Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2024 – 11:54 AM EST

PDB ID	:	4Q5V
Title	:	Crystal structure of the catalytic core of human DNA polymerase alpha in ternary complex with an RNA-primed DNA template and aphidicolin
Authors	:	Baranovskiy, A.G.; Babayeva, N.D.; Suwa, Y.; Gu, J.; Tahirov, T.H.
Deposited on	:	2014-04-17
Resolution	:	2.52 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

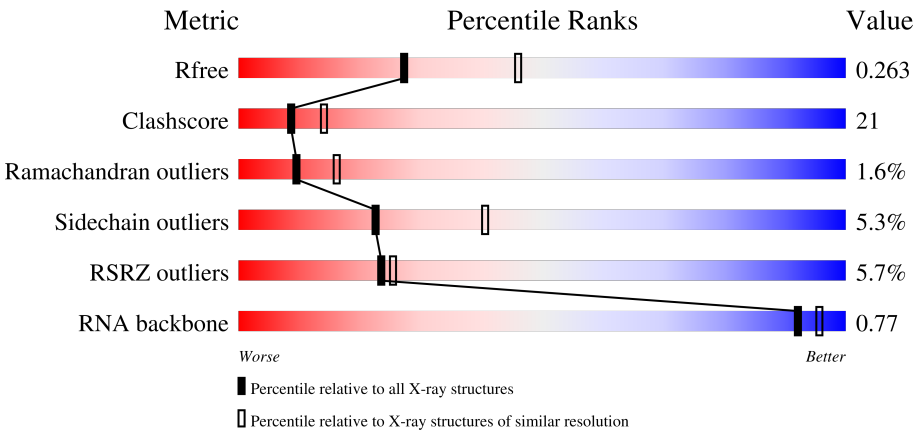
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)
RNA backbone	3102	1020 (2.86-2.18)

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	922	7% 60% 30% • 6%
1	E	922	4% 56% 34% • 6%
2	B	11	9% 82% 9%
2	F	11	36% 55% 9%

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Mol	Chain	Length	Quality of chain
3	C	21	10% 52% 38%
3	G	21	14% 43% 5% 38%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15085 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 DNA polymerase alpha catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	865	6947	4470	1162	1274	41	0	0	0
1	E	865	6947	4470	1162	1274	41	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	ALA	VAL	engineered mutation	UNP P09884
E	516	ALA	VAL	engineered mutation	UNP P09884

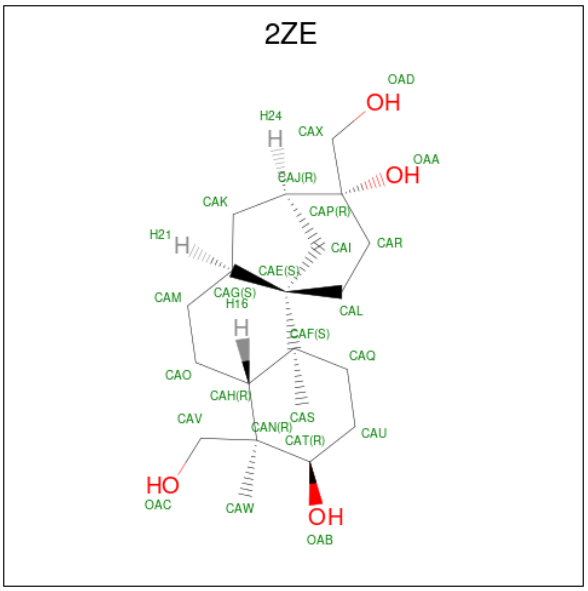
- Molecule 2 is a RNA chain called RNA primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	11	232	105	44	73	10	0	0	0
2	F	11	232	105	44	73	10	0	0	0

- Molecule 3 is a DNA chain called DNA template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	13	264	125	52	75	12	0	0	0
3	G	13	264	125	52	75	12	0	0	0

- Molecule 4 is (3R,4R,4aR,6aS,8R,9R,11aS,11bS)-4,9-bis(hydroxymethyl)-4,11b-dimethyl tetradecahydro-8,11a-methanocyclohepta[a]naphthale ne-3,9-diol (three-letter code: 2ZE) (formula: $C_{20}H_{34}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	24	20	4	0	0
			Total	C	O		
4	E	1	24	20	4	0	0

- Molecule 5 is water.

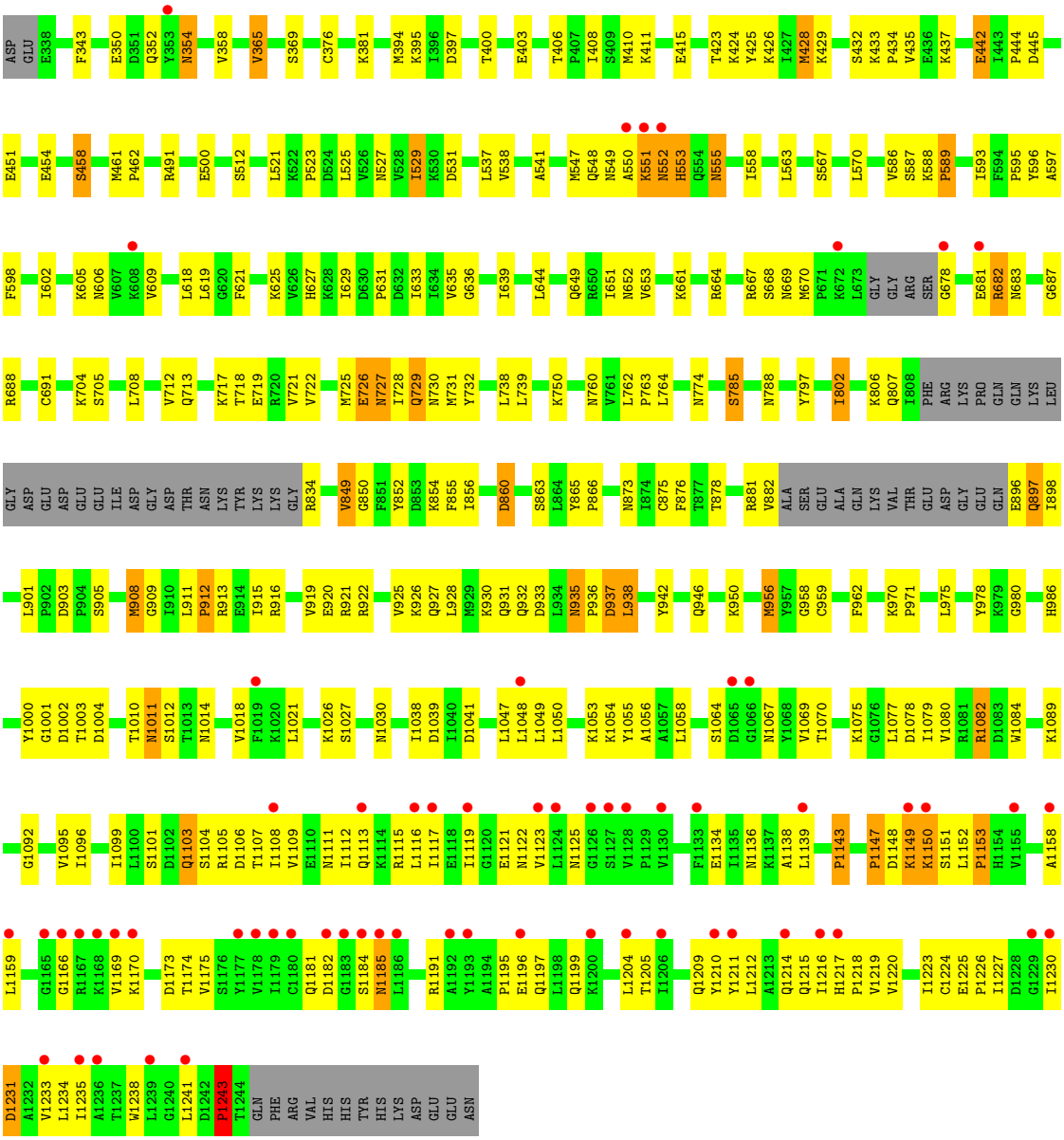
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	80	80	80	0	0
			Total	O		
5	B	1	1	1	0	0
			Total	O		
5	C	3	3	3	0	0
			Total	O		
5	E	62	62	62	0	0
			Total	O		
5	F	3	3	3	0	0
			Total	O		
5	G	2	2	2	0	0

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: DNA polymerase alpha catalytic subunit

Chain A: 7% 60% 30% 6%



• Molecule 1: DNA polymerase alpha catalytic subunit

Chain E: 4% 56% 34% • 6%

ASP GLU E338 Q339 V340 F341 H342 F343 Y344 W345 L346 Q352 Y353 N354 G363 K364 V365 E368 S369 A370 E371 T372 C376 N382 R385 R392 E393 M394 K395 I396 D397 L398 N399 T400 T404 G405 T406 P407 I408 S409 M410 K411 D412 Y425 K426 K429 S432 K433 P434

V435 E436 K437 N438 Y439 A440 F441 E442 T443 P444 D445 Y446 P447 E448 K449 S450 E451 Y452 L453 E454 Y457 P462 T472 V476 E500 V501 K502 S503 P504 Q505 L506 L507 L521 K522 P523 D524 L525 I529 K530 D531 V532 L537 F542 S543 M544 K545 T546 M547 Q548 N549 A550

K551 N552 H553 Q554 N555 A559 M560 A561 A562 L563 V564 S567 L570 P578 F579 F583 V586 S587 K588 P589 C592 I593 F594 F595 Y596 A597 V601 I602 E603 K604 K605 N606 V607 K608 V609 E610 V611 L618 K625 V626 H627 K628 I629 I633 G636 I639

L644 E645 Q649 R650 I651 N652 K661 R667 S668 N669 M670 F671 K672 L673 GLY GLY ARG SER G678 F679 G680 E681 R682 N683 M689 E699 K704 S705 Y706 H707 L708 S709 E710 L711 V712 V721 V722 M725 E726 N727 I728 Q729 N730 M731 Y732 L741 L742 I752 L753

N760 V761 L762 P763 L764 M776 G783 R784 S785 N788 L791 L792 L793 H794 E798 I802 Q807 I808 PHE ARG LYS PRO GLN GLN LYS LEU GLY ASP GLU ASP GLU GLU ILE ASP GLY ASP THR ASN LYS TYR LYS LYS GLY R834 A837 A840 D846 P847 K848 V849

Y852 D853 K854 L857 L858 L859 D860 F861 Y865 P866 Q870 N873 I874 C875 F876 T877 T878 V879 Q880 R881 V882 ALA SER GLU GLU ALA GLN LYS VAL THR GLU ASP GLY GLU GLN E896 Q897 I898 P899 E900 L901 P902 D903 P904 S905 M908 G909 I910 L911 P912 R913 E914 I915 R916

V919 R922 V925 K926 Q927 Q931 D932 D933 L934 N935 P936 D937 L938 I939 L940 Q941 Y942 D943 I944 R945 Q946 M956 C959 S963 Y968 A969 K970 P971 L975 M985 K988 E989 M990 V991 Q992 K993 M994 N995 V998 I999 D1002 T1003 D1004 S1005 I1006 T1010 N1011

S1012 T1013 N1014 V1018 F1019 K1020 L1021 G1022 N1023 K1024 V1025 K1026 S1027 N1030 I1038 D1039 I1040 D1041 S1046 L1047 L1048 L1049 L1050 K1053 K1054 Y1055 A1056 A1057 L1058 D1065 G1066 T1070 L1074 K1075 G1076 L1077 D1078 I1079 R1082 D1083 W1084 K1089 V1095 I1096 G1097 Q1098 I1099 L1100 S1101

D1102 Q1103 S1104 R1105 D1106 T1107 I1108 V1109 I1112 Q1113 K1114 R1115 L1116 I1117 E1118 I1119 G1120 E1121 N1122 V1123 L1124 N1125 V1128 F1133 E1134 I1135 N1136 K1137 A1138 L1139 D1142 P1143 Q1144 D1145 Y1146 P1147 D1148 K1149 K1150 S1151 L1152 P1153 H1154 V1155 A1158 L1159 N1162 G1166 R1167 K1168 V1169 K1170

D1173 T1174 Y1177 V1178 I1179 C1180 S1184 N1185 A1188 Y1193 L1198 Q1199 K1200 Q1201 D1202 N1203 L1204 T1205 I1206 Y1210 Y1211 L1212 A1213 Q1214 Q1215 I1216 H1217 P1218 V1219 V1220 A1221 R1222 I1223 C1224 E1225 P1226 I1227 I1230 D1231 A1232 V1233 L1234 T1237 W1238 L1241 D1242 P1243 T1244 GLN PHE ARG

VAL HIS HIS TYR HIS LYS ASP GLU GLU ASN

• Molecule 2: RNA primer

Chain B: 9% 82% 9%

G1 C2 C3 U4 G5 C6 A7 G8 C9 G10 C11

• Molecule 2: RNA primer

Chain F: 36% 55% 9%

G201 C202 C203 G208 C209 G210 C211

• Molecule 3: DNA template

Chain C: 10% 52% 38%

DA DT DT DA DC DT DA DT A109 G110 G111 C112 G113 C114 T115 C116 C117 A118 G119 G120 C121

• Molecule 3: DNA template

Chain G: 14% 43% 5% 38%

DA DT DT DA DC DT DA DT A309 G310 G311 C312 T315 C316 C317 A318 G319 G320 C321

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.05Å 116.43Å 233.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.02 – 2.52 78.02 – 2.52	Depositor EDS
% Data completeness (in resolution range)	96.0 (78.02-2.52) 96.1 (78.02-2.52)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	189.48 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.268 0.228 , 0.263	Depositor DCC
R_{free} test set	4714 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15085	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 2ZE

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	0.45	0/7089	0.68	4/9582 (0.0%)
1	E	0.47	0/7089	0.67	4/9582 (0.0%)
2	B	0.45	0/259	0.89	2/402 (0.5%)
2	F	0.51	0/259	0.86	2/402 (0.5%)
3	C	0.46	0/296	0.81	0/455
3	G	0.45	0/296	0.77	0/455
All	All	0.46	0/15288	0.69	12/20878 (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
3	G	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	553	HIS	N-CA-C	7.66	131.67	111.00
2	B	8	G	O4'-C1'-N9	6.90	113.72	108.20
2	F	208	G	N9-C1'-C2'	6.16	122.01	114.00
1	A	552	ASN	N-CA-C	5.98	127.15	111.00
1	A	442	GLU	N-CA-C	5.67	126.31	111.00
1	E	553	HIS	N-CA-C	5.55	125.99	111.00
1	E	934	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	802	ILE	N-CA-C	-5.47	96.22	111.00
2	B	8	G	C5'-C4'-C3'	-5.39	107.38	116.00
1	E	442	GLU	N-CA-C	5.25	125.16	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	208	G	O4'-C1'-N9	5.23	112.38	108.20
1	E	802	ILE	N-CA-C	-5.06	97.33	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	320	DG	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	6947	0	7092	268	0
1	E	6947	0	7092	297	0
2	B	232	0	120	9	0
2	F	232	0	120	6	0
3	C	264	0	146	15	0
3	G	264	0	146	15	0
4	A	24	0	34	8	0
4	E	24	0	34	6	0
5	A	80	0	0	12	0
5	B	1	0	0	0	0
5	C	3	0	0	2	0
5	E	62	0	0	7	0
5	F	3	0	0	0	0
5	G	2	0	0	2	0
All	All	15085	0	14784	611	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 21.

All (611) 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)
3:G:315:DT:H2"	3:G:316:DC:H5"	1.30	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:908:MET:HE2	1:E:916:ARG:HH11	1.13	1.08
1:A:652:ASN:HD22	1:A:670:MET:HE3	1.19	1.04
1:A:1233:VAL:HG13	1:A:1243:PRO:HB3	1.36	1.03
1:E:555:ASN:H	1:E:555:ASN:HD22	1.08	1.01
1:A:1224:CYS:HA	1:A:1227:ILE:HD13	1.41	1.00
4:A:1301:2ZE:H14	4:A:1301:2ZE:H4	1.41	0.99
1:E:708:LEU:O	1:E:712:VAL:HG23	1.66	0.96
3:G:315:DT:H2"	3:G:316:DC:C5'	1.96	0.96
4:E:1301:2ZE:H14	4:E:1301:2ZE:H4	1.46	0.95
3:C:120:DG:N7	5:C:201:HOH:O	1.99	0.94
1:E:922:ARG:HG3	1:E:946:GLN:HE21	1.32	0.94
1:E:1150:LYS:H	1:E:1150:LYS:HD2	1.31	0.93
1:E:554:GLN:NE2	1:E:650:ARG:HH12	1.68	0.92
1:E:727:ASN:N	1:E:727:ASN:HD22	1.67	0.91
1:E:922:ARG:HG3	1:E:946:GLN:NE2	1.86	0.90
1:A:1150:LYS:HD2	1:A:1150:LYS:H	1.37	0.89
1:A:354:ASN:HD22	1:A:354:ASN:N	1.69	0.89
1:E:908:MET:CE	1:E:916:ARG:HH11	1.88	0.86
1:E:1040:ILE:N	5:E:1447:HOH:O	1.97	0.86
1:E:555:ASN:H	1:E:555:ASN:ND2	1.73	0.85
3:C:113:DG:OP2	5:C:202:HOH:O	1.93	0.85
1:E:908:MET:HE2	1:E:916:ARG:HD3	1.59	0.84
1:E:854:LYS:HG3	1:E:1011:ASN:HD22	1.41	0.84
1:E:1010:THR:HG22	1:E:1021:LEU:HD23	1.58	0.83
1:A:727:ASN:HD22	1:A:727:ASN:N	1.74	0.83
1:A:921:ARG:HD3	5:A:1479:HOH:O	1.79	0.82
1:A:727:ASN:HD22	1:A:727:ASN:H	1.24	0.82
1:E:840:ALA:HB3	5:E:1453:HOH:O	1.78	0.81
1:A:1122:ASN:HA	1:A:1125:ASN:HD21	1.46	0.80
1:E:727:ASN:HD22	1:E:727:ASN:H	1.29	0.80
3:C:118:DA:H2"	3:C:119:DG:H5'	1.62	0.79
1:E:785:SER:HB3	5:G:402:HOH:O	1.83	0.79
1:A:555:ASN:HD22	1:A:555:ASN:H	1.27	0.79
1:E:354:ASN:N	1:E:354:ASN:HD22	1.78	0.78
1:E:1122:ASN:HA	1:E:1125:ASN:HD21	1.49	0.78
3:C:115:DT:H2"	3:C:116:DC:C5'	2.14	0.78
1:E:727:ASN:H	1:E:727:ASN:ND2	1.80	0.77
1:A:1010:THR:HG22	1:A:1021:LEU:HD23	1.66	0.77
1:A:636:GLY:HA3	1:A:639:ILE:HD11	1.65	0.77
1:A:908:MET:CE	1:A:916:ARG:HD2	2.15	0.76
1:E:672:LYS:HG3	1:E:673:LEU:H	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:ASN:H	1:A:555:ASN:ND2	1.85	0.75
1:A:365:VAL:HG22	1:A:376:CYS:HB2	1.69	0.74
1:E:860:ASP:HB2	1:E:1041:ASP:HB2	1.69	0.74
1:E:1233:VAL:HG13	1:E:1243:PRO:HB3	1.68	0.74
1:E:554:GLN:HE22	1:E:650:ARG:HH12	1.34	0.74
1:A:1234:LEU:HG	1:A:1238:TRP:CZ2	2.22	0.73
3:C:115:DT:H2"	3:C:116:DC:H5'	1.69	0.72
1:A:1212:LEU:HD23	1:A:1216:ILE:HD12	1.70	0.72
1:E:340:VAL:HG23	1:E:501:VAL:O	1.88	0.72
1:E:783:GLY:HA2	3:G:310:DG:OP2	1.90	0.71
1:A:1095:VAL:O	1:A:1099:ILE:HG13	1.91	0.71
1:E:1113:GLN:HG3	1:E:1238:TRP:NE1	2.05	0.71
1:E:875:CYS:HB2	1:E:912:PRO:HD3	1.73	0.70
1:A:397:ASP:OD2	1:A:400:THR:HG23	1.90	0.70
3:C:120:DG:H2"	3:C:121:DC:OP2	1.92	0.70
2:F:208:G:H1'	2:F:209:C:C6	2.26	0.70
1:A:956:MET:HE2	1:A:956:MET:HA	1.72	0.70
1:E:529:ILE:HD11	1:E:532:VAL:HG23	1.72	0.70
1:A:1185:ASN:C	1:A:1185:ASN:HD22	1.94	0.70
1:E:730:ASN:N	1:E:730:ASN:HD22	1.90	0.70
1:E:636:GLY:HA3	1:E:639:ILE:HD11	1.74	0.69
1:E:1150:LYS:HD2	1:E:1150:LYS:N	2.06	0.69
1:A:1225:GLU:HB3	1:A:1226:PRO:HD3	1.73	0.69
1:E:667:ARG:NH1	1:E:683:ASN:O	2.25	0.69
1:A:727:ASN:H	1:A:727:ASN:ND2	1.91	0.68
1:E:915:ILE:HD11	1:E:956:MET:HG2	1.75	0.68
1:E:1113:GLN:HG3	1:E:1238:TRP:CE2	2.29	0.68
1:A:1104:SER:HA	5:A:1473:HOH:O	1.93	0.68
3:C:109:DA:H4'	3:C:110:DG:OP2	1.93	0.68
1:E:730:ASN:H	1:E:730:ASN:ND2	1.92	0.67
1:A:1224:CYS:CA	1:A:1227:ILE:HD13	2.20	0.67
1:A:863:SER:HA	5:A:1411:HOH:O	1.95	0.67
1:E:1225:GLU:HB3	1:E:1226:PRO:HD3	1.76	0.67
1:A:354:ASN:N	1:A:354:ASN:ND2	2.43	0.67
1:E:394:MET:CE	1:E:405:GLY:HA2	2.25	0.67
1:E:854:LYS:HG3	1:E:1011:ASN:HA	1.76	0.67
1:E:1122:ASN:HA	1:E:1125:ASN:ND2	2.09	0.67
1:A:908:MET:HE2	1:A:916:ARG:HD2	1.76	0.67
1:A:667:ARG:NH1	1:A:683:ASN:O	2.27	0.66
1:E:865:TYR:HB2	1:E:866:PRO:HD3	1.77	0.66
3:G:318:DA:H2"	3:G:319:DG:H5'	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:G:H2'	2:B:11:DC:C6	2.31	0.66
1:A:1105:ARG:O	1:A:1109:VAL:HG23	1.96	0.65
1:E:935:ASN:HB3	1:E:938:LEU:HD22	1.78	0.65
1:E:595:PRO:HD3	1:E:732:TYR:O	1.97	0.65
1:A:1217:HIS:HB3	1:A:1218:PRO:HD3	1.79	0.65
1:E:1115:ARG:O	1:E:1119:ILE:HG12	1.96	0.65
1:A:618:LEU:HD23	1:A:619:LEU:N	2.12	0.65
1:E:1211:TYR:O	1:E:1216:ILE:HG13	1.96	0.65
1:E:408:ILE:HD13	1:E:472:THR:HA	1.79	0.65
4:A:1301:2ZE:H4	4:A:1301:2ZE:CAS	2.24	0.65
1:E:394:MET:HE3	1:E:405:GLY:HA2	1.79	0.65
1:E:652:ASN:HD22	1:E:670:MET:CE	2.09	0.65
1:E:1026:LYS:HG3	1:E:1030:ASN:ND2	2.11	0.64
1:E:1109:VAL:HG13	1:E:1230:ILE:CD1	2.27	0.64
1:A:352:GLN:HB2	5:A:1438:HOH:O	1.98	0.64
1:A:1109:VAL:HG13	1:A:1230:ILE:CD1	2.28	0.64
1:A:1149:LYS:HG2	1:A:1150:LYS:N	2.11	0.64
1:A:860:ASP:HB2	1:A:1041:ASP:HB2	1.79	0.63
1:E:669:ASN:HD22	1:E:669:ASN:N	1.95	0.63
1:A:410:MET:HE3	1:A:451:GLU:HG2	1.80	0.63
1:A:962:PHE:CZ	3:C:109:DA:H5'	2.34	0.63
1:A:595:PRO:HG3	1:A:732:TYR:O	1.99	0.62
1:A:908:MET:HE1	1:A:916:ARG:HD2	1.81	0.62
1:A:555:ASN:HD22	1:A:555:ASN:N	1.94	0.62
1:A:962:PHE:HZ	3:C:109:DA:H5'	1.64	0.62
1:E:725:MET:SD	1:E:1166:GLY:HA3	2.39	0.62
1:A:806:LYS:HD2	5:A:1480:HOH:O	1.99	0.62
4:A:1301:2ZE:H14	4:A:1301:2ZE:CAW	2.25	0.62
3:C:115:DT:H2"	3:C:116:DC:H5"	1.81	0.62
1:E:507:LEU:HD12	1:E:507:LEU:N	2.15	0.62
1:E:730:ASN:N	1:E:730:ASN:ND2	2.47	0.62
1:A:1111:ASN:N	1:A:1111:ASN:HD22	1.96	0.61
1:E:354:ASN:N	1:E:354:ASN:ND2	2.47	0.61
1:E:909:GLY:C	1:E:912:PRO:HD2	2.21	0.61
1:A:1181:GLN:HB2	1:A:1205:THR:HG23	1.83	0.61
2:B:8:G:H1'	2:B:9:C:C6	2.36	0.61
1:E:857:LEU:HD11	1:E:1022:GLY:CA	2.31	0.61
1:E:1113:GLN:HE21	1:E:1238:TRP:HE1	1.49	0.61
4:E:1301:2ZE:H4	4:E:1301:2ZE:CAS	2.27	0.61
1:A:926:LYS:HE3	1:A:946:GLN:HG3	1.83	0.61
1:E:436:GLU:O	1:E:437:LYS:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1216:ILE:O	1:A:1220:VAL:HG23	2.01	0.61
1:E:785:SER:CB	5:G:402:HOH:O	2.47	0.61
1:E:555:ASN:ND2	1:E:555:ASN:N	2.39	0.60
1:E:1047:LEU:HD12	1:E:1048:LEU:N	2.16	0.60
1:A:570:LEU:HD22	1:A:762:LEU:HB3	1.83	0.60
1:A:788:ASN:ND2	1:A:959:CYS:HB3	2.16	0.60
1:A:1122:ASN:HA	1:A:1125:ASN:ND2	2.13	0.60
1:E:444:PRO:O	1:E:445:ASP:HB2	2.00	0.60
1:A:1231:ASP:OD2	1:A:1234:LEU:HB2	2.01	0.60
1:A:898:ILE:N	1:A:898:ILE:HD13	2.17	0.60
1:E:410:MET:HG2	1:E:434:PRO:HB3	1.82	0.60
1:A:652:ASN:HB2	1:A:670:MET:HE1	1.83	0.60
1:E:365:VAL:HG22	1:E:376:CYS:HB2	1.81	0.60
1:A:911:LEU:HD11	1:A:956:MET:HG2	1.84	0.60
1:E:672:LYS:NZ	1:E:672:LYS:HB2	2.17	0.59
1:E:792:LEU:HD21	1:E:956:MET:CE	2.32	0.59
1:E:1230:ILE:HA	1:E:1234:LEU:HD23	1.84	0.59
1:A:682:ARG:O	1:A:682:ARG:HD3	2.03	0.59
1:E:597:ALA:O	1:E:601:VAL:HG23	2.03	0.59
1:E:849:VAL:HG13	1:E:1049:LEU:O	2.03	0.59
1:E:1010:THR:HG22	1:E:1021:LEU:CD2	2.29	0.59
1:A:652:ASN:HD22	1:A:670:MET:CE	2.04	0.58
1:A:1148:ASP:OD1	1:A:1151:SER:HB3	2.03	0.58
1:E:398:LEU:O	1:E:399:ASN:HB2	2.02	0.58
1:E:1170:LYS:O	1:E:1173:ASP:HB2	2.03	0.58
1:A:555:ASN:ND2	1:A:555:ASN:N	2.48	0.58
1:E:588:LYS:HD3	1:E:594:PHE:CE1	2.37	0.58
1:A:935:ASN:ND2	1:A:937:ASP:OD1	2.34	0.58
1:E:438:ASN:HA	1:E:448:GLU:O	2.02	0.58
1:E:607:VAL:HB	1:E:609:VAL:HG12	1.85	0.58
1:E:760:ASN:O	1:E:763:PRO:HD2	2.04	0.58
1:E:963:SER:HA	1:E:968:TYR:CE1	2.38	0.58
1:E:1227:ILE:N	1:E:1227:ILE:HD12	2.18	0.58
1:A:1048:LEU:HG	1:A:1050:LEU:HD21	1.85	0.58
1:E:1109:VAL:HG13	1:E:1230:ILE:HD11	1.86	0.58
1:A:369:SER:HB3	5:A:1424:HOH:O	2.03	0.58
1:E:1185:ASN:HD22	1:E:1185:ASN:C	2.08	0.58
1:E:586:VAL:HB	1:E:742:LEU:HD21	1.86	0.57
1:E:644:LEU:HD23	1:E:681:GLU:HB3	1.86	0.57
1:E:1224:CYS:HA	1:E:1227:ILE:HD13	1.86	0.57
2:F:201:G:H2'	2:F:202:C:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:792:LEU:HD21	1:E:956:MET:HE2	1.86	0.57
1:E:555:ASN:HD22	1:E:555:ASN:N	1.80	0.57
1:A:1233:VAL:CG1	1:A:1243:PRO:HB3	2.22	0.57
1:E:727:ASN:N	1:E:727:ASN:ND2	2.35	0.57
1:A:774:ASN:HB2	5:A:1433:HOH:O	2.04	0.56
1:A:704:LYS:HD2	1:A:1136:ASN:ND2	2.19	0.56
1:E:788:ASN:ND2	1:E:959:CYS:HB3	2.19	0.56
1:A:1010:THR:HG22	1:A:1021:LEU:CD2	2.34	0.56
1:E:382:ASN:ND2	1:E:521:LEU:O	2.34	0.56
1:A:538:VAL:CG1	1:A:631:PRO:HA	2.36	0.56
1:E:554:GLN:NE2	1:E:650:ARG:NH1	2.48	0.56
1:A:410:MET:CE	1:A:451:GLU:HG2	2.35	0.56
1:E:900:GLU:HG3	5:E:1441:HOH:O	2.03	0.56
1:E:1217:HIS:HB3	1:E:1218:PRO:HD3	1.85	0.56
1:E:570:LEU:HD22	1:E:762:LEU:HB3	1.88	0.56
1:E:908:MET:HE2	1:E:916:ARG:NH1	1.99	0.56
1:A:1047:LEU:HD12	1:A:1048:LEU:N	2.21	0.56
4:E:1301:2ZE:H14	4:E:1301:2ZE:CAW	2.29	0.56
1:E:1154:HIS:CE1	1:E:1155:VAL:HG23	2.41	0.56
1:A:875:CYS:HB2	1:A:912:PRO:HD3	1.87	0.55
1:A:395:LYS:HB2	1:A:408:ILE:HD11	1.88	0.55
1:A:411:LYS:HE2	1:A:415:GLU:OE2	2.06	0.55
1:E:408:ILE:HG23	1:E:412:ASP:HB2	1.89	0.55
3:G:311:DG:H2"	3:G:312:DC:H5'	1.88	0.55
1:A:538:VAL:HG12	1:A:631:PRO:HA	1.87	0.55
1:A:970:LYS:HB3	1:A:971:PRO:HD3	1.89	0.55
1:E:1212:LEU:HD23	1:E:1216:ILE:HD12	1.87	0.55
1:E:1058:LEU:HB3	1:E:1070:THR:OG1	2.07	0.55
1:E:1095:VAL:O	1:E:1099:ILE:HG13	2.07	0.55
1:A:1231:ASP:O	1:A:1235:ILE:HG13	2.06	0.55
1:E:500:GLU:OE2	1:E:502:LYS:HE3	2.06	0.55
1:E:908:MET:HE3	1:E:913:ARG:HG3	1.89	0.55
1:E:1002:ASP:O	1:E:1004:ASP:N	2.35	0.55
1:A:708:LEU:O	1:A:712:VAL:HG23	2.07	0.55
1:E:1149:LYS:HE3	1:E:1159:LEU:HD12	1.89	0.54
1:A:394:MET:HG2	1:A:403:GLU:OE1	2.06	0.54
1:A:652:ASN:ND2	1:A:670:MET:HE3	2.03	0.54
1:E:935:ASN:HD22	1:E:935:ASN:C	2.09	0.54
1:E:1119:ILE:O	1:E:1123:VAL:HG23	2.07	0.54
1:E:652:ASN:HD22	1:E:670:MET:HE3	1.72	0.54
1:A:1227:ILE:HD12	1:A:1227:ILE:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:LEU:HB3	1:E:689:MET:HE3	1.89	0.54
1:E:432:SER:HA	1:E:454:GLU:O	2.07	0.54
1:E:669:ASN:N	1:E:669:ASN:ND2	2.55	0.54
1:A:1026:LYS:HG2	1:A:1027:SER:N	2.22	0.54
1:A:1082:ARG:HG2	1:A:1136:ASN:O	2.08	0.54
1:E:1113:GLN:O	1:E:1117:ILE:HG13	2.08	0.54
1:E:903:ASP:OD2	1:E:905:SER:HB3	2.08	0.54
1:A:1184:SER:O	1:A:1185:ASN:ND2	2.40	0.53
1:E:627:HIS:HB2	1:E:661:LYS:HD3	1.90	0.53
1:A:547:MET:HE1	1:A:589:PRO:HG3	1.90	0.53
1:A:1095:VAL:HG13	1:A:1112:ILE:HD13	1.90	0.53
1:A:1211:TYR:O	1:A:1215:GLN:HB2	2.09	0.53
1:E:788:ASN:CB	1:E:959:CYS:SG	2.97	0.53
1:E:911:LEU:HB3	1:E:912:PRO:HD3	1.91	0.53
1:A:442:GLU:HB2	5:A:1463:HOH:O	2.07	0.53
2:B:8:G:HO2'	2:B:9:C:H5	1.54	0.53
1:E:564:VAL:HG21	1:E:629:ILE:HD13	1.91	0.53
1:A:437:LYS:HB3	1:A:802:ILE:HG12	1.91	0.53
1:A:1002:ASP:O	1:A:1004:ASP:N	2.39	0.53
1:E:1084:TRP:O	1:E:1089:LYS:HE2	2.09	0.53
1:A:873:ASN:HD21	1:A:878:THR:HG21	1.74	0.53
1:E:353:TYR:HD2	1:E:354:ASN:ND2	2.07	0.53
3:G:315:DT:C2'	3:G:316:DC:H5"	2.21	0.53
1:A:1064:SER:O	1:A:1067:ASN:HB2	2.08	0.52
1:A:1109:VAL:HG13	1:A:1230:ILE:HD11	1.91	0.52
1:E:854:LYS:HG3	1:E:1011:ASN:ND2	2.18	0.52
1:E:476:VAL:HG12	5:E:1436:HOH:O	2.08	0.52
1:E:728:ILE:HG22	1:E:729:GLN:N	2.23	0.52
1:A:432:SER:HA	1:A:454:GLU:O	2.09	0.52
1:A:935:ASN:HD22	1:A:936:PRO:HD2	1.75	0.52
1:E:365:VAL:HA	5:E:1404:HOH:O	2.08	0.52
1:E:668:SER:C	1:E:669:ASN:HD22	2.13	0.52
1:E:1026:LYS:HG3	1:E:1030:ASN:HD21	1.73	0.52
1:E:1241:LEU:O	1:E:1243:PRO:HD3	2.08	0.52
1:A:428:MET:SD	1:A:428:MET:N	2.83	0.52
1:A:537:LEU:HD12	1:A:633:ILE:HD11	1.92	0.52
1:A:855:PHE:HD2	1:A:1018:VAL:HG21	1.75	0.52
1:A:1084:TRP:O	1:A:1089:LYS:HE2	2.10	0.52
1:E:1138:ALA:HA	1:E:1174:THR:HA	1.92	0.52
1:A:1241:LEU:O	1:A:1243:PRO:HD3	2.10	0.52
1:A:913:ARG:HD2	5:A:1442:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ILE:HD12	1:E:342:HIS:CE1	2.45	0.51
1:A:1111:ASN:N	1:A:1111:ASN:ND2	2.57	0.51
1:E:346:LEU:HB3	1:E:689:MET:CE	2.40	0.51
1:E:1020:LYS:O	1:E:1024:LYS:HB2	2.10	0.51
1:E:1198:LEU:HG	1:E:1199:GLN:N	2.25	0.51
1:A:727:ASN:O	1:A:731:MET:HG3	2.10	0.51
1:A:1116:LEU:CD2	1:A:1235:ILE:HG23	2.40	0.51
1:A:1150:LYS:HD2	1:A:1150:LYS:N	2.15	0.51
1:A:728:ILE:HG22	1:A:729:GLN:N	2.24	0.51
1:A:1196:GLU:HG3	1:A:1197:GLN:N	2.26	0.51
1:E:340:VAL:HG21	1:E:500:GLU:CG	2.41	0.51
1:E:652:ASN:HD22	1:E:670:MET:HE2	1.74	0.51
1:A:854:LYS:HG3	1:A:1011:ASN:HD22	1.75	0.51
1:E:1219:VAL:O	1:E:1223:ILE:HG13	2.10	0.51
1:A:875:CYS:SG	1:A:876:PHE:N	2.84	0.51
1:E:618:LEU:C	1:E:618:LEU:HD23	2.30	0.51
1:E:410:MET:HE2	1:E:451:GLU:HG2	1.93	0.51
1:E:1109:VAL:HG13	1:E:1230:ILE:HD13	1.93	0.51
1:E:704:LYS:HA	1:E:1082:ARG:HE	1.77	0.50
1:E:762:LEU:HB2	1:E:763:PRO:HD3	1.93	0.50
1:E:399:ASN:O	1:E:400:THR:C	2.50	0.50
1:E:794:HIS:O	1:E:798:GLU:HG3	2.10	0.50
1:E:370:ALA:O	1:E:372:THR:HG22	2.11	0.50
1:A:458:SER:HB3	1:A:461:MET:CE	2.42	0.50
1:A:588:LYS:O	1:A:589:PRO:O	2.29	0.50
1:A:652:ASN:HB2	1:A:670:MET:CE	2.41	0.50
1:A:1113:GLN:O	1:A:1117:ILE:HG13	2.12	0.50
1:A:1181:GLN:HA	1:A:1181:GLN:NE2	2.26	0.50
1:A:908:MET:CE	1:A:913:ARG:HG3	2.41	0.50
1:A:1181:GLN:HA	1:A:1181:GLN:HE21	1.77	0.50
1:E:410:MET:CE	1:E:451:GLU:HG2	2.41	0.50
1:E:689:MET:HE2	1:E:776:MET:HB3	1.93	0.50
1:A:1069:VAL:HG12	1:A:1070:THR:H	1.77	0.50
1:A:1210:TYR:CD1	1:A:1214:GLN:HG3	2.47	0.50
2:F:202:C:H2'	2:F:203:C:C6	2.47	0.50
1:A:563:LEU:HD22	1:A:750:LYS:HA	1.94	0.50
1:A:1109:VAL:HG13	1:A:1230:ILE:HD13	1.93	0.50
1:A:1219:VAL:O	1:A:1223:ILE:HG13	2.12	0.50
1:A:986:HIS:CD2	1:A:986:HIS:O	2.65	0.49
1:A:1030:ASN:OD1	1:A:1038:ILE:HG22	2.12	0.49
4:A:1301:2ZE:H18	3:C:111:DG:C2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:672:LYS:CG	1:E:673:LEU:H	2.23	0.49
1:E:1095:VAL:HG13	1:E:1112:ILE:HD13	1.94	0.49
1:E:1096:ILE:HD11	1:E:1223:ILE:HG23	1.93	0.49
1:A:619:LEU:HD13	1:A:651:ILE:HA	1.94	0.49
1:E:652:ASN:ND2	1:E:670:MET:HE2	2.26	0.49
1:E:704:LYS:O	1:E:1174:THR:HG21	2.11	0.49
1:A:854:LYS:HG3	1:A:1011:ASN:HA	1.94	0.49
1:E:340:VAL:HG22	1:E:341:PHE:N	2.27	0.49
1:A:1056:ALA:HB2	1:A:1077:LEU:HD11	1.95	0.49
1:E:672:LYS:HB2	1:E:672:LYS:HZ3	1.76	0.49
1:E:870:GLN:HE22	1:E:919:VAL:HG21	1.76	0.49
1:E:1112:ILE:O	1:E:1116:LEU:HD13	2.12	0.49
1:A:669:ASN:N	1:A:669:ASN:HD22	2.10	0.49
1:A:978:TYR:C	1:A:980:GLY:N	2.66	0.49
1:E:908:MET:O	1:E:913:ARG:NH1	2.44	0.49
1:E:1074:LEU:O	1:E:1075:LYS:HG2	2.13	0.49
1:A:788:ASN:ND2	1:A:959:CYS:CB	2.75	0.49
1:E:837:ALA:HB1	3:G:312:DC:H3'	1.95	0.49
1:A:1115:ARG:O	1:A:1119:ILE:HG12	2.13	0.49
1:E:1030:ASN:OD1	1:E:1038:ILE:HG22	2.13	0.49
1:A:644:LEU:HD23	1:A:681:GLU:HB3	1.94	0.49
1:E:432:SER:HB2	1:E:453:LEU:HD11	1.93	0.49
1:E:602:ILE:HG21	1:E:609:VAL:HG13	1.94	0.49
1:A:865:TYR:HB2	1:A:866:PRO:HD3	1.95	0.49
1:A:1116:LEU:HD22	1:A:1238:TRP:HE3	1.76	0.49
1:E:1105:ARG:O	1:E:1109:VAL:HG23	2.13	0.49
3:G:320:DG:H2"	3:G:321:DC:OP2	2.11	0.49
1:A:834:ARG:NH2	3:C:112:DC:C5	2.81	0.49
1:E:1148:ASP:OD1	1:E:1151:SER:HB3	2.12	0.49
1:A:548:GLN:H	1:A:725:MET:HE2	1.78	0.48
1:A:956:MET:HE2	1:A:956:MET:CA	2.43	0.48
1:E:385:ARG:HD2	1:E:457:TYR:CZ	2.47	0.48
1:A:598:PHE:CZ	1:A:738:LEU:HD13	2.48	0.48
1:A:875:CYS:HB2	1:A:912:PRO:CD	2.43	0.48
1:A:807:GLN:HA	1:A:807:GLN:OE1	2.13	0.48
1:E:908:MET:HE3	1:E:913:ARG:HA	1.94	0.48
1:E:963:SER:HA	1:E:968:TYR:CD1	2.48	0.48
1:E:1053:LYS:O	1:E:1054:LYS:HG3	2.14	0.48
2:F:201:G:H2'	2:F:202:C:H6	1.78	0.48
1:E:672:LYS:HG3	1:E:673:LEU:N	2.22	0.48
1:E:1021:LEU:O	1:E:1025:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:G:O2'	2:B:6:G:H5'	2.14	0.48
1:E:1079:ILE:O	1:E:1089:LYS:HD2	2.14	0.48
1:A:541:ALA:HA	1:A:635:VAL:HG13	1.95	0.48
1:A:760:ASN:O	1:A:763:PRO:HD2	2.13	0.48
1:A:935:ASN:HD22	1:A:936:PRO:CD	2.26	0.48
1:A:854:LYS:O	1:A:856:ILE:HD12	2.13	0.48
1:A:909:GLY:C	1:A:912:PRO:HD2	2.33	0.48
1:E:846:ASP:OD1	1:E:847:PRO:HD2	2.14	0.48
1:E:385:ARG:HD2	1:E:457:TYR:CE2	2.49	0.48
1:E:1010:THR:CG2	1:E:1021:LEU:HD23	2.37	0.48
1:A:586:VAL:HG22	1:A:587:SER:N	2.29	0.47
1:A:727:ASN:N	1:A:727:ASN:ND2	2.47	0.47
1:A:785:SER:O	1:A:788:ASN:HB3	2.14	0.47
1:E:523:PRO:C	1:E:525:LEU:H	2.18	0.47
1:E:858:LEU:HD12	1:E:859:LEU:N	2.28	0.47
1:E:1162:ASN:OD1	1:E:1169:VAL:N	2.44	0.47
1:A:550:ALA:O	1:A:551:LYS:O	2.32	0.47
1:A:873:ASN:ND2	1:A:878:THR:HG21	2.28	0.47
1:A:922:ARG:HE	1:A:946:GLN:HG2	1.79	0.47
1:A:1211:TYR:O	1:A:1216:ILE:HG13	2.14	0.47
1:E:429:LYS:HA	5:E:1428:HOH:O	2.13	0.47
1:E:728:ILE:HA	1:E:731:MET:SD	2.54	0.47
1:E:931:GLN:HG2	1:E:932:GLN:N	2.29	0.47
1:A:548:GLN:H	1:A:725:MET:CE	2.28	0.47
1:A:423:THR:OG1	1:A:424:LYS:N	2.46	0.47
1:E:548:GLN:HE21	1:E:548:GLN:HB2	1.45	0.47
1:A:491:ARG:NH2	1:A:527:ASN:OD1	2.48	0.47
1:A:664:ARG:HB2	1:A:687:GLY:HA3	1.95	0.47
1:A:849:VAL:HG13	1:A:1049:LEU:O	2.14	0.47
1:A:1079:ILE:CD1	1:A:1096:ILE:HG13	2.45	0.47
1:E:1128:VAL:HB	1:E:1133:PHE:CZ	2.50	0.47
1:A:547:MET:HE2	1:A:589:PRO:HB3	1.97	0.47
1:A:903:ASP:OD2	1:A:905:SER:HB3	2.14	0.47
1:A:1078:ASP:HB3	1:A:1084:TRP:CD1	2.50	0.47
1:A:1105:ARG:NH2	1:A:1108:ILE:CD1	2.77	0.47
1:E:935:ASN:O	1:E:938:LEU:HB2	2.13	0.47
1:E:1227:ILE:N	1:E:1227:ILE:CD1	2.77	0.47
1:E:394:MET:HE2	1:E:405:GLY:HA2	1.94	0.47
1:E:728:ILE:O	1:E:731:MET:HB2	2.15	0.47
1:E:1215:GLN:C	1:E:1218:PRO:HD2	2.35	0.47
1:A:927:GLN:NE2	1:A:930:LYS:HD2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1112:ILE:HG22	1:A:1116:LEU:HD13	1.97	0.47
1:A:1134:GLU:HG2	1:A:1195:PRO:HG3	1.96	0.47
1:E:529:ILE:HD11	1:E:532:VAL:CG2	2.43	0.47
1:E:1216:ILE:O	1:E:1220:VAL:HG23	2.15	0.46
3:G:315:DT:H2"	3:G:316:DC:H5'	1.90	0.46
1:A:537:LEU:N	1:A:537:LEU:HD23	2.29	0.46
1:A:881:ARG:HG2	1:A:881:ARG:HH11	1.80	0.46
1:E:404:THR:OG1	1:E:405:GLY:N	2.49	0.46
1:E:873:ASN:ND2	1:E:878:THR:HG21	2.30	0.46
1:A:395:LYS:HD2	5:A:1453:HOH:O	2.14	0.46
1:A:618:LEU:HD23	1:A:618:LEU:C	2.35	0.46
1:A:911:LEU:HB3	1:A:912:PRO:HD3	1.96	0.46
1:E:353:TYR:HD2	1:E:354:ASN:HD21	1.63	0.46
1:E:506:LEU:C	1:E:507:LEU:HD12	2.35	0.46
1:E:563:LEU:HD23	1:E:579:PHE:CD1	2.50	0.46
1:E:990:MET:HG2	1:E:994:MET:CE	2.45	0.46
1:A:986:HIS:O	1:A:986:HIS:HD2	1.99	0.46
2:B:2:C:H2'	2:B:3:C:C6	2.51	0.46
1:A:433:LYS:HE3	1:A:435:VAL:CG1	2.45	0.46
1:A:1152:LEU:HA	1:A:1153:PRO:HD2	1.81	0.46
1:E:908:MET:CE	1:E:913:ARG:HA	2.46	0.46
1:A:410:MET:HG2	1:A:434:PRO:HB3	1.97	0.46
1:A:425:TYR:C	1:A:426:LYS:HG2	2.36	0.46
1:E:1148:ASP:CG	1:E:1148:ASP:O	2.54	0.46
1:A:458:SER:HB3	1:A:461:MET:HE3	1.97	0.46
1:A:512:SER:HB2	1:A:664:ARG:O	2.15	0.46
1:E:875:CYS:SG	1:E:876:PHE:N	2.89	0.46
1:A:921:ARG:CD	5:A:1479:HOH:O	2.49	0.46
1:A:928:LEU:O	1:A:931:GLN:HB2	2.16	0.46
1:A:1050:LEU:N	1:A:1050:LEU:HD23	2.31	0.46
1:E:531:ASP:OD1	1:E:531:ASP:N	2.49	0.46
1:E:857:LEU:HD22	1:E:859:LEU:HD21	1.98	0.46
1:A:1119:ILE:O	1:A:1123:VAL:HG23	2.15	0.46
1:E:652:ASN:HB2	1:E:670:MET:CE	2.46	0.46
1:A:500:GLU:HG2	5:A:1454:HOH:O	2.16	0.46
1:A:932:GLN:NE2	1:A:932:GLN:HA	2.31	0.46
1:E:542:PHE:HE2	1:E:544:MET:HE2	1.81	0.46
1:E:562:ALA:C	1:E:563:LEU:HD12	2.36	0.45
1:E:589:PRO:HG2	1:E:592:CYS:SG	2.56	0.45
1:E:940:LEU:O	1:E:944:ILE:HD12	2.16	0.45
1:A:602:ILE:HD13	1:A:609:VAL:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:TYR:CZ	1:A:1075:LYS:HG3	2.50	0.45
1:E:938:LEU:HD12	1:E:938:LEU:HA	1.80	0.45
1:A:705:SER:HA	1:A:1174:THR:HG21	1.98	0.45
1:A:1010:THR:C	1:A:1012:SER:H	2.18	0.45
1:A:682:ARG:HD3	1:A:682:ARG:C	2.36	0.45
1:A:882:VAL:HG22	1:A:882:VAL:O	2.16	0.45
1:E:783:GLY:CA	3:G:310:DG:OP2	2.64	0.45
1:A:730:ASN:N	1:A:730:ASN:HD22	2.13	0.45
1:E:397:ASP:HB2	1:E:404:THR:HG22	1.99	0.45
1:E:559:ALA:O	1:E:560:MET:HG3	2.17	0.45
1:E:1112:ILE:HG22	1:E:1116:LEU:HD13	1.97	0.45
1:A:958:GLY:O	3:C:110:DG:H2"	2.17	0.45
1:A:1181:GLN:HB2	1:A:1205:THR:CG2	2.46	0.45
1:E:340:VAL:HG21	1:E:500:GLU:HG3	1.98	0.45
1:E:985:MET:O	1:E:989:GLU:HG3	2.17	0.45
4:A:1301:2ZE:CAS	4:A:1301:2ZE:CAW	2.91	0.45
1:E:408:ILE:CD1	1:E:472:THR:HA	2.46	0.45
1:E:605:LYS:HB2	1:E:607:VAL:HG23	1.99	0.45
1:E:784:ARG:HG2	1:E:784:ARG:HH11	1.82	0.45
1:E:788:ASN:ND2	1:E:959:CYS:CB	2.79	0.45
1:E:858:LEU:HD12	1:E:858:LEU:C	2.37	0.45
1:E:859:LEU:CD2	1:E:1040:ILE:HD13	2.46	0.45
1:A:896:GLU:O	1:A:897:GLN:HB2	2.16	0.45
1:E:583:PHE:CD2	1:E:625:LYS:HE2	2.51	0.45
1:E:601:VAL:O	1:E:605:LYS:HG2	2.17	0.45
1:A:1000:TYR:CG	1:A:1001:GLY:N	2.85	0.44
1:E:861:PHE:HA	1:E:1038:ILE:HA	1.98	0.44
1:A:1048:LEU:HG	1:A:1050:LEU:CD2	2.47	0.44
1:A:358:VAL:HG22	1:A:381:LYS:HG2	1.98	0.44
1:E:727:ASN:O	1:E:731:MET:HG3	2.17	0.44
1:E:1128:VAL:HB	1:E:1133:PHE:HZ	1.81	0.44
1:A:935:ASN:O	1:A:938:LEU:HB2	2.17	0.44
1:E:529:ILE:C	1:E:529:ILE:HD12	2.38	0.44
1:E:596:TYR:O	1:E:597:ALA:HB3	2.18	0.44
1:E:1231:ASP:OD2	1:E:1233:VAL:HB	2.17	0.44
1:E:368:GLU:OE2	1:E:368:GLU:HA	2.16	0.44
1:A:718:THR:HG22	1:A:719:GLU:N	2.32	0.44
1:A:1215:GLN:C	1:A:1218:PRO:HD2	2.38	0.44
1:E:1142:ASP:O	1:E:1144:GLN:N	2.51	0.44
1:A:806:LYS:HE2	1:A:806:LYS:HB3	1.80	0.44
1:A:1139:LEU:N	1:A:1139:LEU:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:705:SER:HB2	1:E:707:HIS:CD2	2.52	0.44
1:E:852:TYR:CE1	1:E:999:ILE:HG21	2.52	0.44
1:E:901:LEU:CD2	1:E:975:LEU:HD11	2.48	0.44
1:A:925:VAL:HG13	1:A:942:TYR:HB3	2.00	0.44
1:A:1196:GLU:CG	1:A:1197:GLN:N	2.81	0.44
1:E:636:GLY:HA2	1:E:752:ILE:HG21	2.00	0.44
1:E:925:VAL:HG21	1:E:945:ARG:HG2	2.00	0.44
1:E:937:ASP:HB3	5:E:1462:HOH:O	2.18	0.44
1:E:963:SER:HA	1:E:968:TYR:CZ	2.53	0.44
1:E:1056:ALA:HB2	1:E:1077:LEU:HD11	2.00	0.44
1:A:1069:VAL:HG12	1:A:1070:THR:N	2.31	0.43
1:A:1139:LEU:HD23	1:A:1143:PRO:HD3	1.99	0.43
1:E:425:TYR:O	1:E:426:LYS:HB2	2.18	0.43
1:E:859:LEU:HD22	1:E:1040:ILE:HD13	2.00	0.43
1:E:1149:LYS:HG2	1:E:1150:LYS:N	2.32	0.43
1:E:1210:TYR:CD1	1:E:1214:GLN:HG3	2.53	0.43
1:E:875:CYS:HB2	1:E:912:PRO:CD	2.44	0.43
1:A:1149:LYS:HE3	1:A:1159:LEU:HD12	1.99	0.43
1:E:1184:SER:O	1:E:1185:ASN:ND2	2.52	0.43
1:A:688:ARG:HH11	1:A:688:ARG:HG2	1.83	0.43
1:A:916:ARG:O	1:A:920:GLU:HG2	2.18	0.43
1:A:1010:THR:CG2	1:A:1021:LEU:HD23	2.44	0.43
1:A:1182:ASP:OD1	1:A:1191:ARG:HG2	2.18	0.43
2:B:3:C:H2'	2:B:4:U:C6	2.54	0.43
1:E:645:GLU:O	1:E:649:GLN:HG3	2.18	0.43
1:E:672:LYS:NZ	1:E:672:LYS:CB	2.81	0.43
1:E:679:PHE:CD2	1:E:680:GLY:N	2.86	0.43
1:E:1215:GLN:O	1:E:1218:PRO:HD2	2.19	0.43
1:A:762:LEU:HB2	1:A:763:PRO:HD3	2.01	0.43
1:E:412:ASP:HB3	1:E:472:THR:HG21	2.01	0.43
1:E:578:PRO:HB2	1:E:753:LEU:HD21	2.01	0.43
1:E:925:VAL:CG1	1:E:942:TYR:HB3	2.49	0.43
1:E:992:GLN:O	1:E:995:ASN:N	2.51	0.43
1:E:1018:VAL:O	1:E:1021:LEU:HB3	2.19	0.43
1:A:395:LYS:CB	1:A:408:ILE:HD11	2.48	0.43
1:A:429:LYS:N	1:A:429:LYS:HD2	2.33	0.43
1:A:531:ASP:OD1	1:A:531:ASP:N	2.45	0.43
1:A:570:LEU:CD2	1:A:762:LEU:HB3	2.46	0.43
1:A:625:LYS:O	1:A:629:ILE:HG13	2.18	0.43
1:A:901:LEU:HD23	1:A:975:LEU:HD21	2.01	0.43
1:A:1053:LYS:O	1:A:1054:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1103:GLN:HB3	1:A:1107:THR:HB	1.99	0.43
3:G:316:DC:H2"	3:G:317:DC:H5'	1.99	0.43
1:A:1107:THR:O	1:A:1111:ASN:ND2	2.51	0.43
4:A:1301:2ZE:H28	4:A:1301:2ZE:H16	1.80	0.43
1:E:392:ARG:HB2	1:E:408:ILE:HD12	2.00	0.43
1:E:1139:LEU:N	1:E:1139:LEU:HD12	2.34	0.43
1:A:1234:LEU:CG	1:A:1238:TRP:CZ2	2.99	0.43
1:E:537:LEU:HD11	1:E:570:LEU:HD11	2.00	0.43
1:E:1026:LYS:HG2	1:E:1027:SER:N	2.34	0.43
1:A:915:ILE:O	1:A:919:VAL:HG23	2.19	0.43
2:B:1:G:H2'	2:B:2:C:C6	2.53	0.43
1:A:444:PRO:O	1:A:445:ASP:HB2	2.18	0.42
1:A:1121:GLU:O	1:A:1125:ASN:ND2	2.52	0.42
1:E:1046:SER:OG	1:E:1058:LEU:HD12	2.19	0.42
1:A:428:MET:C	1:A:429:LYS:HD2	2.39	0.42
1:E:857:LEU:HD11	1:E:1022:GLY:N	2.34	0.42
1:E:898:ILE:HA	1:E:899:PRO:HD2	1.90	0.42
1:E:1201:GLN:HG2	1:E:1203:ASN:OD1	2.19	0.42
1:A:908:MET:HE1	1:A:913:ARG:HG3	2.00	0.42
1:A:1148:ASP:OD1	1:A:1148:ASP:O	2.36	0.42
1:E:699:GLU:HG3	1:E:784:ARG:HH21	1.85	0.42
1:E:922:ARG:CG	1:E:946:GLN:NE2	2.71	0.42
1:E:1222:ARG:NH1	3:G:317:DC:OP1	2.49	0.42
3:G:315:DT:C2'	3:G:316:DC:C5'	2.84	0.42
1:A:621:PHE:O	1:A:625:LYS:HG2	2.19	0.42
1:A:1139:LEU:HD11	1:A:1175:VAL:CG2	2.50	0.42
1:E:503:SER:N	1:E:504:PRO:CD	2.82	0.42
1:A:713:GLN:O	1:A:717:LYS:HA	2.20	0.42
1:A:1197:GLN:O	1:A:1204:LEU:HD12	2.20	0.42
1:A:726:GLU:H	1:A:726:GLU:HG3	1.62	0.42
1:A:922:ARG:O	1:A:926:LYS:HG3	2.20	0.42
1:E:721:VAL:HG12	1:E:722:VAL:N	2.34	0.42
1:E:392:ARG:HD3	1:E:396:ILE:HD13	2.02	0.42
1:E:545:LYS:HG3	1:E:741:LEU:HD11	2.01	0.42
1:E:807:GLN:HG2	1:E:808:ILE:N	2.34	0.42
1:A:635:VAL:HA	1:A:691:CYS:O	2.20	0.42
1:A:1158:ALA:HB2	1:A:1175:VAL:HG21	2.01	0.42
1:A:558:ILE:C	1:A:558:ILE:HD12	2.40	0.42
1:A:678:GLY:O	1:A:682:ARG:HB2	2.19	0.42
1:E:439:TYR:CZ	1:E:441:PHE:HB2	2.54	0.42
1:E:593:ILE:O	1:E:593:ILE:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:784:ARG:HG3	3:G:310:DG:C5	2.55	0.42
4:E:1301:2ZE:H30	4:E:1301:2ZE:H22	1.82	0.42
1:A:523:PRO:C	1:A:525:LEU:H	2.24	0.41
1:A:1011:ASN:HD22	1:A:1011:ASN:HA	1.68	0.41
1:A:1147:PRO:HG2	1:A:1148:ASP:H	1.83	0.41
1:E:522:LYS:O	1:E:525:LEU:HB2	2.20	0.41
1:E:908:MET:CE	1:E:916:ARG:NH1	2.68	0.41
1:A:593:ILE:O	1:A:593:ILE:HG13	2.19	0.41
1:A:605:LYS:HE2	1:A:739:LEU:HD23	2.01	0.41
1:A:1209:GLN:HE22	1:A:1241:LEU:HD22	1.84	0.41
1:E:1152:LEU:HA	1:E:1153:PRO:HD2	1.79	0.41
3:G:311:DG:H2'	3:G:312:DC:C6	2.54	0.41
1:A:922:ARG:NH2	1:A:950:LYS:HD2	2.35	0.41
1:A:978:TYR:C	1:A:980:GLY:H	2.22	0.41
1:A:1058:LEU:HB3	1:A:1070:THR:OG1	2.21	0.41
1:A:1139:LEU:HD11	1:A:1175:VAL:HG23	2.02	0.41
4:A:1301:2ZE:H22	4:A:1301:2ZE:H30	1.72	0.41
1:E:730:ASN:HD22	1:E:730:ASN:H	1.55	0.41
1:E:788:ASN:HB2	1:E:959:CYS:SG	2.60	0.41
1:A:627:HIS:HB2	1:A:661:LYS:HD3	2.03	0.41
1:A:1010:THR:C	1:A:1012:SER:N	2.73	0.41
1:A:1092:GLY:O	1:A:1096:ILE:HG12	2.20	0.41
1:E:667:ARG:HH22	1:E:683:ASN:HB3	1.84	0.41
1:E:988:LYS:HG3	1:E:998:VAL:HG11	2.01	0.41
1:E:1082:ARG:HG3	1:E:1136:ASN:HB2	2.02	0.41
1:E:1148:ASP:O	1:E:1149:LYS:C	2.59	0.41
1:A:908:MET:HB3	1:A:913:ARG:HD3	2.03	0.41
1:A:1054:LYS:HA	1:A:1075:LYS:O	2.21	0.41
1:A:1170:LYS:HG2	1:A:1173:ASP:OD2	2.21	0.41
1:E:791:LEU:HD12	1:E:791:LEU:O	2.20	0.41
1:E:865:TYR:CB	1:E:866:PRO:HD3	2.49	0.41
1:E:873:ASN:HD21	1:E:878:THR:HG21	1.85	0.41
1:E:1006:ILE:HA	1:E:1006:ILE:HD13	1.81	0.41
1:A:721:VAL:HG12	1:A:722:VAL:N	2.36	0.41
1:A:1082:ARG:HG3	1:A:1136:ASN:HB2	2.02	0.41
3:C:110:DG:N3	3:C:110:DG:H3'	2.36	0.41
1:A:596:TYR:O	1:A:597:ALA:HB3	2.21	0.41
4:A:1301:2ZE:H13	4:A:1301:2ZE:H21	1.87	0.41
1:E:1103:GLN:HB3	1:E:1107:THR:HB	2.03	0.41
1:A:588:LYS:HA	1:A:732:TYR:HE2	1.85	0.41
1:A:667:ARG:HH22	1:A:683:ASN:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:SER:HB3	1:A:1174:THR:OG1	2.20	0.41
1:A:1138:ALA:HA	1:A:1174:THR:HA	2.02	0.41
1:A:1152:LEU:HD13	2:B:6:G:H4'	2.03	0.41
2:B:2:C:O2'	2:B:3:C:H5'	2.21	0.41
3:C:118:DA:H2"	3:C:119:DG:C5'	2.43	0.41
1:E:340:VAL:HG23	1:E:501:VAL:C	2.41	0.41
1:E:1053:LYS:HD3	2:F:210:G:H1'	2.03	0.41
4:E:1301:2ZE:CAS	4:E:1301:2ZE:CAW	2.94	0.41
1:A:649:GLN:O	1:A:653:VAL:HG23	2.21	0.41
1:A:849:VAL:HG12	1:A:850:GLY:N	2.36	0.41
1:A:1169:VAL:HG13	1:A:1173:ASP:HB2	2.03	0.41
1:E:586:VAL:CB	1:E:742:LEU:HD21	2.51	0.41
1:A:549:ASN:OD1	1:A:552:ASN:O	2.39	0.40
1:A:922:ARG:NH2	1:A:946:GLN:OE1	2.51	0.40
1:E:433:LYS:HB3	1:E:433:LYS:HE2	1.92	0.40
1:E:970:LYS:N	1:E:971:PRO:CD	2.85	0.40
1:E:1142:ASP:HB2	1:E:1145:ASP:OD2	2.21	0.40
4:E:1301:2ZE:H21	4:E:1301:2ZE:H13	1.90	0.40
1:E:678:GLY:HA2	1:E:681:GLU:OE1	2.22	0.40
1:E:854:LYS:HB3	1:E:1012:SER:O	2.21	0.40
1:E:1050:LEU:HD13	1:E:1222:ARG:O	2.21	0.40
1:E:1082:ARG:CG	1:E:1136:ASN:HB2	2.51	0.40
1:E:1179:ILE:HD12	1:E:1188:ALA:O	2.21	0.40
2:F:210:G:H2'	2:F:211:DC:C6	2.56	0.40
1:A:588:LYS:HA	1:A:732:TYR:CE2	2.56	0.40
1:E:705:SER:OG	1:E:710:GLU:HG2	2.21	0.40
1:E:1237:THR:HG23	1:E:1243:PRO:HG3	2.02	0.40
1:E:633:ILE:HD13	1:E:762:LEU:HD22	2.04	0.40
1:A:521:LEU:HD23	1:A:521:LEU:HA	1.94	0.40
1:A:669:ASN:N	1:A:669:ASN:ND2	2.69	0.40
1:A:1139:LEU:CD2	1:A:1143:PRO:HD3	2.51	0.40
1:A:1149:LYS:HE3	1:A:1159:LEU:CD1	2.51	0.40
1:E:345:TRP:HA	1:E:363:GLY:HA3	2.04	0.40
1:E:353:TYR:C	1:E:354:ASN:HD22	2.25	0.40
1:E:447:PRO:HB2	1:E:449:LYS:O	2.21	0.40
1:E:1116:LEU:HD22	1:E:1238:TRP:HE3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	857/922 (93%)	785 (92%)	56 (6%)	16 (2%)	8 12
1	E	857/922 (93%)	783 (91%)	62 (7%)	12 (1%)	11 19
All	All	1714/1844 (93%)	1568 (92%)	118 (7%)	28 (2%)	9 16

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	551	LYS
1	A	553	HIS
1	A	589	PRO
1	A	1101	SER
1	A	1149	LYS
1	E	551	LYS
1	E	1101	SER
1	E	1149	LYS
1	A	849	VAL
1	A	897	GLN
1	A	1003	THR
1	A	1150	LYS
1	E	589	PRO
1	E	1150	LYS
1	E	1003	THR
1	A	1103	GLN
1	E	1143	PRO
1	E	1166	GLY
1	A	1243	PRO
1	E	462	PRO
1	A	1153	PRO
1	E	399	ASN
1	E	1026	LYS
1	A	1166	GLY
1	A	462	PRO

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Mol	Chain	Res	Type
1	A	1143	PRO
1	A	1147	PRO
1	E	1243	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	778/827 (94%)	740 (95%)	38 (5%)	25	45
1	E	778/827 (94%)	734 (94%)	44 (6%)	20	37
All	All	1556/1654 (94%)	1474 (95%)	82 (5%)	22	40

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	PHE
1	A	350	GLU
1	A	354	ASN
1	A	365	VAL
1	A	406	THR
1	A	428	MET
1	A	458	SER
1	A	529	ILE
1	A	555	ASN
1	A	567	SER
1	A	606	ASN
1	A	668	SER
1	A	682	ARG
1	A	726	GLU
1	A	727	ASN
1	A	729	GLN
1	A	764	LEU
1	A	785	SER
1	A	797	TYR
1	A	852	TYR

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Mol	Chain	Res	Type
1	A	860	ASP
1	A	908	MET
1	A	912	PRO
1	A	933	ASP
1	A	935	ASN
1	A	937	ASP
1	A	938	LEU
1	A	956	MET
1	A	1011	ASN
1	A	1014	ASN
1	A	1039	ASP
1	A	1080	VAL
1	A	1082	ARG
1	A	1106	ASP
1	A	1185	ASN
1	A	1199	GLN
1	A	1231	ASP
1	A	1243	PRO
1	E	343	PHE
1	E	352	GLN
1	E	354	ASN
1	E	365	VAL
1	E	372	THR
1	E	393	GLU
1	E	406	THR
1	E	529	ILE
1	E	546	THR
1	E	548	GLN
1	E	552	ASN
1	E	555	ASN
1	E	567	SER
1	E	596	TYR
1	E	609	VAL
1	E	611	VAL
1	E	672	LYS
1	E	682	ARG
1	E	727	ASN
1	E	730	ASN
1	E	742	LEU
1	E	764	LEU
1	E	784	ARG
1	E	857	LEU

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Mol	Chain	Res	Type
1	E	860	ASP
1	E	880	GLN
1	E	896	GLU
1	E	916	ARG
1	E	927	GLN
1	E	933	ASP
1	E	935	ASN
1	E	938	LEU
1	E	943	ASP
1	E	945	ARG
1	E	1011	ASN
1	E	1014	ASN
1	E	1039	ASP
1	E	1098	GLN
1	E	1106	ASP
1	E	1173	ASP
1	E	1185	ASN
1	E	1199	GLN
1	E	1231	ASP
1	E	1242	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	ASN
1	A	548	GLN
1	A	554	GLN
1	A	555	ASN
1	A	566	HIS
1	A	606	ASN
1	A	652	ASN
1	A	669	ASN
1	A	683	ASN
1	A	727	ASN
1	A	729	GLN
1	A	730	ASN
1	A	760	ASN
1	A	770	ASN
1	A	870	GLN
1	A	880	GLN
1	A	897	GLN
1	A	927	GLN

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Mol	Chain	Res	Type
1	A	931	GLN
1	A	932	GLN
1	A	935	ASN
1	A	954	ASN
1	A	986	HIS
1	A	1011	ASN
1	A	1014	ASN
1	A	1098	GLN
1	A	1103	GLN
1	A	1111	ASN
1	A	1122	ASN
1	A	1125	ASN
1	A	1132	GLN
1	A	1144	GLN
1	A	1181	GLN
1	A	1185	ASN
1	A	1199	GLN
1	A	1201	GLN
1	A	1209	GLN
1	E	354	ASN
1	E	548	GLN
1	E	554	GLN
1	E	555	ASN
1	E	606	ASN
1	E	652	ASN
1	E	669	ASN
1	E	683	ASN
1	E	707	HIS
1	E	727	ASN
1	E	729	GLN
1	E	730	ASN
1	E	770	ASN
1	E	788	ASN
1	E	870	GLN
1	E	880	GLN
1	E	897	GLN
1	E	924	GLN
1	E	931	GLN
1	E	932	GLN
1	E	935	ASN
1	E	946	GLN
1	E	954	ASN

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Mol	Chain	Res	Type
1	E	1011	ASN
1	E	1014	ASN
1	E	1111	ASN
1	E	1113	GLN
1	E	1122	ASN
1	E	1132	GLN
1	E	1156	HIS
1	E	1181	GLN
1	E	1185	ASN
1	E	1199	GLN
1	E	1201	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	9/11 (81%)	0	0
2	F	9/11 (81%)	0	0
All	All	18/22 (81%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
4	2ZE	E	1301	-	27,27,27	1.02	3 (11%)	43,46,46	1.65	5 (11%)
4	2ZE	A	1301	-	27,27,27	1.02	4 (14%)	43,46,46	1.63	7 (16%)

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
4	2ZE	E	1301	-	-	3/6/72/72	0/5/4/4
4	2ZE	A	1301	-	-	3/6/72/72	0/5/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1301	2ZE	CAF-CAE	-2.50	1.52	1.57
4	A	1301	2ZE	CAF-CAE	-2.45	1.52	1.57
4	A	1301	2ZE	CAF-CAH	-2.32	1.52	1.56
4	E	1301	2ZE	CAE-CAG	-2.27	1.51	1.55
4	E	1301	2ZE	CAN-CAH	-2.20	1.53	1.56
4	A	1301	2ZE	CAN-CAH	-2.16	1.53	1.56
4	A	1301	2ZE	CAE-CAG	-2.07	1.52	1.55

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1301	2ZE	CAL-CAE-CAI	6.16	111.50	105.08
4	E	1301	2ZE	CAL-CAE-CAI	6.11	111.46	105.08
4	A	1301	2ZE	CAK-CAJ-CAP	-3.41	107.84	111.07
4	E	1301	2ZE	CAK-CAJ-CAP	-3.36	107.89	111.07
4	A	1301	2ZE	CAU-CAT-CAN	-2.93	110.00	113.15
4	E	1301	2ZE	CAF-CAH-CAN	-2.82	113.37	116.74
4	A	1301	2ZE	CAF-CAH-CAN	-2.82	113.37	116.74
4	E	1301	2ZE	CAU-CAT-CAN	-2.67	110.28	113.15
4	E	1301	2ZE	CAI-CAJ-CAP	-2.23	108.31	110.16
4	A	1301	2ZE	CAO-CAH-CAN	-2.06	111.53	114.31
4	A	1301	2ZE	CAU-CAQ-CAF	-2.03	109.35	112.84
4	A	1301	2ZE	CAI-CAE-CAG	-2.00	97.28	100.07

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1301	2ZE	CAJ-CAP-CAX-OAD
4	E	1301	2ZE	CAR-CAP-CAX-OAD
4	E	1301	2ZE	OAA-CAP-CAX-OAD
4	A	1301	2ZE	OAA-CAP-CAX-OAD
4	A	1301	2ZE	CAR-CAP-CAX-OAD
4	A	1301	2ZE	CAJ-CAP-CAX-OAD

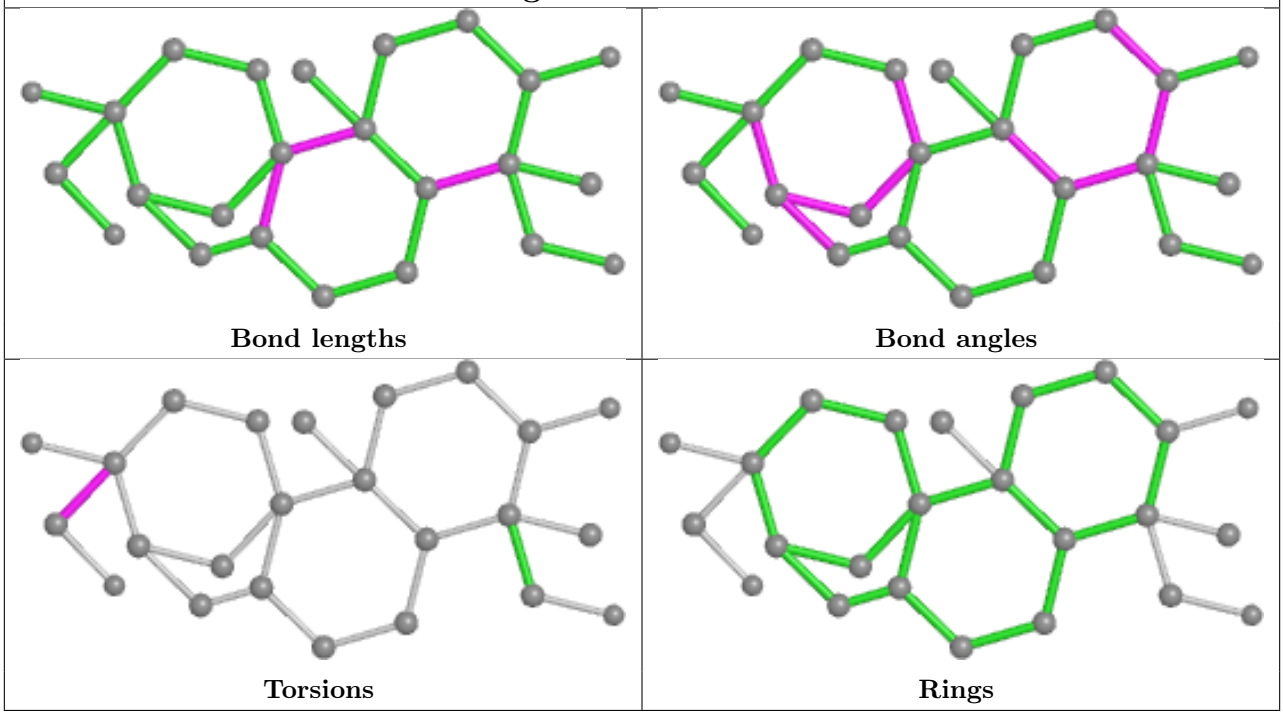
There are no ring outliers.

2 monomers are involved in 14 short contacts:

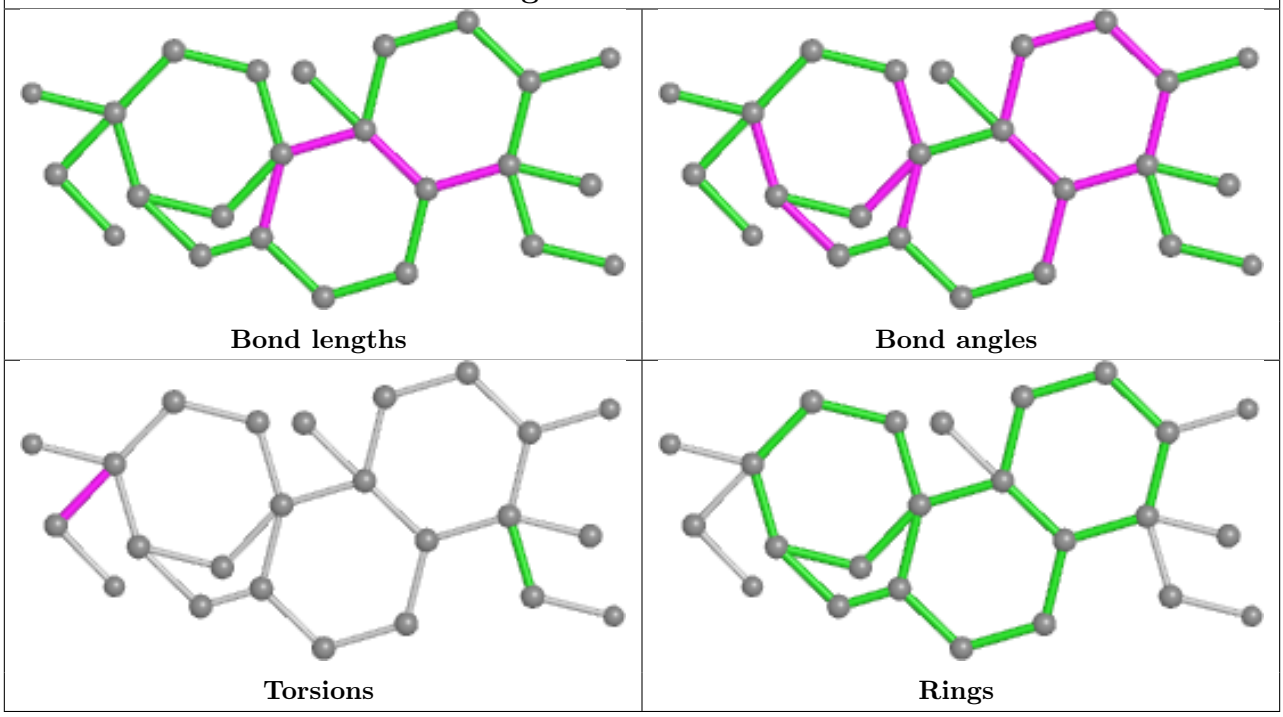
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1301	2ZE	6	0
4	A	1301	2ZE	8	0

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.

Ligand 2ZE E 1301



Ligand 2ZE A 1301



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	865/922 (93%)	0.38	63 (7%)	15	16	15, 54, 113, 128	0
1	E	865/922 (93%)	0.27	39 (4%)	33	36	18, 52, 105, 129	0
2	B	11/11 (100%)	-0.83	0	100	100	48, 62, 78, 87	0
2	F	11/11 (100%)	-0.63	0	100	100	43, 52, 79, 81	0
3	C	13/21 (61%)	-0.29	0	100	100	37, 59, 92, 101	0
3	G	13/21 (61%)	-0.34	0	100	100	42, 57, 76, 85	0
All	All	1778/1908 (93%)	0.30	102 (5%)	23	25	15, 53, 111, 129	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1241	LEU	9.0
1	A	1239	LEU	8.1
1	E	550	ALA	7.2
1	A	1180	CYS	6.8
1	A	1193	TYR	5.8
1	A	1233	VAL	5.7
1	A	1119	ILE	5.7
1	E	1204	LEU	5.4
1	A	678	GLY	5.3
1	A	1186	LEU	5.2
1	A	1210	TYR	5.0
1	A	1124	LEU	4.9
1	E	399	ASN	4.7
1	A	1150	LYS	4.5
1	A	672	LYS	4.3
1	E	1149	LYS	4.2
1	A	1204	LEU	4.2
1	A	1127	SER	4.1
1	A	1167	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	1206	ILE	4.0
1	A	1133	PHE	3.8
1	E	1202	ASP	3.8
1	A	1123	VAL	3.8
1	A	1158	ALA	3.7
1	E	1128	VAL	3.7
1	A	1149	LYS	3.6
1	E	1065	ASP	3.6
1	A	353	TYR	3.5
1	A	1179	ILE	3.5
1	E	1150	LYS	3.4
1	A	1117	ILE	3.4
1	E	681	GLU	3.3
1	A	1177	TYR	3.3
1	A	550	ALA	3.3
1	E	1198	LEU	3.2
1	E	1146	TYR	3.2
1	A	1196	GLU	3.1
1	A	552	ASN	3.1
1	E	1205	THR	3.1
1	A	1128	VAL	3.1
1	A	1065	ASP	3.1
1	A	1116	LEU	3.0
1	E	1124	LEU	3.0
1	E	1158	ALA	3.0
1	A	1230	ILE	3.0
1	A	1066	GLY	2.9
1	E	1180	CYS	2.8
1	E	1120	GLY	2.8
1	A	551	LYS	2.8
1	E	1179	ILE	2.8
1	A	1211	TYR	2.7
1	A	1183	GLY	2.7
1	A	681	GLU	2.6
1	A	1113	GLN	2.6
1	E	1109	VAL	2.6
1	A	1170	LYS	2.6
1	E	682	ARG	2.6
1	A	1108	ILE	2.6
1	A	1206	ILE	2.6
1	E	592	CYS	2.6
1	E	1066	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1159	LEU	2.6
1	A	1166	GLY	2.5
1	E	1210	TYR	2.5
1	A	1235	ILE	2.5
1	E	1211	TYR	2.5
1	A	1165	GLY	2.5
1	E	1123	VAL	2.5
1	A	1182	ASP	2.5
1	A	1169	VAL	2.5
1	E	1079	ILE	2.5
1	E	604	LYS	2.4
1	E	730	ASN	2.4
1	E	1121	GLU	2.4
1	E	1199	GLN	2.4
1	A	1185	ASN	2.4
1	E	1200	LYS	2.4
1	A	1155	VAL	2.3
1	A	1217	HIS	2.3
1	A	1019	PHE	2.3
1	A	1048	LEU	2.3
1	E	1167	ARG	2.3
1	E	551	LYS	2.3
1	A	1214	GLN	2.2
1	A	1192	ALA	2.2
1	E	1177	TYR	2.2
1	E	1105	ARG	2.2
1	E	1193	TYR	2.2
1	A	1216	ILE	2.1
1	E	1108	ILE	2.1
1	A	1130	VAL	2.1
1	A	1236	ALA	2.1
1	A	1184	SER	2.1
1	A	1229	GLY	2.1
1	A	1178	VAL	2.1
1	A	608	LYS	2.1
1	E	1135	ILE	2.1
1	A	1139	LEU	2.1
1	A	1168	LYS	2.1
1	A	1126	GLY	2.1
1	E	445	ASP	2.1
1	A	1200	LYS	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)

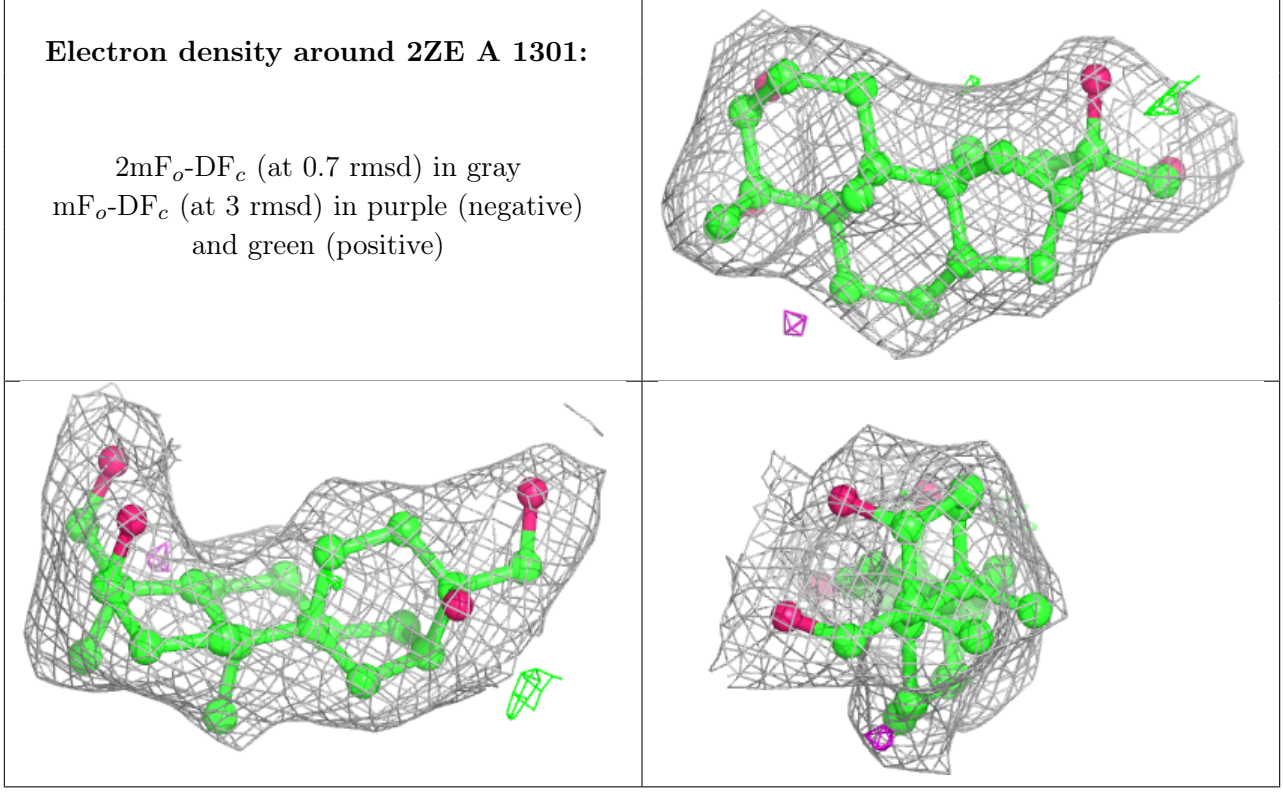
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	2ZE	A	1301	24/24	0.95	0.14	20,29,34,42	0
4	2ZE	E	1301	24/24	0.96	0.14	30,37,43,43	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.

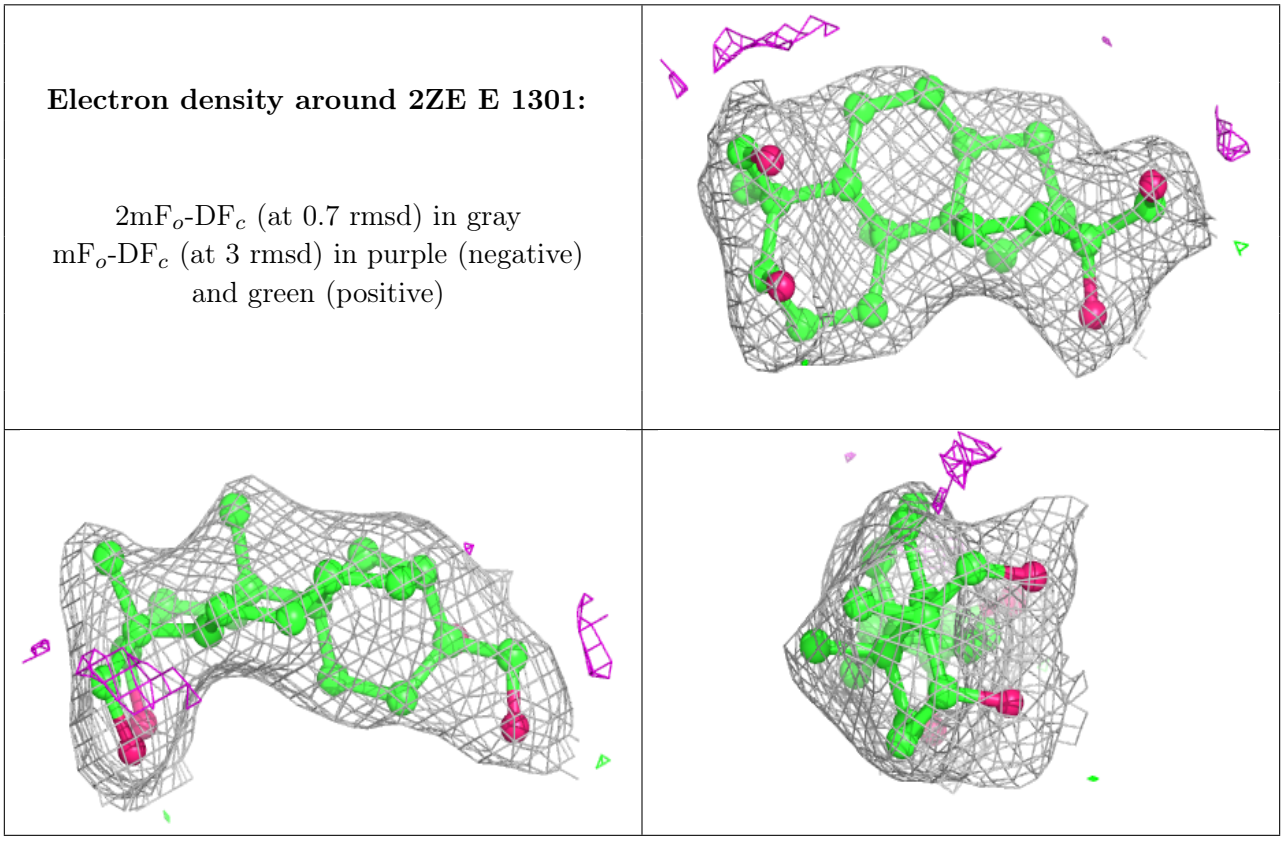
Electron density around 2ZE A 1301:

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



Electron density around 2ZE E 1301:

$2mF_o$-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.