1:D:1213:LEU:N	2.38	0.53
1:B:1165:LYS:HZ3	1:B:1219:LEU:HD13	1.73	0.53
1:B:1260:ILE:O	1:B:1264:LYS:N	2.41	0.53
1:B:1018:VAL:HG12	1:B:1019:VAL:CG2	2.35	0.53
1:B:1054:PHE:HE1	1:B:1151:PHE:CE2	2.26	0.53
1:A:1118:ASP:HA	1:A:1260:ILE:HD11	1.90	0.53
1:B:1239:PHE:O	1:B:1242:MET:HB2	2.08	0.53
1:C:1179:GLU:OE1	1:C:1253:ARG:NH2	2.41	0.53
1:B:985:VAL:HG11	1:C:1049:SER:CB	2.39	0.53
1:B:1018:VAL:HG13	1:B:1063:LEU:HD22	1.90	0.53
1:C:1025:THR:O	1:C:1027:VAL:HG13	2.08	0.53
1:D:989:TRP:HD1	1:D:1064:GLY:HA2	1.73	0.53
1:C:1182:LYS:HG2	1:C:1183:ASP:OD1	2.09	0.53
1:D:1027:VAL:HG12	1:D:1063:LEU:HD12	1.90	0.53
1:A:1136:ARG:NH1	1:A:1161:ASP:OD1	2.42	0.53
1:A:1181:LEU:HD22	1:A:1219:LEU:CD2	2.39	0.53
1:D:993:ARG:HH22	1:D:1071:PRO:C	2.11	0.53
1:D:1164:ARG:HA	1:D:1169:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:996:ILE:HD13	1:A:1075:ILE:CD1	2.39	0.52
1:B:1181:LEU:HD22	1:B:1219:LEU:CD2	2.37	0.52
1:D:1120:MET:HG2	1:D:1148:ILE:HD11	1.91	0.52
1:A:1019:VAL:CG1	1:A:1020:LYS:N	2.72	0.52
1:A:1129:VAL:CG2	1:A:1129:VAL:O	2.57	0.52
1:C:986:PRO:O	1:C:987:ASP:CB	2.56	0.52
2:C:1:01P:C3	2:C:1:01P:O2	2.56	0.52
1:C:993:ARG:HH21	1:C:1069:GLY:C	2.12	0.52
1:C:1187:THR:HG1	1:C:1189:TYR:HD2	1.55	0.52
1:B:1075:ILE:O	1:B:1076:MET:HG2	2.09	0.52
1:B:1190:SER:O	1:B:1193:TRP:HB3	2.09	0.52
1:C:1022:GLU:O	1:C:1023:PRO:C	2.48	0.52
1:D:993:ARG:NH2	1:D:1071:PRO:O	2.43	0.52
1:D:1031:THR:HG22	1:D:1073:LEU:HD22	1.92	0.52
1:A:1029:ILE:HG23	1:A:1075:ILE:CD1	2.39	0.52
1:C:1018:VAL:HG11	1:C:1063:LEU:CB	2.33	0.52
1:D:1157:ILE:HD11	1:D:1158:TYR:CE2	2.44	0.52
1:A:1152:GLY:O	1:A:1153:MET:HB2	2.10	0.52
1:B:1136:ARG:NE	1:B:1162:TYR:OH	2.30	0.52
1:C:1037:SER:C	1:C:1039:ARG:H	2.13	0.52
1:C:990:GLU:HA	1:C:1065:VAL:O	2.10	0.52
1:C:1001:GLU:HG2	1:C:1011:TYR:CD2	2.44	0.51
1:D:1084:LEU:HB3	1:D:1135:ALA:O	2.11	0.51
1:D:1249:ASN:ND2	1:D:1251:LYS:HB2	2.25	0.51
1:D:1106:LEU:O	1:D:1110:ILE:HG12	2.10	0.51
1:A:996:ILE:HD13	1:A:1075:ILE:HG13	1.91	0.51
1:B:1019:VAL:O	1:B:1022:GLU:HB3	2.10	0.51
1:B:1054:PHE:HE1	1:B:1151:PHE:HE2	1.59	0.51
1:A:1120:MET:SD	1:A:1148:ILE:HD13	2.51	0.51
1:B:1006:SER:HB3	1:B:1154:THR:CB	2.40	0.51
1:C:1194:SER:O	1:C:1198:VAL:HG23	2.09	0.51
1:D:1118:ASP:CA	1:D:1260:ILE:HD11	2.38	0.51
1:A:1214:SER:H	1:A:1217:GLN:HB2	1.75	0.51
1:B:991:VAL:HG12	1:B:992:ALA:N	2.25	0.51
1:D:1012:GLU:HG3	1:D:1078:LEU:HD21	1.93	0.51
1:D:1179:GLU:CD	1:D:1253:ARG:HH22	2.13	0.51
1:A:1083:ASP:OD1	1:A:1086:SER:OG	2.26	0.51
1:B:1079:MET:HB3	1:B:1140:VAL:O	2.11	0.51
1:C:1015:ALA:HB1	1:C:1018:VAL:HG23	1.93	0.51
1:C:993:ARG:NH2	1:C:1069:GLY:O	2.44	0.51
1:D:1210:TYR:O	1:D:1213:LEU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1031:THR:HG22	1:A:1073:LEU:CD2	2.40	0.51
1:A:1164:ARG:HA	1:A:1169:GLY:O	2.10	0.51
1:C:1114:GLY:HA3	1:C:1267:MET:SD	2.50	0.51
1:D:1077:GLU:OE1	1:D:1147:LYS:NZ	2.35	0.51
1:D:1105:SER:HB2	1:D:1108:LYS:H	1.76	0.51
1:B:1031:THR:HG22	1:B:1073:LEU:HD23	1.93	0.50
1:B:1134:ALA:HA	1:B:1198:VAL:CG2	2.40	0.50
1:C:993:ARG:NH1	1:C:1071:PRO:HD2	2.26	0.50
1:C:1079:MET:HE1	1:C:1147:LYS:HD2	1.93	0.50
1:C:1197:VAL:O	1:C:1200:TRP:HB3	2.12	0.50
1:C:1009:MET:HE2	1:C:1009:MET:HA	1.92	0.50
1:A:1219:LEU:O	1:A:1223:MET:HB2	2.11	0.50
1:A:1054:PHE:HE1	1:A:1151:PHE:CE2	2.30	0.50
1:B:1237:MET:CE	1:B:1266:GLU:OE2	2.59	0.50
1:C:1231:PRO:HG2	1:C:1234:CYS:SG	2.50	0.50
1:D:1120:MET:HB3	1:D:1256:PHE:CE2	2.46	0.50
1:A:1208:GLN:HG2	3:A:25:HOH:O	2.12	0.50
1:B:1039:ARG:O	1:B:1043:GLU:HG3	2.12	0.50
1:B:1153:MET:CE	2:B:1:01P:H17	2.41	0.50
1:C:1242:MET:HB3	1:C:1246:TRP:CH2	2.46	0.50
1:A:993:ARG:NH2	1:A:1071:PRO:O	2.44	0.50
1:B:1026:ARG:HB3	1:B:1078:LEU:HD23	1.93	0.50
1:B:990:GLU:OE2	1:B:1066:VAL:HA	2.11	0.50
1:B:1124:ASN:OD1	1:B:1188:THR:HG22	2.11	0.50
1:B:1174:ARG:NH1	1:B:1210:TYR:O	2.45	0.50
1:C:1060:VAL:HB	1:C:1150:ASP:H	1.76	0.50
1:A:1260:ILE:O	1:A:1264:LYS:N	2.45	0.49
1:B:1000:ARG:NH1	1:D:1233:ASN:O	2.41	0.49
1:A:997:THR:O	1:A:998:MET:CB	2.60	0.49
1:B:1130:HIS:O	1:B:1191:ASP:OD1	2.30	0.49
1:C:1033:ASN:HD22	1:C:1033:ASN:C	2.13	0.49
1:D:1034:GLU:HG2	1:D:1070:GLN:NE2	2.27	0.49
1:D:1174:ARG:NH1	1:D:1210:TYR:HB2	2.27	0.49
1:D:1102:ALA:HB1	1:D:1103:PRO:HD2	1.94	0.49
1:D:1272:ARG:HG3	1:D:1273:GLU:OE2	2.13	0.49
1:B:1237:MET:HG3	1:B:1238:LEU:N	2.27	0.49
1:B:1085:LYS:HD3	1:B:1158:TYR:CE2	2.47	0.49
1:B:1111:GLN:HA	1:B:1267:MET:HE3	1.95	0.49
1:D:1060:VAL:HG11	2:D:1:01P:H23	1.93	0.49
1:D:1249:ASN:HD22	1:D:1250:PRO:N	2.11	0.49
1:A:1041:ARG:HG3	1:A:1041:ARG:NH1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1077:GLU:OE1	1:A:1079:MET:HE1	2.13	0.49
1:A:1195:PHE:CZ	1:A:1199:LEU:HD21	2.48	0.49
1:C:1106:LEU:HD23	1:C:1106:LEU:O	2.12	0.49
1:D:1033:ASN:C	1:D:1035:ALA:N	2.64	0.49
1:D:1106:LEU:HD12	1:D:1235:PRO:CG	2.43	0.49
1:B:993:ARG:NH2	1:B:1069:GLY:O	2.36	0.49
1:A:1174:ARG:HD3	1:A:1209:PRO:O	2.12	0.49
1:B:1015:ALA:O	1:B:1024:GLU:HA	2.13	0.49
1:B:1188:THR:O	1:B:1192:VAL:HG23	2.13	0.49
1:C:1103:PRO:O	1:C:1104:PRO:O	2.31	0.49
1:D:993:ARG:NH2	1:D:1070:GLN:CA	2.76	0.49
1:A:993:ARG:HG3	1:A:1066:VAL:HG11	1.95	0.48
1:B:1122:TYR:O	1:B:1126:ASN:ND2	2.46	0.48
1:D:1060:VAL:CG2	1:D:1149:GLY:HA2	2.42	0.48
1:B:1002:LEU:HD21	1:B:1012:GLU:HB2	1.94	0.48
1:B:993:ARG:HG3	3:B:5:HOH:O	2.12	0.48
1:B:993:ARG:NH2	1:B:1070:GLN:C	2.66	0.48
1:B:1054:PHE:CE1	1:B:1151:PHE:HE2	2.32	0.48
1:B:1152:GLY:O	1:B:1153:MET:HB2	2.13	0.48
1:B:1174:ARG:HD3	1:B:1209:PRO:O	2.13	0.48
1:D:1056:CYS:HB2	1:D:1122:TYR:CD2	2.49	0.48
1:D:1267:MET:O	1:D:1268:GLU:C	2.51	0.48
1:A:1129:VAL:O	1:A:1129:VAL:HG23	2.13	0.48
1:D:1204:THR:HG22	1:D:1231:PRO:HB3	1.94	0.48
1:A:1060:VAL:CG2	1:A:1149:GLY:HA3	2.44	0.48
1:B:1007:PHE:HZ	1:B:1043:GLU:HB3	1.78	0.48
1:C:993:ARG:NH2	1:C:1070:GLN:C	2.66	0.48
1:D:1042:ILE:HD11	3:D:30:HOH:O	2.14	0.48
1:D:1106:LEU:HD23	1:D:1106:LEU:C	2.34	0.48
1:D:1198:VAL:O	1:D:1202:ILE:HG13	2.14	0.48
1:D:1204:THR:OG1	1:D:1207:GLU:HB2	2.13	0.48
1:A:1085:LYS:HE2	1:A:1089:ARG:NH2	2.28	0.48
1:B:1165:LYS:HZ3	1:B:1219:LEU:HD22	1.78	0.48
1:C:1101:LEU:CD2	1:C:1101:LEU:N	2.76	0.48
1:A:1069:GLY:O	1:A:1070:GLN:HG2	2.14	0.48
1:B:1069:GLY:H	1:C:1053:GLU:CD	2.16	0.48
1:D:989:TRP:CD2	1:D:1052:LYS:HD3	2.48	0.48
1:A:1134:ALA:HA	1:A:1198:VAL:HG22	1.95	0.47
1:C:997:THR:O	1:C:998:MET:CB	2.62	0.47
1:D:1170:LEU:HD12	1:D:1170:LEU:HA	1.75	0.47
1:A:1019:VAL:CG1	1:A:1020:LYS:H	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1164:ARG:CG	1:C:1164:ARG:HH11	2.26	0.47
1:A:1006:SER:HB3	1:A:1154:THR:CB	2.44	0.47
1:C:1033:ASN:C	1:C:1035:ALA:N	2.66	0.47
1:C:1204:THR:HG22	1:C:1231:PRO:HB3	1.96	0.47
1:D:1010:VAL:HG12	1:D:1011:TYR:N	2.29	0.47
1:C:1060:VAL:HG12	1:C:1076:MET:HE2	1.96	0.47
1:D:1033:ASN:O	1:D:1035:ALA:N	2.47	0.47
1:D:1058:HIS:HA	1:D:1147:LYS:HG2	1.97	0.47
1:A:1109:MET:HE3	3:A:11:HOH:O	2.15	0.47
1:D:993:ARG:NH2	1:D:1070:GLN:C	2.68	0.47
1:D:1154:THR:HG22	1:D:1155:ARG:H	1.78	0.47
1:A:1182:LYS:HG2	1:A:1183:ASP:N	2.29	0.47
1:C:1014:VAL:HG11	1:C:1024:GLU:CD	2.35	0.47
1:A:1018:VAL:CG1	1:A:1063:LEU:HB3	2.45	0.47
1:A:1077:GLU:HG2	1:A:1079:MET:HE2	1.96	0.47
1:A:1122:TYR:HE1	1:A:1281:GLU:OE2	1.98	0.47
1:D:1019:VAL:HG12	1:D:1020:LYS:N	2.28	0.47
1:A:990:GLU:OE2	1:A:1067:SER:N	2.47	0.47
1:C:1033:ASN:C	1:C:1035:ALA:H	2.18	0.47
1:C:1079:MET:HE3	1:C:1147:LYS:HD2	1.96	0.47
1:D:1014:VAL:HA	1:D:1025:THR:O	2.14	0.47
1:D:1128:PHE:CD1	1:D:1128:PHE:C	2.89	0.47
1:A:1016:LYS:HG2	1:A:1024:GLU:HG2	1.97	0.47
1:A:1130:HIS:CD2	1:A:1132:ASP:C	2.89	0.47
1:B:1059:VAL:O	1:B:1060:VAL:C	2.51	0.47
1:B:1171:LEU:HB3	1:B:1176:MET:SD	2.55	0.47
1:C:1180:SER:O	1:C:1184:GLY:HA2	2.15	0.47
1:C:1263:ILE:O	1:C:1264:LYS:C	2.51	0.47
1:D:1272:ARG:CG	1:D:1273:GLU:OE2	2.63	0.47
1:A:1106:LEU:HD23	1:A:1110:ILE:HG12	1.98	0.46
1:A:1110:ILE:HD11	1:A:1237:MET:SD	2.55	0.46
1:A:1116:ILE:O	1:A:1148:ILE:HD11	2.16	0.46
1:B:1089:ARG:CD	1:B:1092:ARG:NH1	2.77	0.46
1:D:996:ILE:HD11	1:D:1075:ILE:HG13	1.96	0.46
1:A:1157:ILE:CG1	1:A:1157:ILE:O	2.63	0.46
1:A:1029:ILE:HG23	1:A:1075:ILE:HD13	1.98	0.46
1:B:1163:TYR:HD1	1:B:1215:ASN:HD22	1.54	0.46
1:D:1027:VAL:CG1	1:D:1063:LEU:HD12	2.45	0.46
1:A:1046:ASN:HD22	1:A:1046:ASN:N	2.13	0.46
1:A:1195:PHE:CE2	1:A:1199:LEU:HD11	2.50	0.46
1:B:1157:ILE:HG12	1:B:1157:ILE:O	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1237:MET:HG3	1:C:1238:LEU:N	2.31	0.46
1:C:1240:GLU:OE2	1:C:1240:GLU:HA	2.16	0.46
1:D:1092:ARG:HG2	1:D:1205:LEU:CD1	2.43	0.46
2:C:1:01P:H19	2:C:1:01P:N5	2.31	0.46
1:C:1109:MET:CE	1:C:1202:ILE:HG22	2.45	0.46
1:D:1016:LYS:HG2	1:D:1024:GLU:HG2	1.97	0.46
1:D:1249:ASN:HD21	1:D:1251:LYS:CB	2.25	0.46
1:A:1249:ASN:HD21	1:A:1251:LYS:H	1.63	0.46
1:A:1172:PRO:O	1:A:1176:MET:HG3	2.16	0.46
1:B:1204:THR:HG22	1:B:1231:PRO:HB3	1.98	0.46
1:C:1249:ASN:O	1:C:1250:PRO:C	2.54	0.46
1:D:1091:LEU:CD1	1:D:1104:PRO:HG3	2.45	0.46
1:D:1018:VAL:HG13	1:D:1063:LEU:HB3	1.90	0.45
1:A:1039:ARG:O	1:A:1043:GLU:HG3	2.16	0.45
1:A:1130:HIS:HD2	1:A:1132:ASP:N	2.08	0.45
1:B:1030:LYS:HD3	1:B:1150:ASP:OD2	2.16	0.45
1:B:1204:THR:O	1:B:1205:LEU:C	2.53	0.45
1:B:1243:ARG:HG3	1:B:1243:ARG:NH1	2.30	0.45
1:C:991:VAL:O	1:C:1066:VAL:HG22	2.15	0.45
1:D:1033:ASN:O	1:D:1036:ALA:N	2.49	0.45
1:C:1245:CYS:O	1:C:1253:ARG:HD3	2.16	0.45
1:D:1029:ILE:HG12	1:D:1075:ILE:CD1	2.45	0.45
1:D:1182:LYS:O	1:D:1182:LYS:HD2	2.16	0.45
1:D:1200:TRP:CD1	1:D:1228:LEU:HD13	2.52	0.45
1:B:1001:GLU:OE1	1:B:1009:MET:HE1	2.16	0.45
1:D:1156:ASP:HB3	1:D:1157:ILE:H	1.46	0.45
1:A:1077:GLU:OE1	1:A:1079:MET:CE	2.65	0.45
1:D:1165:LYS:NZ	1:D:1181:LEU:O	2.50	0.45
1:A:1133:LEU:O	1:A:1194:SER:HB3	2.17	0.45
1:B:1065:VAL:HG12	1:B:1066:VAL:N	2.32	0.45
1:C:1078:LEU:HG	1:C:1079:MET:N	2.32	0.45
1:D:1155:ARG:HD3	1:D:1162:TYR:CD2	2.51	0.45
1:B:997:THR:O	1:B:998:MET:HB2	2.17	0.45
1:C:1033:ASN:CG	1:C:1035:ALA:HB3	2.37	0.45
1:D:1200:TRP:CD2	1:D:1228:LEU:HD13	2.51	0.45
1:A:1128:PHE:CZ	1:A:1151:PHE:CE2	3.05	0.45
1:B:993:ARG:NH2	1:B:1070:GLN:CA	2.80	0.45
1:C:1001:GLU:OE2	1:C:1009:MET:SD	2.75	0.45
1:C:1156:ASP:OD2	1:C:1157:ILE:CG2	2.64	0.45
1:B:1241:LEU:HD21	1:B:1259:ILE:HG23	1.98	0.45
1:B:987:ASP:OD1	1:B:988:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:LEU:O	1:A:1126:ASN:N	2.48	0.44
1:C:1215:ASN:O	1:C:1218:VAL:HB	2.16	0.44
1:D:1120:MET:SD	1:D:1148:ILE:HD13	2.57	0.44
1:B:1027:VAL:HG12	1:B:1063:LEU:HD12	1.99	0.44
1:B:1214:SER:O	1:B:1217:GLN:N	2.50	0.44
1:B:1111:GLN:CD	1:B:1267:MET:HE3	2.37	0.44
1:C:1015:ALA:HB1	1:C:1018:VAL:HG21	1.97	0.44
1:C:1133:LEU:HD12	1:C:1134:ALA:N	2.31	0.44
1:C:1155:ARG:HH11	1:C:1159:GLU:CG	2.30	0.44
1:D:994:GLU:H	1:D:994:GLU:HG3	1.56	0.44
1:D:1079:MET:CE	1:D:1147:LYS:HD2	2.48	0.44
1:D:1080:THR:OG1	1:D:1142:GLU:HB2	2.16	0.44
1:D:997:THR:O	1:D:998:MET:CB	2.65	0.44
1:C:1043:GLU:O	1:C:1047:GLU:N	2.42	0.44
1:D:1012:GLU:HG3	1:D:1078:LEU:HD22	1.99	0.44
1:D:1142:GLU:C	1:D:1144:PHE:H	2.19	0.44
1:A:1004:GLN:HB3	1:A:1004:GLN:HE21	1.51	0.44
1:A:1005:GLY:O	1:A:1006:SER:C	2.56	0.44
1:D:1139:MET:CE	1:D:1153:MET:SD	3.06	0.44
1:B:1014:VAL:CG1	1:B:1024:GLU:HB3	2.48	0.44
1:D:1042:ILE:CG2	1:D:1042:ILE:O	2.55	0.44
1:D:1245:CYS:O	1:D:1253:ARG:HD3	2.18	0.44
1:A:988:GLU:N	3:A:4:HOH:O	2.50	0.44
1:B:1018:VAL:CG1	1:B:1063:LEU:HD22	2.47	0.44
1:C:1249:ASN:ND2	1:C:1251:LYS:HB2	2.33	0.44
1:C:1268:GLU:O	1:C:1270:GLY:N	2.51	0.44
1:A:1165:LYS:NZ	1:A:1171:LEU:CD1	2.80	0.44
1:B:1018:VAL:CG1	1:B:1063:LEU:HB3	2.47	0.44
1:A:1011:TYR:HE1	1:A:1031:THR:HG21	1.83	0.44
1:A:1042:ILE:HG22	1:A:1042:ILE:O	2.17	0.44
1:A:1057:HIS:O	1:A:1147:LYS:NZ	2.50	0.44
1:A:1161:ASP:OD2	1:A:1208:GLN:OE1	2.36	0.44
1:C:1155:ARG:HH11	1:C:1159:GLU:CD	2.21	0.44
1:D:1034:GLU:HB3	1:D:1070:GLN:HE22	1.82	0.44
1:A:1084:LEU:O	1:A:1088:LEU:HG	2.17	0.43
1:B:1165:LYS:O	1:B:1165:LYS:CG	2.65	0.43
1:C:1204:THR:OG1	1:C:1207:GLU:HB2	2.17	0.43
1:A:1029:ILE:HG22	1:A:1073:LEU:HD22	2.00	0.43
1:C:1030:LYS:O	1:C:1044:PHE:HZ	2.02	0.43
1:C:1200:TRP:CG	1:C:1228:LEU:HD13	2.53	0.43
1:A:1030:LYS:O	1:A:1044:PHE:HZ	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1150:ASP:C	1:C:1152:GLY:N	2.72	0.43
1:D:1041:ARG:O	1:D:1045:LEU:HD12	2.18	0.43
1:A:1130:HIS:O	1:A:1191:ASP:OD1	2.35	0.43
1:B:1237:MET:HG3	1:B:1238:LEU:H	1.82	0.43
1:A:1019:VAL:HB	1:A:1022:GLU:HB3	2.01	0.43
1:B:1085:LYS:HD3	1:B:1158:TYR:CZ	2.52	0.43
1:B:1168:LYS:HB2	1:B:1168:LYS:HE3	1.79	0.43
1:A:1036:ALA:HB1	1:A:1040:GLU:HB2	2.00	0.43
1:B:1068:GLN:HB2	1:B:1068:GLN:HE21	1.50	0.43
1:C:1174:ARG:HD3	1:C:1209:PRO:O	2.18	0.43
1:D:1102:ALA:HB1	1:D:1103:PRO:CD	2.48	0.43
1:D:1174:ARG:HB2	1:D:1175:TRP:CE3	2.54	0.43
1:A:1064:GLY:O	1:A:1075:ILE:N	2.41	0.43
1:B:1129:VAL:O	1:B:1129:VAL:CG2	2.67	0.43
1:B:1214:SER:H	1:B:1217:GLN:HB2	1.83	0.43
1:B:985:VAL:O	1:B:985:VAL:HG23	2.19	0.43
1:D:1157:ILE:CG1	1:D:1158:TYR:CE2	3.02	0.43
1:A:1018:VAL:HG13	1:A:1063:LEU:HB3	2.01	0.43
1:A:993:ARG:CG	1:A:1066:VAL:HG11	2.49	0.43
1:B:1139:MET:HE1	1:B:1150:ASP:H	1.84	0.43
1:C:1133:LEU:O	1:C:1134:ALA:HB2	2.19	0.43
1:D:1182:LYS:HG3	1:D:1183:ASP:OD1	2.19	0.43
1:A:1059:VAL:O	1:A:1060:VAL:C	2.55	0.43
1:B:1172:PRO:O	1:B:1176:MET:HG3	2.19	0.43
1:D:1249:ASN:HD22	1:D:1251:LYS:N	2.16	0.43
1:A:1027:VAL:HG12	1:A:1063:LEU:HD12	2.01	0.42
1:A:999:SER:O	1:A:1000:ARG:CB	2.65	0.42
1:B:1004:GLN:HE22	1:B:1009:MET:CG	2.30	0.42
1:B:1128:PHE:CZ	1:B:1151:PHE:CE2	3.07	0.42
1:C:1187:THR:OG1	1:C:1189:TYR:HD2	2.02	0.42
1:C:1120:MET:HB3	1:C:1256:PHE:CE2	2.53	0.42
1:D:1035:ALA:O	1:D:1036:ALA:O	2.37	0.42
1:B:1071:PRO:O	1:B:1072:THR:C	2.57	0.42
1:B:1076:MET:O	1:B:1077:GLU:C	2.57	0.42
1:B:1164:ARG:HG2	1:B:1164:ARG:H	1.55	0.42
1:C:1037:SER:C	1:C:1039:ARG:N	2.73	0.42
1:A:1036:ALA:O	1:A:1041:ARG:NH2	2.52	0.42
1:A:1045:LEU:HD12	1:A:1045:LEU:HA	1.85	0.42
1:B:1075:ILE:O	1:B:1076:MET:CG	2.67	0.42
1:B:1237:MET:HE1	1:B:1266:GLU:OE2	2.19	0.42
1:C:1052:LYS:HE2	1:C:1052:LYS:HB2	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1250:PRO:HA	1:C:1253:ARG:CZ	2.49	0.42
1:D:1047:GLU:C	1:D:1049:SER:N	2.73	0.42
1:A:1066:VAL:HB	1:A:1073:LEU:HB2	2.01	0.42
1:B:1204:THR:O	1:B:1206:ALA:N	2.52	0.42
1:C:1041:ARG:HE	1:C:1041:ARG:HB2	1.58	0.42
1:B:1037:SER:HB3	1:C:1131:ARG:CD	2.50	0.42
1:C:1190:SER:O	1:C:1193:TRP:HB3	2.19	0.42
1:C:1268:GLU:HA	1:C:1269:PRO:HD3	1.88	0.42
1:C:1272:ARG:HB3	1:C:1273:GLU:OE2	2.19	0.42
1:D:1034:GLU:HG2	1:D:1070:GLN:CD	2.40	0.42
1:D:1029:ILE:HG12	1:D:1075:ILE:HD12	2.00	0.42
1:D:1081:ARG:HG2	1:D:1081:ARG:HH11	1.83	0.42
1:D:1120:MET:SD	1:D:1148:ILE:CD1	3.07	0.42
1:B:1165:LYS:CE	1:B:1181:LEU:O	2.68	0.42
1:C:1033:ASN:ND2	1:C:1033:ASN:C	2.73	0.42
1:C:1230:LYS:HA	1:C:1239:PHE:CE1	2.55	0.42
1:A:1031:THR:HG22	1:A:1073:LEU:HD23	2.01	0.42
1:B:1046:ASN:O	1:B:1050:VAL:HG23	2.20	0.42
1:C:996:ILE:CD1	1:C:1066:VAL:HG21	2.48	0.42
1:C:1177:SER:HA	1:C:1193:TRP:CD1	2.55	0.42
1:D:1165:LYS:HD3	1:D:1171:LEU:HD12	2.01	0.42
1:D:1244:MET:O	1:D:1247:GLN:HG2	2.20	0.42
1:A:1059:VAL:HA	1:A:1148:ILE:O	2.19	0.42
1:A:1150:ASP:OD2	2:A:1:01P:N2	2.45	0.42
1:C:1153:MET:CE	2:C:1:01P:H17	2.50	0.42
1:C:1122:TYR:CE1	1:C:1126:ASN:ND2	2.87	0.42
1:D:1018:VAL:HG12	1:D:1063:LEU:HD13	2.02	0.42
1:D:1123:LEU:HA	1:D:1123:LEU:HD12	1.86	0.42
1:D:1186:PHE:CD1	1:D:1186:PHE:N	2.88	0.42
1:C:993:ARG:HH12	1:C:1071:PRO:CD	2.33	0.42
1:D:1211:GLN:C	1:D:1213:LEU:H	2.24	0.42
1:D:1204:THR:CG2	1:D:1231:PRO:HB3	2.50	0.42
1:A:1131:ARG:HH11	1:A:1186:PHE:HB2	1.84	0.42
1:B:1015:ALA:O	1:B:1025:THR:N	2.47	0.42
1:A:1015:ALA:O	1:A:1024:GLU:HA	2.19	0.41
1:A:1143:ASP:O	1:A:1144:PHE:HB2	2.20	0.41
1:C:1157:ILE:HG13	1:C:1157:ILE:O	2.19	0.41
1:A:1085:LYS:HD3	1:A:1158:TYR:CZ	2.55	0.41
1:B:1053:GLU:OE1	1:B:1053:GLU:HA	2.20	0.41
1:B:1150:ASP:OD2	2:B:1:01P:H1	2.20	0.41
1:C:1260:ILE:HG21	1:C:1277:TYR:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1165:LYS:HB3	1:D:1165:LYS:HE2	1.87	0.41
1:D:1179:GLU:HG2	1:D:1180:SER:N	2.36	0.41
1:D:1106:LEU:HD12	1:D:1235:PRO:HG2	2.01	0.41
1:A:1214:SER:OG	1:A:1217:GLN:HG3	2.19	0.41
1:B:1005:GLY:HA2	2:B:1:01P:H10	2.02	0.41
1:B:993:ARG:NH2	1:B:1070:GLN:HA	2.35	0.41
1:C:1181:LEU:HD22	1:C:1219:LEU:HD22	2.02	0.41
1:D:1157:ILE:HG12	1:D:1158:TYR:CD2	2.55	0.41
1:A:1174:ARG:HG2	1:A:1218:VAL:HG21	2.02	0.41
1:A:1234:CYS:HA	1:A:1235:PRO:HD3	1.96	0.41
1:C:1034:GLU:CG	1:C:1070:GLN:NE2	2.82	0.41
1:C:1247:GLN:HB2	1:C:1253:ARG:HG2	2.03	0.41
1:D:1047:GLU:C	1:D:1049:SER:H	2.24	0.41
1:D:1157:ILE:HG12	1:D:1158:TYR:CE2	2.56	0.41
1:B:1027:VAL:C	1:B:1078:LEU:HB2	2.41	0.41
1:B:992:ALA:O	1:B:993:ARG:C	2.59	0.41
1:C:1153:MET:HE1	2:C:1:01P:H17	2.03	0.41
1:C:1029:ILE:HG12	1:C:1075:ILE:CD1	2.51	0.41
1:C:1193:TRP:CE3	1:C:1246:TRP:HA	2.56	0.41
1:A:1077:GLU:CD	1:A:1079:MET:CE	2.89	0.41
1:B:1057:HIS:O	1:B:1057:HIS:ND1	2.53	0.41
1:B:1162:TYR:HB3	1:B:1170:LEU:HB3	2.01	0.41
1:B:1235:PRO:HD2	1:B:1238:LEU:HD12	2.02	0.41
1:C:1058:HIS:ND1	1:C:1118:ASP:OD2	2.48	0.41
1:D:1033:ASN:ND2	1:D:1035:ALA:H	2.19	0.41
1:D:1114:GLY:O	1:D:1118:ASP:N	2.44	0.41
1:D:1176:MET:HE3	1:D:1180:SER:HB3	2.02	0.41
1:A:996:ILE:HD11	1:A:1075:ILE:HG13	2.03	0.41
1:C:1007:PHE:CE1	1:C:1040:GLU:HB3	2.56	0.41
1:C:1263:ILE:O	1:C:1266:GLU:N	2.35	0.41
1:D:1035:ALA:O	1:D:1036:ALA:C	2.59	0.41
1:D:1058:HIS:ND1	1:D:1118:ASP:CB	2.77	0.41
1:A:1007:PHE:HZ	1:A:1043:GLU:HB3	1.86	0.41
1:A:1106:LEU:HD23	1:A:1110:ILE:CG1	2.51	0.41
1:D:1034:GLU:CG	1:D:1070:GLN:NE2	2.84	0.41
1:D:1106:LEU:HA	1:D:1109:MET:HB2	2.02	0.41
1:D:1210:TYR:O	1:D:1211:GLN:C	2.60	0.41
1:A:1065:VAL:HG12	1:A:1066:VAL:N	2.36	0.41
1:B:1227:LEU:HD13	1:B:1243:ARG:HE	1.83	0.41
1:C:1019:VAL:CG1	1:C:1020:LYS:N	2.65	0.41
1:C:1080:THR:OG1	1:C:1142:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1179:GLU:HG2	1:C:1180:SER:N	2.36	0.41
1:C:1250:PRO:O	1:C:1252:MET:N	2.54	0.41
1:C:1111:GLN:NE2	1:C:1267:MET:HE2	2.35	0.41
1:A:1033:ASN:HD22	1:A:1033:ASN:HA	1.76	0.40
1:A:1188:THR:O	1:A:1191:ASP:HB2	2.21	0.40
1:C:1150:ASP:O	1:C:1152:GLY:N	2.53	0.40
1:D:1043:GLU:HG2	1:D:1043:GLU:O	2.21	0.40
1:A:1116:ILE:HD13	1:A:1198:VAL:HG11	2.04	0.40
1:C:1060:VAL:HG12	1:C:1076:MET:CE	2.51	0.40
1:C:1264:LYS:O	1:C:1266:GLU:N	2.55	0.40
1:D:1001:GLU:HB3	1:D:1009:MET:SD	2.62	0.40
1:D:1155:ARG:O	1:D:1156:ASP:O	2.39	0.40
1:A:1060:VAL:HG23	1:A:1149:GLY:HA3	2.03	0.40
1:A:1218:VAL:O	1:A:1219:LEU:C	2.60	0.40
1:B:1139:MET:CE	1:B:1150:ASP:H	2.33	0.40
1:C:1031:THR:HG22	1:C:1073:LEU:HD22	2.03	0.40
1:D:1063:LEU:HD23	1:D:1063:LEU:HA	1.81	0.40
1:B:1058:HIS:O	1:B:1059:VAL:HG23	2.21	0.40
1:B:1083:ASP:HA	1:B:1139:MET:HA	2.03	0.40
1:B:1187:THR:HG1	1:B:1189:TYR:HD2	1.64	0.40
1:C:998:MET:HE2	1:C:1029:ILE:HG21	2.03	0.40
1:D:1159:GLU:C	1:D:1161:ASP:N	2.75	0.40
2:B:1:01P:H3	2:B:1:01P:H17B	2.04	0.40
1:C:1084:LEU:N	1:C:1138:CYS:O	2.41	0.40
1:C:1120:MET:SD	1:C:1148:ILE:HD13	2.62	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	281/301 (93%)	241 (86%)	31 (11%)	9 (3%)	<b>4</b> <b>16</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	284/301 (94%)	236 (83%)	33 (12%)	15 (5%)	2	6
1	C	289/301 (96%)	241 (83%)	32 (11%)	16 (6%)	2	5
1	D	288/301 (96%)	238 (83%)	36 (12%)	14 (5%)	2	8
All	All	1142/1204 (95%)	956 (84%)	132 (12%)	54 (5%)	2	8

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1106	LEU
1	A	1150	ASP
1	B	1154	THR
1	B	1156	ASP
1	B	1165	LYS
1	C	987	ASP
1	C	988	GLU
1	C	998	MET
1	C	1036	ALA
1	C	1104	PRO
1	C	1150	ASP
1	D	1036	ALA
1	D	1094	GLU
1	D	1105	SER
1	D	1106	LEU
1	D	1156	ASP
1	A	1000	ARG
1	A	1091	LEU
1	A	1182	LYS
1	B	1036	ALA
1	B	1082	GLY
1	B	1106	LEU
1	B	1149	GLY
1	B	1205	LEU
1	B	1232	ASP
1	C	999	SER
1	C	1106	LEU
1	C	1251	LYS
1	C	1269	PRO
1	A	1017	GLY
1	B	1023	PRO
1	C	1080	THR
1	C	1151	PHE

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Mol	Chain	Res	Type
1	C	1153	MET
1	D	999	SER
1	D	1023	PRO
1	D	1103	PRO
1	D	1211	GLN
1	A	1023	PRO
1	A	1055	ASN
1	B	998	MET
1	B	1151	PHE
1	C	1265	GLU
1	D	998	MET
1	D	1154	THR
1	A	998	MET
1	B	1155	ARG
1	C	1077	GLU
1	C	1264	LYS
1	D	1034	GLU
1	D	1165	LYS
1	B	1152	GLY
1	D	1263	ILE
1	B	1059	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	232/263 (88%)	208 (90%)	24 (10%)	7	22
1	B	238/263 (90%)	215 (90%)	23 (10%)	8	25
1	C	234/263 (89%)	216 (92%)	18 (8%)	13	35
1	D	235/263 (89%)	214 (91%)	21 (9%)	9	29
All	All	939/1052 (89%)	853 (91%)	86 (9%)	9	27

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	988	GLU
1	A	989	TRP
1	A	1004	GLN
1	A	1006	SER
1	A	1018	VAL
1	A	1033	ASN
1	A	1046	ASN
1	A	1070	GLN
1	A	1104	PRO
1	A	1107	SER
1	A	1123	LEU
1	A	1129	VAL
1	A	1150	ASP
1	A	1157	ILE
1	A	1160	THR
1	A	1164	ARG
1	A	1208	GLN
1	A	1227	LEU
1	A	1241	LEU
1	A	1249	ASN
1	A	1264	LYS
1	A	1265	GLU
1	A	1273	GLU
1	A	1282	ASN
1	B	988	GLU
1	B	989	TRP
1	B	1009	MET
1	B	1041	ARG
1	B	1045	LEU
1	B	1049	SER
1	B	1068	GLN
1	B	1070	GLN
1	B	1104	PRO
1	B	1123	LEU
1	B	1129	VAL
1	B	1153	MET
1	B	1156	ASP
1	B	1157	ILE
1	B	1164	ARG
1	B	1211	GLN
1	B	1237	MET
1	B	1243	ARG
1	B	1249	ASN

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Mol	Chain	Res	Type
1	B	1258	GLU
1	B	1264	LYS
1	B	1266	GLU
1	B	1280	GLU
1	C	988	GLU
1	C	989	TRP
1	C	999	SER
1	C	1033	ASN
1	C	1038	MET
1	C	1050	VAL
1	C	1062	LEU
1	C	1094	GLU
1	C	1101	LEU
1	C	1131	ARG
1	C	1157	ILE
1	C	1159	GLU
1	C	1205	LEU
1	C	1241	LEU
1	C	1243	ARG
1	C	1249	ASN
1	C	1272	ARG
1	C	1273	GLU
1	D	989	TRP
1	D	997	THR
1	D	1023	PRO
1	D	1045	LEU
1	D	1050	VAL
1	D	1055	ASN
1	D	1062	LEU
1	D	1070	GLN
1	D	1123	LEU
1	D	1131	ARG
1	D	1139	MET
1	D	1154	THR
1	D	1156	ASP
1	D	1157	ILE
1	D	1173	VAL
1	D	1213	LEU
1	D	1233	ASN
1	D	1237	MET
1	D	1241	LEU
1	D	1249	ASN

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Mol	Chain	Res	Type
1	D	1272	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1004	GLN
1	A	1033	ASN
1	A	1046	ASN
1	A	1068	GLN
1	A	1124	ASN
1	A	1130	HIS
1	A	1208	GLN
1	A	1249	ASN
1	A	1282	ASN
1	B	1004	GLN
1	B	1046	ASN
1	B	1068	GLN
1	B	1130	HIS
1	B	1208	GLN
1	B	1211	GLN
1	C	1033	ASN
1	C	1046	ASN
1	C	1111	GLN
1	C	1208	GLN
1	C	1249	ASN
1	D	1033	ASN
1	D	1046	ASN
1	D	1057	HIS
1	D	1130	HIS
1	D	1208	GLN
1	D	1249	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	01P	C	1	-	36,36,36	2.55	14 (38%)	49,49,49	3.01	20 (40%)
2	01P	A	1	-	36,36,36	2.39	14 (38%)	49,49,49	3.23	17 (34%)
2	01P	D	1	-	36,36,36	2.83	17 (47%)	49,49,49	2.94	17 (34%)
2	01P	B	1	-	36,36,36	2.76	19 (52%)	49,49,49	3.20	22 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	01P	C	1	-	-	4/14/22/22	0/5/5/5
2	01P	A	1	-	-	4/14/22/22	0/5/5/5
2	01P	D	1	-	-	3/14/22/22	0/5/5/5
2	01P	B	1	-	-	5/14/22/22	0/5/5/5

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	01P	C20-C21	6.91	1.52	1.42
2	D	1	01P	C20-C21	6.81	1.52	1.42
2	A	1	01P	C20-C21	5.86	1.51	1.42
2	C	1	01P	C20-C21	5.23	1.50	1.42
2	D	1	01P	C9-C10	5.23	1.48	1.36
2	C	1	01P	C8-C7	5.13	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	01P	C8-C7	4.89	1.47	1.36
2	D	1	01P	C8-C7	4.89	1.47	1.36
2	D	1	01P	C22-N3	4.85	1.39	1.31
2	D	1	01P	C19-C18	4.83	1.48	1.37
2	C	1	01P	C19-C18	4.73	1.47	1.37
2	C	1	01P	C13-C12	4.66	1.47	1.39
2	B	1	01P	C21-N3	4.48	1.45	1.37
2	D	1	01P	C21-N3	4.43	1.45	1.37
2	C	1	01P	C9-C10	4.32	1.46	1.36
2	B	1	01P	C8-C7	4.32	1.46	1.36
2	B	1	01P	C13-C12	4.21	1.46	1.39
2	A	1	01P	C19-C18	4.20	1.46	1.37
2	B	1	01P	C10-C21	4.13	1.49	1.41
2	B	1	01P	C15-C14	4.03	1.47	1.40
2	A	1	01P	C9-C10	4.01	1.45	1.36
2	B	1	01P	C19-C18	3.95	1.46	1.37
2	B	1	01P	C9-C10	3.95	1.45	1.36
2	D	1	01P	C16-C15	3.91	1.46	1.39
2	C	1	01P	C22-N3	3.88	1.38	1.31
2	B	1	01P	C13-C14	3.80	1.45	1.38
2	D	1	01P	C10-C21	3.78	1.48	1.41
2	C	1	01P	C13-C14	3.67	1.45	1.38
2	D	1	01P	C13-C12	3.61	1.45	1.39
2	D	1	01P	C9-C8	3.60	1.47	1.38
2	C	1	01P	C9-C8	3.50	1.47	1.38
2	C	1	01P	C15-C14	3.49	1.46	1.40
2	A	1	01P	C10-C21	3.46	1.47	1.41
2	A	1	01P	C9-C8	3.45	1.47	1.38
2	B	1	01P	O2-C14	3.44	1.42	1.37
2	B	1	01P	C11-C12	3.41	1.45	1.39
2	A	1	01P	C11-C12	3.39	1.45	1.39
2	C	1	01P	C21-N3	3.33	1.43	1.37
2	C	1	01P	O2-C14	3.31	1.42	1.37
2	A	1	01P	C21-N3	3.31	1.43	1.37
2	C	1	01P	C16-C15	3.28	1.45	1.39
2	D	1	01P	C13-C14	3.18	1.44	1.38
2	A	1	01P	C16-C15	3.11	1.44	1.39
2	A	1	01P	C15-C14	3.10	1.45	1.40
2	C	1	01P	C10-C21	3.08	1.47	1.41
2	D	1	01P	C22-C18	3.03	1.44	1.39
2	B	1	01P	C16-C15	3.03	1.44	1.39
2	B	1	01P	C9-C8	3.02	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	01P	C16-C11	2.98	1.44	1.38
2	A	1	01P	C16-C11	2.95	1.44	1.38
2	B	1	01P	C22-N3	2.95	1.36	1.31
2	A	1	01P	C22-N3	2.91	1.36	1.31
2	D	1	01P	C11-C12	2.84	1.44	1.39
2	A	1	01P	C22-C18	2.66	1.44	1.39
2	B	1	01P	C1-C23	2.49	1.43	1.38
2	B	1	01P	C7-C20	2.49	1.48	1.41
2	B	1	01P	C16-C11	2.37	1.43	1.38
2	C	1	01P	C1-C23	2.35	1.43	1.38
2	B	1	01P	C22-C18	2.28	1.43	1.39
2	D	1	01P	C3-N1	2.27	1.50	1.46
2	B	1	01P	C15-N1	-2.22	1.36	1.41
2	D	1	01P	C5-N1	2.10	1.50	1.46
2	D	1	01P	C18-N2	-2.07	1.36	1.40
2	A	1	01P	C13-C14	2.03	1.42	1.38

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	01P	C23-N4-C4	10.64	124.88	115.45
2	D	1	01P	C18-C22-N3	-10.62	116.41	124.49
2	C	1	01P	C18-C22-N3	-10.20	116.73	124.49
2	B	1	01P	C18-C22-N3	-9.67	117.13	124.49
2	A	1	01P	C18-C22-N3	-9.61	117.18	124.49
2	A	1	01P	N4-C4-N5	-9.15	117.88	126.55
2	C	1	01P	C22-N3-C21	8.45	127.08	116.91
2	B	1	01P	C23-N4-C4	7.78	122.35	115.45
2	D	1	01P	C23-N4-C4	7.62	122.20	115.45
2	A	1	01P	C22-N3-C21	7.37	125.78	116.91
2	B	1	01P	C22-N3-C21	7.37	125.78	116.91
2	D	1	01P	N4-C4-N5	-7.35	119.58	126.55
2	D	1	01P	C22-N3-C21	7.13	125.50	116.91
2	C	1	01P	N4-C4-N5	-6.68	120.22	126.55
2	C	1	01P	C23-N4-C4	6.35	121.08	115.45
2	B	1	01P	O2-C14-C15	6.28	124.63	116.06
2	B	1	01P	N4-C4-N5	-5.69	121.15	126.55
2	B	1	01P	O1-C6-C5	-4.95	100.90	111.80
2	C	1	01P	O2-C14-C15	4.43	122.10	116.06
2	B	1	01P	C1-C23-N4	-4.26	118.67	123.96
2	C	1	01P	C18-C19-C20	4.24	126.51	120.29
2	B	1	01P	C16-C15-N1	-4.22	115.58	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	01P	C1-C23-N4	-4.19	118.76	123.96
2	C	1	01P	C19-C20-C21	-4.17	112.82	118.27
2	B	1	01P	O2-C14-C13	-4.16	116.97	124.12
2	D	1	01P	C6-C5-N1	4.07	117.54	110.02
2	C	1	01P	C2-C3-N1	3.90	117.21	110.02
2	B	1	01P	C19-C20-C21	-3.83	113.27	118.27
2	D	1	01P	C17-O2-C14	3.74	123.17	117.53
2	B	1	01P	C16-C11-C12	3.72	124.59	120.30
2	B	1	01P	C10-C21-N3	3.61	124.44	118.52
2	A	1	01P	C19-C20-C21	-3.56	113.61	118.27
2	A	1	01P	O2-C14-C15	3.50	120.84	116.06
2	D	1	01P	C5-N1-C3	3.40	119.03	111.52
2	A	1	01P	O2-C14-C13	-3.25	118.53	124.12
2	A	1	01P	C18-C19-C20	3.24	125.04	120.29
2	B	1	01P	C18-C19-C20	3.24	125.04	120.29
2	C	1	01P	C16-C15-N1	-3.20	117.19	122.30
2	D	1	01P	C1-C23-N4	-3.18	120.00	123.96
2	D	1	01P	C19-C20-C21	-3.17	114.13	118.27
2	A	1	01P	O1-C6-C5	-3.11	104.96	111.80
2	C	1	01P	C1-C23-N4	-3.02	120.21	123.96
2	D	1	01P	C18-C19-C20	2.98	124.67	120.29
2	A	1	01P	C17-O2-C14	2.97	122.01	117.53
2	D	1	01P	C10-C21-N3	2.92	123.30	118.52
2	C	1	01P	C4-N5-C24	2.90	122.05	116.28
2	A	1	01P	C10-C21-N3	2.86	123.21	118.52
2	C	1	01P	C5-N1-C3	2.85	117.82	111.52
2	B	1	01P	C5-N1-C3	2.82	117.75	111.52
2	C	1	01P	C7-C20-C19	2.80	126.95	122.02
2	A	1	01P	C5-N1-C3	2.77	117.64	111.52
2	D	1	01P	C19-C18-C22	2.64	120.17	118.20
2	A	1	01P	C4-N5-C24	2.60	121.46	116.28
2	B	1	01P	C16-C15-C14	2.59	122.94	118.73
2	A	1	01P	C5-N1-C15	2.57	122.35	116.27
2	C	1	01P	C10-C21-N3	2.52	122.65	118.52
2	C	1	01P	C13-C14-C15	-2.52	117.13	120.42
2	B	1	01P	C19-C18-C22	2.48	120.05	118.20
2	C	1	01P	C5-N1-C15	2.41	121.99	116.27
2	B	1	01P	C7-C20-C19	2.41	126.27	122.02
2	A	1	01P	C2-C3-N1	2.41	114.46	110.02
2	D	1	01P	C4-N5-C24	2.37	121.00	116.28
2	D	1	01P	C2-C3-N1	2.35	114.35	110.02
2	A	1	01P	C16-C15-N1	-2.33	118.59	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	01P	C5-N1-C15	2.33	121.78	116.27
2	D	1	01P	C16-C15-C14	2.27	122.42	118.73
2	D	1	01P	C3-N1-C15	2.27	121.65	116.27
2	C	1	01P	C6-C5-N1	2.25	114.17	110.02
2	B	1	01P	C20-C21-N3	-2.22	118.73	122.02
2	C	1	01P	C20-C21-N3	-2.22	118.73	122.02
2	C	1	01P	C16-C15-C14	2.18	122.27	118.73
2	D	1	01P	C22-C18-N2	-2.16	112.76	120.19
2	B	1	01P	C10-C21-C20	-2.10	116.83	119.04
2	B	1	01P	C4-N5-C24	2.07	120.41	116.28
2	B	1	01P	C6-C5-N1	2.02	113.74	110.02
2	C	1	01P	O2-C14-C13	-2.02	120.65	124.12

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	01P	C14-C15-N1-C3
2	A	1	01P	C14-C15-N1-C3
2	B	1	01P	C14-C15-N1-C3
2	B	1	01P	C15-C14-O2-C17
2	C	1	01P	C16-C15-N1-C3
2	B	1	01P	C13-C14-O2-C17
2	D	1	01P	C14-C15-N1-C3
2	D	1	01P	C14-C15-N1-C5
2	B	1	01P	C14-C15-N1-C5
2	C	1	01P	C15-C14-O2-C17
2	C	1	01P	C13-C14-O2-C17
2	A	1	01P	C14-C15-N1-C5
2	A	1	01P	C15-C14-O2-C17
2	D	1	01P	C16-C15-N1-C5
2	A	1	01P	C13-C14-O2-C17
2	B	1	01P	C16-C15-N1-C5

There are no ring outliers.

4 monomers are involved in 15 short contacts:

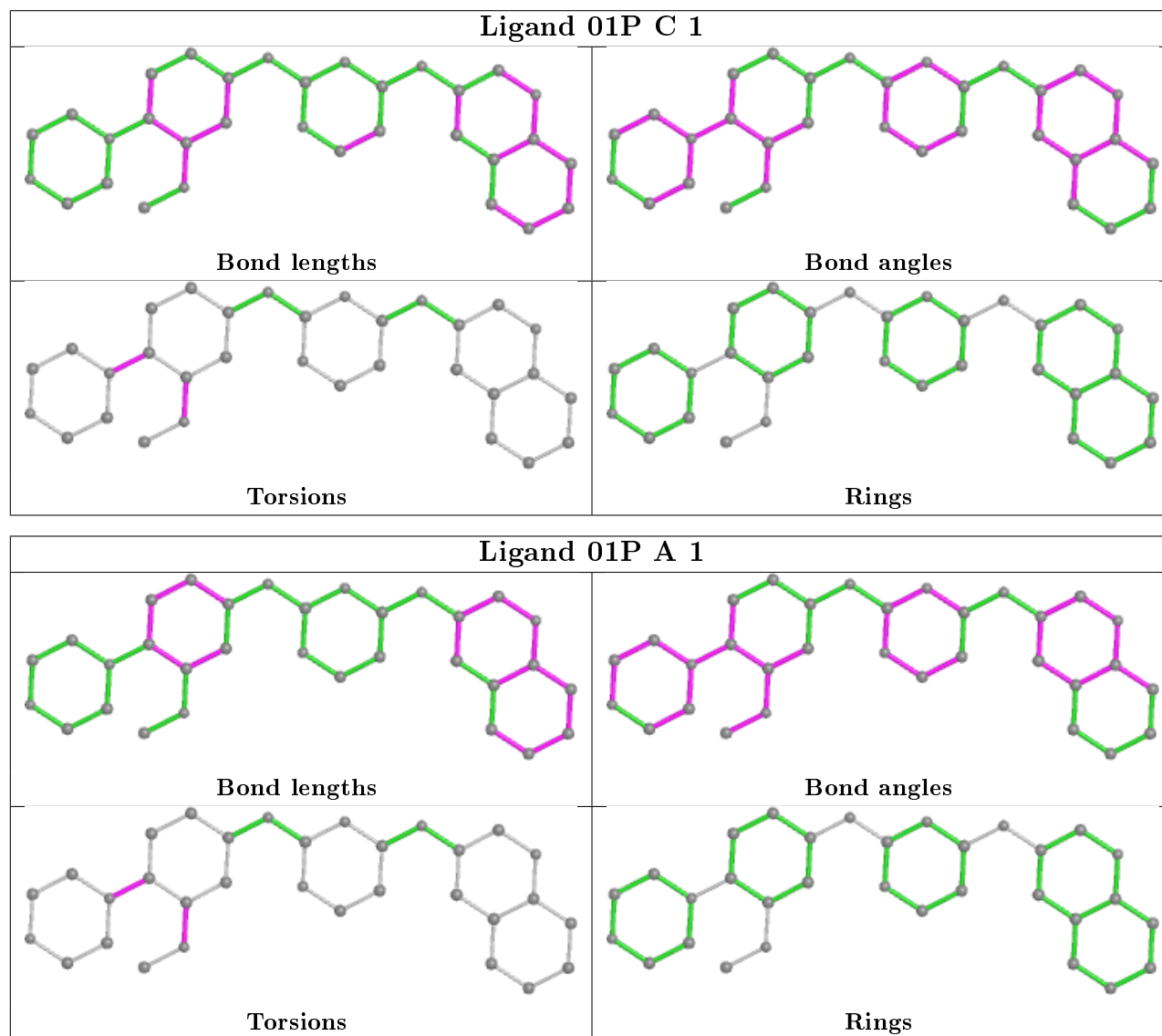
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	01P	5	0
2	A	1	01P	3	0
2	D	1	01P	3	0

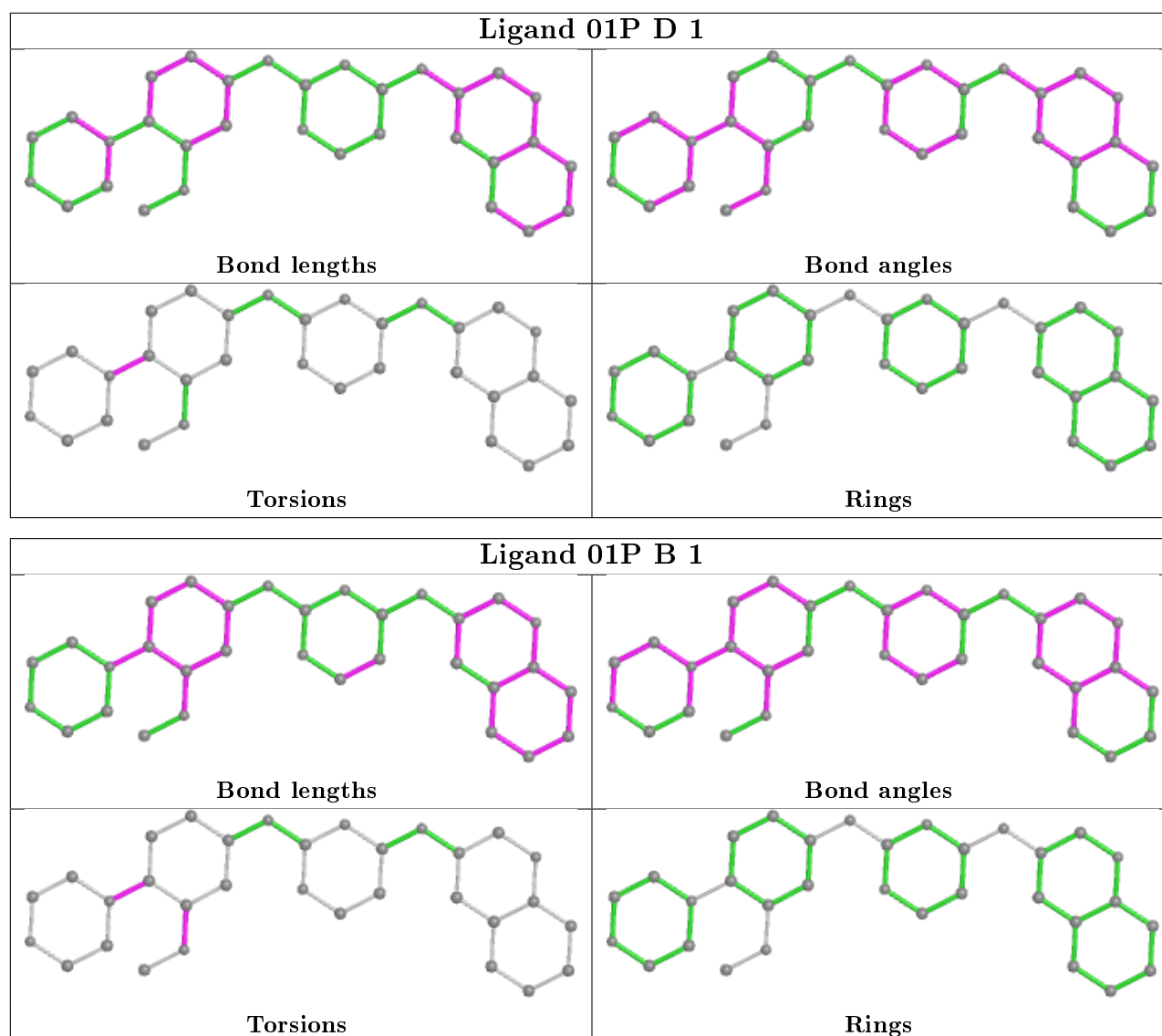
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	01P	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	285/301 (94%)	-0.16	1 (0%) 92 93	19, 36, 59, 81	0
1	B	288/301 (95%)	-0.14	4 (1%) 75 75	18, 36, 63, 85	0
1	C	293/301 (97%)	0.07	9 (3%) 49 44	17, 45, 71, 85	0
1	D	292/301 (97%)	0.03	9 (3%) 49 44	19, 44, 73, 84	0
All	All	1158/1204 (96%)	-0.05	23 (1%) 65 63	17, 40, 70, 85	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1152	GLY	5.3
1	D	986	PRO	4.5
1	C	1038	MET	4.1
1	C	987	ASP	4.0
1	C	986	PRO	3.8
1	B	1153	MET	3.3
1	C	1278	TYR	3.0
1	D	1034	GLU	2.9
1	D	987	ASP	2.8
1	C	1016	LYS	2.7
1	C	1018	VAL	2.6
1	D	1269	PRO	2.5
1	A	1154	THR	2.5
1	D	1183	ASP	2.5
1	D	1040	GLU	2.4
1	B	1154	THR	2.3
1	B	1021	ASP	2.3
1	C	1249	ASN	2.2
1	D	1023	PRO	2.2
1	C	1272	ARG	2.1
1	C	1273	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	1278	TYR	2.0
1	D	1095	MET	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

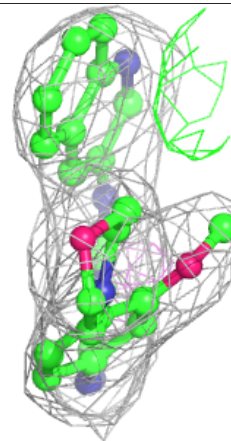
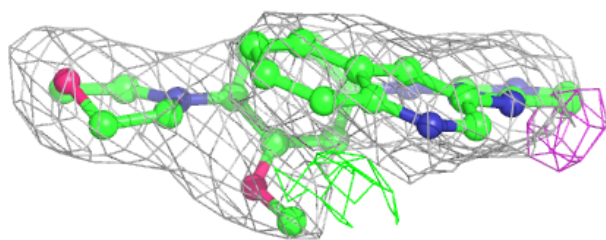
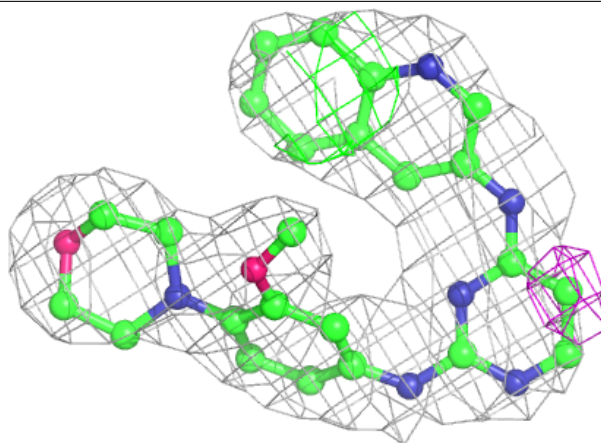
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	01P	D	1	32/32	0.93	0.18	25,33,38,39	0
2	01P	B	1	32/32	0.93	0.19	26,34,42,47	0
2	01P	C	1	32/32	0.95	0.18	30,34,42,44	0
2	01P	A	1	32/32	0.96	0.16	24,30,39,40	0

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.



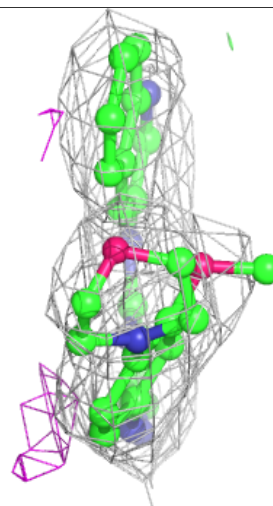
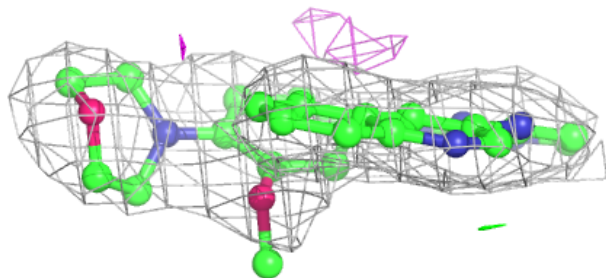
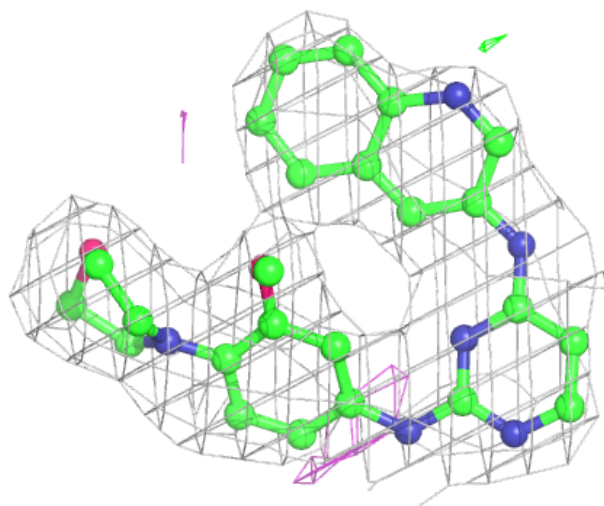
**Electron density around 01P D 1:**

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



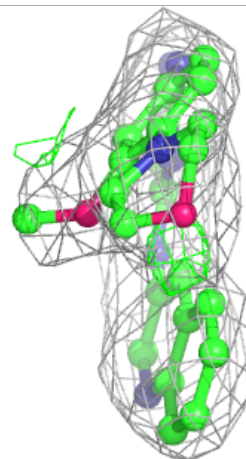
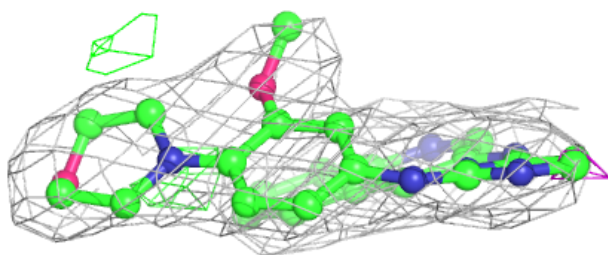
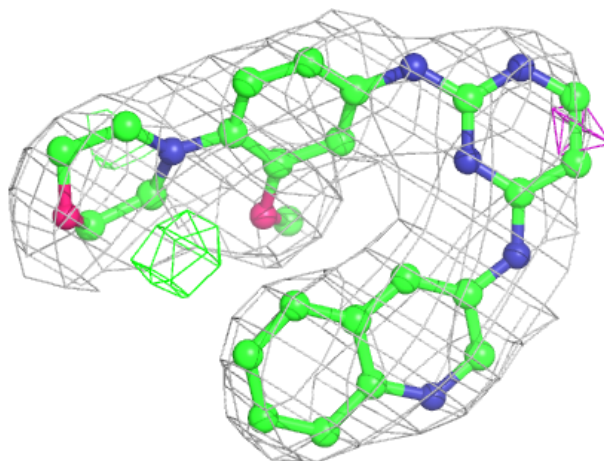
**Electron density around 01P B 1:**

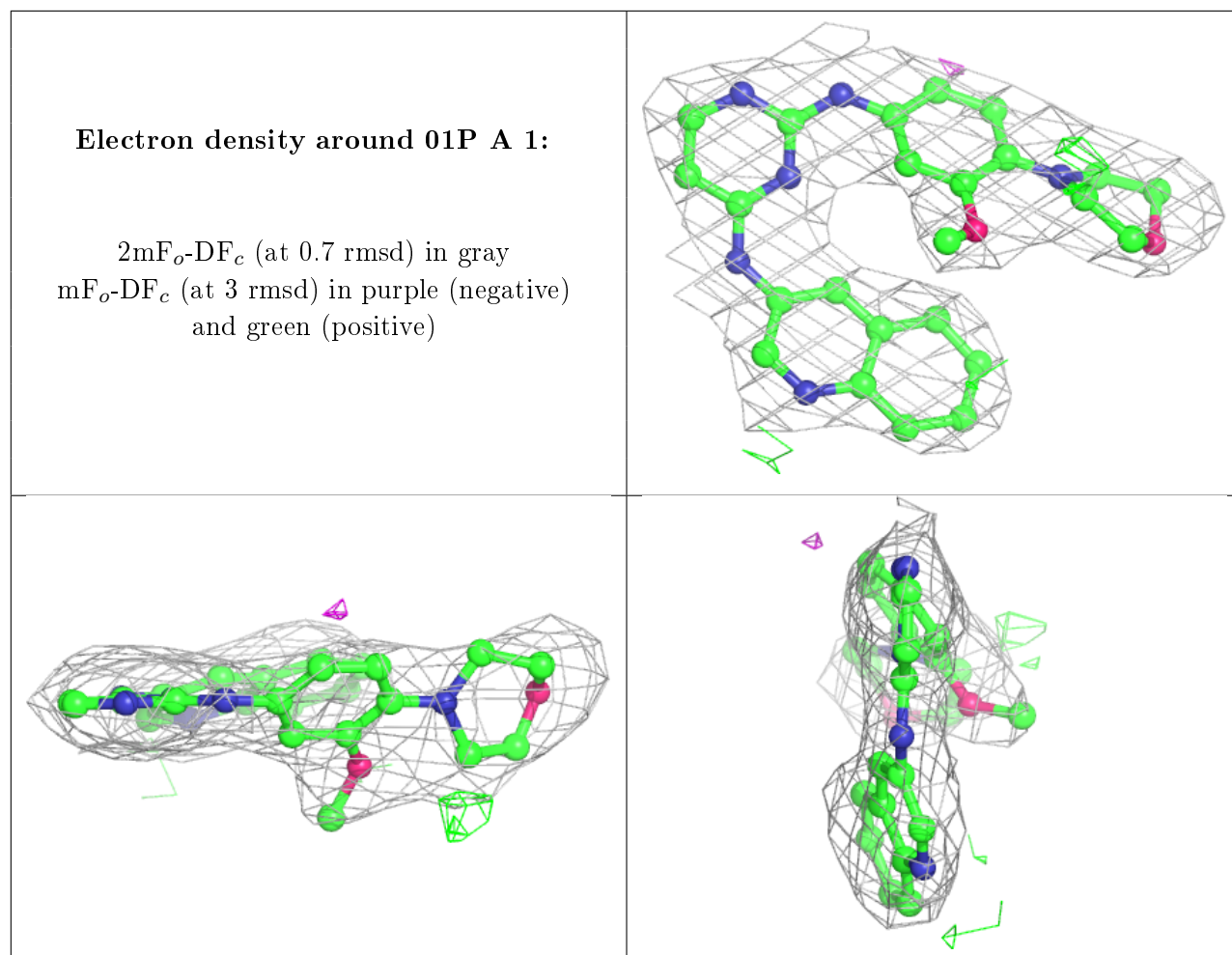
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 01P C 1:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.