Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 10:33 PM EST

PDB ID	:	1N35
Title	:	lambda3 elongation complex with four phosphodiester bond formed
Authors	:	Tao, Y.; Farsetta, D.L.; Nibert, M.L.; Harrison, S.C.
Deposited on	:	2002-10-25
Resolution	:	2.50 Å(reported)

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 ⓘ

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

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
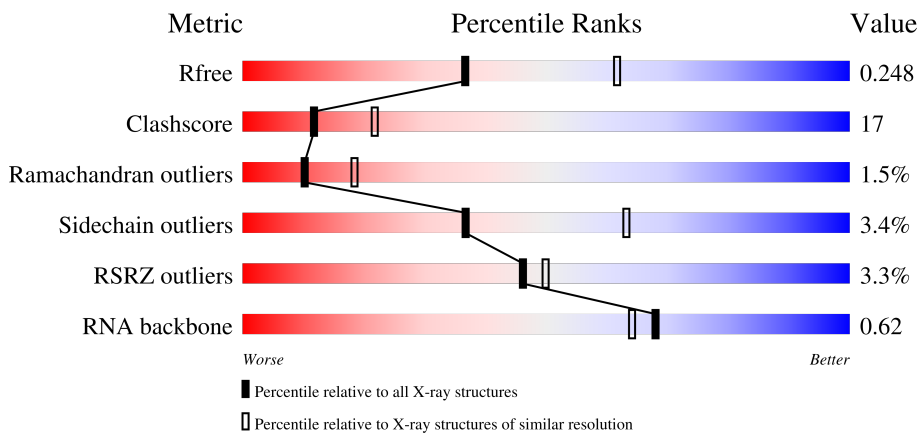
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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	B	5	100% / 20% 80%
2	C	10	20% / 60% 20% 20%
3	A	1267	3% / 69% 29% ·

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10703 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 RNA chain called 5'-R(P*GP*GP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	5	Total	C	N	O	P	0	0	0
			116	50	25	36	5			

- Molecule 2 is a RNA chain called 5'-R(*AP*UP*UP*AP*GP*CP*CP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	P	0	0	0
			165	74	27	56	8			

- Molecule 3 is a protein called Minor core protein lambda 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1264	Total	C	N	O	S	0	0	0
			9986	6369	1712	1841	64			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

- Molecule 5 is 3'-DEOXY-CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CH1) (formula: $C_9H_{16}N_3O_{13}P_3$).

CH1

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 28	C 9	N 3	O 13	P 3	0	0
5	A	1	Total 28	C 9	N 3	O 13	P 3	0	0
5	A	1	Total 28	C 9	N 3	O 13	P 3	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total 4	O 4	0	0
6	C	6	Total 6	O 6	0	0
6	A	340	Total 340	O 340	0	0

3 Residue-property plots ⓘ

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 gr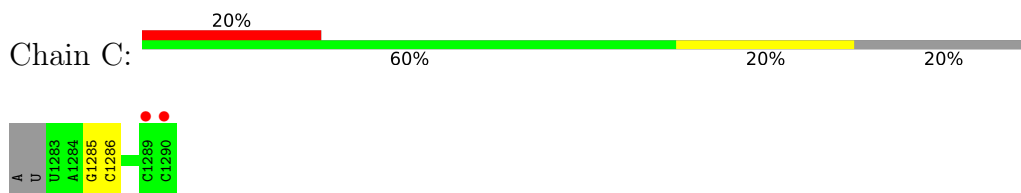aphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a 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.
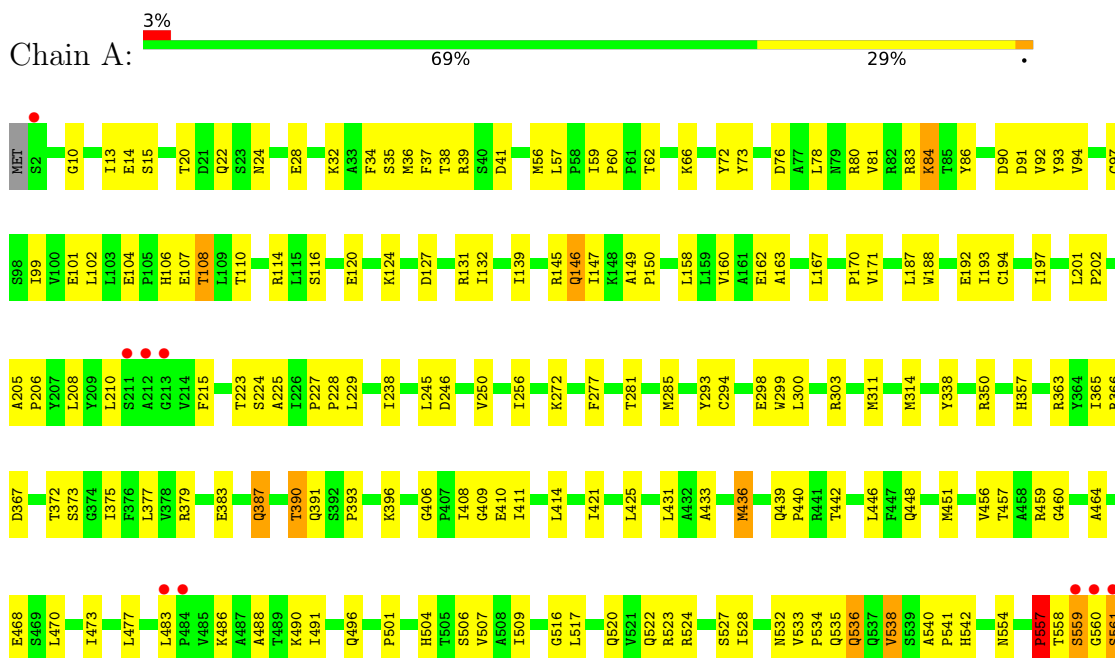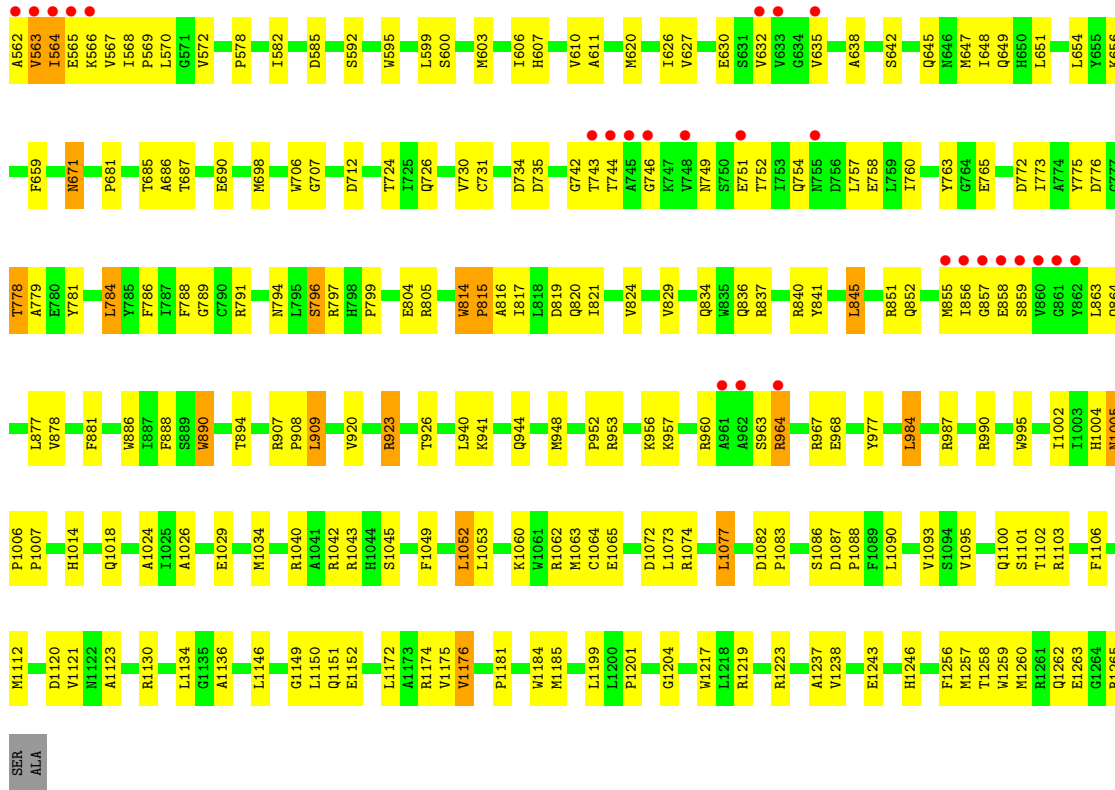
- Molecule 1: 5'-R(P*GP*GP*GP*GP*G)-3'

Chain B:
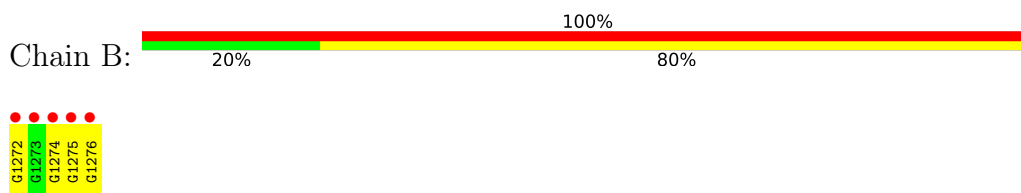
- Molecule 2: 5'-R(*AP*UP*UP*AP*GP*CP*CP*CP*CP*C)-3'

Chain C:

- Molecule 3: Minor core protein lambda 3

Chain A:

A562 V563 I564 E565 K566 V567 I568 P569 L570 G571 V572 P578 I582 D585 S592 S600 W595 L599 S600 M603 I606 H607 V610 A611 M620 I626 V627 E630 S631 V632 V633 G634 V635 A638 S642 Q645 N646 M647 I648 Q649 H650 L651 L654 Y655 K656

F659 N671 P681 T685 A686 T687 E690 M698 W706 G707 D712 T724 I725 Q726 V730 C731 D734 D735 G742 T743 T744 A745 G746 K747 V748 N749 S750 E751 T752 I753 Q754 N755 D756 L757 E758 L759 I760 Y763 G764 E765 D772 I773 A774 Y775 D776 G777

T778 A779 E780 Y781 L784 Y785 F786 I787 F788 G789 C790 R791 N794 L795 S796 R797 H798 P799 E804 R805 W814 P815 A816 I817 L818 D819 Q820 I821 V824 V829 Q834 W835 Q836 R837 R840 Y841 L845 R851 Q852 M855 I856 G857 E858 S859 V860 G861 Y862 L863 Q864

L877 V878 F881 W886 I887 F888 S889 W890 T894 R907 P908 L909 V920 R923 T926 L940 K941 Q944 M948 P952 R953 K956 K957 R960 A961 A962 S963 R964 R967 E968 Y977 L984 R987 R990 W995 I1002 I1003 H1004 N1005

P1006 P1007 H1014 Q1018 A1024 I1025 A1026 E1029 M1034 R1040 A1041 R1042 R1043 H1044 S1045 F1049 L1052 L1053 K1060 W1061 R1062 M1063 C1064 E1065 D1072 L1073 R1074 L1077 D1082 P1083 S1086 D1087 P1088 F1089 L1090 V1093 S1094 V1095 Q1100 S1101 T1102 R1103 F1106

M1112 D1120 V1121 N1122 A1123 R1130 L1134 G1135 A1136 L1146 G1149 L1150 Q1151 E1152 L1172 A1173 R1174 V1175 V1176 P1181 W1184 M1185 L1199 L1200 P1201 G1204 L1217 L1218 R1219 R1223 A1237 V1238 E1243 H1246 F1256 M1257 T1258 W1259 M1260 R1261 Q1262 E1263 G1264 R1265

SER ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.88Å 85.01Å 249.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.01 – 2.50 43.01 – 2.49	Depositor EDS
% Data completeness (in resolution range)	89.9 (43.01-2.50) 89.4 (43.01-2.49)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.259 0.198 , 0.248	Depositor DCC
R_{free} test set	2767 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.1	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10703	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MN, CH1

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	B	0.81	1/130 (0.8%)	0.68	0/201
2	C	0.52	0/182	0.71	0/280
3	A	0.38	0/10239	0.61	1/13905 (0.0%)
All	All	0.39	1/10551 (0.0%)	0.61	1/14386 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1272	G	OP3-P	-7.10	1.52	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	408	ILE	N-CA-C	-5.48	96.19	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	116	0	56	8	0
2	C	165	0	88	4	0
3	A	9986	0	9903	354	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
5	A	84	0	36	3	0
6	A	340	0	0	8	0
6	B	4	0	0	0	0
6	C	6	0	0	0	0
All	All	10703	0	10083	356	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 17.

All (356) 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:A:223:THR:HG22	3:A:225:ALA:H	1.14	1.07
3:A:1112:MET:HE1	3:A:1150:LEU:HD11	1.33	1.05
3:A:410:GLU:H	3:A:649:GLN:NE2	1.58	1.01
1:B:1274:G:H21	3:A:562:ALA:HB2	1.22	1.01
3:A:81:VAL:H	3:A:671:ASN:HD21	1.09	0.99
3:A:749:ASN:HD21	3:A:751:GLU:HB3	1.31	0.95
3:A:724:THR:HG22	3:A:726:GLN:H	1.31	0.94
3:A:146:GLN:HE22	3:A:805:ARG:H	1.08	0.92
3:A:22:GLN:NE2	3:A:878:VAL:H	1.66	0.92
3:A:410:GLU:H	3:A:649:GLN:HE22	1.12	0.90
3:A:561:SER:HB3	3:A:566:LYS:HE2	1.54	0.88
3:A:743:THR:HG22	3:A:744:THR:H	1.37	0.86
1:B:1274:G:N2	3:A:562:ALA:HB2	1.91	0.84
3:A:1005:ASN:HB2	3:A:1130:ARG:HH22	1.41	0.84
3:A:856:ILE:HB	3:A:859:SER:HB2	1.61	0.83
3:A:563:VAL:O	3:A:564:ILE:HG22	1.80	0.82
3:A:851:ARG:HH11	3:A:864:GLN:HE21	1.29	0.80
3:A:78:LEU:HD12	3:A:80:ARG:NH2	1.96	0.80
3:A:522:GLN:HE22	3:A:796:SER:HB3	1.48	0.78
3:A:907:ARG:HB3	3:A:908:PRO:HD3	1.64	0.78
3:A:1201:PRO:HB2	3:A:1204:GLY:O	1.84	0.77
3:A:1004:HIS:C	3:A:1006:PRO:HD3	2.05	0.77
3:A:536:GLN:HE22	3:A:685:THR:H	1.30	0.76
3:A:1005:ASN:HD21	3:A:1263:GLU:HB3	1.49	0.76
3:A:749:ASN:HD22	3:A:752:THR:H	1.33	0.76
3:A:167:LEU:HD23	3:A:837:ARG:HD2	1.68	0.75
3:A:603:MET:HE3	3:A:648:ILE:HG23	1.69	0.75
3:A:379:ARG:HH12	3:A:387:GLN:NE2	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:814:TRP:HB3	3:A:815:PRO:HD3	1.70	0.74
3:A:821:ILE:HG23	3:A:845:LEU:HD13	1.70	0.74
3:A:39:ARG:HH11	3:A:39:ARG:HG2	1.53	0.73
3:A:425:LEU:HD13	3:A:698:MET:HE3	1.70	0.73
3:A:285:MET:HG3	3:A:365:ILE:HD11	1.70	0.73
3:A:114:ARG:HB2	3:A:215:PHE:CE1	2.24	0.73
3:A:1072:ASP:OD1	3:A:1074:ARG:HD3	1.89	0.72
3:A:104:GLU:HG3	3:A:116:SER:HA	1.71	0.72
3:A:1087:ASP:HB3	3:A:1088:PRO:HD3	1.72	0.71
3:A:167:LEU:HD21	3:A:840:ARG:CZ	2.20	0.71
3:A:363:ARG:HH22	3:A:834:GLN:HE22	1.38	0.71
3:A:957:LYS:HE3	3:A:1026:ALA:HB2	1.73	0.71
3:A:561:SER:HB3	3:A:566:LYS:CE	2.21	0.70
3:A:749:ASN:ND2	3:A:752:THR:H	1.89	0.70
3:A:81:VAL:H	3:A:671:ASN:ND2	1.85	0.70
3:A:114:ARG:HB2	3:A:215:PHE:HE1	1.56	0.69
3:A:743:THR:HG22	3:A:744:THR:N	2.07	0.69
3:A:22:GLN:HE21	3:A:878:VAL:H	1.38	0.69
3:A:223:THR:HG22	3:A:225:ALA:N	1.99	0.68
3:A:227:PRO:HB2	3:A:228:PRO:HD3	1.75	0.68
3:A:81:VAL:N	3:A:671:ASN:HD21	1.89	0.68
3:A:536:GLN:HA	3:A:536:GLN:HE21	1.58	0.68
3:A:557:PRO:HD2	3:A:731:CYS:O	1.93	0.68
3:A:776:ASP:OD1	3:A:778:THR:HB	1.93	0.68
3:A:410:GLU:N	3:A:649:GLN:HE22	1.90	0.67
3:A:410:GLU:N	3:A:649:GLN:NE2	2.37	0.67
3:A:171:VAL:HG11	3:A:1090:LEU:HD11	1.77	0.67
3:A:1005:ASN:ND2	3:A:1263:GLU:HB3	2.09	0.67
3:A:66:LYS:HB3	3:A:97:CYS:HA	1.77	0.66
3:A:92:VAL:HG11	3:A:383:GLU:HB3	1.77	0.66
3:A:94:VAL:HG22	3:A:139:ILE:HG23	1.78	0.66
3:A:73:TYR:HB3	3:A:132:ILE:HD12	1.78	0.65
3:A:779:ALA:HB3	3:A:786:PHE:HB2	1.78	0.65
3:A:754:GLN:HE21	3:A:775:TYR:HD2	1.41	0.65
3:A:926:THR:HG21	3:A:1246:HIS:CG	2.31	0.65
3:A:281:THR:O	3:A:285:MET:HG2	1.96	0.65
3:A:532:ASN:OD1	3:A:535:GLN:HG3	1.97	0.65
3:A:815:PRO:HG2	3:A:1034:MET:CE	2.27	0.64
3:A:24:ASN:O	3:A:28:GLU:HG3	1.98	0.64
3:A:1064:CYS:HB3	3:A:1065:GLU:OE2	1.98	0.64
3:A:393:PRO:HG3	3:A:592:SER:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:995:TRP:CZ2	3:A:1006:PRO:HG3	2.33	0.64
3:A:754:GLN:O	3:A:758:GLU:HG3	1.98	0.63
3:A:92:VAL:CG1	3:A:383:GLU:HB3	2.27	0.63
3:A:76:ASP:OD2	3:A:80:ARG:NH1	2.32	0.63
3:A:1062:ARG:HG3	3:A:1243:GLU:HB2	1.81	0.63
3:A:393:PRO:CG	3:A:592:SER:HA	2.29	0.62
3:A:558:THR:O	3:A:559:SER:HB3	2.00	0.62
3:A:146:GLN:HE22	3:A:805:ARG:N	1.90	0.61
3:A:146:GLN:NE2	3:A:805:ARG:H	1.88	0.61
3:A:433:ALA:HB1	3:A:610:VAL:HG23	1.81	0.61
3:A:542:HIS:NE2	3:A:690:GLU:CG	2.63	0.61
3:A:851:ARG:HH11	3:A:864:GLN:NE2	1.96	0.61
3:A:120:GLU:O	3:A:124:LYS:HG3	1.99	0.61
3:A:167:LEU:HD21	3:A:840:ARG:NH2	2.16	0.61
3:A:570:LEU:HD21	3:A:730:VAL:HG21	1.82	0.61
3:A:724:THR:HG22	3:A:726:GLN:N	2.09	0.60
3:A:83:ARG:HG2	3:A:92:VAL:HA	1.82	0.60
3:A:372:THR:HB	3:A:796:SER:OG	2.00	0.60
3:A:952:PRO:HG2	3:A:956:LYS:HE3	1.83	0.60
3:A:542:HIS:NE2	3:A:690:GLU:HG3	2.17	0.60
3:A:377:LEU:HD12	3:A:377:LEU:H	1.67	0.59
1:B:1274:G:H21	3:A:562:ALA:CB	2.07	0.58
3:A:501:PRO:HD2	3:A:504:HIS:HD2	1.67	0.58
3:A:409:GLY:HA3	3:A:649:GLN:NE2	2.19	0.58
3:A:293:TYR:CZ	3:A:1074:ARG:NH2	2.71	0.58
3:A:797:ARG:C	3:A:799:PRO:HD3	2.24	0.58
1:B:1276:G:H1'	3:A:560:GLY:O	2.04	0.57
3:A:724:THR:HG23	3:A:726:GLN:OE1	2.04	0.57
3:A:1029:GLU:N	3:A:1029:GLU:OE1	2.36	0.57
3:A:194:CYS:SG	3:A:206:PRO:HG2	2.45	0.57
3:A:501:PRO:HD2	3:A:504:HIS:CD2	2.40	0.57
3:A:829:VAL:HG13	3:A:890:TRP:CE2	2.39	0.57
3:A:836:GLN:HG2	3:A:886:TRP:CE3	2.40	0.57
3:A:451:MET:HA	3:A:451:MET:CE	2.34	0.57
3:A:566:LYS:HD2	3:A:784:LEU:HD23	1.86	0.57
3:A:794:ASN:OD1	3:A:796:SER:HB2	2.04	0.56
3:A:1040:ARG:HG3	3:A:1043:ARG:NH2	2.21	0.56
3:A:193:ILE:HD13	3:A:229:LEU:HD21	1.88	0.56
3:A:926:THR:CG2	3:A:1246:HIS:CG	2.89	0.56
3:A:855:MET:CE	3:A:858:GLU:H	2.19	0.55
3:A:562:ALA:O	3:A:565:GLU:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:856:ILE:HB	3:A:859:SER:CB	2.35	0.55
3:A:957:LYS:O	3:A:960:ARG:HG3	2.06	0.55
3:A:522:GLN:NE2	3:A:796:SER:HB3	2.19	0.55
3:A:1065:GLU:H	3:A:1065:GLU:CD	2.09	0.55
3:A:20:THR:HG21	6:A:1413:HOH:O	2.06	0.55
3:A:819:ASP:OD1	3:A:953:ARG:NH1	2.40	0.55
3:A:851:ARG:NH1	3:A:864:GLN:HE21	2.01	0.55
3:A:926:THR:HG21	3:A:1246:HIS:ND1	2.21	0.55
3:A:659:PHE:CZ	3:A:681:PRO:HG2	2.42	0.55
3:A:944:GLN:HB3	3:A:948:MET:CE	2.37	0.55
3:A:202:PRO:HD2	6:A:1484:HOH:O	2.05	0.55
2:C:1285:G:H1	5:A:1291:CH1:HN41	1.55	0.55
3:A:107:GLU:O	3:A:108:THR:CB	2.55	0.55
3:A:815:PRO:HG2	3:A:1034:MET:HE1	1.89	0.55
3:A:532:ASN:OD1	3:A:534:PRO:HD2	2.07	0.54
3:A:425:LEU:HB2	3:A:698:MET:HE3	1.88	0.54
3:A:957:LYS:HE2	3:A:1024:ALA:O	2.06	0.54
3:A:1082:ASP:HB2	3:A:1083:PRO:CD	2.37	0.54
3:A:566:LYS:CD	3:A:784:LEU:HD23	2.37	0.54
3:A:1176:VAL:O	3:A:1176:VAL:HG13	2.06	0.54
3:A:13:ILE:HD13	3:A:163:ALA:HB3	1.88	0.54
3:A:92:VAL:HG13	3:A:383:GLU:CG	2.38	0.54
3:A:595:TRP:CE2	3:A:600:SER:HB3	2.42	0.54
3:A:516:GLY:HA3	3:A:528:ILE:HG22	1.89	0.54
3:A:814:TRP:O	3:A:815:PRO:C	2.45	0.54
3:A:1073:LEU:HG	3:A:1093:VAL:HG11	1.90	0.54
3:A:561:SER:O	3:A:565:GLU:HB3	2.08	0.54
3:A:606:ILE:O	3:A:610:VAL:HB	2.08	0.54
3:A:188:TRP:CZ2	3:A:192:GLU:HG3	2.43	0.53
3:A:193:ILE:O	3:A:197:ILE:HG13	2.08	0.53
3:A:540:ALA:HB3	3:A:541:PRO:HD3	1.91	0.53
3:A:603:MET:CE	3:A:648:ILE:HG23	2.38	0.53
3:A:1052:LEU:HD21	3:A:1176:VAL:HG22	1.91	0.53
3:A:22:GLN:HE22	3:A:878:VAL:H	1.51	0.53
3:A:81:VAL:HG13	3:A:132:ILE:HD13	1.91	0.53
3:A:170:PRO:HG3	3:A:886:TRP:HB2	1.91	0.52
3:A:607:HIS:HB2	3:A:648:ILE:HG21	1.89	0.52
3:A:446:LEU:HD13	3:A:1149:GLY:HA3	1.91	0.52
3:A:564:ILE:HG21	3:A:1185:MET:HB3	1.89	0.52
3:A:944:GLN:HB3	3:A:948:MET:HE2	1.89	0.52
3:A:167:LEU:HD23	3:A:837:ARG:CD	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:743:THR:CG2	3:A:744:THR:H	2.16	0.52
3:A:1174:ARG:HB2	6:A:1323:HOH:O	2.10	0.52
3:A:62:THR:O	3:A:66:LYS:HE2	2.09	0.51
3:A:436:MET:O	3:A:436:MET:HE2	2.09	0.51
3:A:724:THR:CG2	3:A:726:GLN:H	2.13	0.51
3:A:406:GLY:HA3	3:A:630:GLU:O	2.10	0.51
3:A:377:LEU:HD12	3:A:377:LEU:N	2.24	0.51
3:A:1005:ASN:N	3:A:1006:PRO:HD3	2.24	0.51
3:A:566:LYS:HD2	3:A:784:LEU:CD2	2.40	0.51
3:A:784:LEU:HD12	3:A:786:PHE:CZ	2.46	0.51
3:A:940:LEU:O	3:A:941:LYS:HB2	2.11	0.51
3:A:578:PRO:HB2	3:A:742:GLY:HA3	1.93	0.51
3:A:14:GLU:C	3:A:20:THR:HG22	2.31	0.51
3:A:245:LEU:HD22	3:A:367:ASP:HA	1.93	0.51
3:A:34:PHE:CZ	3:A:160:VAL:HG21	2.46	0.51
3:A:814:TRP:O	3:A:817:ILE:HG22	2.10	0.51
3:A:984:LEU:O	3:A:987:ARG:HB2	2.11	0.51
1:B:1275:G:H2'	3:A:561:SER:HB2	1.93	0.50
3:A:1219:ARG:O	3:A:1223:ARG:HG3	2.10	0.50
3:A:470:LEU:HD23	3:A:477:LEU:HD21	1.93	0.50
3:A:1002:ILE:HD13	3:A:1136:ALA:HB2	1.93	0.50
3:A:1258:THR:HG23	3:A:1262:GLN:NE2	2.27	0.50
3:A:411:ILE:C	3:A:411:ILE:HD12	2.32	0.50
3:A:32:LYS:O	3:A:36:MET:HG3	2.11	0.50
3:A:686:ALA:O	3:A:690:GLU:HB2	2.12	0.50
3:A:881:PHE:O	3:A:909:LEU:HD12	2.12	0.50
3:A:572:VAL:HG13	3:A:789:GLY:O	2.12	0.50
3:A:303:ARG:HG3	3:A:303:ARG:HH11	1.77	0.49
3:A:436:MET:HE2	3:A:436:MET:C	2.32	0.49
3:A:948:MET:HE1	3:A:1042:ARG:HG3	1.94	0.49
3:A:298:GLU:HB2	3:A:311:MET:CE	2.42	0.49
3:A:92:VAL:HG13	3:A:383:GLU:HG3	1.94	0.49
3:A:464:ALA:O	3:A:468:GLU:HG2	2.12	0.49
3:A:409:GLY:HA3	3:A:627:VAL:HG21	1.95	0.49
3:A:542:HIS:NE2	3:A:690:GLU:HG2	2.28	0.49
3:A:523:ARG:HG2	3:A:524:ARG:H	1.77	0.49
3:A:778:THR:CG2	3:A:779:ALA:N	2.75	0.49
3:A:1120:ASP:HB3	3:A:1123:ALA:CB	2.43	0.49
3:A:557:PRO:HG3	3:A:781:TYR:OH	2.13	0.49
3:A:561:SER:CB	3:A:566:LYS:HE2	2.34	0.48
3:A:1199:LEU:HD12	3:A:1219:ARG:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:568:ILE:N	3:A:569:PRO:CD	2.76	0.48
3:A:749:ASN:ND2	3:A:751:GLU:HB3	2.14	0.48
3:A:538:VAL:HG13	3:A:651:LEU:HB2	1.96	0.48
3:A:582:ILE:HG21	3:A:757:LEU:CD2	2.42	0.48
3:A:223:THR:HG21	6:A:1418:HOH:O	2.13	0.48
3:A:523:ARG:HG2	3:A:524:ARG:N	2.28	0.48
3:A:599:LEU:O	3:A:603:MET:HG2	2.14	0.48
3:A:436:MET:HE1	3:A:442:THR:HG21	1.94	0.48
3:A:857:GLY:C	3:A:859:SER:H	2.15	0.48
3:A:1082:ASP:HB2	3:A:1083:PRO:HD2	1.95	0.48
3:A:446:LEU:HD22	3:A:1149:GLY:C	2.34	0.48
3:A:815:PRO:HB2	3:A:953:ARG:O	2.14	0.48
3:A:1172:LEU:O	3:A:1175:VAL:HG13	2.14	0.48
3:A:299:TRP:CD2	3:A:303:ARG:HG2	2.49	0.47
3:A:35:SER:HB3	5:A:1294:CH1:H1'	1.96	0.47
3:A:509:ILE:HD13	3:A:538:VAL:HG21	1.95	0.47
3:A:396:LYS:HD2	3:A:765:GLU:HB3	1.96	0.47
3:A:39:ARG:HH11	3:A:39:ARG:CG	2.23	0.47
3:A:470:LEU:CD2	3:A:477:LEU:HD21	2.44	0.47
3:A:272:LYS:HD3	3:A:338:TYR:OH	2.14	0.47
3:A:957:LYS:HD2	3:A:957:LYS:N	2.30	0.47
3:A:477:LEU:HB3	3:A:496:GLN:HB3	1.97	0.47
3:A:760:ILE:O	3:A:763:TYR:HB3	2.14	0.47
3:A:451:MET:HA	3:A:451:MET:HE2	1.97	0.47
3:A:582:ILE:HG21	3:A:757:LEU:HD21	1.96	0.47
3:A:13:ILE:HD13	3:A:163:ALA:CB	2.45	0.46
3:A:149:ALA:HB1	3:A:150:PRO:CD	2.45	0.46
3:A:886:TRP:HA	6:A:1409:HOH:O	2.15	0.46
3:A:83:ARG:NH1	3:A:84:LYS:O	2.48	0.46
3:A:632:VAL:HB	3:A:635:VAL:HB	1.96	0.46
3:A:995:TRP:HZ2	3:A:1006:PRO:HG3	1.79	0.46
3:A:15:SER:N	3:A:20:THR:HG22	2.31	0.46
3:A:565:GLU:OE1	3:A:1103:ARG:HB2	2.16	0.46
1:B:1275:G:O2'	3:A:561:SER:HB3	2.16	0.46
2:C:1285:G:C5	3:A:528:ILE:HG12	2.50	0.46
3:A:238:ILE:HD12	3:A:841:TYR:CZ	2.51	0.46
3:A:246:ASP:O	3:A:250:VAL:HG23	2.16	0.46
3:A:457:THR:O	3:A:491:ILE:HG13	2.16	0.46
3:A:856:ILE:O	3:A:856:ILE:HG22	2.16	0.46
3:A:1005:ASN:O	3:A:1007:PRO:HD3	2.15	0.46
3:A:1172:LEU:HD21	3:A:1217:TRP:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:92:VAL:CG1	3:A:92:VAL:O	2.64	0.46
3:A:595:TRP:HA	3:A:599:LEU:HB2	1.97	0.46
3:A:101:GLU:HG2	3:A:102:LEU:HG	1.97	0.45
3:A:734:ASP:OD1	5:A:1291:CH1:H5'2	2.16	0.45
3:A:149:ALA:HB1	3:A:150:PRO:HD2	1.98	0.45
3:A:1146:LEU:HD21	3:A:1152:GLU:HG2	1.98	0.45
3:A:59:ILE:HA	3:A:60:PRO:HD3	1.84	0.45
3:A:784:LEU:CD1	3:A:791:ARG:HD2	2.46	0.45
2:C:1286:C:OP2	3:A:459:ARG:HG3	2.16	0.45
3:A:72:TYR:O	3:A:83:ARG:HD2	2.16	0.45
3:A:749:ASN:HD22	3:A:752:THR:N	2.07	0.45
3:A:106:HIS:CE1	3:A:108:THR:HB	2.51	0.45
3:A:90:ASP:O	3:A:92:VAL:N	2.50	0.45
3:A:964:ARG:O	3:A:968:GLU:HG3	2.16	0.45
3:A:855:MET:HE3	3:A:858:GLU:H	1.81	0.45
3:A:104:GLU:CG	3:A:116:SER:HA	2.43	0.45
3:A:256:ILE:HD12	3:A:277:PHE:CE2	2.52	0.45
3:A:814:TRP:CG	3:A:815:PRO:N	2.82	0.45
3:A:15:SER:HA	3:A:20:THR:HG22	1.99	0.44
3:A:162:GLU:OE1	3:A:837:ARG:NH2	2.50	0.44
3:A:486:LYS:HE2	3:A:488:ALA:HB3	1.98	0.44
3:A:561:SER:O	3:A:562:ALA:HB3	2.16	0.44
3:A:706:TRP:O	3:A:707:GLY:C	2.55	0.44
3:A:814:TRP:O	3:A:816:ALA:N	2.50	0.44
3:A:127:ASP:O	3:A:131:ARG:HG3	2.17	0.44
3:A:303:ARG:HH11	3:A:303:ARG:CG	2.30	0.44
3:A:563:VAL:O	3:A:564:ILE:CG2	2.60	0.44
3:A:907:ARG:HH12	3:A:1060:LYS:HE3	1.82	0.44
3:A:820:GLN:O	3:A:824:VAL:HG23	2.18	0.44
3:A:1112:MET:HE3	3:A:1150:LEU:HD21	1.99	0.44
3:A:73:TYR:HB2	3:A:132:ILE:HG23	1.99	0.44
3:A:757:LEU:HD22	3:A:773:ILE:HG21	1.99	0.44
3:A:1095:VAL:HG23	3:A:1237:ALA:HB2	1.99	0.44
3:A:107:GLU:O	3:A:108:THR:HB	2.16	0.44
3:A:1150:LEU:HD12	3:A:1150:LEU:N	2.32	0.44
3:A:1134:LEU:HA	3:A:1257:MET:HE3	1.98	0.44
3:A:84:LYS:HD2	3:A:86:TYR:CZ	2.53	0.44
3:A:373:SER:OG	3:A:375:ILE:HG12	2.18	0.44
3:A:554:ASN:HB2	6:A:1412:HOH:O	2.17	0.44
3:A:1102:THR:O	3:A:1106:PHE:HD2	2.00	0.44
3:A:38:THR:O	3:A:41:ASP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:642:SER:OG	3:A:645:GLN:HG3	2.18	0.44
3:A:784:LEU:HD22	3:A:784:LEU:HA	1.79	0.44
3:A:73:TYR:CB	3:A:132:ILE:HD12	2.47	0.43
3:A:201:LEU:HA	3:A:202:PRO:HD3	1.78	0.43
3:A:457:THR:C	3:A:491:ILE:HG13	2.38	0.43
3:A:585:ASP:HB3	3:A:772:ASP:HB3	1.98	0.43
3:A:208:LEU:HB2	3:A:210:LEU:HD21	1.99	0.43
3:A:425:LEU:HB2	3:A:698:MET:CE	2.48	0.43
3:A:1052:LEU:HD13	3:A:1259:TRP:CG	2.53	0.43
3:A:814:TRP:CD2	3:A:852:GLN:HB2	2.53	0.43
3:A:877:LEU:HB2	3:A:888:PHE:CD2	2.54	0.43
3:A:106:HIS:HE1	3:A:108:THR:HB	1.83	0.43
3:A:814:TRP:CB	3:A:815:PRO:HD3	2.45	0.43
3:A:223:THR:CG2	3:A:224:SER:N	2.81	0.43
3:A:533:VAL:HB	3:A:534:PRO:HD3	1.99	0.43
2:C:1285:G:H5"	3:A:460:GLY:N	2.34	0.43
3:A:39:ARG:CG	3:A:39:ARG:NH1	2.80	0.43
3:A:139:ILE:HD12	3:A:139:ILE:HA	1.86	0.43
3:A:448:GLN:NE2	3:A:620:MET:H	2.16	0.43
1:B:1275:G:N2	3:A:560:GLY:HA3	2.34	0.43
3:A:855:MET:O	3:A:856:ILE:HD13	2.18	0.43
3:A:39:ARG:HG2	3:A:39:ARG:NH1	2.28	0.43
3:A:473:ILE:HG21	3:A:507:VAL:HG11	2.01	0.43
3:A:294:CYS:SG	3:A:314:MET:HB3	2.59	0.42
3:A:557:PRO:O	3:A:557:PRO:HG2	2.18	0.42
3:A:245:LEU:CD2	3:A:367:ASP:HA	2.50	0.42
3:A:350:ARG:HD2	6:A:1524:HOH:O	2.19	0.42
3:A:517:LEU:HD23	3:A:527:SER:HA	2.00	0.42
3:A:659:PHE:CZ	3:A:681:PRO:CG	3.02	0.42
3:A:170:PRO:CG	3:A:886:TRP:HB2	2.49	0.42
3:A:1086:SER:O	3:A:1090:LEU:HG	2.19	0.42
3:A:907:ARG:CB	3:A:908:PRO:HD3	2.43	0.42
3:A:1014:HIS:O	3:A:1018:GLN:HG3	2.19	0.42
3:A:357:HIS:CE1	3:A:788:PHE:HB2	2.54	0.42
3:A:439:GLN:HA	3:A:440:PRO:HD3	1.94	0.42
3:A:855:MET:HE1	3:A:858:GLU:H	1.83	0.42
3:A:1049:PHE:CG	3:A:1053:LEU:HD23	2.55	0.42
3:A:390:THR:HG22	3:A:391:GLN:N	2.34	0.42
3:A:158:LEU:HD22	3:A:238:ILE:HD13	2.02	0.42
3:A:456:VAL:HG21	3:A:977:TYR:CE2	2.54	0.42
3:A:541:PRO:HB2	3:A:648:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:829:VAL:HG13	3:A:890:TRP:NE1	2.34	0.42
3:A:814:TRP:HB3	3:A:815:PRO:CD	2.44	0.42
3:A:1120:ASP:HB3	3:A:1123:ALA:HB2	2.00	0.42
3:A:93:TYR:CD1	3:A:379:ARG:HB3	2.55	0.42
3:A:114:ARG:HH11	3:A:114:ARG:HG3	1.85	0.42
3:A:814:TRP:CB	3:A:815:PRO:CD	2.98	0.42
3:A:460:GLY:O	3:A:490:LYS:NZ	2.53	0.41
3:A:1256:PHE:O	3:A:1260:MET:HG3	2.21	0.41
3:A:393:PRO:HG2	3:A:592:SER:HA	2.03	0.41
3:A:923:ARG:HH11	3:A:923:ARG:CB	2.33	0.41
3:A:147:ILE:HD12	3:A:149:ALA:O	2.20	0.41
3:A:626:ILE:CG2	3:A:638:ALA:HB1	2.50	0.41
3:A:863:LEU:HD23	3:A:863:LEU:HA	1.92	0.41
3:A:538:VAL:HG22	3:A:647:MET:HA	2.02	0.41
3:A:1262:GLN:HG2	3:A:1265:ARG:NH1	2.36	0.41
3:A:56:MET:HG2	3:A:188:TRP:CE2	2.55	0.41
3:A:83:ARG:HG3	3:A:83:ARG:HH11	1.85	0.41
3:A:523:ARG:HG2	3:A:523:ARG:HH11	1.85	0.41
3:A:817:ILE:O	3:A:821:ILE:HG12	2.21	0.41
3:A:145:ARG:O	3:A:805:ARG:HD2	2.20	0.41
3:A:528:ILE:HD12	3:A:528:ILE:HA	1.88	0.41
3:A:744:THR:C	3:A:746:GLY:H	2.24	0.41
3:A:542:HIS:CE1	3:A:690:GLU:HG3	2.54	0.41
3:A:595:TRP:CE2	3:A:656:LYS:HG2	2.56	0.41
3:A:654:LEU:HD21	3:A:659:PHE:CE1	2.55	0.41
3:A:926:THR:HG23	3:A:1246:HIS:CD2	2.56	0.41
3:A:1077:LEU:HD13	3:A:1077:LEU:HA	1.79	0.41
3:A:187:LEU:HD23	3:A:187:LEU:HA	1.91	0.41
3:A:520:GLN:NE2	3:A:523:ARG:HD3	2.35	0.41
3:A:387:GLN:HE21	3:A:387:GLN:HB3	1.73	0.40
3:A:749:ASN:ND2	3:A:752:THR:N	2.62	0.40
3:A:1181:PRO:HD2	3:A:1184:TRP:CE3	2.57	0.40
3:A:167:LEU:HD22	3:A:167:LEU:N	2.36	0.40
3:A:1043:ARG:HD3	6:A:1425:HOH:O	2.20	0.40
1:B:1274:G:H2'	1:B:1275:G:O4'	2.21	0.40
3:A:205:ALA:HA	3:A:206:PRO:HD3	1.83	0.40
3:A:421:ILE:HD12	3:A:421:ILE:HA	1.87	0.40
3:A:483:LEU:HD21	3:A:967:ARG:HA	2.04	0.40
3:A:941:LYS:HA	3:A:944:GLN:OE1	2.22	0.40
3:A:1100:GLN:CG	3:A:1101:SER:N	2.84	0.40
3:A:66:LYS:HA	3:A:66:LYS:HD3	1.84	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
3	A	1262/1267 (100%)	1169 (93%)	74 (6%)	19 (2%)	10 18

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	108	THR
3	A	559	SER
3	A	561	SER
3	A	814	TRP
3	A	564	ILE
3	A	963	SER
3	A	91	ASP
3	A	557	PRO
3	A	567	VAL
3	A	687	THR
3	A	964	ARG
3	A	110	THR
3	A	99	ILE
3	A	146	GLN
3	A	611	ALA
3	A	815	PRO
3	A	10	GLY
3	A	1005	ASN
3	A	563	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	
3	A	1081/1083 (100%)	1044 (97%)	37 (3%)	37	63

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	37	PHE
3	A	57	LEU
3	A	84	LYS
3	A	300	LEU
3	A	366	ARG
3	A	387	GLN
3	A	390	THR
3	A	414	LEU
3	A	431	LEU
3	A	436	MET
3	A	506	SER
3	A	536	GLN
3	A	538	VAL
3	A	557	PRO
3	A	671	ASN
3	A	712	ASP
3	A	735	ASP
3	A	778	THR
3	A	784	LEU
3	A	796	SER
3	A	804	GLU
3	A	845	LEU
3	A	890	TRP
3	A	894	THR
3	A	909	LEU
3	A	920	VAL
3	A	923	ARG
3	A	984	LEU
3	A	990	ARG
3	A	1045	SER
3	A	1052	LEU
3	A	1063	MET
3	A	1077	LEU
3	A	1121	VAL
3	A	1151	GLN

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Mol	Chain	Res	Type
3	A	1176	VAL
3	A	1238	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	22	GLN
3	A	121	ASN
3	A	146	GLN
3	A	283	HIS
3	A	296	ASN
3	A	387	GLN
3	A	448	GLN
3	A	504	HIS
3	A	520	GLN
3	A	522	GLN
3	A	536	GLN
3	A	649	GLN
3	A	664	ASN
3	A	671	ASN
3	A	675	HIS
3	A	710	HIS
3	A	728	ASN
3	A	749	ASN
3	A	754	GLN
3	A	834	GLN
3	A	864	GLN
3	A	969	GLN
3	A	980	GLN
3	A	1004	HIS
3	A	1005	ASN
3	A	1165	GLN
3	A	1177	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	4/5 (80%)	0	0
2	C	7/10 (70%)	0	0
All	All	11/15 (73%)	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	#$|Z| > 2$
5	CH1	A	1291	4	24,29,29	1.15	1 (4%)	33,45,45	2.84	15 (45%)
5	CH1	A	1295	-	24,29,29	1.14	2 (8%)	33,45,45	2.72	15 (45%)
5	CH1	A	1294	-	24,29,29	1.16	2 (8%)	33,45,45	2.79	15 (45%)

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
5	CH1	A	1291	4	-	5/22/34/34	0/2/2/2
5	CH1	A	1295	-	-	8/22/34/34	0/2/2/2
5	CH1	A	1294	-	-	6/22/34/34	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1294	CH1	C6-C5	2.64	1.41	1.35
5	A	1291	CH1	C6-C5	2.58	1.41	1.35
5	A	1295	CH1	C6-C5	2.46	1.40	1.35
5	A	1294	CH1	PG-O1G	2.15	1.57	1.50
5	A	1295	CH1	PB-O1B	2.01	1.58	1.50

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1295	CH1	O3G-PG-O1G	-7.66	80.69	110.68
5	A	1294	CH1	O3G-PG-O1G	-7.38	81.79	110.68
5	A	1291	CH1	O3G-PG-O1G	-7.34	81.95	110.68
5	A	1291	CH1	O3G-PG-O3B	-6.68	82.22	104.64
5	A	1294	CH1	O3G-PG-O3B	-6.61	82.48	104.64
5	A	1295	CH1	O3G-PG-O3B	-6.31	83.48	104.64
5	A	1291	CH1	O3G-PG-O2G	-5.16	87.92	107.64
5	A	1295	CH1	O3G-PG-O2G	-5.11	88.09	107.64
5	A	1294	CH1	O3G-PG-O2G	-5.11	88.12	107.64
5	A	1294	CH1	O2-C2-N3	-4.99	114.22	122.33
5	A	1291	CH1	O2-C2-N3	-4.95	114.28	122.33
5	A	1295	CH1	O2-C2-N3	-4.81	114.51	122.33
5	A	1294	CH1	C3'-C4'-C5'	-4.20	104.83	113.11
5	A	1291	CH1	C3'-C4'-C5'	-4.11	105.00	113.11
5	A	1291	CH1	O4'-C1'-C2'	-3.94	102.80	106.51
5	A	1295	CH1	C3'-C4'-C5'	-3.84	105.52	113.11
5	A	1294	CH1	O4'-C1'-C2'	-3.80	102.93	106.51
5	A	1291	CH1	PB-O3A-PA	-3.50	120.81	132.83
5	A	1291	CH1	O4'-C4'-C5'	3.32	114.98	109.52
5	A	1294	CH1	PB-O3B-PG	-3.13	122.07	132.83
5	A	1295	CH1	PB-O3A-PA	-3.11	122.16	132.83
5	A	1295	CH1	O4'-C4'-C5'	3.01	114.47	109.52
5	A	1294	CH1	PB-O3A-PA	-3.01	122.50	132.83
5	A	1291	CH1	PB-O3B-PG	-2.98	122.60	132.83
5	A	1295	CH1	O4'-C1'-C2'	-2.96	103.73	106.51
5	A	1294	CH1	C6-N1-C2	-2.84	115.57	120.49
5	A	1291	CH1	C6-N1-C2	-2.81	115.62	120.49
5	A	1295	CH1	C6-N1-C2	-2.75	115.72	120.49
5	A	1294	CH1	O4'-C4'-C5'	2.75	114.03	109.52
5	A	1291	CH1	O2G-PG-O3B	2.71	113.72	104.64
5	A	1294	CH1	O2G-PG-O3B	2.71	113.72	104.64
5	A	1295	CH1	O3B-PG-O1G	2.53	125.21	111.19
5	A	1295	CH1	O2G-PG-O3B	2.43	112.80	104.64
5	A	1295	CH1	PB-O3B-PG	-2.39	124.61	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1294	CH1	O3B-PG-O1G	2.35	124.21	111.19
5	A	1291	CH1	O3B-PG-O1G	2.31	123.98	111.19
5	A	1291	CH1	O4'-C1'-N1	2.28	113.58	108.36
5	A	1294	CH1	N1-C2-N3	2.27	122.94	118.81
5	A	1294	CH1	O4'-C1'-N1	2.24	113.49	108.36
5	A	1295	CH1	N1-C2-N3	2.24	122.89	118.81
5	A	1291	CH1	N1-C2-N3	2.20	122.81	118.81
5	A	1291	CH1	O2G-PG-O1G	2.11	118.95	110.68
5	A	1294	CH1	O2G-PG-O1G	2.08	118.82	110.68
5	A	1295	CH1	O4'-C1'-N1	2.03	113.01	108.36
5	A	1295	CH1	O2G-PG-O1G	2.03	118.64	110.68

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1291	CH1	C3'-C4'-C5'-O5'
5	A	1291	CH1	O4'-C4'-C5'-O5'
5	A	1291	CH1	C5'-O5'-PA-O1A
5	A	1294	CH1	C3'-C4'-C5'-O5'
5	A	1294	CH1	O4'-C4'-C5'-O5'
5	A	1294	CH1	C5'-O5'-PA-O2A
5	A	1294	CH1	C5'-O5'-PA-O3A
5	A	1295	CH1	C3'-C4'-C5'-O5'
5	A	1295	CH1	O4'-C4'-C5'-O5'
5	A	1295	CH1	C5'-O5'-PA-O1A
5	A	1295	CH1	C5'-O5'-PA-O3A
5	A	1294	CH1	C4'-C5'-O5'-PA
5	A	1295	CH1	PG-O3B-PB-O3A
5	A	1291	CH1	C5'-O5'-PA-O3A
5	A	1294	CH1	C5'-O5'-PA-O1A
5	A	1291	CH1	PB-O3A-PA-O2A
5	A	1295	CH1	PB-O3A-PA-O1A
5	A	1295	CH1	PG-O3B-PB-O1B
5	A	1295	CH1	PG-O3B-PB-O2B

There are no ring outliers.

2 monomers are involved in 3 short contacts:
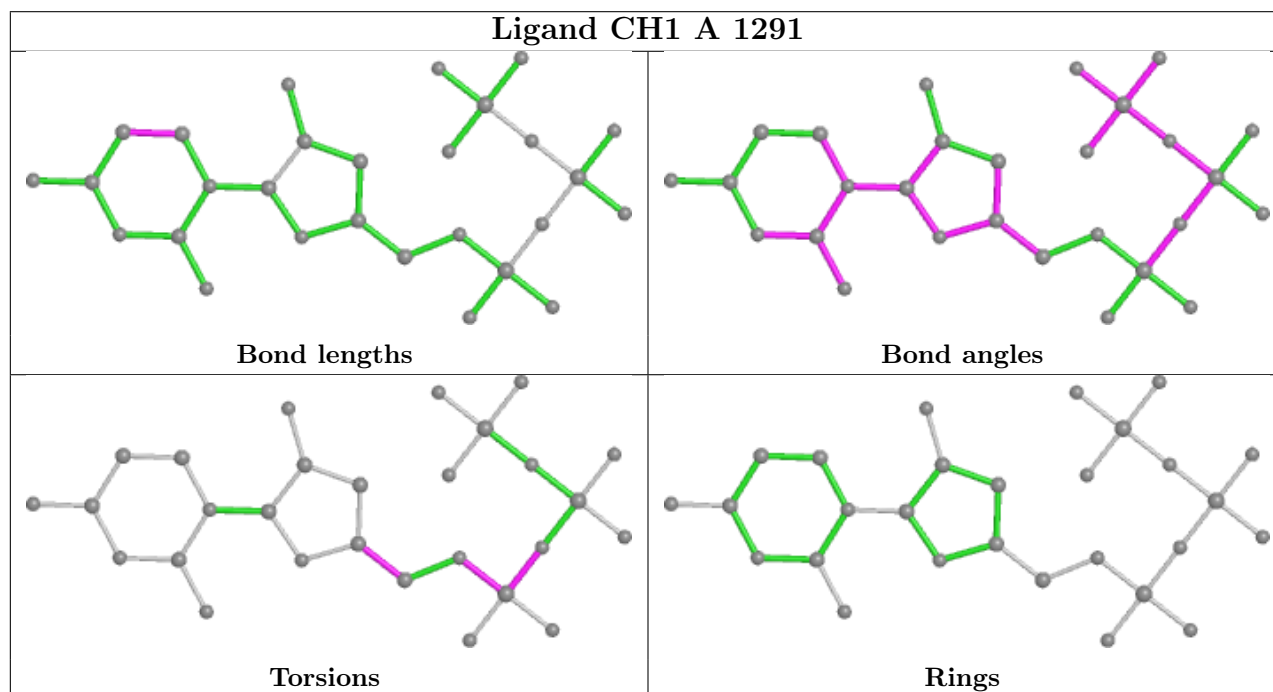
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1291	CH1	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1294	CH1	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 CH1 A 1291

Ligand CH1 A 1295

Bond lengths

Bond angles

Torsions

Rings

Ligand CH1 A 1294

Bond lengths

Bond angles

Torsions

Rings
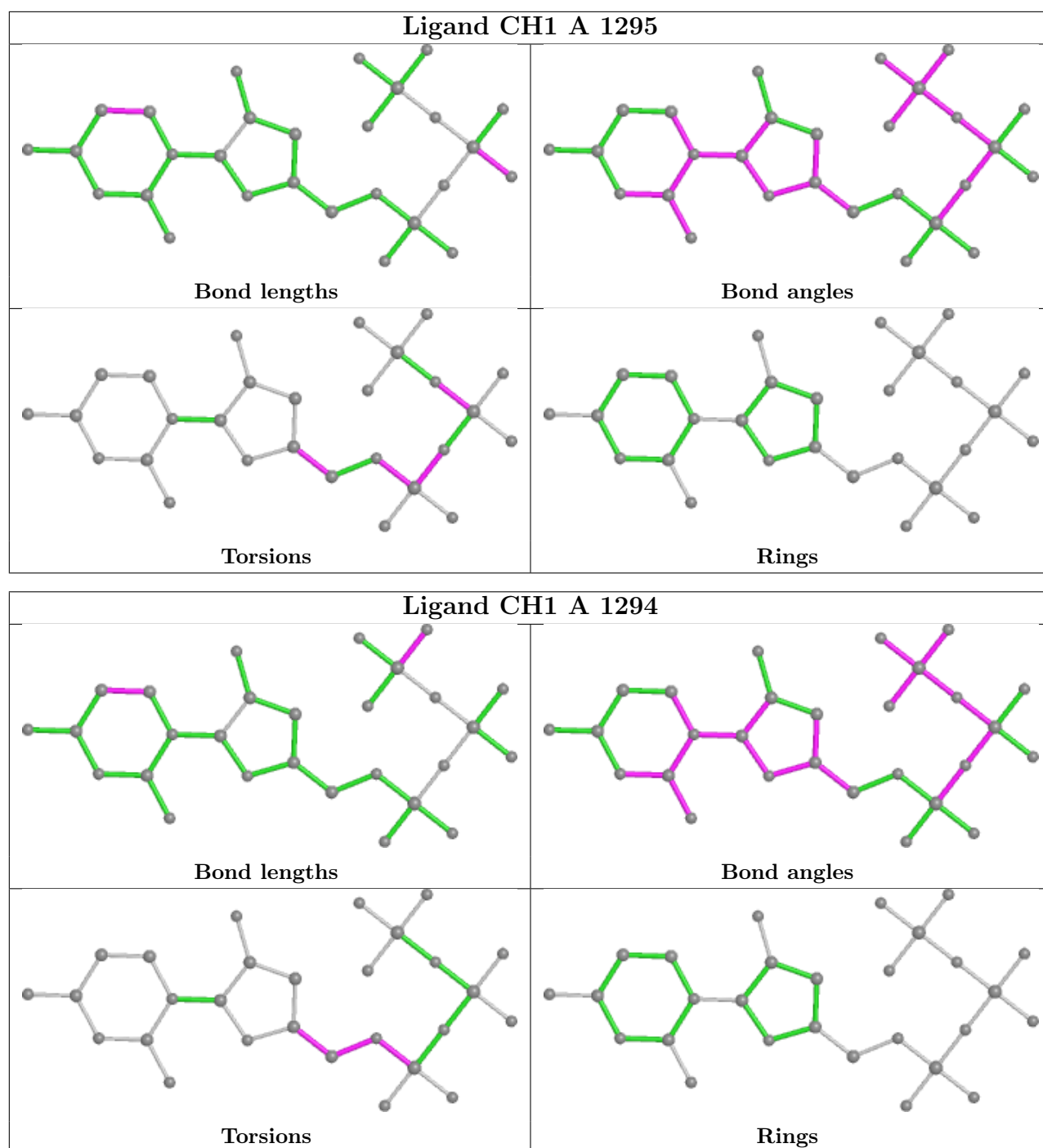
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	B	5/5 (100%)	4.45	5 (100%)	0	0	108, 119, 124, 124	0
2	C	8/10 (80%)	2.28	2 (25%)	0	0	35, 69, 127, 133	0
3	A	1264/1267 (99%)	-0.04	35 (2%)	53	56	17, 32, 53, 98	0
All	All	1277/1282 (99%)	-0.00	42 (3%)	46	50	17, 32, 54, 133	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1290	C	10.1
3	A	2	SER	8.1
3	A	211	SER	6.7
3	A	561	SER	6.6
2	C	1289	C	6.5
1	B	1272	G	5.8
3	A	563	VAL	5.6
1	B	1276	G	5.3
3	A	856	ILE	5.2
3	A	744	THR	4.9
3	A	633	VAL	4.9
3	A	961	ALA	4.4
3	A	858	GLU	4.2
1	B	1275	G	4.1
3	A	746	GLY	4.0
1	B	1273	G	3.8
3	A	855	MET	3.4
3	A	484	PRO	3.4
1	B	1274	G	3.2
3	A	860	VAL	3.2
3	A	748	VAL	3.2
3	A	559	SER	3.1
3	A	560	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
3	A	213	GLY	2.8
3	A	859	SER	2.7
3	A	964	ARG	2.7
3	A	857	GLY	2.6
3	A	566	LYS	2.6
3	A	565	GLU	2.5
3	A	862	TYR	2.5
3	A	564	ILE	2.4
3	A	562	ALA	2.4
3	A	745	ALA	2.4
3	A	743	THR	2.4
3	A	635	VAL	2.3
3	A	751	GLU	2.3
3	A	962	ALA	2.2
3	A	483	LEU	2.1
3	A	212	ALA	2.1
3	A	755	ASN	2.0
3	A	861	GLY	2.0
3	A	632	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
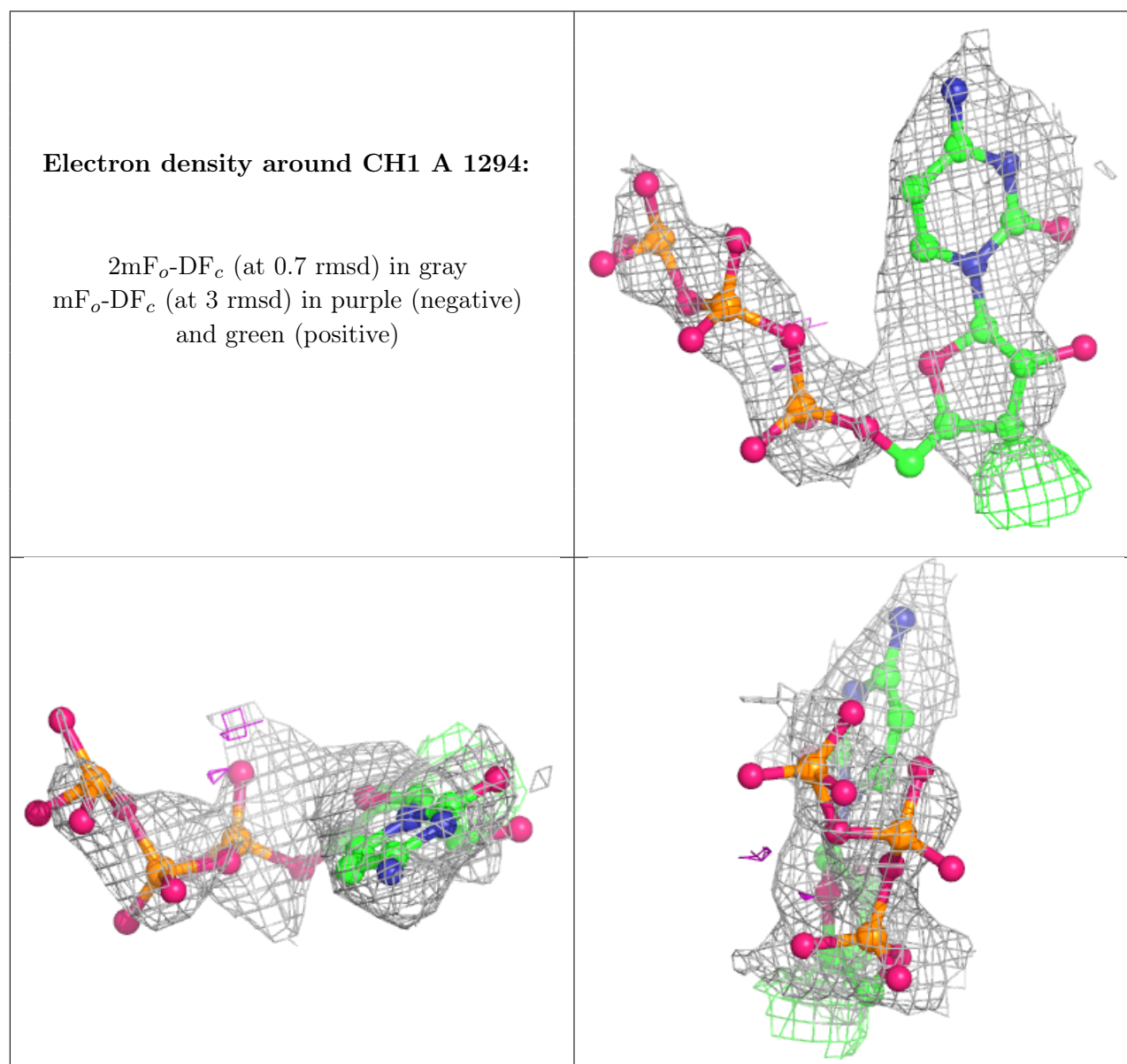
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CH1	A	1294	28/28	0.65	0.33	86,99,118,119	0
5	CH1	A	1291	28/28	0.83	0.21	83,93,100,100	0
5	CH1	A	1295	28/28	0.88	0.20	44,59,81,81	0
4	MN	A	1301	1/1	0.90	0.06	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MN	A	1302	1/1	0.98	0.11	60,60,60,60	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 CH1 A 1294:

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

Electron density around CH1 A 1291:

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

Electron density around CH1 A 1295:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.