



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:58 PM GMT

PDB ID : 3VNV  
Title : Complex structure of viral RNA polymerase II  
Authors : Takeshita, D.; Tomita, K.  
Deposited on : 2012-01-18  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

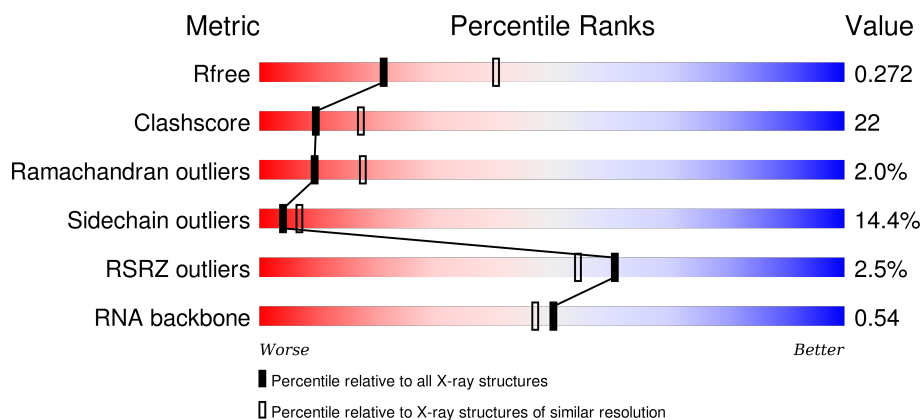
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)
RNA backbone	2183	1022 (3.00-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1289	
2	G	7	
3	T	8	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9680 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
1	A	1203	Total	C	N	O	S	0	0	0
			9287	5865	1605	1772	45			

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

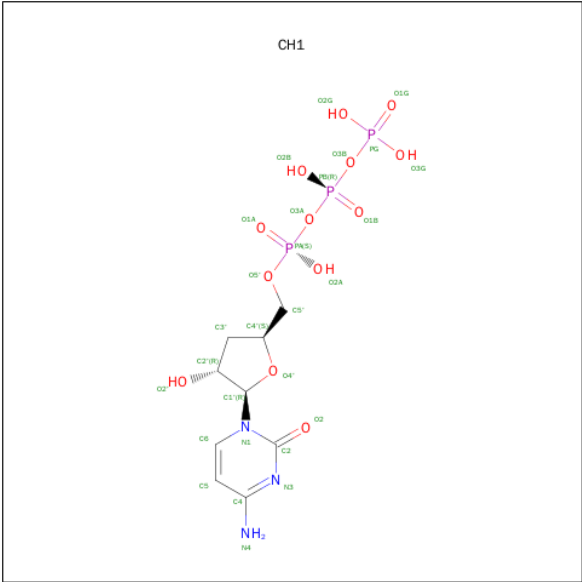
- Molecule 2 is a RNA chain called RNA (5'-R(\*CP\*CP\*CP\*UP\*AP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	7	Total	C	N	O	P	0	0	0
			139	64	22	47	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	8	Total	C	N	O	P	8	0	0
			177	79	37	54	7			

- Molecule 4 is 3'-DEOXY-CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CH1) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>).



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

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

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

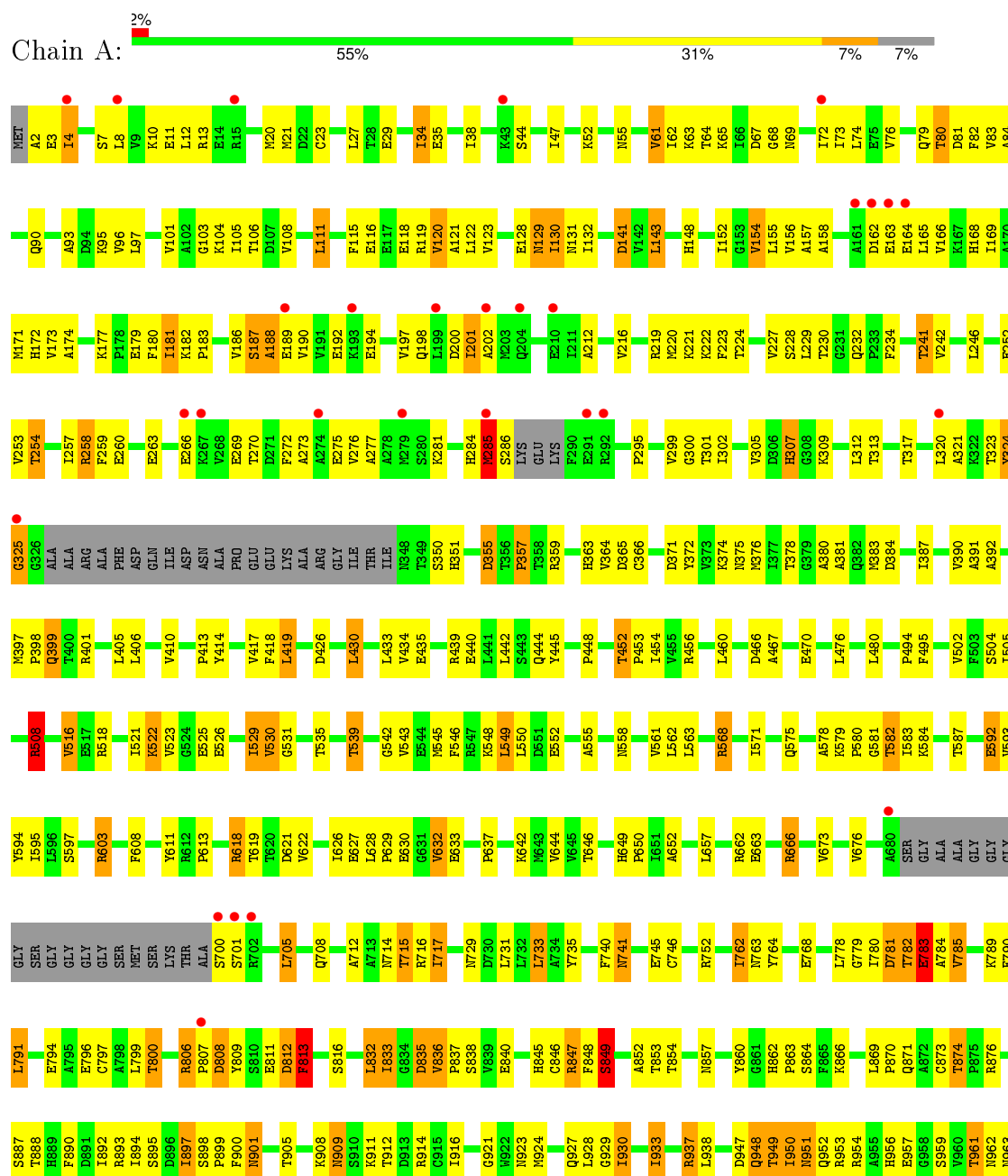
- Molecule 6 is water.

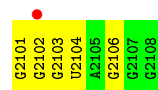
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total	O	0	0
			47	47		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.73Å 256.04Å 101.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.60 48.08 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.94-2.60) 99.3 (48.08-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.25 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.220 , 0.279 0.213 , 0.272	Depositor DCC
$R_{free}$ test set	2821 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.5	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 40.3	EDS
Estimated twinning fraction	0.024 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 55782 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9680	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.49	1/9456 (0.0%)	0.63	0/12787
2	G	0.46	0/153	0.84	0/235
3	T	0.64	0/199	1.20	0/311
All	All	0.50	1/9808 (0.0%)	0.65	0/13333

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	981	CYS	CB-SG	-6.00	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	849	SER	Peptide

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen



atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9287	0	9273	421	0
2	G	139	0	78	5	0
3	T	177	0	89	7	0
4	A	28	0	12	2	0
5	A	2	0	0	0	0
6	A	47	0	0	2	0
All	All	9680	0	9452	428	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 22.

All (428) 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)
2:G:2003:C:H42	3:T:2106:G:H1	1.07	0.98
1:A:1157:ILE:HG12	1:A:1165:ALA:HB3	1.43	0.97
1:A:1100:ASP:OD1	1:A:1102:THR:HG23	1.62	0.97
1:A:961:THR:HG22	1:A:963:ASN:H	1.28	0.97
1:A:741:ASN:HD21	1:A:745:GLU:HB2	1.33	0.93
1:A:1019:ASN:HB3	1:A:1022:THR:HG22	1.48	0.91
1:A:729:ASN:HD21	1:A:740:PHE:H	1.16	0.90
1:A:582:THR:HB	1:A:583:ILE:HD12	1.55	0.89
1:A:871:GLN:HE21	1:A:921:GLY:HA3	1.37	0.89
1:A:467:ALA:HA	1:A:470:GLU:HB2	1.52	0.89
1:A:1173:ASN:ND2	1:A:1175:PHE:H	1.70	0.88
1:A:448:PRO:O	1:A:452:THR:HG22	1.75	0.85
1:A:1049:THR:HG22	1:A:1056:ILE:HB	1.57	0.84
1:A:1019:ASN:HB3	1:A:1022:THR:CG2	2.08	0.84
1:A:782:THR:HG23	1:A:783:GLU:H	1.45	0.82
1:A:516:VAL:HG22	1:A:555:ALA:HA	1.58	0.82
1:A:522:LYS:HB2	1:A:525:GLU:OE1	1.79	0.81
1:A:806:ARG:H	1:A:807:PRO:HD3	1.44	0.80
1:A:80:THR:HG22	1:A:83:VAL:H	1.46	0.79
1:A:183:PRO:HD3	1:A:230:THR:HB	1.65	0.79
1:A:324:TYR:CD1	1:A:357:PRO:HD3	2.18	0.79
1:A:618:ARG:HG2	1:A:618:ARG:HH21	1.46	0.78
1:A:1143:LYS:HD3	1:A:1144:TYR:CE1	2.19	0.77
1:A:93:ALA:HA	1:A:96:VAL:HG12	1.64	0.77
1:A:103:GLY:O	1:A:105:ILE:HG13	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:VAL:HG22	1:A:561:VAL:HG22	1.67	0.76
1:A:44:SER:O	1:A:47:ILE:HG22	1.86	0.76
1:A:1077:ASN:O	1:A:1081:THR:HG23	1.84	0.76
1:A:212:ALA:O	1:A:216:VAL:HG23	1.85	0.76
1:A:163:GLU:HG2	1:A:164:GLU:H	1.49	0.75
1:A:148:HIS:HB3	1:A:152:ILE:HG23	1.69	0.75
1:A:8:LEU:HG	1:A:27:LEU:HD21	1.69	0.74
1:A:1173:ASN:HD22	1:A:1175:PHE:H	1.34	0.74
1:A:666:ARG:HA	1:A:666:ARG:HH21	1.53	0.74
1:A:1182:ILE:HD12	1:A:1183:ARG:N	2.02	0.73
1:A:838:SER:HB2	1:A:840:GLU:OE1	1.88	0.73
1:A:714:ASN:HD21	1:A:1254:PHE:H	1.37	0.73
1:A:579:LYS:HG3	1:A:580:PRO:HD2	1.71	0.73
1:A:782:THR:HG23	1:A:783:GLU:N	2.03	0.73
1:A:419:LEU:HD11	1:A:434:VAL:HG11	1.71	0.73
1:A:1245:THR:O	1:A:1246:LYS:HE3	1.88	0.72
1:A:372:TYR:HE1	1:A:410:VAL:HG21	1.54	0.72
1:A:914:ARG:HD3	1:A:1017:MET:HE2	1.69	0.72
1:A:916:ILE:HD12	3:T:2101:G:C8	2.24	0.72
1:A:309:LYS:HE3	1:A:365:ASP:OD1	1.90	0.72
1:A:156:VAL:HG12	1:A:166:VAL:HG13	1.72	0.71
1:A:741:ASN:ND2	1:A:745:GLU:HB2	2.03	0.71
1:A:956:HIS:O	1:A:959:SER:HB3	1.89	0.71
1:A:273:ALA:O	1:A:276:VAL:HG12	1.90	0.71
1:A:494:PRO:HB2	1:A:582:THR:HG21	1.73	0.71
1:A:937:ARG:HH21	1:A:937:ARG:HG3	1.55	0.71
1:A:80:THR:HG23	1:A:82:PHE:H	1.54	0.71
1:A:729:ASN:ND2	1:A:740:PHE:H	1.87	0.70
1:A:307:HIS:CD2	1:A:391:ALA:H	2.10	0.70
1:A:849:SER:HA	1:A:863:PRO:HG3	1.74	0.69
2:G:2003:C:N4	3:T:2106:G:H1	1.86	0.69
1:A:853:THR:HG23	1:A:866:LYS:HE2	1.75	0.69
1:A:129:ASN:HD22	1:A:130:ILE:N	1.91	0.69
1:A:592:GLU:HG3	1:A:642:LYS:HG2	1.75	0.69
1:A:405:LEU:HD13	1:A:445:TYR:CE2	2.28	0.69
1:A:1193:ARG:HD2	1:A:1249:ARG:HH11	1.56	0.68
1:A:1149:PRO:HG2	1:A:1152:LEU:HD22	1.75	0.68
1:A:840:GLU:CD	1:A:840:GLU:H	1.96	0.68
1:A:558:ASN:HB3	1:A:1210:ARG:HD3	1.76	0.68
1:A:181:ILE:HD13	1:A:182:LYS:HG3	1.76	0.68
1:A:806:ARG:N	1:A:807:PRO:HD3	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ASN:HA	1:A:378:THR:HG22	1.75	0.68
1:A:163:GLU:HG2	1:A:164:GLU:N	2.09	0.67
1:A:947:ASP:OD1	1:A:949:THR:HB	1.94	0.67
1:A:949:THR:HG23	1:A:953:ARG:NH1	2.10	0.67
1:A:119:ARG:HE	1:A:131:ASN:HB3	1.60	0.67
1:A:80:THR:HG23	1:A:82:PHE:N	2.10	0.67
1:A:916:ILE:HD12	3:T:2101:G:N9	2.09	0.66
1:A:968:ASP:H	1:A:1081:THR:HG22	1.59	0.66
1:A:72:ILE:HD12	1:A:101:VAL:HA	1.77	0.66
1:A:961:THR:CG2	1:A:963:ASN:H	2.05	0.66
1:A:1094:HIS:H	1:A:1102:THR:HG22	1.61	0.66
1:A:806:ARG:N	1:A:807:PRO:CD	2.59	0.66
1:A:494:PRO:CB	1:A:582:THR:HG21	2.25	0.66
1:A:168:HIS:HA	1:A:171:MET:HE2	1.75	0.65
1:A:417:VAL:HB	1:A:454:ILE:HG12	1.78	0.65
1:A:1121:ASN:HD21	1:A:1167:VAL:H	1.45	0.65
1:A:120:VAL:HA	1:A:123:VAL:HG12	1.79	0.65
1:A:281:LYS:HA	1:A:284:HIS:CD2	2.32	0.65
1:A:187:SER:HB3	1:A:190:VAL:HG12	1.78	0.65
1:A:924:MET:HE3	1:A:928:LEU:HG	1.79	0.65
1:A:833:ILE:HD12	1:A:937:ARG:HG2	1.79	0.64
4:A:2501:CH1:H5'2	2:G:2007:C:H2'	1.80	0.64
1:A:629:PRO:HG2	1:A:632:VAL:HG11	1.79	0.64
1:A:4:ILE:H	1:A:4:ILE:HD13	1.62	0.64
1:A:1173:ASN:HD22	1:A:1174:PRO:N	1.95	0.64
1:A:442:LEU:HD13	1:A:452:THR:HG21	1.78	0.64
1:A:836:VAL:HG22	1:A:837:PRO:HD2	1.80	0.64
1:A:73:ILE:HB	1:A:155:LEU:HD12	1.80	0.64
1:A:735:TYR:CG	1:A:762:ILE:HG13	2.33	0.64
1:A:806:ARG:H	1:A:807:PRO:CD	2.10	0.64
1:A:1173:ASN:HD22	1:A:1173:ASN:C	2.00	0.63
1:A:399:GLN:HE21	1:A:399:GLN:H	1.44	0.63
1:A:562:LEU:N	1:A:562:LEU:HD12	2.12	0.63
1:A:1057:LEU:H	1:A:1057:LEU:HD23	1.63	0.63
1:A:384:ASP:O	1:A:413:PRO:HG2	1.98	0.63
1:A:1016:SER:O	1:A:1022:THR:HG21	1.98	0.63
1:A:909:ASN:HD22	1:A:911:LYS:H	1.45	0.63
1:A:229:LEU:HD11	1:A:242:VAL:HG11	1.81	0.63
1:A:73:ILE:HD13	1:A:259:PHE:CD1	2.34	0.62
1:A:272:PHE:CZ	1:A:313:THR:HG21	2.34	0.62
1:A:324:TYR:CG	1:A:357:PRO:HD3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ILE:HG21	1:A:508:ARG:HD2	1.82	0.62
1:A:916:ILE:CD1	3:T:2101:G:C8	2.83	0.61
1:A:847:ARG:HH21	1:A:849:SER:HB2	1.66	0.61
1:A:949:THR:HG23	1:A:953:ARG:HH12	1.64	0.61
1:A:929:GLY:O	1:A:933:ILE:HG23	2.00	0.61
1:A:1243:ASN:CB	1:A:1244:PRO:HD2	2.30	0.61
1:A:1003:LEU:HB3	1:A:1004:PRO:HD2	1.82	0.61
1:A:300:GLY:HA3	1:A:383:MET:SD	2.40	0.61
1:A:716:ARG:HD3	1:A:1111:VAL:HG23	1.83	0.61
1:A:63:LYS:NZ	1:A:90:GLN:HE22	1.99	0.60
1:A:529:ILE:HD11	1:A:575:GLN:CD	2.21	0.60
1:A:874:THR:HG21	6:A:3503:HOH:O	2.01	0.60
2:G:2002:C:H2'	2:G:2003:C:H5''	1.84	0.60
1:A:1124:TYR:O	1:A:1128:THR:HB	2.02	0.60
1:A:740:PHE:CE2	1:A:746:CYS:HA	2.37	0.60
1:A:120:VAL:HA	1:A:123:VAL:CG1	2.32	0.60
1:A:35:GLU:O	1:A:38:ILE:HG12	2.01	0.59
1:A:1154:ARG:HH11	1:A:1154:ARG:HG3	1.66	0.59
1:A:611:TYR:HB3	1:A:626:ILE:HD13	1.83	0.59
1:A:796:GLU:O	1:A:800:THR:HG23	2.01	0.59
1:A:712:ALA:O	1:A:715:THR:HB	2.03	0.59
1:A:526:GLU:HG2	1:A:539:THR:HB	1.84	0.59
1:A:281:LYS:HA	1:A:284:HIS:CG	2.37	0.59
1:A:272:PHE:HZ	1:A:313:THR:HG21	1.66	0.59
1:A:63:LYS:HZ3	1:A:90:GLN:HE22	1.51	0.59
1:A:930:ILE:C	1:A:930:ILE:HD12	2.23	0.59
1:A:165:LEU:O	1:A:169:ILE:HG12	2.03	0.59
1:A:260:GLU:HB3	1:A:263:GLU:HG3	1.84	0.59
1:A:1157:ILE:HG12	1:A:1165:ALA:CB	2.26	0.58
1:A:320:LEU:HD12	1:A:355:ASP:O	2.03	0.58
1:A:21:MET:HE2	1:A:21:MET:HA	1.84	0.58
1:A:387:ILE:HD11	1:A:476:LEU:HD21	1.85	0.58
1:A:158:ALA:HB1	1:A:252:GLU:O	2.03	0.58
1:A:937:ARG:NH2	1:A:937:ARG:HG3	2.15	0.58
1:A:399:GLN:HE21	1:A:399:GLN:N	2.01	0.58
1:A:740:PHE:HD2	1:A:745:GLU:HG3	1.69	0.58
1:A:187:SER:HB3	1:A:190:VAL:CG1	2.34	0.58
1:A:806:ARG:CG	1:A:806:ARG:O	2.51	0.57
1:A:321:ALA:O	1:A:325:GLY:HA2	2.04	0.57
1:A:783:GLU:O	1:A:783:GLU:HG3	2.03	0.57
1:A:177:LYS:HG2	1:A:258:ARG:CZ	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:LYS:HG3	1:A:580:PRO:CD	2.33	0.57
1:A:1182:ILE:HG13	1:A:1184:TYR:CE2	2.40	0.56
1:A:502:VAL:HG11	1:A:571:ILE:HB	1.86	0.56
1:A:951:ASN:OD1	1:A:1049:THR:HG23	2.05	0.56
1:A:833:ILE:HG23	1:A:989:TRP:NE1	2.19	0.56
1:A:301:THR:HB	1:A:363:HIS:NE2	2.20	0.56
1:A:836:VAL:CG2	1:A:837:PRO:HD2	2.35	0.56
1:A:629:PRO:HD3	1:A:642:LYS:O	2.05	0.56
1:A:74:LEU:HD21	1:A:96:VAL:HG13	1.88	0.56
1:A:847:ARG:NH2	1:A:849:SER:HB2	2.21	0.56
1:A:611:TYR:HB3	1:A:626:ILE:CD1	2.36	0.56
1:A:701:SER:N	1:A:1177:LYS:HE2	2.20	0.56
1:A:399:GLN:H	1:A:399:GLN:NE2	2.03	0.55
1:A:948:GLN:O	1:A:952:GLN:HG3	2.06	0.55
1:A:21:MET:CE	1:A:21:MET:HA	2.36	0.55
1:A:595:ILE:HG22	1:A:637:PRO:HA	1.87	0.55
1:A:65:LYS:HD3	1:A:101:VAL:HG21	1.88	0.55
1:A:529:ILE:HG13	1:A:529:ILE:O	2.06	0.55
1:A:1121:ASN:ND2	1:A:1167:VAL:H	2.04	0.54
1:A:961:THR:HG22	1:A:963:ASN:N	2.11	0.54
1:A:967:VAL:HG23	1:A:968:ASP:N	2.21	0.54
1:A:809:TYR:CE1	1:A:811:GLU:O	2.61	0.54
1:A:156:VAL:CG1	1:A:166:VAL:HG13	2.38	0.54
1:A:806:ARG:HG3	1:A:806:ARG:O	2.08	0.54
1:A:708:GLN:HB3	1:A:1151:GLN:HE22	1.73	0.54
1:A:705:LEU:HD11	1:A:1175:PHE:CD2	2.43	0.54
1:A:874:THR:HG22	1:A:876:ARG:H	1.72	0.53
1:A:874:THR:HG22	1:A:876:ARG:N	2.22	0.53
1:A:419:LEU:HD11	1:A:434:VAL:CG1	2.38	0.53
1:A:837:PRO:HD3	1:A:989:TRP:CE2	2.43	0.53
1:A:862:HIS:HD2	1:A:864:SER:H	1.56	0.53
1:A:914:ARG:HD3	1:A:1017:MET:CE	2.38	0.53
1:A:398:PRO:O	1:A:401:ARG:HG3	2.08	0.53
1:A:1050:VAL:HG22	1:A:1055:ILE:HG12	1.90	0.53
1:A:152:ILE:HD11	1:A:258:ARG:NH1	2.23	0.53
1:A:387:ILE:CD1	1:A:476:LEU:HD21	2.38	0.53
1:A:779:GLY:C	1:A:781:ASP:H	2.10	0.53
1:A:933:ILE:HD12	1:A:933:ILE:C	2.30	0.53
1:A:969:LEU:HD21	1:A:1069:PHE:CD2	2.44	0.53
1:A:4:ILE:HB	1:A:8:LEU:HD23	1.91	0.53
1:A:116:GLU:O	1:A:120:VAL:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:LEU:N	1:A:1057:LEU:HD23	2.23	0.53
1:A:700:SER:O	1:A:1177:LYS:HB2	2.08	0.52
1:A:930:ILE:HD11	1:A:1021:TYR:HB2	1.90	0.52
1:A:529:ILE:HD11	1:A:575:GLN:OE1	2.08	0.52
1:A:1093:LYS:HB3	1:A:1095:TYR:CE1	2.44	0.52
1:A:797:CYS:HB2	1:A:1012:GLU:HB3	1.89	0.52
1:A:752:ARG:H	1:A:763:ASN:ND2	2.08	0.52
1:A:568:ARG:HG3	1:A:568:ARG:O	2.10	0.52
1:A:619:THR:HG22	1:A:1241:ARG:HG3	1.92	0.52
1:A:954:ARG:NH1	1:A:1049:THR:HB	2.25	0.52
1:A:558:ASN:HD22	1:A:1210:ARG:HH21	1.57	0.52
1:A:351:HIS:CG	1:A:351:HIS:O	2.62	0.52
1:A:376:MET:CE	1:A:410:VAL:HG23	2.39	0.52
1:A:741:ASN:ND2	1:A:745:GLU:CB	2.73	0.52
1:A:1077:ASN:HD22	1:A:1077:ASN:C	2.14	0.51
1:A:852:ALA:H	3:T:2101:G:H5"	1.75	0.51
1:A:227:VAL:HG22	1:A:227:VAL:O	2.09	0.51
1:A:269:GLU:HG3	1:A:270:THR:N	2.25	0.51
1:A:790:PHE:HD1	1:A:791:LEU:HD13	1.74	0.51
1:A:132:ILE:N	1:A:132:ILE:HD12	2.26	0.51
1:A:93:ALA:HA	1:A:96:VAL:CG1	2.36	0.51
1:A:608:PHE:HD1	1:A:633:GLU:O	1.93	0.51
1:A:156:VAL:HG12	1:A:166:VAL:CG1	2.40	0.51
1:A:435:GLU:O	1:A:439:ARG:HG3	2.11	0.51
1:A:611:TYR:CE2	1:A:613:PRO:HG3	2.45	0.51
1:A:901:ASN:HD22	1:A:901:ASN:C	2.14	0.51
1:A:809:TYR:CD1	1:A:811:GLU:O	2.64	0.51
1:A:649:HIS:HB2	1:A:650:PRO:CD	2.41	0.51
1:A:950:ILE:O	1:A:954:ARG:HG3	2.10	0.50
1:A:837:PRO:HD3	1:A:989:TRP:CD2	2.46	0.50
1:A:618:ARG:NH2	1:A:618:ARG:HG2	2.20	0.50
1:A:232:GLN:O	1:A:242:VAL:HG23	2.12	0.50
1:A:61:VAL:HG12	1:A:84:ALA:HB1	1.93	0.50
1:A:782:THR:HG21	1:A:784:ALA:HB3	1.93	0.50
1:A:157:ALA:O	1:A:254:THR:HG23	2.12	0.50
1:A:897:ILE:O	1:A:897:ILE:HG12	2.11	0.50
1:A:129:ASN:C	1:A:129:ASN:HD22	2.13	0.50
1:A:3:GLU:HB2	1:A:4:ILE:HD13	1.94	0.50
1:A:300:GLY:O	1:A:387:ILE:HG22	2.12	0.50
1:A:162:ASP:O	1:A:166:VAL:HG23	2.11	0.49
1:A:1243:ASN:HB2	1:A:1244:PRO:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:SER:C	1:A:189:GLU:H	2.14	0.49
1:A:971:ALA:O	1:A:972:ALA:C	2.50	0.49
1:A:198:GLN:HA	1:A:201:ILE:HG12	1.94	0.49
1:A:1239:ILE:O	1:A:1239:ILE:HG22	2.12	0.49
1:A:376:MET:HG3	1:A:410:VAL:CG2	2.42	0.49
1:A:169:ILE:O	1:A:173:VAL:HG23	2.12	0.49
1:A:522:LYS:HE2	1:A:552:GLU:OE1	2.13	0.49
1:A:701:SER:CA	1:A:1177:LYS:HE2	2.42	0.49
1:A:323:THR:C	1:A:325:GLY:H	2.16	0.48
1:A:924:MET:CE	1:A:928:LEU:HG	2.43	0.48
1:A:997:ARG:O	6:A:3503:HOH:O	2.20	0.48
1:A:1185:VAL:HG23	1:A:1186:PRO:HD2	1.95	0.48
1:A:782:THR:HG22	1:A:785:VAL:HG13	1.95	0.48
1:A:968:ASP:N	1:A:1081:THR:HG22	2.26	0.48
1:A:782:THR:CG2	1:A:785:VAL:HG13	2.44	0.48
1:A:961:THR:CG2	1:A:963:ASN:HB2	2.44	0.48
1:A:143:LEU:HA	1:A:156:VAL:O	2.14	0.48
1:A:627:GLU:HG2	1:A:644:VAL:HB	1.96	0.48
1:A:951:ASN:OD1	1:A:1049:THR:CG2	2.61	0.47
1:A:67:ASP:O	1:A:69:ASN:N	2.46	0.47
1:A:495:PHE:HA	1:A:518:ARG:O	2.14	0.47
1:A:603:ARG:HD2	1:A:663:GLU:OE1	2.14	0.47
1:A:705:LEU:HD11	1:A:1175:PHE:HD2	1.77	0.47
1:A:80:THR:CG2	1:A:83:VAL:H	2.21	0.47
1:A:392:ALA:HB2	1:A:419:LEU:CD1	2.44	0.47
1:A:275:GLU:O	1:A:275:GLU:OE2	2.32	0.47
1:A:378:THR:HG23	1:A:380:ALA:H	1.79	0.47
1:A:180:PHE:CD2	1:A:186:VAL:HG12	2.49	0.47
1:A:899:PRO:HG2	1:A:900:PHE:CE1	2.49	0.47
1:A:181:ILE:O	1:A:181:ILE:HD13	2.15	0.47
1:A:179:GLU:HB3	1:A:227:VAL:HG22	1.97	0.47
1:A:768:GLU:HB3	1:A:1105:TYR:CE1	2.50	0.47
1:A:890:PHE:CG	1:A:1204:LEU:HD21	2.49	0.47
1:A:34:ILE:HG22	1:A:35:GLU:N	2.30	0.46
1:A:430:LEU:O	1:A:433:LEU:HB3	2.15	0.46
1:A:397:MET:HA	1:A:397:MET:HE2	1.97	0.46
1:A:740:PHE:CD2	1:A:745:GLU:HG3	2.49	0.46
1:A:1019:ASN:CB	1:A:1022:THR:HG22	2.33	0.46
1:A:105:ILE:HG22	1:A:106:THR:N	2.30	0.46
1:A:187:SER:O	1:A:190:VAL:HG12	2.14	0.46
1:A:833:ILE:HG23	1:A:989:TRP:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:ILE:O	1:A:1014:ILE:HG22	2.16	0.46
1:A:21:MET:HE1	1:A:430:LEU:HD23	1.96	0.46
1:A:812:ASP:O	1:A:813:PHE:C	2.54	0.46
1:A:276:VAL:CG1	1:A:277:ALA:N	2.78	0.46
1:A:949:THR:HG23	1:A:953:ARG:CZ	2.46	0.46
1:A:1071:TYR:HD1	1:A:1072:VAL:HG12	1.81	0.46
1:A:299:VAL:O	1:A:363:HIS:HA	2.15	0.46
1:A:270:THR:HG23	1:A:270:THR:O	2.16	0.46
1:A:923:ASN:O	1:A:927:GLN:HG3	2.16	0.46
1:A:581:GLY:HA2	1:A:584:LYS:NZ	2.31	0.46
1:A:10:LYS:HG3	1:A:11:GLU:N	2.31	0.46
1:A:95:LYS:C	1:A:97:LEU:H	2.19	0.46
1:A:806:ARG:O	1:A:808:ASP:N	2.49	0.45
1:A:80:THR:HG22	1:A:83:VAL:N	2.25	0.45
1:A:899:PRO:HG2	1:A:900:PHE:CD1	2.51	0.45
1:A:417:VAL:HG12	1:A:454:ILE:HG23	1.98	0.45
1:A:221:LYS:HD3	1:A:222:LYS:N	2.30	0.45
1:A:546:PHE:O	1:A:888:THR:OG1	2.24	0.45
1:A:714:ASN:ND2	1:A:1254:PHE:H	2.08	0.45
1:A:181:ILE:O	1:A:182:LYS:HG3	2.17	0.45
1:A:716:ARG:CD	1:A:1111:VAL:HG23	2.45	0.45
1:A:194:GLU:O	1:A:197:VAL:HG12	2.16	0.45
1:A:141:ASP:OD1	1:A:141:ASP:N	2.49	0.45
1:A:717:ILE:C	1:A:717:ILE:HD12	2.36	0.45
1:A:1121:ASN:CG	1:A:1167:VAL:HG23	2.37	0.45
1:A:870:PRO:O	1:A:895:SER:HB3	2.15	0.45
1:A:530:VAL:HG22	1:A:652:ALA:HB2	1.99	0.45
1:A:174:ALA:O	1:A:258:ARG:NH1	2.50	0.45
1:A:187:SER:O	1:A:189:GLU:N	2.50	0.45
1:A:794:GLU:OE1	1:A:794:GLU:HA	2.16	0.45
1:A:1157:ILE:CG1	1:A:1165:ALA:HB3	2.31	0.45
1:A:832:LEU:HD13	1:A:833:ILE:HD13	1.99	0.45
1:A:72:ILE:CD1	1:A:101:VAL:HA	2.45	0.45
1:A:132:ILE:H	1:A:132:ILE:HD12	1.81	0.45
1:A:200:ASP:O	1:A:201:ILE:C	2.54	0.45
1:A:957:GLU:O	1:A:961:THR:HB	2.17	0.45
1:A:4:ILE:N	1:A:4:ILE:HD13	2.30	0.45
1:A:666:ARG:HA	1:A:666:ARG:HD3	1.75	0.45
1:A:228:SER:O	1:A:229:LEU:C	2.55	0.45
1:A:229:LEU:HD12	1:A:242:VAL:HG21	1.99	0.45
1:A:1149:PRO:HG2	1:A:1152:LEU:CD2	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:GLN:NE2	1:A:921:GLY:HA3	2.17	0.44
1:A:597:SER:HA	1:A:637:PRO:HB3	1.98	0.44
1:A:901:ASN:ND2	1:A:1001:GLY:HA2	2.33	0.44
1:A:892:ILE:O	1:A:892:ILE:HG22	2.16	0.44
1:A:200:ASP:O	1:A:202:ALA:N	2.51	0.44
1:A:985:LEU:HD13	1:A:993:LEU:HD12	1.98	0.44
1:A:1157:ILE:HG22	1:A:1185:VAL:HG11	1.99	0.44
1:A:108:VAL:O	1:A:111:LEU:HD23	2.17	0.44
1:A:62:ILE:HD12	1:A:152:ILE:HA	1.99	0.44
1:A:949:THR:CG2	1:A:953:ARG:HH22	2.29	0.44
1:A:222:LYS:O	1:A:224:THR:N	2.51	0.44
1:A:374:LYS:HE3	1:A:594:TYR:CZ	2.52	0.44
1:A:996:LEU:HD12	1:A:996:LEU:HA	1.70	0.44
1:A:1157:ILE:O	1:A:1167:VAL:HA	2.18	0.44
1:A:23:CYS:O	1:A:27:LEU:HB2	2.17	0.44
1:A:863:PRO:HB2	1:A:1205:TYR:CD2	2.52	0.44
1:A:1057:LEU:CD2	1:A:1057:LEU:N	2.81	0.44
1:A:1154:ARG:HG3	1:A:1154:ARG:NH1	2.32	0.44
1:A:363:HIS:C	1:A:363:HIS:CD2	2.91	0.44
1:A:1074:PHE:N	1:A:1074:PHE:CD2	2.81	0.44
1:A:466:ASP:C	1:A:466:ASP:OD1	2.55	0.44
1:A:1087:PHE:O	1:A:1088:ARG:HD3	2.17	0.44
1:A:701:SER:HA	1:A:1177:LYS:HG3	1.98	0.44
1:A:957:GLU:C	1:A:959:SER:N	2.71	0.44
1:A:894:ILE:O	1:A:895:SER:C	2.56	0.44
1:A:985:LEU:HD13	1:A:993:LEU:CD1	2.48	0.43
1:A:302:ILE:HD13	1:A:366:CYS:HB2	1.99	0.43
1:A:118:GLU:O	1:A:121:ALA:HB3	2.18	0.43
1:A:578:ALA:CB	1:A:583:ILE:HD13	2.48	0.43
4:A:2501:CH1:H6	4:A:2501:CH1:H5'2	2.00	0.43
1:A:701:SER:HA	1:A:1177:LYS:HE2	1.99	0.43
1:A:397:MET:CE	1:A:397:MET:HA	2.47	0.43
1:A:188:ALA:O	1:A:192:GLU:HB2	2.19	0.43
1:A:52:LYS:O	1:A:55:ASN:HB2	2.18	0.43
1:A:908:LYS:HB3	1:A:912:THR:O	2.18	0.43
1:A:111:LEU:O	1:A:115:PHE:HD1	2.01	0.43
1:A:833:ILE:HA	1:A:833:ILE:HD12	1.68	0.43
1:A:405:LEU:HD13	1:A:445:TYR:HE2	1.79	0.43
1:A:782:THR:HG23	1:A:784:ALA:N	2.33	0.43
1:A:105:ILE:HD13	1:A:111:LEU:HB3	2.00	0.43
1:A:187:SER:C	1:A:189:GLU:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ALA:HA	1:A:254:THR:HG23	2.00	0.43
1:A:562:LEU:N	1:A:562:LEU:CD1	2.81	0.43
1:A:295:PRO:HG2	1:A:359:ARG:HB3	2.00	0.43
1:A:105:ILE:CD1	1:A:111:LEU:HB3	2.48	0.43
3:T:2102:G:O5'	3:T:2102:G:H8	2.02	0.43
1:A:521:ILE:O	1:A:552:GLU:HA	2.17	0.43
1:A:158:ALA:HB2	1:A:253:VAL:HG22	2.01	0.43
1:A:392:ALA:HB2	1:A:419:LEU:HD12	2.01	0.43
1:A:1068:VAL:O	1:A:1072:VAL:HG13	2.18	0.43
1:A:73:ILE:HG23	1:A:259:PHE:CE1	2.54	0.42
1:A:549:LEU:HD23	1:A:550:LEU:H	1.84	0.42
1:A:846:CYS:SG	1:A:929:GLY:HA3	2.59	0.42
1:A:731:LEU:HA	1:A:731:LEU:HD12	1.85	0.42
1:A:119:ARG:O	1:A:123:VAL:HG12	2.19	0.42
1:A:876:ARG:NH2	1:A:995:ASP:OD2	2.49	0.42
1:A:63:LYS:NZ	1:A:90:GLN:NE2	2.65	0.42
1:A:323:THR:HG22	1:A:324:TYR:CD2	2.54	0.42
1:A:73:ILE:HD11	1:A:259:PHE:HB2	2.02	0.42
1:A:984:LEU:HD12	1:A:984:LEU:HA	1.81	0.42
1:A:27:LEU:HA	1:A:27:LEU:HD12	1.87	0.42
1:A:853:THR:CG2	1:A:866:LYS:HE2	2.48	0.42
1:A:452:THR:HA	1:A:453:PRO:HD3	1.94	0.42
1:A:618:ARG:NH2	1:A:618:ARG:CG	2.79	0.42
1:A:413:PRO:HB2	1:A:414:TYR:CD1	2.55	0.42
1:A:764:TYR:OH	1:A:1094:HIS:CD2	2.72	0.42
1:A:95:LYS:C	1:A:97:LEU:N	2.72	0.42
1:A:862:HIS:CD2	1:A:864:SER:H	2.35	0.42
1:A:862:HIS:HD2	1:A:864:SER:OG	2.03	0.42
1:A:494:PRO:HG2	1:A:582:THR:HG21	2.02	0.41
1:A:234:PHE:H	1:A:241:THR:HA	1.85	0.41
1:A:1015:SER:OG	1:A:1022:THR:HB	2.19	0.41
1:A:12:LEU:HG	1:A:23:CYS:SG	2.59	0.41
1:A:132:ILE:CD1	1:A:132:ILE:H	2.33	0.41
1:A:627:GLU:CG	1:A:644:VAL:HB	2.50	0.41
1:A:857:ASN:O	1:A:860:TYR:N	2.48	0.41
1:A:621:ASP:OD1	1:A:662:ARG:HD3	2.20	0.41
2:G:2007:C:O5'	2:G:2007:C:H6	2.02	0.41
1:A:418:PHE:CD1	1:A:476:LEU:HD22	2.55	0.41
1:A:523:VAL:HG12	1:A:542:GLY:HA2	2.02	0.41
1:A:83:VAL:HG21	1:A:128:GLU:CD	2.41	0.41
1:A:845:HIS:C	1:A:929:GLY:HA2	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:PHE:CD1	1:A:791:LEU:HD13	2.53	0.41
1:A:733:LEU:HD12	1:A:733:LEU:HA	1.79	0.41
1:A:735:TYR:CB	1:A:762:ILE:HG13	2.50	0.41
1:A:969:LEU:HD23	1:A:1076:THR:HA	2.03	0.41
1:A:285:MET:HB3	1:A:286:SER:H	1.68	0.41
1:A:172:HIS:CD2	1:A:172:HIS:C	2.93	0.41
1:A:806:ARG:C	1:A:808:ASP:H	2.24	0.41
1:A:148:HIS:HB3	1:A:152:ILE:CG2	2.46	0.41
1:A:97:LEU:O	1:A:101:VAL:HG23	2.21	0.41
1:A:1177:LYS:HB3	1:A:1177:LYS:HE3	1.92	0.41
1:A:154:VAL:HA	1:A:257:ILE:O	2.20	0.41
1:A:740:PHE:HD2	1:A:745:GLU:CG	2.32	0.41
1:A:1182:ILE:C	1:A:1182:ILE:HD12	2.40	0.41
1:A:558:ASN:CB	1:A:1210:ARG:HB3	2.51	0.41
1:A:380:ALA:O	1:A:381:ALA:HB2	2.21	0.41
1:A:779:GLY:C	1:A:781:ASP:N	2.74	0.41
1:A:657:LEU:O	1:A:673:VAL:HG22	2.21	0.41
1:A:13:ARG:HD2	1:A:20:MET:CE	2.50	0.41
1:A:835:ASP:OD1	1:A:835:ASP:N	2.54	0.41
1:A:130:ILE:O	1:A:130:ILE:HG13	2.15	0.41
1:A:1057:LEU:HB2	1:A:1058:PRO:CD	2.51	0.41
1:A:583:ILE:N	1:A:583:ILE:HD12	2.36	0.40
1:A:312:LEU:HD22	1:A:418:PHE:CD2	2.56	0.40
1:A:930:ILE:HD11	1:A:1021:TYR:CB	2.51	0.40
1:A:430:LEU:HD12	1:A:430:LEU:HA	1.86	0.40
1:A:630:GLU:HA	1:A:630:GLU:OE1	2.20	0.40
1:A:229:LEU:CD1	1:A:242:VAL:HG11	2.49	0.40
1:A:583:ILE:CG2	1:A:652:ALA:HB1	2.51	0.40
1:A:93:ALA:CA	1:A:96:VAL:HG12	2.44	0.40
1:A:163:GLU:CG	1:A:164:GLU:H	2.26	0.40
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.95	0.40
1:A:2:ALA:N	1:A:426:ASP:OD1	2.54	0.40
1:A:929:GLY:O	1:A:933:ILE:CG2	2.70	0.40
1:A:545:MET:CE	1:A:548:LYS:HE3	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1193/1289 (93%)	1079 (90%)	90 (8%)	24 (2%)	9	18

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	GLU
1	A	285	MET
1	A	325	GLY
1	A	806	ARG
1	A	972	ALA
1	A	34	ILE
1	A	68	GLY
1	A	188	ALA
1	A	223	PHE
1	A	350	SER
1	A	508	ARG
1	A	778	LEU
1	A	780	ILE
1	A	783	GLU
1	A	849	SER
1	A	962	ASN
1	A	104	LYS
1	A	813	PHE
1	A	187	SER
1	A	324	TYR
1	A	782	THR
1	A	201	ILE
1	A	357	PRO
1	A	531	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	995/1060 (94%)	852 (86%)	143 (14%)	4 7

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	7	SER
1	A	29	GLU
1	A	61	VAL
1	A	64	THR
1	A	76	VAL
1	A	79	GLN
1	A	80	THR
1	A	81	ASP
1	A	111	LEU
1	A	120	VAL
1	A	129	ASN
1	A	130	ILE
1	A	141	ASP
1	A	143	LEU
1	A	154	VAL
1	A	181	ILE
1	A	219	ARG
1	A	220	MET
1	A	241	THR
1	A	246	LEU
1	A	254	THR
1	A	258	ARG
1	A	285	MET
1	A	305	VAL
1	A	307	HIS
1	A	317	THR
1	A	355	ASP
1	A	364	VAL
1	A	371	ASP

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Mol	Chain	Res	Type
1	A	390	VAL
1	A	399	GLN
1	A	406	LEU
1	A	419	LEU
1	A	430	LEU
1	A	440	GLU
1	A	444	GLN
1	A	452	THR
1	A	456	ARG
1	A	460	LEU
1	A	480	LEU
1	A	504	SER
1	A	508	ARG
1	A	516	VAL
1	A	522	LYS
1	A	529	ILE
1	A	530	VAL
1	A	535	THR
1	A	539	THR
1	A	549	LEU
1	A	563	LEU
1	A	568	ARG
1	A	582	THR
1	A	587	THR
1	A	592	GLU
1	A	593	VAL
1	A	603	ARG
1	A	618	ARG
1	A	622	VAL
1	A	628	LEU
1	A	632	VAL
1	A	646	THR
1	A	666	ARG
1	A	676	VAL
1	A	705	LEU
1	A	715	THR
1	A	717	ILE
1	A	733	LEU
1	A	741	ASN
1	A	762	ILE
1	A	781	ASP
1	A	783	GLU

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Mol	Chain	Res	Type
1	A	785	VAL
1	A	789	LYS
1	A	791	LEU
1	A	799	LEU
1	A	800	THR
1	A	808	ASP
1	A	812	ASP
1	A	813	PHE
1	A	816	SER
1	A	832	LEU
1	A	833	ILE
1	A	835	ASP
1	A	836	VAL
1	A	847	ARG
1	A	848	PHE
1	A	854	THR
1	A	869	LEU
1	A	873	CYS
1	A	874	THR
1	A	887	SER
1	A	893	ARG
1	A	897	ILE
1	A	898	SER
1	A	901	ASN
1	A	905	THR
1	A	909	ASN
1	A	930	ILE
1	A	933	ILE
1	A	937	ARG
1	A	938	LEU
1	A	948	GLN
1	A	949	THR
1	A	950	ILE
1	A	951	ASN
1	A	961	THR
1	A	967	VAL
1	A	970	SER
1	A	976	ILE
1	A	984	LEU
1	A	991	GLU
1	A	996	LEU
1	A	1012	GLU

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Mol	Chain	Res	Type
1	A	1013	LYS
1	A	1021	TYR
1	A	1022	THR
1	A	1033	LEU
1	A	1035	ARG
1	A	1044	ASP
1	A	1049	THR
1	A	1053	ASP
1	A	1075	THR
1	A	1076	THR
1	A	1077	ASN
1	A	1089	GLU
1	A	1093	LYS
1	A	1102	THR
1	A	1111	VAL
1	A	1116	LEU
1	A	1128	THR
1	A	1150	LYS
1	A	1152	LEU
1	A	1173	ASN
1	A	1177	LYS
1	A	1182	ILE
1	A	1183	ARG
1	A	1193	ARG
1	A	1200	LEU
1	A	1207	LEU
1	A	1237	GLN
1	A	1246	LYS
1	A	1251	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	114	GLN
1	A	129	ASN
1	A	168	HIS
1	A	284	HIS
1	A	298	ASN
1	A	307	HIS
1	A	399	GLN
1	A	444	GLN

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Mol	Chain	Res	Type
1	A	558	ASN
1	A	640	ASN
1	A	714	ASN
1	A	729	ASN
1	A	741	ASN
1	A	763	ASN
1	A	857	ASN
1	A	862	HIS
1	A	871	GLN
1	A	901	ASN
1	A	909	ASN
1	A	948	GLN
1	A	1077	ASN
1	A	1094	HIS
1	A	1121	ASN
1	A	1122	ASN
1	A	1151	GLN
1	A	1155	ASN
1	A	1173	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	6/7 (85%)	2 (33%)	0
3	T	7/8 (87%)	2 (28%)	0
All	All	13/15 (86%)	4 (30%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	2003	C
2	G	2004	U
3	T	2103	G
3	T	2104	U

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 carbohydrates 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	21,29,29	2.21	3 (14%)	27,45,45	1.73	9 (33%)

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	-	0/18/34/34	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	C2'-C1'	-6.57	1.42	1.53
4	A	2501	CH1	C3'-C4'	-4.58	1.41	1.52
4	A	2501	CH1	C4-N4	4.83	1.49	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2501	CH1	C5-C4-N3	-2.53	118.61	121.80
4	A	2501	CH1	PB-O3B-PG	-2.16	125.42	132.67
4	A	2501	CH1	O4'-C4'-C3'	2.11	107.93	105.04
4	A	2501	CH1	O2B-PB-O3B	2.15	114.86	105.09
4	A	2501	CH1	O2B-PB-O3A	2.44	116.17	105.09
4	A	2501	CH1	O3G-PG-O3B	2.48	116.34	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2501	CH1	O3A-PA-O5'	2.83	110.44	102.94
4	A	2501	CH1	N4-C4-N3	2.85	121.70	116.50
4	A	2501	CH1	C2-N3-C4	3.26	120.21	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2501	CH1	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1203/1289 (93%)	-0.07	29 (2%) 62 56	16, 49, 97, 122	0
2	G	7/7 (100%)	-0.14	0 100 100	59, 76, 99, 105	0
3	T	8/8 (100%)	0.73	1 (12%) 5 3	45, 69, 117, 122	1 (12%)
All	All	1218/1304 (93%)	-0.07	30 (2%) 61 54	16, 50, 99, 122	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	700	SER	5.4
1	A	701	SER	5.3
1	A	189	GLU	4.7
1	A	8	LEU	4.7
1	A	193	LYS	4.5
1	A	680	ALA	3.8
1	A	204	GLN	3.4
1	A	292	ARG	3.3
1	A	162	ASP	2.9
1	A	267	LYS	2.8
1	A	291	GLU	2.8
1	A	274	ALA	2.8
1	A	199	LEU	2.7
1	A	202	ALA	2.6
1	A	320	LEU	2.5
1	A	163	GLU	2.5
1	A	43	LYS	2.5
1	A	15	ARG	2.5
1	A	285	MET	2.4
1	A	4	ILE	2.4
1	A	161	ALA	2.4
3	T	2102	G	2.3
1	A	807	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	702	ARG	2.2
1	A	279	MET	2.2
1	A	210	GLU	2.1
1	A	325	GLY	2.1
1	A	164	GLU	2.1
1	A	266	GLU	2.1
1	A	72	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CH1	A	2501	28/28	0.96	0.14	-0.51	35,48,53,57	0
5	CA	A	2502	1/1	0.99	0.17	-	31,31,31,31	0
5	CA	A	2503	1/1	0.92	0.20	-	53,53,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.