



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:58 PM UTC

PDB ID : 1N35 / pdb_00001n35
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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

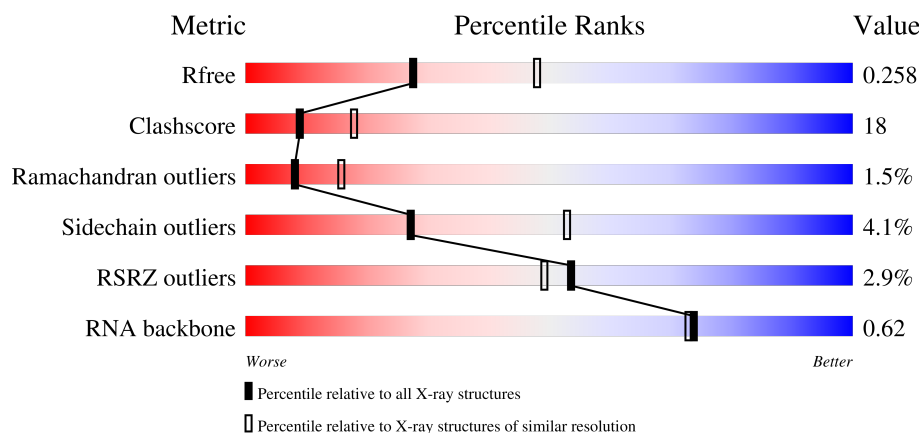
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	5	100% 40% 60%
2	C	10	30% 50% 30% 20%
3	A	1267	2% 66% 30% .

2 Entry composition

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			

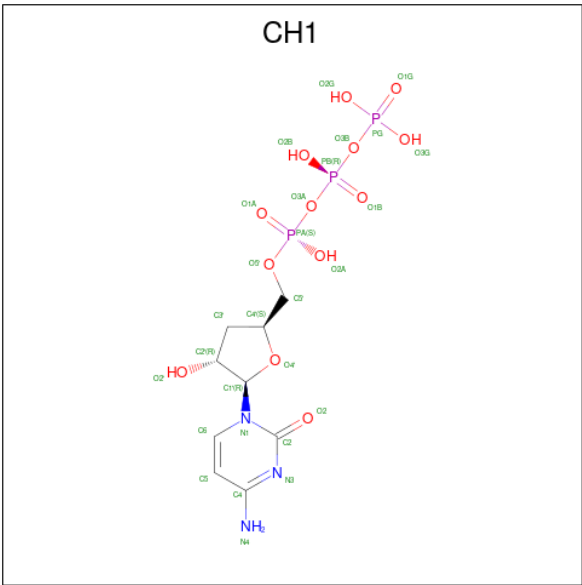
- Molecule 3 is a protein called Minor core protein lambda 3.

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 (CCD ID: 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 (CCD ID: CH1) (formula: C₉H₁₆N₃O₁₃P₃).



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

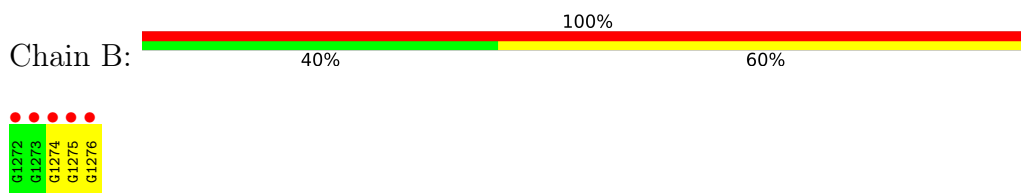
- Molecule 6 is water.

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

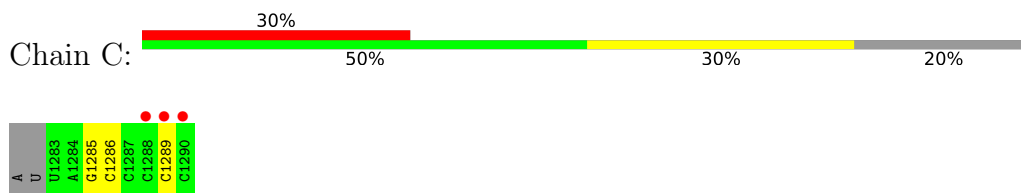
3 Residue-property plots

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 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.

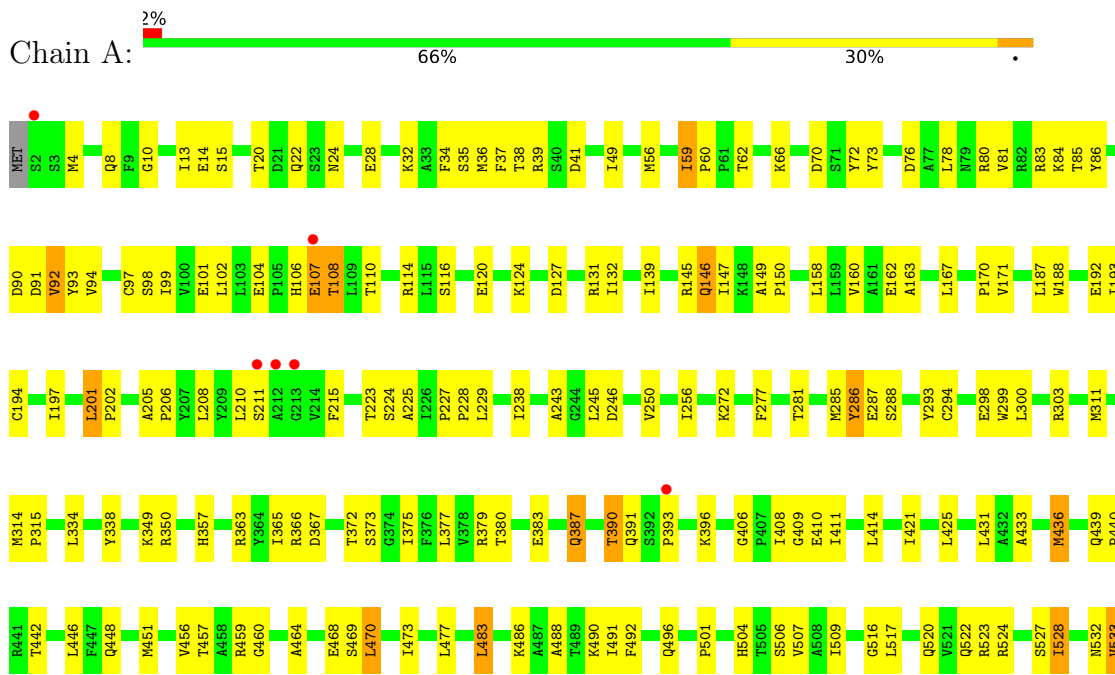
- Molecule 1: 5'-R(P*GP*GP*GP*GP*G)-3'

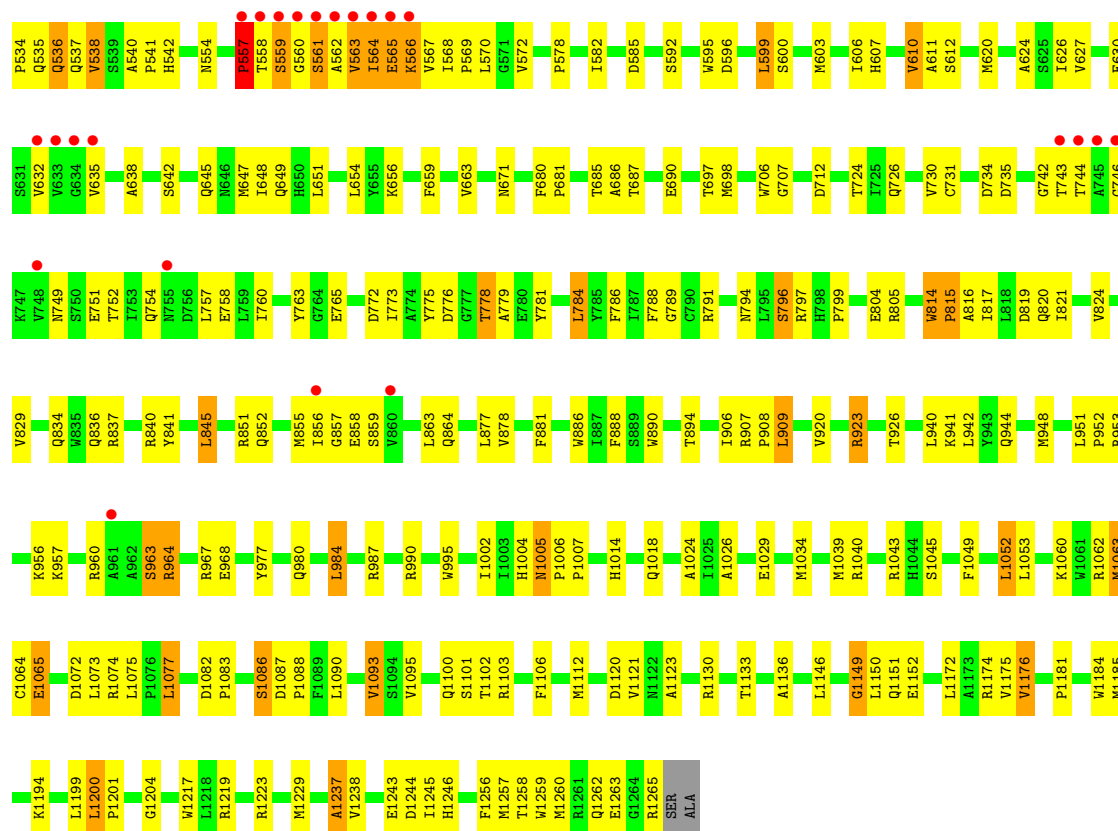


- Molecule 2: 5'-R(*AP*UP*UP*AP*GP*CP*CP*CP*CP*C)-3'



- Molecule 3: Minor core protein lambda 3





4 Data and refinement statistics

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 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.9 (43.01-2.50) 89.9 (43.01-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.259 0.207 , 0.258	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 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.50	0/130	0.53	0/201
2	C	0.44	0/182	0.54	0/280
3	A	0.45	0/10239	0.95	39/13905 (0.3%)
All	All	0.45	0/10551	0.94	39/14386 (0.3%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	243	ALA	N-CA-C	-7.57	103.63	113.17
3	A	287	GLU	N-CA-C	-7.30	103.48	112.38
3	A	49	ILE	N-CA-C	7.27	115.10	107.76
3	A	565	GLU	N-CA-C	-7.15	104.53	113.18
3	A	70	ASP	N-CA-C	6.76	120.41	111.75
3	A	612	SER	N-CA-C	6.46	120.02	111.75
3	A	408	ILE	N-CA-C	-6.32	96.19	109.34
3	A	1194	LYS	N-CA-C	6.26	119.39	111.69
3	A	566	LYS	N-CA-C	-6.22	105.54	112.57
3	A	1149	GLY	N-CA-C	6.17	123.88	115.00
3	A	624	ALA	N-CA-C	-6.15	102.59	110.53
3	A	951	LEU	CA-C-N	5.99	126.34	119.93
3	A	951	LEU	C-N-CA	5.99	126.34	119.93
3	A	201	LEU	CA-C-N	5.96	125.83	119.28
3	A	201	LEU	C-N-CA	5.96	125.83	119.28
3	A	286	TYR	N-CA-C	5.96	119.78	111.74
3	A	211	SER	N-CA-C	-5.92	105.72	113.12
3	A	8	GLN	N-CA-C	5.90	117.71	111.28
3	A	680	PHE	CA-C-N	5.85	125.61	119.76
3	A	680	PHE	C-N-CA	5.85	125.61	119.76
3	A	380	THR	CA-C-N	5.70	125.16	119.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	380	THR	C-N-CA	5.70	125.16	119.24
3	A	59	ILE	CA-C-N	5.51	126.05	120.38
3	A	59	ILE	C-N-CA	5.51	126.05	120.38
3	A	663	VAL	N-CA-C	5.50	115.70	107.51
3	A	599	LEU	N-CA-C	5.47	117.94	111.33
3	A	4	MET	N-CA-C	-5.38	105.31	111.07
3	A	483	LEU	CA-C-N	5.26	126.42	119.84
3	A	483	LEU	C-N-CA	5.26	126.42	119.84
3	A	1093	VAL	N-CA-C	5.25	116.03	110.72
3	A	1244	ASP	N-CA-C	5.24	116.49	108.52
3	A	1086	SER	N-CA-C	5.24	121.96	110.80
3	A	469	SER	N-CA-C	-5.24	106.15	112.54
3	A	492	PHE	N-CA-C	-5.21	105.68	111.36
3	A	596	ASP	N-CA-C	5.21	118.42	111.75
3	A	1075	LEU	N-CA-C	5.17	117.73	108.47
3	A	1237	ALA	N-CA-C	-5.17	102.64	110.28
3	A	98	SER	N-CA-C	-5.06	104.18	110.41
3	A	533	VAL	CB-CA-C	-5.05	108.90	113.70

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	5	0
3	A	9986	0	9903	376	0
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	378	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 18.

All (378) 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	1.32	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:451:MET:HE2	3:A:451:MET:HA	1.54	0.90
3:A:855:MET:HE1	3:A:858:GLU:H	1.38	0.89
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
3:A:603:MET:HE3	3:A:648:ILE:HG23	1.57	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:1004:HIS:C	3:A:1006:PRO:HD3	2.05	0.81
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:425:LEU:HB2	3:A:698:MET:HE1	1.64	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:1063:MET:HE1	3:A:1229:MET:HE2	1.68	0.74
3:A:379:ARG:HH12	3:A:387:GLN:NE2	1.84	0.74
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: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:298:GLU:HB2	3:A:311:MET:HE2	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:425:LEU:HD13	3:A:698:MET:HE3	1.72	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:815:PRO:HG2	3:A:1034:MET:HE1	1.79	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:797:ARG:C	3:A:799:PRO:HD3	2.24	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:436:MET:C	3:A:436:MET:HE2	2.26	0.61
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:1065:GLU:H	3:A:1065:GLU:CD	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
3:A:814:TRP:O	3:A:815:PRO:C	2.45	0.58
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
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:566:LYS:HD2	3:A:784:LEU:HD23	1.86	0.57
3:A:314:MET:HE3	3:A:315:PRO:HD2	1.87	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:14:GLU:C	3:A:20:THR:HG22	2.31	0.55
3:A:562:ALA:O	3:A:565:GLU:HB3	2.06	0.55
3:A:856:ILE:HB	3:A:859:SER:CB	2.35	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:411:ILE:C	3:A:411:ILE:HD12	2.32	0.55
3:A:107:GLU:O	3:A:108:THR:CB	2.55	0.55
3:A:532:ASN:OD1	3:A:534:PRO:HD2	2.07	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: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:436:MET:HE2	3:A:436:MET:O	2.08	0.53
3:A:540:ALA:HB3	3:A:541:PRO:HD3	1.91	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:857:GLY:C	3:A:859:SER:H	2.15	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:1133:THR:O	3:A:1257:MET:HE3	2.09	0.52
3:A:167:LEU:HD23	3:A:837:ARG:CD	2.37	0.52
3:A:446:LEU:HD22	3:A:1149:GLY:C	2.34	0.52
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:62:THR:O	3:A:66:LYS: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:944:GLN:HB3	3:A:948:MET:HE2	1.92	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:245:LEU:HD22	3:A:367:ASP:HA	1.93	0.51
3:A:1005:ASN:N	3:A:1006:PRO:HD3	2.24	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: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:836:GLN:HE21	3:A:886:TRP:CG	2.30	0.50
3:A:303:ARG:HG3	3:A:303:ARG:HH11	1.77	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:706:TRP:O	3:A:707:GLY:C	2.55	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: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
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:778:THR:CG2	3:A:779:ALA:N	2.75	0.48
2:C:1289:C:O2'	3:A:1185:MET:HE3	2.13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:457:THR:C	3:A:491:ILE:HG13	2.38	0.48
3:A:599:LEU:O	3:A:603:MET:HG2	2.14	0.48
3:A:1082:ASP:HB2	3:A:1083:PRO:HD2	1.95	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:1063:MET:HE1	3:A:1229:MET:CE	2.43	0.47
3:A:451:MET:HA	3:A:451:MET:CE	2.34	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:298:GLU:HB2	3:A:311:MET:CE	2.42	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
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:744:THR:C	3:A:746:GLY:H	2.24	0.46
3:A:101:GLU:HG2	3:A:102:LEU:HG	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:537:GLN:O	3:A:647:MET:HE2	2.16	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: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: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: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:1039:MET:HE3	3:A:1039:MET:HB2	1.86	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
3:A:603:MET:CE	3:A:648:ILE:HG23	2.38	0.44
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:A:857:GLY:C	3:A:859:SER:N	2.76	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:286:TYR:C	3:A:288:SER:N	2.71	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:436:MET:HE1	3:A:442:THR:HG21	2.01	0.43
3:A:603:MET:HE1	3:A:651:LEU:HD23	2.00	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:836:GLN:HE21	3:A:886:TRP:CD1	2.36	0.43
3:A:1112:MET:HE3	3:A:1150:LEU:HD21	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:532:ASN:CG	3:A:535:GLN:HG3	2.44	0.42
3:A:1063:MET:HE3	3:A:1063:MET:HB2	1.86	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:CE	3:A:858:GLU:H	2.19	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:697:THR:HG22	3:A:698:MET:HE2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:829:VAL:HG13	3:A:890:TRP:NE1	2.34	0.42
3:A:944:GLN:CD	3:A:944:GLN:H	2.27	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:562:ALA:O	3:A:563:VAL:C	2.63	0.41
3:A:1200:LEU:C	3:A:1200:LEU:HD23	2.45	0.41
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:334:LEU:HD23	3:A:334:LEU:C	2.46	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:855:MET:HE1	3:A:858:GLU:N	2.20	0.41
3:A:906:ILE:O	3:A:907:ARG:C	2.64	0.41
3:A:942:LEU:HD23	3:A:942:LEU:C	2.46	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:372:THR:O	3:A:373:SER:C	2.62	0.41
3:A:528:ILE:HD12	3:A:528:ILE:HA	1.88	0.41
3:A:1245:ILE:O	3:A:1246:HIS:C	2.64	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:863:LEU:HG	3:A:1039:MET:HE2	2.03	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	
3	A	1262/1267 (100%)	1169 (93%)	74 (6%)	19 (2%)	8	16

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 [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
3	A	1081/1083 (100%)	1037 (96%)	44 (4%)	27 53

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	37	PHE
3	A	85	THR
3	A	92	VAL
3	A	107	GLU
3	A	300	LEU
3	A	349	LYS
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	470	LEU
3	A	506	SER
3	A	528	ILE
3	A	536	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	538	VAL
3	A	557	PRO
3	A	610	VAL
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	894	THR
3	A	909	LEU
3	A	920	VAL
3	A	923	ARG
3	A	963	SER
3	A	980	GLN
3	A	984	LEU
3	A	990	ARG
3	A	1045	SER
3	A	1052	LEU
3	A	1063	MET
3	A	1065	GLU
3	A	1077	LEU
3	A	1121	VAL
3	A	1151	GLN
3	A	1176	VAL
3	A	1200	LEU
3	A	1238	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	22	GLN
3	A	121	ASN
3	A	146	GLN
3	A	196	HIS
3	A	283	HIS
3	A	296	ASN
3	A	387	GLN
3	A	439	GLN
3	A	448	GLN
3	A	499	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	504	HIS
3	A	520	GLN
3	A	522	GLN
3	A	536	GLN
3	A	550	ASN
3	A	554	ASN
3	A	646	ASN
3	A	649	GLN
3	A	650	HIS
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	917	ASN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	27,29,29	2.80	6 (22%)	37,45,45	2.69	16 (43%)
5	CH1	A	1295	-	27,29,29	3.01	6 (22%)	37,45,45	2.61	15 (40%)
5	CH1	A	1294	-	27,29,29	2.99	6 (22%)	37,45,45	2.65	16 (43%)

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	-	4/22/34/34	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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1295	CH1	PB-O3B	10.25	1.70	1.59
5	A	1294	CH1	PA-O3A	9.05	1.69	1.59
5	A	1294	CH1	PB-O3B	8.45	1.68	1.59
5	A	1291	CH1	PB-O3B	8.35	1.68	1.59
5	A	1291	CH1	PA-O3A	8.30	1.68	1.59
5	A	1295	CH1	PA-O3A	7.72	1.67	1.59
5	A	1294	CH1	PB-O3A	7.37	1.67	1.59
5	A	1295	CH1	PB-O3A	6.91	1.67	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1291	CH1	PB-O3A	6.33	1.66	1.59
5	A	1294	CH1	C6-C5	2.62	1.41	1.35
5	A	1291	CH1	C6-C5	2.57	1.41	1.35
5	A	1295	CH1	C6-C5	2.44	1.40	1.35
5	A	1294	CH1	PG-O1G	2.25	1.57	1.50
5	A	1295	CH1	PB-O1B	2.08	1.58	1.50
5	A	1294	CH1	PB-O1B	2.06	1.58	1.50
5	A	1295	CH1	PG-O1G	2.01	1.56	1.50
5	A	1291	CH1	PG-O1G	2.01	1.56	1.50
5	A	1291	CH1	PB-O1B	2.00	1.57	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1295	CH1	O3G-PG-O1G	-7.74	80.69	110.83
5	A	1294	CH1	O3G-PG-O1G	-7.45	81.79	110.83
5	A	1291	CH1	O3G-PG-O1G	-7.41	81.95	110.83
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	-5.30	87.92	107.80
5	A	1295	CH1	O3G-PG-O2G	-5.26	88.09	107.80
5	A	1294	CH1	O3G-PG-O2G	-5.25	88.12	107.80
5	A	1294	CH1	O2-C2-N3	-5.15	114.22	122.33
5	A	1291	CH1	O2-C2-N3	-5.11	114.28	122.33
5	A	1295	CH1	O2-C2-N3	-4.96	114.51	122.33
5	A	1294	CH1	C3'-C4'-C5'	-4.11	104.83	113.30
5	A	1291	CH1	C3'-C4'-C5'	-4.03	105.00	113.30
5	A	1291	CH1	O4'-C1'-C2'	-3.94	102.80	106.51
5	A	1294	CH1	O4'-C1'-C2'	-3.80	102.93	106.51
5	A	1295	CH1	C3'-C4'-C5'	-3.78	105.52	113.30
5	A	1291	CH1	O4'-C4'-C5'	3.13	114.98	109.34
5	A	1295	CH1	O4'-C1'-C2'	-2.96	103.73	106.51
5	A	1294	CH1	C6-N1-C2	-2.89	115.57	120.46
5	A	1291	CH1	C6-N1-C2	-2.87	115.62	120.46
5	A	1295	CH1	O4'-C4'-C5'	2.85	114.47	109.34
5	A	1295	CH1	C6-N1-C2	-2.81	115.72	120.46
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	2.69	125.21	111.04
5	A	1294	CH1	O4'-C4'-C5'	2.60	114.03	109.34
5	A	1291	CH1	O2A-PA-O3A	2.56	114.19	107.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1294	CH1	O3B-PG-O1G	2.50	124.21	111.04
5	A	1291	CH1	O3B-PG-O1G	2.46	123.98	111.04
5	A	1291	CH1	O2B-PB-O3B	2.45	113.91	107.27
5	A	1295	CH1	O2G-PG-O3B	2.43	112.80	104.64
5	A	1294	CH1	O2A-PA-O3A	2.42	113.82	107.27
5	A	1295	CH1	O2A-PA-O3A	2.42	113.81	107.27
5	A	1294	CH1	N1-C2-N3	2.39	122.94	118.80
5	A	1295	CH1	O2B-PB-O3B	2.38	113.70	107.27
5	A	1295	CH1	N1-C2-N3	2.35	122.89	118.80
5	A	1291	CH1	N1-C2-N3	2.31	122.81	118.80
5	A	1291	CH1	O4'-C1'-N1	2.30	113.58	108.36
5	A	1294	CH1	O4'-C1'-N1	2.26	113.49	108.36
5	A	1294	CH1	O2B-PB-O3B	2.11	112.97	107.27
5	A	1291	CH1	O2G-PG-O1G	2.08	118.95	110.83
5	A	1295	CH1	O4'-C1'-N1	2.05	113.01	108.36
5	A	1291	CH1	O2-C2-N1	2.05	122.92	118.90
5	A	1294	CH1	O2G-PG-O1G	2.05	118.82	110.83
5	A	1294	CH1	O2-C2-N1	2.01	122.84	118.90
5	A	1295	CH1	O2G-PG-O1G	2.00	118.64	110.83

There are no chirality outliers.

All (18) torsion outliers are listed below:

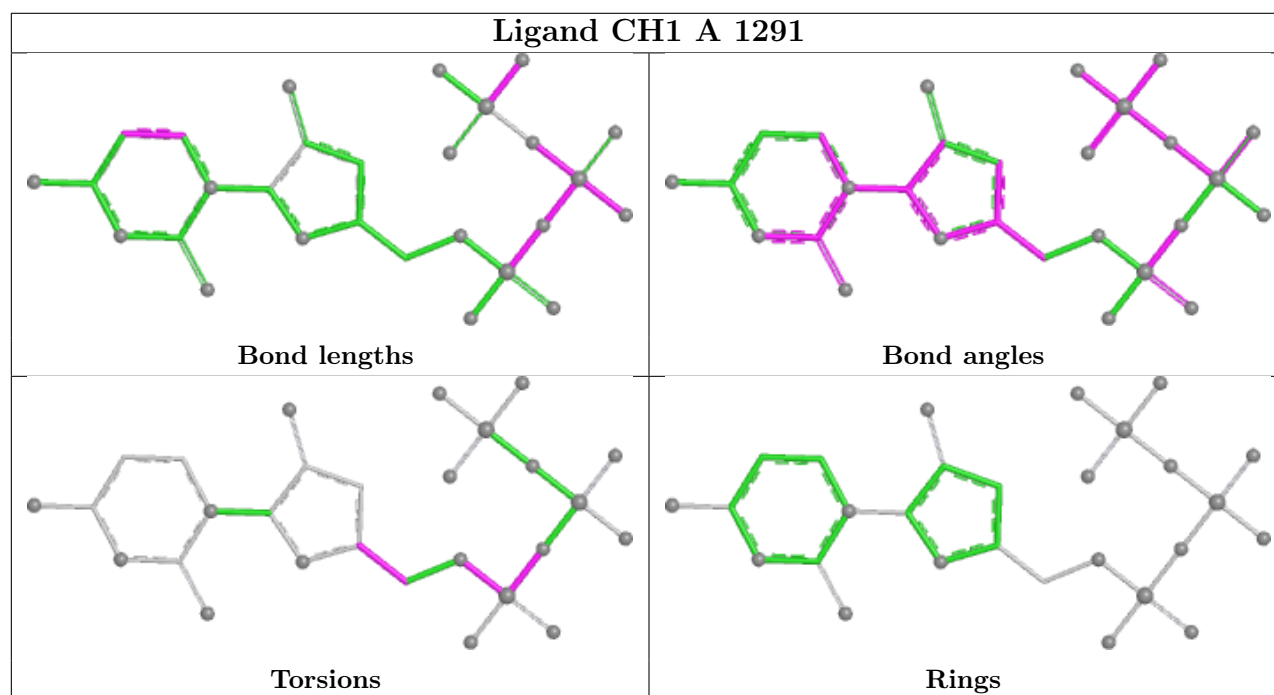
Mol	Chain	Res	Type	Atoms
5	A	1291	CH1	C3'-C4'-C5'-O5'
5	A	1291	CH1	O4'-C4'-C5'-O5'
5	A	1291	CH1	C5'-O5'-PA-O1A
5	A	1294	CH1	C3'-C4'-C5'-O5'
5	A	1294	CH1	O4'-C4'-C5'-O5'
5	A	1294	CH1	C5'-O5'-PA-O2A
5	A	1294	CH1	C5'-O5'-PA-O3A
5	A	1295	CH1	C3'-C4'-C5'-O5'
5	A	1295	CH1	O4'-C4'-C5'-O5'
5	A	1295	CH1	C5'-O5'-PA-O1A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

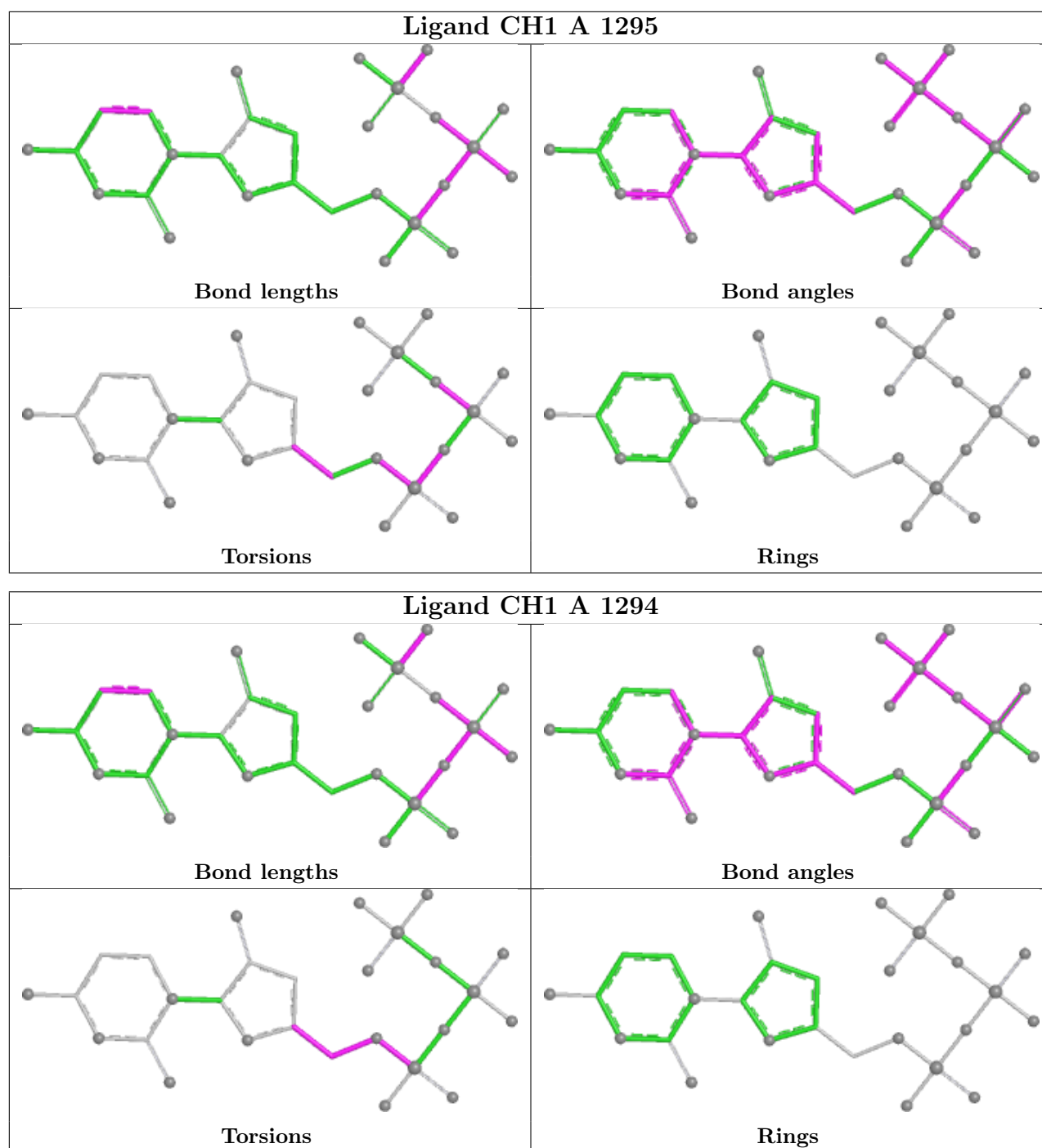
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1291	CH1	2	0
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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	B	5/5 (100%)	3.24	5 (100%) 0 0	108, 119, 124, 124	0
2	C	8/10 (80%)	1.67	3 (37%) 1 1	35, 69, 127, 133	0
3	A	1264/1267 (99%)	-0.06	29 (2%) 61 57	17, 32, 53, 98	0
All	All	1277/1282 (99%)	-0.03	37 (2%) 53 49	17, 32, 54, 133	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	563	VAL	6.3
1	B	1276	G	5.1
2	C	1290	C	5.0
3	A	2	SER	4.8
3	A	211	SER	4.8
3	A	561	SER	4.3
3	A	562	ALA	4.2
3	A	212	ALA	4.2
2	C	1289	C	4.0
3	A	565	GLU	4.0
3	A	856	ILE	3.9
3	A	560	GLY	3.8
3	A	744	THR	3.7
3	A	564	ILE	3.5
3	A	566	LYS	3.5
3	A	633	VAL	3.5
1	B	1275	G	3.4
3	A	213	GLY	3.4
3	A	745	ALA	3.0
3	A	559	SER	2.9
3	A	746	GLY	2.8
3	A	107	GLU	2.7
1	B	1272	G	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1273	G	2.6
3	A	632	VAL	2.6
2	C	1288	C	2.5
3	A	860	VAL	2.5
1	B	1274	G	2.4
3	A	755	ASN	2.3
3	A	557	PRO	2.3
3	A	748	VAL	2.3
3	A	635	VAL	2.3
3	A	393	PRO	2.2
3	A	558	THR	2.2
3	A	743	THR	2.2
3	A	961	ALA	2.1
3	A	634	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

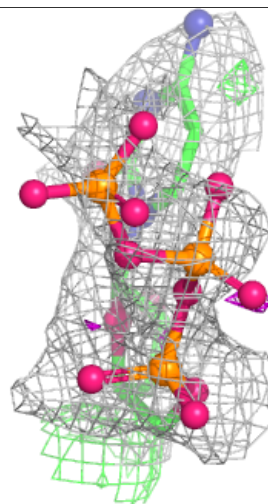
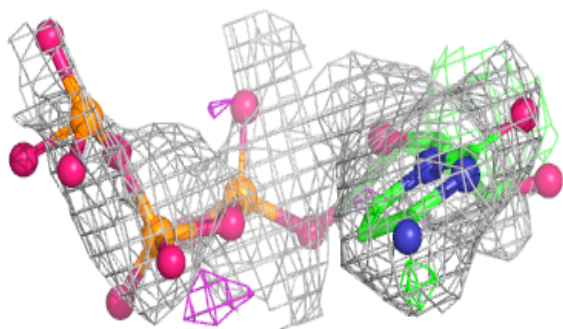
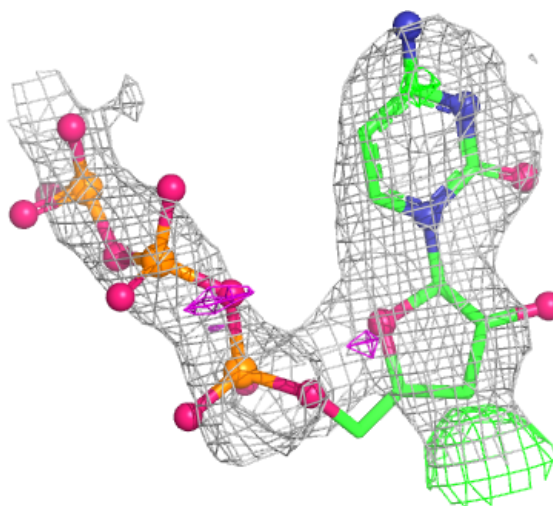
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CH1	A	1294	28/28	0.53	0.18	86,99,118,119	0
5	CH1	A	1291	28/28	0.78	0.17	83,93,100,100	0
5	CH1	A	1295	28/28	0.82	0.14	44,59,81,81	0
4	MN	A	1301	1/1	0.96	0.10	63,63,63,63	0
4	MN	A	1302	1/1	0.97	0.04	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.

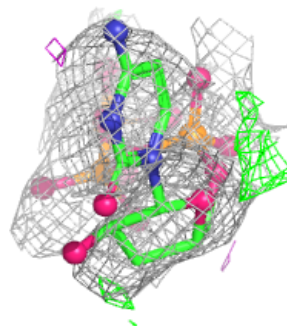
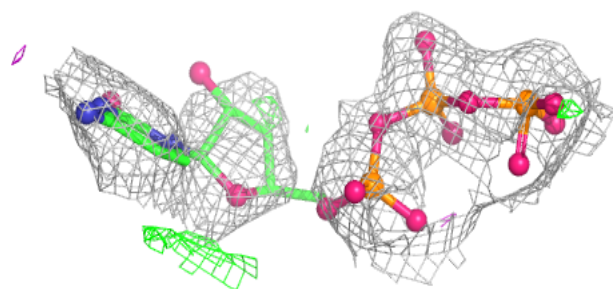
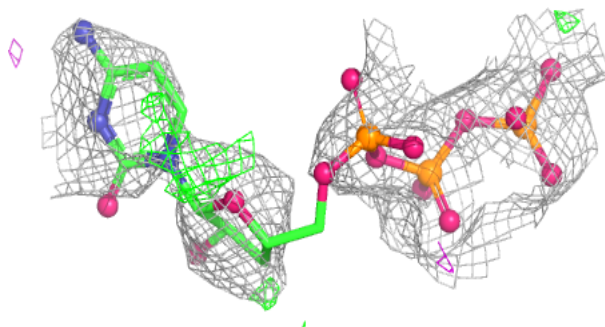
Electron density around CH1 A 1294:

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



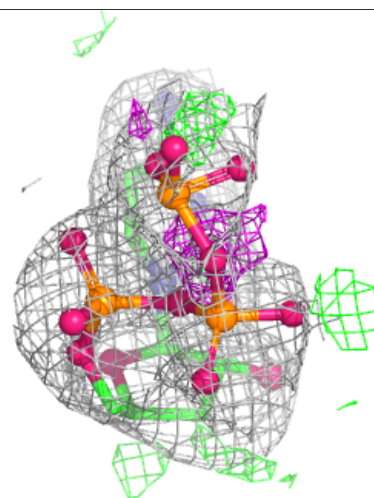
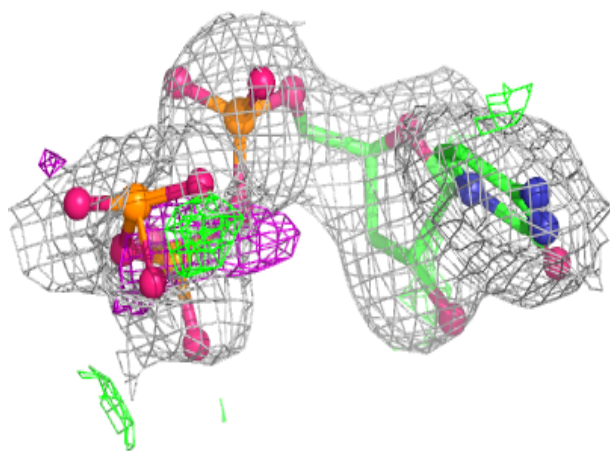
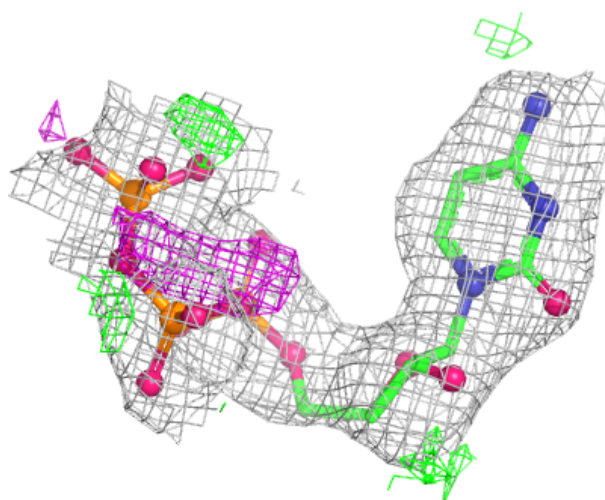
Electron density around CH1 A 1291:

$2mF_o-DF_c$ (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:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.