Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2023 – 02:39 PM EDT

PDB ID	:	3AVY
Title	:	Structure of viral RNA polymerase complex 6
Authors	:	Takeshita, D.; Tomita, K.
Deposited on	:	2011-03-08
Resolution	:	2.62 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:

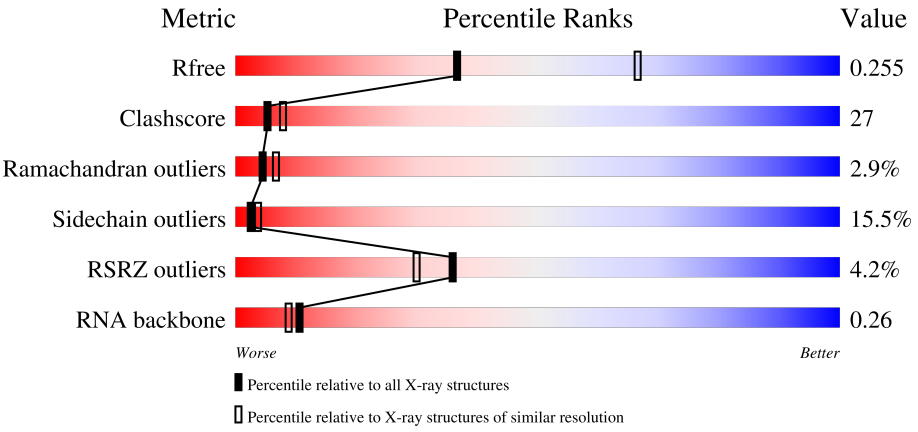
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)
RNA backbone	3102	1062 (2.94-2.30)

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	1289	2% 51% 34% 8% 7%
2	G	13	54% 15% 38% 8% 38%
3	T	18	78% 6% 39% 28% 6% 22%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9871 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 Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1203	9287	5865	1605	1772	45	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	HIS	-	linker	UNP P0A6P3
A	1284	HIS	-	expression tag	UNP Q8LTE0
A	1285	HIS	-	expression tag	UNP Q8LTE0
A	1286	HIS	-	expression tag	UNP Q8LTE0
A	1287	HIS	-	expression tag	UNP Q8LTE0
A	1288	HIS	-	expression tag	UNP Q8LTE0
A	1289	HIS	-	expression tag	UNP Q8LTE0

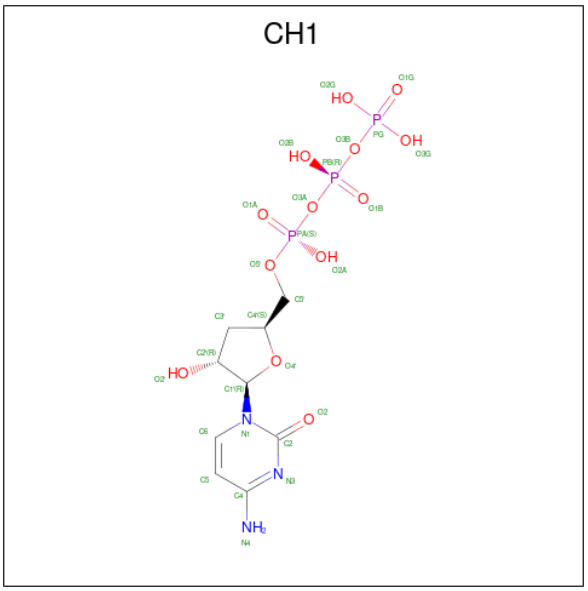
- Molecule 2 is a RNA chain called RNA (5'-R(*GP*GP*GP*UP*CP*CP*AP*UP*AP*AP*AP*AP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	G	8	169	77	32	52	8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	T	14	297	133	51	99	14	0	0	0

- Molecule 4 is 3'-DEOXY-CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CH1) (formula: $C_9H_{16}N_3O_{13}P_3$).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Ca 2 2	0	0

- Molecule 6 is water.

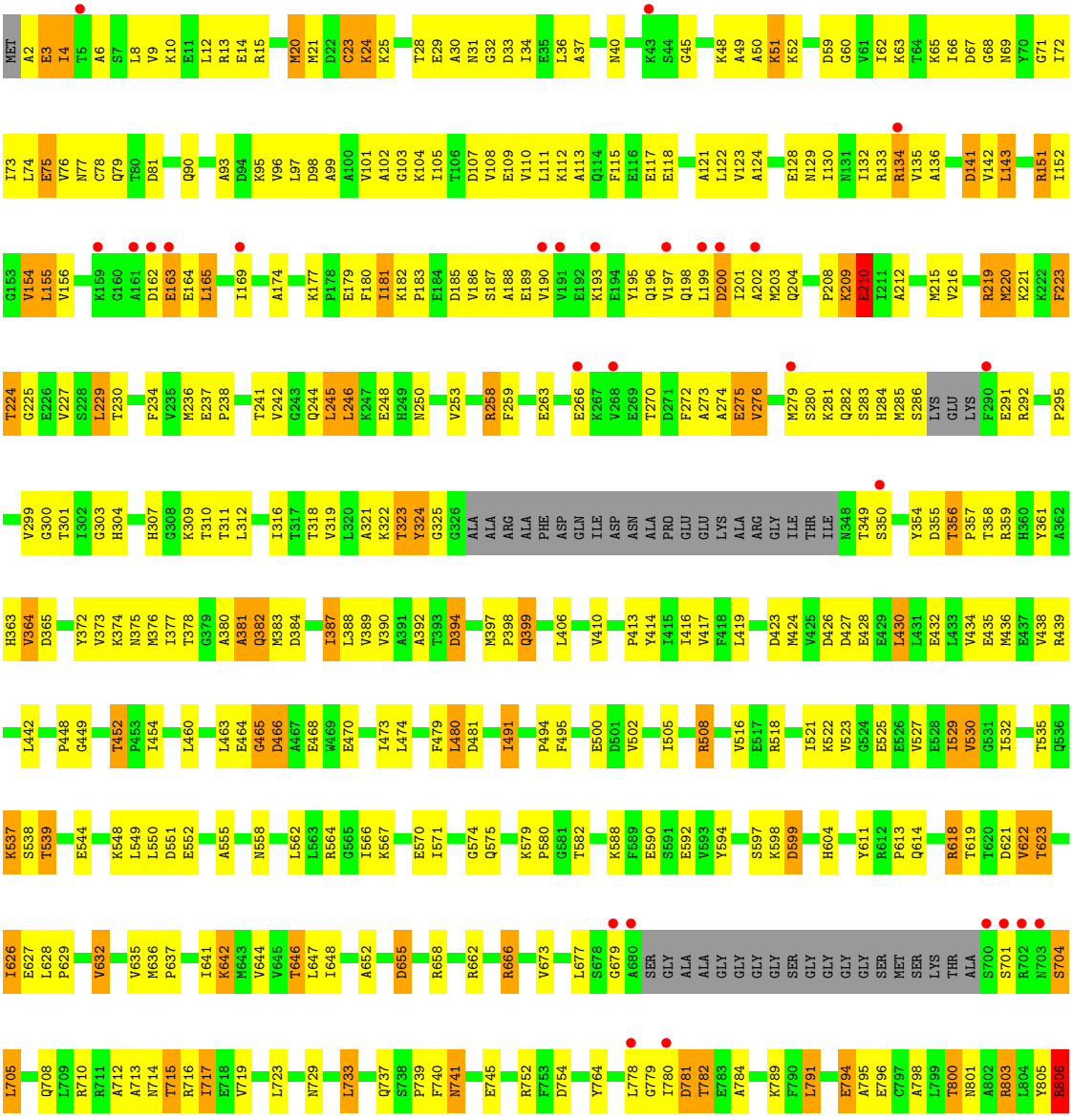
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	85	Total O 85 85	0	0
6	T	3	Total O 3 3	0	0

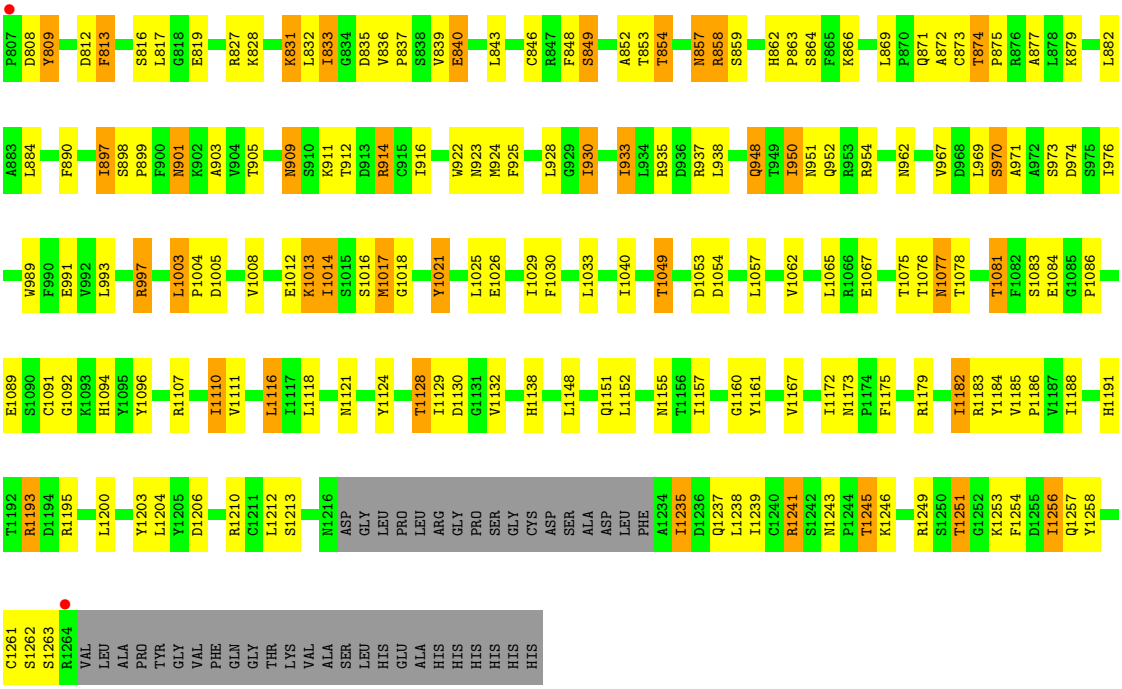
3 Residue-property plots (i)

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.

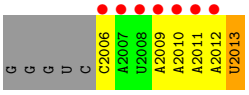
• Molecule 1: Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase

Chain A:

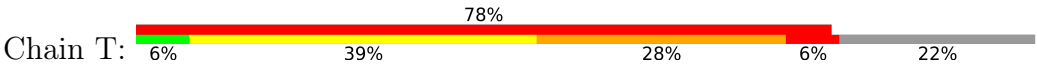


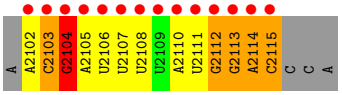


• Molecule 2: RNA (5'-R(*GP*GP*GP*UP*CP*CP*AP*UP*AP*AP*AP*AP*U)-3')



• Molecule 3: RNA (5'-R(*AP*AP*CP*GP*AP*UP*UP*UP*UP*AP*UP*GP*GP*AP*CP*CP *CP*A)-3')





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	140.07Å 257.22Å 101.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.62 48.29 – 2.61	Depositor EDS
% Data completeness (in resolution range)	97.3 (19.99-2.62) 99.4 (48.29-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.214 , 0.262 0.212 , 0.255	Depositor DCC
R_{free} test set	2812 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.022 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9871	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	A	0.48	0/9456	0.63	0/12787
2	G	0.50	0/189	0.80	1/291 (0.3%)
3	T	0.59	0/331	0.92	1/513 (0.2%)
All	All	0.49	0/9976	0.64	2/13591 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	2013	U	O4'-C1'-N1	5.40	112.52	108.20
3	T	2104	G	C8-N9-C4	-5.34	104.26	106.40

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	A	9287	0	9273	492	0
2	G	169	0	85	12	0
3	T	297	0	150	32	0
4	A	28	0	12	6	0
5	A	2	0	0	0	0
6	A	85	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	3	0	0	0	0
All	All	9871	0	9520	512	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 27.

All (512) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:ILE:HD11	1:A:1021:TYR:HD1	1.13	1.12
1:A:858:ARG:HG3	1:A:858:ARG:HH11	1.15	1.08
1:A:930:ILE:HD11	1:A:1021:TYR:CD1	1.87	1.07
3:T:2104:G:H2'	3:T:2105:A:C8	1.93	1.03
1:A:79:GLN:HE21	1:A:129:ASN:H	1.03	0.94
1:A:954:ARG:NH1	1:A:1049:THR:HB	1.82	0.93
1:A:21:MET:HA	1:A:21:MET:HE2	1.50	0.93
1:A:399:GLN:H	1:A:399:GLN:HE21	1.17	0.93
1:A:79:GLN:NE2	1:A:129:ASN:H	1.70	0.90
1:A:280:SER:O	1:A:284:HIS:HB2	1.74	0.88
1:A:1092:GLY:HA3	2:G:2012:A:H5"	1.54	0.87
1:A:163:GLU:CD	1:A:163:GLU:H	1.76	0.87
1:A:79:GLN:HE21	1:A:129:ASN:N	1.75	0.84
1:A:1193:ARG:HD3	1:A:1249:ARG:HH21	1.43	0.84
1:A:916:ILE:HD12	3:T:2104:G:H1'	1.58	0.83
1:A:51:LYS:H	1:A:51:LYS:HD2	1.44	0.83
1:A:372:TYR:HE1	1:A:410:VAL:HG11	1.44	0.83
1:A:28:THR:HG23	1:A:29:GLU:HG3	1.61	0.82
1:A:419:LEU:HD11	1:A:434:VAL:HG11	1.60	0.81
1:A:98:ASP:O	1:A:101:VAL:HG12	1.79	0.81
1:A:614:GLN:HE21	1:A:621:ASP:HB3	1.42	0.81
1:A:382:GLN:H	1:A:382:GLN:HE21	1.27	0.80
1:A:714:ASN:HD21	1:A:1254:PHE:H	1.28	0.80
1:A:1160:GLY:O	3:T:2110:A:H4'	1.82	0.80
1:A:105:ILE:HD12	1:A:111:LEU:HD13	1.65	0.79
1:A:779:GLY:C	1:A:781:ASP:H	1.85	0.79
1:A:618:ARG:HH21	1:A:618:ARG:HG3	1.46	0.78
1:A:858:ARG:N	3:T:2103:C:OP1	2.16	0.78
1:A:967:VAL:HA	1:A:1081:THR:HB	1.66	0.78
1:A:1110:ILE:HD12	1:A:1116:LEU:HA	1.66	0.77
1:A:705:LEU:HD11	1:A:1175:PHE:HD2	1.49	0.77
1:A:1121:ASN:HD21	1:A:1167:VAL:H	1.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:ARG:HH11	1:A:1049:THR:HB	1.48	0.77
3:T:2114:A:H5'	3:T:2115:C:OP2	1.84	0.77
1:A:729:ASN:ND2	1:A:740:PHE:H	1.82	0.76
1:A:796:GLU:O	1:A:800:THR:HG23	1.85	0.76
1:A:618:ARG:HH21	1:A:618:ARG:CG	1.99	0.76
1:A:853:THR:HG23	1:A:866:LYS:HE2	1.69	0.75
1:A:300:GLY:HA3	1:A:383:MET:SD	2.27	0.75
1:A:951:ASN:OD1	1:A:1049:THR:HG23	1.87	0.75
1:A:180:PHE:CD2	1:A:186:VAL:HG12	2.22	0.74
1:A:37:ALA:HA	1:A:40:ASN:ND2	2.02	0.74
1:A:848:PHE:O	1:A:849:SER:C	2.25	0.74
1:A:1235:ILE:H	1:A:1235:ILE:HD12	1.53	0.73
1:A:1246:LYS:HG2	3:T:2113:G:O2'	1.89	0.73
1:A:705:LEU:HD11	1:A:1175:PHE:CD2	2.24	0.73
1:A:1245:THR:O	1:A:1246:LYS:HD3	1.89	0.72
1:A:392:ALA:HB2	1:A:419:LEU:HD12	1.70	0.72
1:A:244:GLN:O	1:A:248:GLU:HG3	1.89	0.72
1:A:1092:GLY:CA	2:G:2012:A:H5"	2.19	0.71
1:A:103:GLY:O	1:A:105:ILE:HG13	1.90	0.71
1:A:72:ILE:HG13	1:A:136:ALA:O	1.89	0.71
1:A:502:VAL:HG11	1:A:571:ILE:HB	1.73	0.71
1:A:604:HIS:CE1	1:A:1262:SER:HB3	2.25	0.71
1:A:567:LYS:HG3	1:A:570:GLU:OE1	1.91	0.71
1:A:49:ALA:O	1:A:52:LYS:HB2	1.91	0.70
1:A:73:ILE:HB	1:A:155:LEU:CD2	2.22	0.70
1:A:442:LEU:HD13	1:A:452:THR:HG21	1.73	0.70
1:A:187:SER:C	1:A:189:GLU:H	1.95	0.69
1:A:272:PHE:O	1:A:276:VAL:HG12	1.91	0.69
1:A:382:GLN:H	1:A:382:GLN:NE2	1.91	0.69
1:A:63:LYS:NZ	1:A:90:GLN:HE22	1.89	0.69
1:A:324:TYR:CD1	1:A:357:PRO:HD3	2.26	0.69
1:A:210:GLU:CD	1:A:210:GLU:H	1.97	0.69
1:A:101:VAL:HG13	1:A:102:ALA:H	1.58	0.68
1:A:618:ARG:HG3	1:A:618:ARG:NH2	2.08	0.68
1:A:950:ILE:HD13	1:A:951:ASN:N	2.08	0.68
1:A:729:ASN:HD21	1:A:740:PHE:H	1.40	0.68
1:A:1110:ILE:HD12	1:A:1116:LEU:CA	2.24	0.68
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.59	0.67
1:A:399:GLN:H	1:A:399:GLN:NE2	1.91	0.67
1:A:494:PRO:HB2	1:A:582:THR:HG21	1.75	0.67
1:A:101:VAL:HG13	1:A:102:ALA:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:GLU:HB3	1:A:549:LEU:HD23	1.76	0.67
1:A:779:GLY:C	1:A:781:ASP:N	2.48	0.67
1:A:1124:TYR:O	1:A:1128:THR:HB	1.94	0.67
1:A:574:GLY:HA2	1:A:619:THR:CG2	2.25	0.67
1:A:151:ARG:HG2	1:A:151:ARG:NH1	2.10	0.67
1:A:212:ALA:O	1:A:216:VAL:HG23	1.94	0.67
1:A:862:HIS:HD2	1:A:864:SER:H	1.43	0.66
1:A:238:PRO:HG2	1:A:1183:ARG:HH11	1.60	0.66
1:A:655:ASP:HA	1:A:673:VAL:HG23	1.75	0.66
1:A:200:ASP:HB3	1:A:204:GLN:HE21	1.60	0.66
1:A:909:ASN:HD22	1:A:911:LYS:H	1.43	0.66
1:A:1193:ARG:HD3	1:A:1249:ARG:NH2	2.11	0.65
1:A:198:GLN:HA	1:A:201:ILE:HG12	1.78	0.65
1:A:858:ARG:HG3	1:A:858:ARG:NH1	1.91	0.65
1:A:494:PRO:CB	1:A:582:THR:HG21	2.27	0.65
1:A:1110:ILE:HD11	1:A:1116:LEU:HG	1.78	0.65
1:A:522:LYS:HE3	1:A:552:GLU:OE1	1.97	0.65
2:G:2012:A:H2	3:T:2106:U:H3	1.45	0.64
1:A:862:HIS:CE1	3:T:2113:G:H22	2.15	0.64
1:A:373:VAL:O	1:A:377:ILE:HG12	1.98	0.64
1:A:901:ASN:C	1:A:901:ASN:HD22	1.99	0.64
1:A:897:ILE:HD13	1:A:897:ILE:C	2.18	0.64
1:A:874:THR:HG21	6:A:3508:HOH:O	1.97	0.64
1:A:801:ASN:HD22	1:A:1012:GLU:HG3	1.63	0.63
1:A:588:LYS:HG3	1:A:646:THR:HB	1.79	0.63
1:A:618:ARG:HD2	1:A:618:ARG:N	2.14	0.63
1:A:112:LYS:O	1:A:112:LYS:HG2	1.99	0.63
1:A:592:GLU:OE2	1:A:642:LYS:HG3	1.99	0.63
1:A:1017:MET:HB2	4:A:2501:CH1:C4	2.29	0.63
1:A:574:GLY:HA2	1:A:619:THR:HG23	1.81	0.63
1:A:857:ASN:HD22	1:A:857:ASN:C	2.02	0.62
1:A:63:LYS:HZ3	1:A:90:GLN:HE22	1.46	0.62
1:A:713:ALA:HB2	1:A:1188:ILE:HD12	1.81	0.62
3:T:2102:A:O2'	3:T:2103:C:OP2	2.16	0.62
1:A:789:LYS:NZ	1:A:912:THR:HG21	2.14	0.62
1:A:1017:MET:HB2	4:A:2501:CH1:N3	2.15	0.62
1:A:714:ASN:ND2	1:A:1254:PHE:H	1.97	0.62
1:A:1121:ASN:ND2	1:A:1167:VAL:H	1.98	0.61
1:A:187:SER:O	1:A:189:GLU:N	2.32	0.61
1:A:73:ILE:HB	1:A:155:LEU:HD22	1.83	0.61
1:A:833:ILE:HG23	1:A:989:TRP:NE1	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:GLN:HE21	1:A:382:GLN:N	1.97	0.61
1:A:529:ILE:HD11	1:A:575:GLN:NE2	2.14	0.61
1:A:162:ASP:HB2	1:A:163:GLU:OE2	2.01	0.61
1:A:516:VAL:HG22	1:A:555:ALA:HA	1.82	0.61
1:A:764:TYR:OH	1:A:1094:HIS:HD2	1.84	0.61
1:A:372:TYR:CE1	1:A:410:VAL:HG11	2.30	0.61
3:T:2110:A:H2'	3:T:2111:U:C6	2.35	0.61
1:A:948:GLN:O	1:A:952:GLN:HG3	2.00	0.61
1:A:33:ASP:HB2	1:A:36:LEU:HD23	1.83	0.60
1:A:1186:PRO:HG3	1:A:1258:TYR:CE2	2.36	0.60
1:A:1182:ILE:HG13	1:A:1184:TYR:CE2	2.36	0.60
1:A:4:ILE:HD12	1:A:4:ILE:H	1.66	0.60
1:A:794:GLU:HA	1:A:794:GLU:OE1	2.01	0.60
1:A:238:PRO:HG2	1:A:1183:ARG:NH1	2.17	0.60
1:A:384:ASP:O	1:A:413:PRO:HG2	2.01	0.60
3:T:2104:G:H2'	3:T:2105:A:N7	2.15	0.60
1:A:712:ALA:O	1:A:715:THR:HB	2.02	0.60
1:A:20:MET:HE3	1:A:20:MET:HA	1.83	0.60
1:A:165:LEU:O	1:A:169:ILE:HG12	2.02	0.60
1:A:598:LYS:HG2	1:A:604:HIS:HA	1.84	0.60
1:A:909:ASN:HD22	1:A:909:ASN:C	2.04	0.60
1:A:181:ILE:CD1	1:A:253:VAL:HB	2.32	0.59
1:A:356:THR:HG22	1:A:358:THR:H	1.66	0.59
1:A:523:VAL:HG13	1:A:551:ASP:O	2.02	0.59
1:A:183:PRO:HD3	1:A:230:THR:HB	1.84	0.59
1:A:1155:ASN:ND2	1:A:1173:ASN:HD21	1.98	0.59
1:A:187:SER:HB3	1:A:190:VAL:HB	1.84	0.59
1:A:618:ARG:HD2	1:A:618:ARG:H	1.66	0.59
1:A:2:ALA:O	1:A:3:GLU:HB2	2.03	0.59
1:A:375:ASN:HA	1:A:378:THR:HG22	1.84	0.59
1:A:622:VAL:HG22	1:A:647:LEU:HD22	1.84	0.59
1:A:849:SER:HA	1:A:863:PRO:HG3	1.84	0.59
1:A:21:MET:HA	1:A:21:MET:CE	2.31	0.59
1:A:558:ASN:HB3	1:A:1210:ARG:HD3	1.85	0.58
1:A:862:HIS:HE1	3:T:2113:G:H22	1.50	0.58
1:A:1193:ARG:NH2	1:A:1249:ARG:HE	2.01	0.58
1:A:316:ILE:HD13	1:A:473:ILE:HG23	1.84	0.58
4:A:2501:CH1:H4'	2:G:2013:U:O2'	2.03	0.58
1:A:51:LYS:HD2	1:A:51:LYS:N	2.17	0.58
1:A:399:GLN:HE21	1:A:399:GLN:N	1.94	0.58
1:A:273:ALA:O	1:A:276:VAL:HG13	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLU:CD	1:A:1241:ARG:HD3	2.24	0.58
1:A:380:ALA:O	1:A:381:ALA:HB2	2.03	0.58
1:A:65:LYS:HB2	1:A:97:LEU:HD11	1.84	0.58
1:A:539:THR:HG23	1:A:564:ARG:HB3	1.86	0.58
1:A:836:VAL:HG22	1:A:837:PRO:HD2	1.86	0.58
1:A:1239:ILE:HG22	1:A:1239:ILE:O	2.03	0.58
1:A:301:THR:CG2	1:A:365:ASP:HA	2.34	0.58
1:A:862:HIS:CD2	1:A:864:SER:H	2.22	0.58
1:A:77:ASN:HD21	1:A:133:ARG:HD2	1.68	0.57
1:A:394:ASP:HB3	1:A:397:MET:HE1	1.85	0.57
1:A:950:ILE:O	1:A:954:ARG:HG3	2.05	0.57
1:A:914:ARG:O	1:A:914:ARG:HG3	2.03	0.57
1:A:530:VAL:HG22	1:A:652:ALA:HB2	1.86	0.57
1:A:227:VAL:HG22	1:A:227:VAL:O	2.05	0.56
1:A:387:ILE:HD11	1:A:389:VAL:HG12	1.86	0.56
1:A:219:ARG:O	1:A:219:ARG:HD3	2.04	0.56
1:A:448:PRO:O	1:A:452:THR:HG22	2.05	0.56
1:A:611:TYR:HB3	1:A:626:ILE:HD11	1.87	0.56
1:A:8:LEU:HD11	1:A:10:LYS:HE2	1.87	0.56
1:A:562:LEU:N	1:A:562:LEU:HD12	2.20	0.56
1:A:875:PRO:HA	1:A:897:ILE:HD11	1.86	0.56
1:A:4:ILE:HB	1:A:6:ALA:O	2.06	0.56
1:A:529:ILE:HD11	1:A:575:GLN:CD	2.25	0.56
1:A:741:ASN:OD1	1:A:745:GLU:HB2	2.05	0.56
1:A:874:THR:HB	1:A:923:ASN:HD21	1.71	0.56
1:A:954:ARG:HH11	1:A:1049:THR:CB	2.17	0.56
1:A:1077:ASN:C	1:A:1077:ASN:HD22	2.09	0.56
1:A:122:LEU:HD23	1:A:130:ILE:HD12	1.87	0.56
1:A:463:LEU:HD12	1:A:464:GLU:N	2.20	0.56
1:A:812:ASP:O	1:A:813:PHE:HD1	1.88	0.56
1:A:1193:ARG:HH21	1:A:1249:ARG:HE	1.54	0.56
1:A:181:ILE:HD13	1:A:253:VAL:HB	1.86	0.56
1:A:163:GLU:HG2	1:A:164:GLU:H	1.71	0.56
1:A:413:PRO:HB2	1:A:414:TYR:CD1	2.40	0.56
1:A:909:ASN:ND2	1:A:911:LYS:H	2.02	0.55
1:A:134:ARG:HD3	1:A:259:PHE:CE2	2.40	0.55
1:A:292:ARG:HD2	1:A:292:ARG:N	2.21	0.55
1:A:460:LEU:HD23	1:A:463:LEU:HD11	1.88	0.55
1:A:930:ILE:HA	1:A:933:ILE:HG23	1.88	0.55
1:A:997:ARG:HD2	1:A:1014:ILE:O	2.06	0.55
1:A:151:ARG:HH11	1:A:151:ARG:CG	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:ILE:O	1:A:897:ILE:HG23	2.07	0.55
1:A:874:THR:HG22	1:A:877:ALA:H	1.71	0.55
1:A:210:GLU:CD	1:A:210:GLU:N	2.60	0.55
1:A:666:ARG:HE	1:A:666:ARG:HA	1.71	0.55
1:A:318:THR:O	1:A:321:ALA:HB3	2.07	0.55
1:A:285:MET:O	1:A:286:SER:HB2	2.07	0.55
1:A:658:ARG:HH21	1:A:658:ARG:HG3	1.72	0.55
1:A:234:PHE:CE1	1:A:236:MET:HB2	2.42	0.54
1:A:187:SER:C	1:A:189:GLU:N	2.61	0.54
1:A:9:VAL:CG1	1:A:23:CYS:HB3	2.37	0.54
1:A:764:TYR:OH	1:A:1094:HIS:CD2	2.60	0.54
1:A:195:TYR:HB2	1:A:220:MET:CE	2.37	0.54
2:G:2011:A:H2'	2:G:2012:A:H5'	1.90	0.54
1:A:299:VAL:O	1:A:363:HIS:HA	2.08	0.54
1:A:951:ASN:OD1	1:A:1049:THR:CG2	2.53	0.54
1:A:442:LEU:CD1	1:A:452:THR:HG21	2.38	0.54
1:A:465:GLY:O	1:A:466:ASP:HB2	2.08	0.54
1:A:4:ILE:C	1:A:6:ALA:H	2.12	0.53
1:A:245:LEU:O	1:A:245:LEU:HD22	2.09	0.53
1:A:279:MET:C	1:A:281:LYS:H	2.12	0.53
1:A:295:PRO:HG2	1:A:359:ARG:HG2	1.90	0.53
1:A:377:ILE:CD1	1:A:592:GLU:HB2	2.38	0.53
1:A:833:ILE:HG23	1:A:989:TRP:CE2	2.44	0.53
1:A:857:ASN:HD21	1:A:859:SER:HB2	1.72	0.53
1:A:1155:ASN:HD22	1:A:1173:ASN:HD21	1.57	0.53
1:A:1062:VAL:HG21	1:A:1083:SER:HB3	1.89	0.53
1:A:133:ARG:NH2	1:A:263:GLU:O	2.30	0.53
1:A:717:ILE:HD11	1:A:723:LEU:HD22	1.90	0.53
1:A:971:ALA:HB1	1:A:974:ASP:HB2	1.90	0.53
1:A:1026:GLU:OE1	4:A:2501:CH1:H3'	2.08	0.53
1:A:221:LYS:O	1:A:224:THR:HG22	2.09	0.53
1:A:924:MET:HE3	1:A:928:LEU:HG	1.91	0.53
1:A:1025:LEU:O	1:A:1029:ILE:HG12	2.08	0.53
3:T:2105:A:O2'	3:T:2106:U:H5'	2.09	0.53
1:A:387:ILE:HD12	1:A:388:LEU:N	2.24	0.53
1:A:423:ASP:OD2	1:A:424:MET:HG2	2.08	0.53
1:A:604:HIS:HE1	1:A:1262:SER:HB3	1.74	0.53
1:A:954:ARG:HH12	1:A:1049:THR:HB	1.70	0.53
1:A:36:LEU:HG	1:A:40:ASN:HD21	1.75	0.52
1:A:281:LYS:C	1:A:283:SER:H	2.13	0.52
1:A:199:LEU:HD23	1:A:203:MET:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:ALA:HA	1:A:1012:GLU:HG2	1.91	0.52
1:A:174:ALA:O	1:A:258:ARG:NH1	2.42	0.52
1:A:229:LEU:HD22	1:A:242:VAL:HG11	1.92	0.52
1:A:590:GLU:HG3	1:A:677:LEU:HD11	1.91	0.52
1:A:840:GLU:H	1:A:840:GLU:CD	2.13	0.52
1:A:199:LEU:CD2	1:A:203:MET:HG3	2.39	0.52
1:A:933:ILE:HG12	1:A:989:TRP:HH2	1.74	0.52
1:A:805:TYR:O	1:A:806:ARG:HB2	2.09	0.51
1:A:1182:ILE:HD12	1:A:1183:ARG:N	2.26	0.51
1:A:374:LYS:HE3	1:A:594:TYR:CZ	2.45	0.51
1:A:417:VAL:HB	1:A:454:ILE:HG12	1.93	0.51
1:A:154:VAL:HG12	1:A:258:ARG:HB2	1.91	0.51
1:A:890:PHE:CG	1:A:1204:LEU:HD21	2.46	0.51
1:A:323:THR:HG22	1:A:324:TYR:CD2	2.45	0.51
1:A:387:ILE:HD12	1:A:387:ILE:C	2.31	0.51
1:A:410:VAL:O	1:A:410:VAL:CG1	2.59	0.51
1:A:897:ILE:C	1:A:897:ILE:CD1	2.79	0.51
1:A:701:SER:OG	1:A:1179:ARG:NH1	2.43	0.51
1:A:394:ASP:HB3	1:A:397:MET:CE	2.41	0.51
1:A:101:VAL:CG1	1:A:102:ALA:H	2.22	0.50
1:A:323:THR:HG22	1:A:324:TYR:N	2.25	0.50
1:A:419:LEU:HD23	1:A:454:ILE:CG2	2.41	0.50
1:A:74:LEU:HD21	1:A:96:VAL:HG13	1.92	0.50
1:A:215:MET:O	1:A:219:ARG:HB2	2.10	0.50
1:A:272:PHE:HE1	1:A:310:THR:HG22	1.74	0.50
1:A:789:LYS:HZ2	1:A:912:THR:HG21	1.76	0.50
1:A:143:LEU:HB2	1:A:156:VAL:O	2.11	0.50
1:A:719:VAL:HG21	1:A:723:LEU:HB2	1.92	0.50
1:A:62:ILE:HG12	1:A:75:GLU:HG2	1.93	0.50
1:A:180:PHE:CE2	1:A:186:VAL:HG12	2.46	0.50
1:A:435:GLU:O	1:A:439:ARG:HG3	2.12	0.50
1:A:4:ILE:HG12	1:A:24:LYS:HD2	1.93	0.50
1:A:163:GLU:CD	1:A:163:GLU:N	2.54	0.50
1:A:854:THR:HG21	1:A:872:ALA:HB3	1.94	0.50
1:A:1092:GLY:HA3	2:G:2012:A:C5'	2.34	0.50
1:A:301:THR:HB	1:A:363:HIS:NE2	2.27	0.50
1:A:1257:GLN:HE22	3:T:2112:G:H4'	1.77	0.50
4:A:2501:CH1:C5'	2:G:2013:U:H2'	2.42	0.49
1:A:272:PHE:CE1	1:A:310:THR:HG22	2.48	0.49
1:A:976:ILE:HD11	1:A:1026:GLU:HG2	1.94	0.49
1:A:715:THR:HG23	1:A:716:ARG:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:ARG:HH22	3:T:2114:A:H2'	1.78	0.49
1:A:1246:LYS:HG2	3:T:2113:G:HO2'	1.78	0.49
1:A:312:LEU:O	1:A:316:ILE:HG12	2.12	0.49
1:A:356:THR:HG21	1:A:481:ASP:CG	2.33	0.49
1:A:494:PRO:CG	1:A:582:THR:HG21	2.43	0.49
1:A:710:ARG:HA	1:A:1256:ILE:HD13	1.95	0.49
1:A:741:ASN:OD1	1:A:745:GLU:CB	2.61	0.49
1:A:60:GLY:HA2	1:A:78:CYS:SG	2.53	0.48
1:A:389:VAL:HG23	1:A:389:VAL:O	2.11	0.48
1:A:508:ARG:NH1	1:A:544:GLU:OE1	2.46	0.48
1:A:229:LEU:CD2	1:A:242:VAL:HG11	2.43	0.48
1:A:1118:LEU:HD21	2:G:2010:A:H5"	1.96	0.48
1:A:128:GLU:O	1:A:130:ILE:HG13	2.13	0.48
1:A:449:GLY:O	1:A:452:THR:HG23	2.13	0.48
1:A:93:ALA:HA	1:A:96:VAL:HG12	1.94	0.48
1:A:733:LEU:HD11	1:A:739:PRO:HD3	1.95	0.48
1:A:177:LYS:HB3	1:A:258:ARG:CZ	2.44	0.48
1:A:1206:ASP:OD1	1:A:1210:ARG:NH2	2.46	0.48
1:A:122:LEU:HD23	1:A:130:ILE:CD1	2.43	0.48
1:A:301:THR:HG23	1:A:365:ASP:OD2	2.13	0.48
1:A:529:ILE:HD13	1:A:529:ILE:O	2.14	0.48
1:A:1003:LEU:HB3	1:A:1004:PRO:HD2	1.95	0.48
1:A:1017:MET:SD	1:A:1017:MET:N	2.81	0.48
1:A:4:ILE:HD12	1:A:4:ILE:N	2.29	0.48
1:A:798:ALA:CA	1:A:1012:GLU:HG2	2.43	0.48
1:A:1086:PRO:HG2	1:A:1096:TYR:CE1	2.48	0.48
1:A:103:GLY:O	1:A:105:ILE:N	2.47	0.48
1:A:356:THR:HG22	1:A:359:ARG:H	1.79	0.48
1:A:948:GLN:HE21	1:A:1091:CYS:HB3	1.78	0.48
1:A:1128:THR:O	1:A:1128:THR:HG22	2.14	0.48
1:A:21:MET:HE1	1:A:430:LEU:HD23	1.96	0.47
1:A:203:MET:SD	1:A:209:LYS:HA	2.53	0.47
1:A:181:ILE:HG23	1:A:185:ASP:OD1	2.14	0.47
1:A:828:LYS:O	1:A:831:LYS:HG3	2.14	0.47
1:A:1157:ILE:HG22	1:A:1185:VAL:HG21	1.96	0.47
1:A:1191:HIS:HD2	1:A:1251:THR:OG1	1.97	0.47
1:A:20:MET:HA	1:A:20:MET:CE	2.42	0.47
1:A:141:ASP:O	1:A:142:VAL:HG23	2.14	0.47
1:A:187:SER:O	1:A:190:VAL:HG12	2.14	0.47
1:A:924:MET:CE	1:A:928:LEU:HG	2.45	0.47
1:A:195:TYR:HB2	1:A:220:MET:HE3	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLY:CA	1:A:383:MET:SD	3.00	0.47
1:A:636:MET:O	1:A:637:PRO:C	2.53	0.47
1:A:733:LEU:CD1	1:A:739:PRO:HD3	2.45	0.47
1:A:416:ILE:HD13	1:A:479:PHE:HB3	1.96	0.47
1:A:537:LYS:HB3	1:A:537:LYS:HE2	1.67	0.47
1:A:852:ALA:HB3	3:T:2104:G:H5"	1.96	0.47
1:A:862:HIS:HD2	1:A:864:SER:OG	1.98	0.47
1:A:1243:ASN:HB2	3:T:2113:G:N7	2.29	0.47
1:A:4:ILE:HG22	1:A:6:ALA:N	2.30	0.46
1:A:189:GLU:HA	1:A:189:GLU:OE1	2.14	0.46
1:A:301:THR:HG22	1:A:365:ASP:HA	1.97	0.46
1:A:618:ARG:HH21	1:A:618:ARG:CB	2.28	0.46
1:A:909:ASN:HD22	1:A:911:LYS:N	2.12	0.46
1:A:1057:LEU:N	1:A:1057:LEU:HD23	2.31	0.46
1:A:51:LYS:H	1:A:51:LYS:CD	2.20	0.46
1:A:181:ILE:HG13	1:A:182:LYS:HG3	1.98	0.46
1:A:372:TYR:CE1	1:A:410:VAL:HG21	2.51	0.46
1:A:279:MET:SD	1:A:311:THR:HG22	2.55	0.46
1:A:9:VAL:HG11	1:A:23:CYS:HB3	1.97	0.46
1:A:522:LYS:HB2	1:A:525:GLU:OE2	2.15	0.46
1:A:538:SER:OG	1:A:539:THR:N	2.49	0.46
1:A:1161:TYR:CZ	1:A:1261:CYS:HB2	2.50	0.46
1:A:13:ARG:HD2	1:A:20:MET:CE	2.46	0.46
1:A:274:ALA:O	1:A:275:GLU:C	2.55	0.46
3:T:2110:A:H2'	3:T:2111:U:H6	1.79	0.46
1:A:862:HIS:CD2	1:A:864:SER:OG	2.69	0.46
1:A:1057:LEU:HD23	1:A:1057:LEU:H	1.81	0.46
3:T:2112:G:H2'	3:T:2113:G:H5"	1.97	0.46
1:A:629:PRO:HG2	1:A:632:VAL:CG1	2.46	0.45
1:A:852:ALA:HB3	3:T:2104:G:C5'	2.46	0.45
1:A:202:ALA:HB3	1:A:212:ALA:HB1	1.99	0.45
1:A:301:THR:HG23	1:A:365:ASP:HA	1.97	0.45
1:A:319:VAL:HG12	1:A:474:LEU:HD21	1.98	0.45
1:A:532:ILE:N	1:A:532:ILE:HD12	2.31	0.45
1:A:803:ARG:HG3	1:A:806:ARG:NH2	2.32	0.45
3:T:2102:A:O2'	3:T:2102:A:N3	2.50	0.45
1:A:349:THR:HG22	1:A:350:SER:H	1.81	0.45
1:A:816:SER:OG	1:A:819:GLU:HB2	2.17	0.45
1:A:107:ASP:HB3	1:A:110:VAL:HG23	1.98	0.45
1:A:179:GLU:OE2	1:A:227:VAL:HG21	2.16	0.45
1:A:242:VAL:HG12	1:A:246:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:THR:HG23	1:A:357:PRO:HD2	1.97	0.45
1:A:397:MET:HB3	1:A:398:PRO:HD2	1.97	0.45
1:A:950:ILE:HD13	1:A:951:ASN:H	1.80	0.45
1:A:795:ALA:O	1:A:798:ALA:HB3	2.17	0.45
1:A:954:ARG:HH11	1:A:1049:THR:CG2	2.29	0.45
1:A:1013:LYS:NZ	1:A:1013:LYS:HB3	2.31	0.45
1:A:316:ILE:HD13	1:A:473:ILE:CG2	2.47	0.45
1:A:219:ARG:HD3	1:A:219:ARG:C	2.37	0.45
1:A:629:PRO:O	1:A:632:VAL:HG13	2.17	0.45
1:A:833:ILE:HD12	1:A:833:ILE:HA	1.59	0.45
1:A:1077:ASN:O	1:A:1081:THR:HG23	2.17	0.45
1:A:901:ASN:C	1:A:901:ASN:ND2	2.67	0.45
1:A:224:THR:CG2	1:A:225:GLY:N	2.80	0.45
1:A:349:THR:HG22	1:A:350:SER:N	2.32	0.45
1:A:186:VAL:HG23	1:A:186:VAL:O	2.18	0.44
1:A:372:TYR:CD1	1:A:410:VAL:HG21	2.52	0.44
1:A:794:GLU:OE1	1:A:1013:LYS:NZ	2.42	0.44
1:A:30:ALA:C	1:A:32:GLY:H	2.21	0.44
1:A:48:LYS:C	1:A:50:ALA:H	2.20	0.44
1:A:301:THR:HG22	1:A:364:VAL:O	2.17	0.44
1:A:846:CYS:HB3	1:A:925:PHE:CE2	2.52	0.44
1:A:21:MET:CE	1:A:24:LYS:HG2	2.48	0.44
1:A:281:LYS:O	1:A:283:SER:N	2.50	0.44
1:A:491:ILE:HG23	1:A:555:ALA:HB3	1.99	0.44
1:A:13:ARG:C	1:A:15:ARG:H	2.20	0.44
1:A:37:ALA:HA	1:A:40:ASN:HD22	1.77	0.44
1:A:316:ILE:HG21	1:A:354:TYR:CZ	2.52	0.44
1:A:969:LEU:HD12	1:A:1030:PHE:CZ	2.53	0.44
1:A:1110:ILE:CD1	1:A:1116:LEU:HA	2.42	0.44
1:A:361:TYR:CZ	1:A:480:LEU:HB3	2.52	0.44
4:A:2501:CH1:C4'	2:G:2013:U:H2'	2.47	0.44
1:A:234:PHE:CZ	1:A:236:MET:HB2	2.53	0.44
1:A:419:LEU:HD11	1:A:434:VAL:CG1	2.41	0.44
1:A:976:ILE:O	1:A:1014:ILE:HG22	2.18	0.44
1:A:1116:LEU:HD13	1:A:1148:LEU:HG	1.99	0.44
1:A:1193:ARG:HH21	1:A:1249:ARG:HH21	1.65	0.44
1:A:52:LYS:HA	1:A:52:LYS:HD2	1.84	0.44
1:A:219:ARG:HG2	1:A:1132:VAL:HG21	1.98	0.44
1:A:782:THR:HB	1:A:784:ALA:H	1.82	0.44
1:A:801:ASN:ND2	1:A:1012:GLU:HG3	2.29	0.44
1:A:858:ARG:HB2	3:T:2103:C:H5"	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1077:ASN:C	1:A:1077:ASN:ND2	2.70	0.44
1:A:1110:ILE:HD12	1:A:1116:LEU:N	2.33	0.44
1:A:1151:GLN:HE21	1:A:1151:GLN:HB2	1.54	0.44
3:T:2103:C:H5'	3:T:2104:G:OP1	2.18	0.44
1:A:274:ALA:O	1:A:276:VAL:N	2.50	0.44
1:A:322:LYS:HD3	1:A:470:GLU:OE1	2.18	0.44
1:A:304:HIS:HB3	1:A:307:HIS:CG	2.53	0.43
1:A:495:PHE:HA	1:A:518:ARG:O	2.18	0.43
1:A:597:SER:HA	1:A:637:PRO:HB3	2.00	0.43
1:A:629:PRO:HG2	1:A:632:VAL:HG11	2.01	0.43
1:A:997:ARG:NH2	1:A:1013:LYS:O	2.51	0.43
3:T:2107:U:H2'	3:T:2108:U:O4'	2.18	0.43
1:A:118:GLU:O	1:A:121:ALA:HB3	2.18	0.43
1:A:916:ILE:CD1	3:T:2104:G:H1'	2.40	0.43
1:A:12:LEU:HG	1:A:23:CYS:SG	2.58	0.43
1:A:858:ARG:NH1	1:A:858:ARG:CG	2.70	0.43
1:A:1018:GLY:HA2	3:T:2104:G:O2'	2.19	0.43
1:A:704:SER:O	1:A:708:GLN:N	2.41	0.43
1:A:270:THR:HG23	1:A:270:THR:O	2.18	0.43
1:A:281:LYS:C	1:A:283:SER:N	2.71	0.43
1:A:715:THR:CG2	1:A:716:ARG:N	2.81	0.43
1:A:165:LEU:O	1:A:165:LEU:HD13	2.19	0.43
1:A:356:THR:HG21	1:A:481:ASP:OD1	2.18	0.43
1:A:635:VAL:HG22	1:A:641:ILE:HD12	2.01	0.43
1:A:430:LEU:HD12	1:A:430:LEU:HA	1.78	0.43
1:A:752:ARG:HB3	1:A:754:ASP:OD2	2.19	0.43
1:A:623:THR:O	1:A:648:ILE:HG22	2.18	0.43
1:A:627:GLU:HG2	1:A:644:VAL:HB	2.00	0.43
1:A:717:ILE:C	1:A:717:ILE:HD12	2.40	0.43
1:A:875:PRO:CA	1:A:897:ILE:HD11	2.49	0.43
1:A:66:ILE:HG22	1:A:71:GLY:HA3	2.01	0.42
1:A:389:VAL:O	1:A:389:VAL:CG2	2.67	0.42
1:A:96:VAL:HA	1:A:115:PHE:CZ	2.55	0.42
1:A:108:VAL:HG13	1:A:109:GLU:N	2.35	0.42
1:A:898:SER:OG	1:A:899:PRO:HD2	2.19	0.42
3:T:2105:A:H2'	3:T:2106:U:H6	1.84	0.42
1:A:111:LEU:C	1:A:113:ALA:H	2.23	0.42
1:A:1054:ASP:OD2	2:G:2013:U:H5"	2.19	0.42
1:A:729:ASN:HD21	1:A:740:PHE:N	2.13	0.42
1:A:1173:ASN:OD1	1:A:1175:PHE:N	2.45	0.42
1:A:219:ARG:HH21	1:A:223:PHE:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:VAL:O	1:A:410:VAL:HG12	2.19	0.42
1:A:4:ILE:HG12	1:A:24:LYS:CD	2.49	0.42
1:A:4:ILE:CG2	1:A:6:ALA:HB3	2.50	0.42
1:A:73:ILE:HG23	1:A:259:PHE:CE1	2.54	0.42
1:A:134:ARG:HB3	1:A:259:PHE:CZ	2.55	0.42
1:A:566:ILE:HD11	1:A:570:GLU:HG3	2.01	0.42
1:A:598:LYS:CG	1:A:604:HIS:HA	2.47	0.42
1:A:599:ASP:OD1	1:A:599:ASP:N	2.52	0.42
1:A:1185:VAL:HA	1:A:1186:PRO:HD3	1.78	0.42
1:A:303:GLY:N	1:A:309:LYS:HD3	2.34	0.42
1:A:903:ALA:HB3	1:A:1003:LEU:HD12	2.00	0.42
3:T:2113:G:OP2	3:T:2114:A:H5"	2.20	0.42
1:A:74:LEU:CD2	1:A:96:VAL:HG13	2.50	0.42
1:A:198:GLN:HE21	1:A:198:GLN:HB2	1.61	0.42
1:A:935:ARG:NH2	3:T:2106:U:H4'	2.35	0.42
1:A:1237:GLN:C	1:A:1239:ILE:H	2.23	0.42
2:G:2006:C:O2	2:G:2006:C:H2'	2.19	0.42
1:A:673:VAL:HG23	1:A:673:VAL:O	2.20	0.42
1:A:48:LYS:HD2	1:A:124:ALA:HA	2.02	0.42
1:A:93:ALA:HA	1:A:96:VAL:CG1	2.50	0.42
1:A:909:ASN:C	1:A:909:ASN:ND2	2.72	0.42
1:A:115:PHE:O	1:A:118:GLU:N	2.52	0.41
1:A:193:LYS:O	1:A:197:VAL:HG12	2.20	0.41
1:A:279:MET:C	1:A:281:LYS:N	2.73	0.41
1:A:723:LEU:HD23	1:A:1110:ILE:HG12	2.01	0.41
2:G:2009:A:C2	3:T:2110:A:C6	3.08	0.41
1:A:21:MET:HE2	1:A:21:MET:CA	2.35	0.41
1:A:186:VAL:O	1:A:187:SER:C	2.59	0.41
1:A:324:TYR:CG	1:A:357:PRO:HD3	2.54	0.41
1:A:1191:HIS:HA	6:A:3582:HOH:O	2.19	0.41
1:A:208:PRO:O	1:A:209:LYS:C	2.58	0.41
1:A:611:TYR:CE2	1:A:613:PRO:HG3	2.55	0.41
1:A:1212:LEU:HD23	1:A:1212:LEU:HA	1.78	0.41
1:A:45:GLY:O	1:A:48:LYS:HG2	2.20	0.41
1:A:806:ARG:HE	1:A:806:ARG:HB3	1.61	0.41
1:A:1243:ASN:HB2	3:T:2113:G:C8	2.56	0.41
1:A:122:LEU:O	1:A:123:VAL:C	2.59	0.41
1:A:505:ILE:HD11	1:A:1203:TYR:CD1	2.56	0.41
1:A:579:LYS:HA	1:A:580:PRO:HD3	1.81	0.41
1:A:714:ASN:HD21	1:A:1253:LYS:HB3	1.85	0.41
1:A:1186:PRO:HG3	1:A:1258:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:HIS:CD2	1:A:363:HIS:C	2.94	0.41
1:A:25:LYS:HA	1:A:28:THR:HG22	2.03	0.41
1:A:72:ILE:HD11	1:A:135:VAL:CG2	2.51	0.41
1:A:9:VAL:O	1:A:9:VAL:HG12	2.21	0.41
1:A:13:ARG:HD2	1:A:20:MET:HE3	2.02	0.41
1:A:521:ILE:CD1	1:A:527:VAL:HG11	2.51	0.41
1:A:817:LEU:HD23	1:A:1067:GLU:HB3	2.02	0.41
1:A:859:SER:O	1:A:1195:ARG:NH2	2.51	0.41
1:A:195:TYR:HA	1:A:220:MET:HE1	2.02	0.40
1:A:764:TYR:CE2	1:A:1094:HIS:CD2	3.08	0.40
1:A:779:GLY:O	1:A:781:ASP:N	2.41	0.40
1:A:4:ILE:HG22	1:A:6:ALA:H	1.86	0.40
1:A:162:ASP:HB2	1:A:163:GLU:CD	2.41	0.40
1:A:209:LYS:HE2	1:A:209:LYS:HB3	1.80	0.40
1:A:397:MET:HE2	1:A:397:MET:HA	2.03	0.40
1:A:508:ARG:HB3	1:A:508:ARG:HH21	1.87	0.40
1:A:791:LEU:HD12	1:A:791:LEU:HA	1.86	0.40
1:A:871:GLN:HB2	1:A:922:TRP:CD1	2.56	0.40
1:A:962:ASN:OD1	1:A:1084:GLU:HA	2.21	0.40
1:A:1003:LEU:N	1:A:1003:LEU:CD1	2.84	0.40
1:A:59:ASP:OD2	1:A:151:ARG:NH2	2.53	0.40
1:A:223:PHE:CD1	1:A:223:PHE:C	2.94	0.40
1:A:529:ILE:HD13	1:A:529:ILE:C	2.42	0.40
1:A:833:ILE:HD12	1:A:937:ARG:HG3	2.04	0.40
1:A:1129:ILE:HD13	1:A:1129:ILE:HA	1.89	0.40
1:A:67:ASP:O	1:A:69:ASN:N	2.54	0.40
1:A:839:VAL:HG12	1:A:843:LEU:HD23	2.03	0.40
1:A:857:ASN:C	1:A:857:ASN:ND2	2.74	0.40
1:A:1110:ILE:HD11	1:A:1116:LEU:CG	2.49	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	1193/1289 (93%)	1058 (89%)	100 (8%)	35 (3%)	4 7

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	34	ILE
1	A	104	LYS
1	A	188	ALA
1	A	323	THR
1	A	381	ALA
1	A	466	ASP
1	A	780	ILE
1	A	806	ARG
1	A	809	TYR
1	A	1263	SER
1	A	68	GLY
1	A	282	GLN
1	A	325	GLY
1	A	468	GLU
1	A	679	GLY
1	A	849	SER
1	A	1078	THR
1	A	223	PHE
1	A	427	ASP
1	A	1005	ASP
1	A	1238	LEU
1	A	14	GLU
1	A	31	ASN
1	A	99	ALA
1	A	209	LYS
1	A	778	LEU
1	A	803	ARG
1	A	210	GLU
1	A	275	GLU
1	A	970	SER
1	A	81	ASP
1	A	324	TYR
1	A	465	GLY
1	A	237	GLU

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	995/1060 (94%)	841 (84%)	154 (16%)	2 4

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	20	MET
1	A	23	CYS
1	A	24	LYS
1	A	51	LYS
1	A	75	GLU
1	A	76	VAL
1	A	95	LYS
1	A	117	GLU
1	A	132	ILE
1	A	134	ARG
1	A	141	ASP
1	A	143	LEU
1	A	151	ARG
1	A	152	ILE
1	A	154	VAL
1	A	155	LEU
1	A	163	GLU
1	A	165	LEU
1	A	181	ILE
1	A	196	GLN
1	A	200	ASP
1	A	210	GLU
1	A	219	ARG
1	A	220	MET
1	A	224	THR
1	A	229	LEU
1	A	241	THR
1	A	245	LEU
1	A	246	LEU

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Mol	Chain	Res	Type
1	A	250	ASN
1	A	258	ARG
1	A	266	GLU
1	A	276	VAL
1	A	291	GLU
1	A	355	ASP
1	A	356	THR
1	A	364	VAL
1	A	376	MET
1	A	382	GLN
1	A	387	ILE
1	A	390	VAL
1	A	394	ASP
1	A	399	GLN
1	A	406	LEU
1	A	426	ASP
1	A	428	GLU
1	A	430	LEU
1	A	432	GLU
1	A	436	MET
1	A	438	VAL
1	A	452	THR
1	A	480	LEU
1	A	491	ILE
1	A	508	ARG
1	A	529	ILE
1	A	530	VAL
1	A	535	THR
1	A	537	LYS
1	A	539	THR
1	A	548	LYS
1	A	550	LEU
1	A	599	ASP
1	A	618	ARG
1	A	622	VAL
1	A	623	THR
1	A	626	ILE
1	A	628	LEU
1	A	632	VAL
1	A	642	LYS
1	A	646	THR
1	A	655	ASP

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Mol	Chain	Res	Type
1	A	666	ARG
1	A	704	SER
1	A	705	LEU
1	A	715	THR
1	A	717	ILE
1	A	733	LEU
1	A	737	GLN
1	A	741	ASN
1	A	781	ASP
1	A	782	THR
1	A	791	LEU
1	A	794	GLU
1	A	800	THR
1	A	806	ARG
1	A	808	ASP
1	A	809	TYR
1	A	813	PHE
1	A	827	ARG
1	A	831	LYS
1	A	832	LEU
1	A	833	ILE
1	A	835	ASP
1	A	840	GLU
1	A	854	THR
1	A	857	ASN
1	A	858	ARG
1	A	869	LEU
1	A	873	CYS
1	A	874	THR
1	A	879	LYS
1	A	882	LEU
1	A	884	LEU
1	A	897	ILE
1	A	901	ASN
1	A	905	THR
1	A	909	ASN
1	A	914	ARG
1	A	930	ILE
1	A	933	ILE
1	A	938	LEU
1	A	948	GLN
1	A	950	ILE

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Mol	Chain	Res	Type
1	A	970	SER
1	A	973	SER
1	A	991	GLU
1	A	993	LEU
1	A	997	ARG
1	A	1003	LEU
1	A	1008	VAL
1	A	1013	LYS
1	A	1014	ILE
1	A	1016	SER
1	A	1017	MET
1	A	1021	TYR
1	A	1033	LEU
1	A	1040	ILE
1	A	1049	THR
1	A	1053	ASP
1	A	1065	LEU
1	A	1075	THR
1	A	1076	THR
1	A	1077	ASN
1	A	1081	THR
1	A	1089	GLU
1	A	1107	ARG
1	A	1110	ILE
1	A	1111	VAL
1	A	1116	LEU
1	A	1128	THR
1	A	1130	ASP
1	A	1138	HIS
1	A	1152	LEU
1	A	1172	ILE
1	A	1182	ILE
1	A	1193	ARG
1	A	1200	LEU
1	A	1213	SER
1	A	1235	ILE
1	A	1241	ARG
1	A	1245	THR
1	A	1251	THR
1	A	1256	ILE

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

Mol	Chain	Res	Type
1	A	40	ASN
1	A	55	ASN
1	A	77	ASN
1	A	79	GLN
1	A	90	GLN
1	A	147	GLN
1	A	198	GLN
1	A	204	GLN
1	A	375	ASN
1	A	382	GLN
1	A	399	GLN
1	A	409	GLN
1	A	714	ASN
1	A	729	ASN
1	A	857	ASN
1	A	862	HIS
1	A	901	ASN
1	A	909	ASN
1	A	948	GLN
1	A	956	HIS
1	A	963	ASN
1	A	1077	ASN
1	A	1094	HIS
1	A	1121	ASN
1	A	1151	GLN
1	A	1155	ASN
1	A	1191	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	6/13 (46%)	0	0
3	T	13/18 (72%)	6 (46%)	0
All	All	19/31 (61%)	6 (31%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	T	2103	C
3	T	2104	G
3	T	2112	G
3	T	2113	G

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Mol	Chain	Res	Type
3	T	2114	A
3	T	2115	C

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)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
4	CH1	A	2501	5	24,29,29	1.56	3 (12%)	33,45,45	1.45	7 (21%)

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	CH1	A	2501	5	-	8/22/34/34	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2501	CH1	C4-N4	4.74	1.45	1.33
4	A	2501	CH1	C3'-C4'	-4.18	1.43	1.52
4	A	2501	CH1	C3'-C2'	-2.16	1.47	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2501	CH1	O4'-C1'-N1	3.72	116.86	108.36
4	A	2501	CH1	O4'-C4'-C5'	2.66	113.89	109.52
4	A	2501	CH1	O4'-C1'-C2'	-2.65	104.02	106.51
4	A	2501	CH1	PB-O3A-PA	-2.55	124.06	132.83
4	A	2501	CH1	O2G-PG-O3B	2.26	112.20	104.64
4	A	2501	CH1	O3G-PG-O3B	2.06	111.54	104.64
4	A	2501	CH1	C4'-O4'-C1'	-2.02	106.97	109.75

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2501	CH1	C3'-C4'-C5'-O5'
4	A	2501	CH1	O4'-C4'-C5'-O5'
4	A	2501	CH1	C5'-O5'-PA-O1A
4	A	2501	CH1	C5'-O5'-PA-O2A
4	A	2501	CH1	PB-O3A-PA-O5'
4	A	2501	CH1	PG-O3B-PB-O3A
4	A	2501	CH1	C5'-O5'-PA-O3A
4	A	2501	CH1	PB-O3A-PA-O1A

There are no ring outliers.

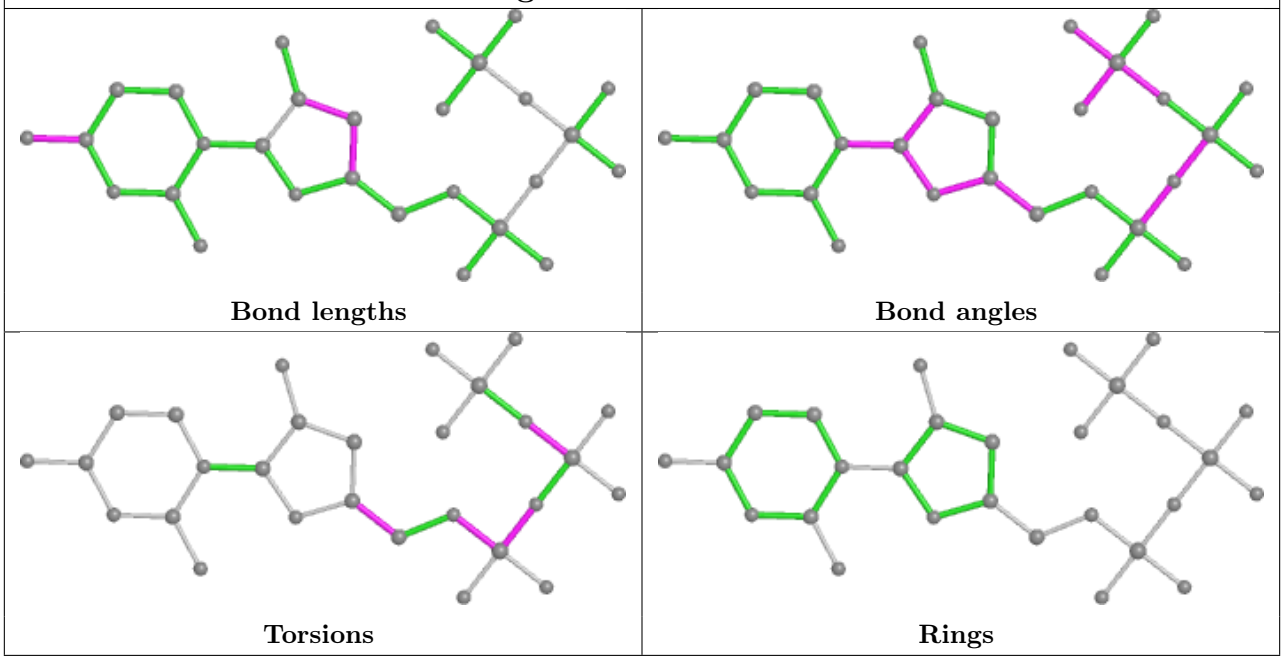
1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2501	CH1	6	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 2501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1203/1289 (93%)	-0.10	30 (2%) 57 51	16, 44, 90, 112	0
2	G	8/13 (61%)	4.67	7 (87%) 0 0	77, 113, 134, 140	0
3	T	14/18 (77%)	6.79	14 (100%) 0 0	86, 106, 118, 128	0
All	All	1225/1320 (92%)	0.01	51 (4%) 36 30	16, 45, 95, 140	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	2114	A	12.7
3	T	2112	G	11.2
3	T	2113	G	10.6
3	T	2104	G	9.9
2	G	2008	U	8.3
3	T	2115	C	7.5
3	T	2102	A	7.3
2	G	2007	A	7.3
3	T	2103	C	6.9
2	G	2009	A	6.8
1	A	700	SER	5.9
3	T	2111	U	5.8
3	T	2108	U	5.6
2	G	2010	A	4.5
2	G	2006	C	4.2
3	T	2110	A	4.2
3	T	2109	U	4.0
1	A	290	PHE	3.9
1	A	197	VAL	3.8
1	A	193	LYS	3.7
1	A	680	ALA	3.6
3	T	2105	A	3.6
1	A	5	THR	3.5

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Mol	Chain	Res	Type	RSRZ
3	T	2107	U	3.4
1	A	268	VAL	3.3
1	A	778	LEU	3.3
1	A	350	SER	3.2
1	A	702	ARG	3.2
1	A	163	GLU	3.0
1	A	279	MET	2.9
1	A	780	ILE	2.9
1	A	200	ASP	2.9
1	A	43	LYS	2.8
1	A	190	VAL	2.7
1	A	701	SER	2.6
1	A	679	GLY	2.6
2	G	2011	A	2.6
1	A	159	LYS	2.6
3	T	2106	U	2.5
2	G	2012	A	2.5
1	A	161	ALA	2.5
1	A	199	LEU	2.4
1	A	266	GLU	2.4
1	A	169	ILE	2.3
1	A	703	ASN	2.3
1	A	134	ARG	2.3
1	A	807	PRO	2.2
1	A	162	ASP	2.2
1	A	1264	ARG	2.1
1	A	202	ALA	2.1
1	A	191	VAL	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

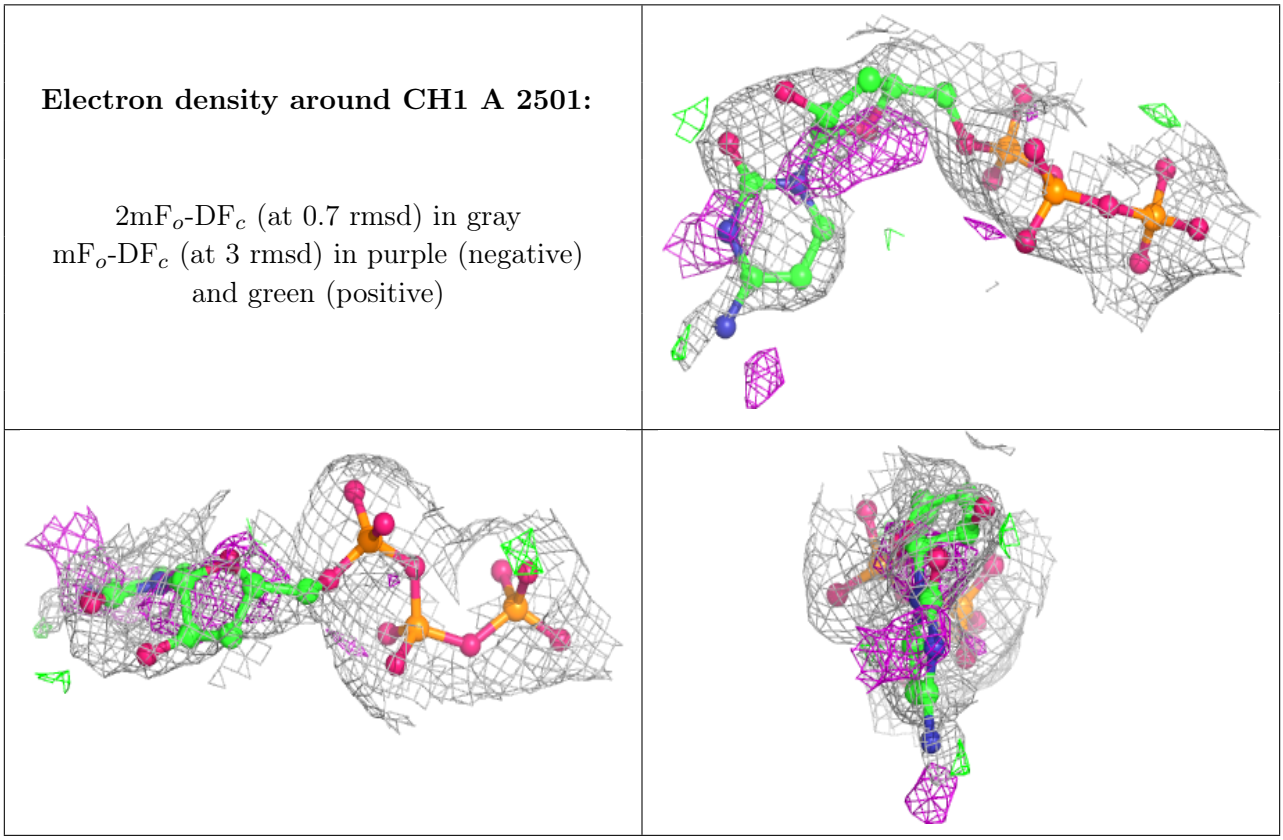
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CH1	A	2501	28/28	0.89	0.19	33,60,77,83	0
5	CA	A	3001	1/1	0.97	0.17	42,42,42,42	0
5	CA	A	3002	1/1	0.98	0.22	46,46,46,46	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 2501:

$2mF_o$-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.