



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:01 PM GMT

PDB ID : 1N38
Title : reovirus polymerase lambda3 elongation complex with one phosphodiester bond formed
Authors : Tao, Y.; Farsetta, D.L.; Nibert, M.L.; Harrison, S.C.
Deposited on : 2002-10-25
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

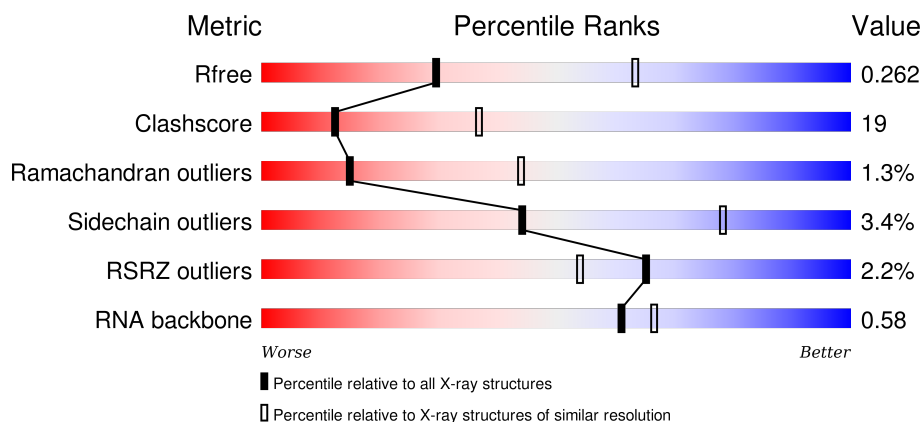
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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 ≥ 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	B	2	<div> <div>100%</div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	C	6	<div> <div>17%</div> <div>33%</div> <div>50%</div> <div>17%</div> </div>
3	A	1267	<div> <div>2%</div> <div>64%</div> <div>33%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	U3H	A	1291	X	-	-	-
6	CH1	A	1294	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10485 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*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	2	Total	C	N	O	P	0	0	0
			43	19	8	14	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	P	0	0	0
			105	47	17	36	5			

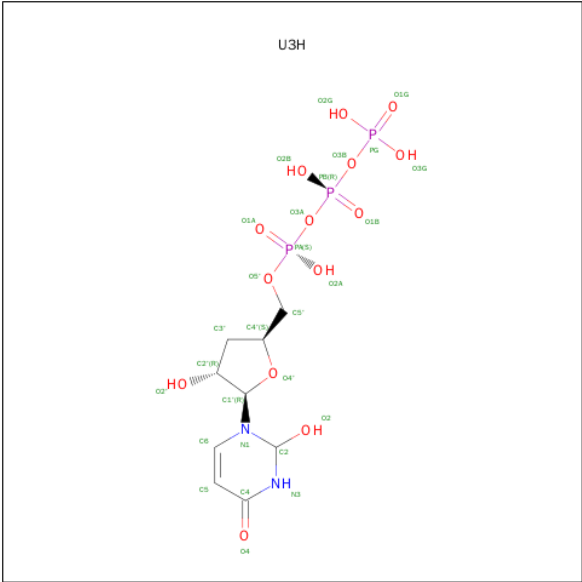
- Molecule 3 is a protein called Minor core protein lambda 3.

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

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

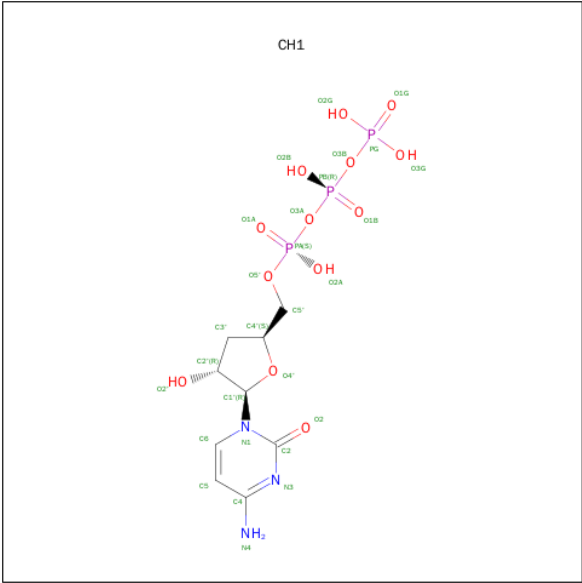
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

- Molecule 5 is 3'-DEOXY-URIDINE 5'-TRIPHOSPHATE (three-letter code: U3H) (formula: C₉H₁₇N₂O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			28	9	2	14	3		

- Molecule 6 is 3'-DEOXY-CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CH1) (formula: C₉H₁₆N₃O₁₃P₃).



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

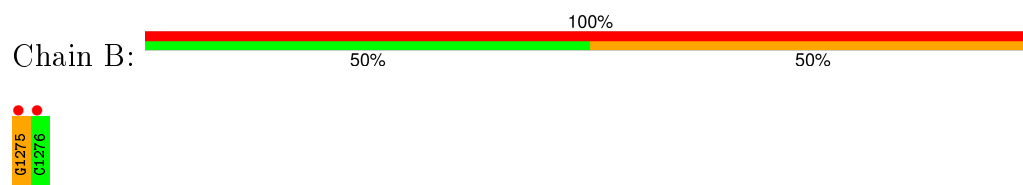
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	261	Total 261	O 261	0	0
7	B	2	Total 2	O 2	0	0
7	C	2	Total 2	O 2	0	0

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.

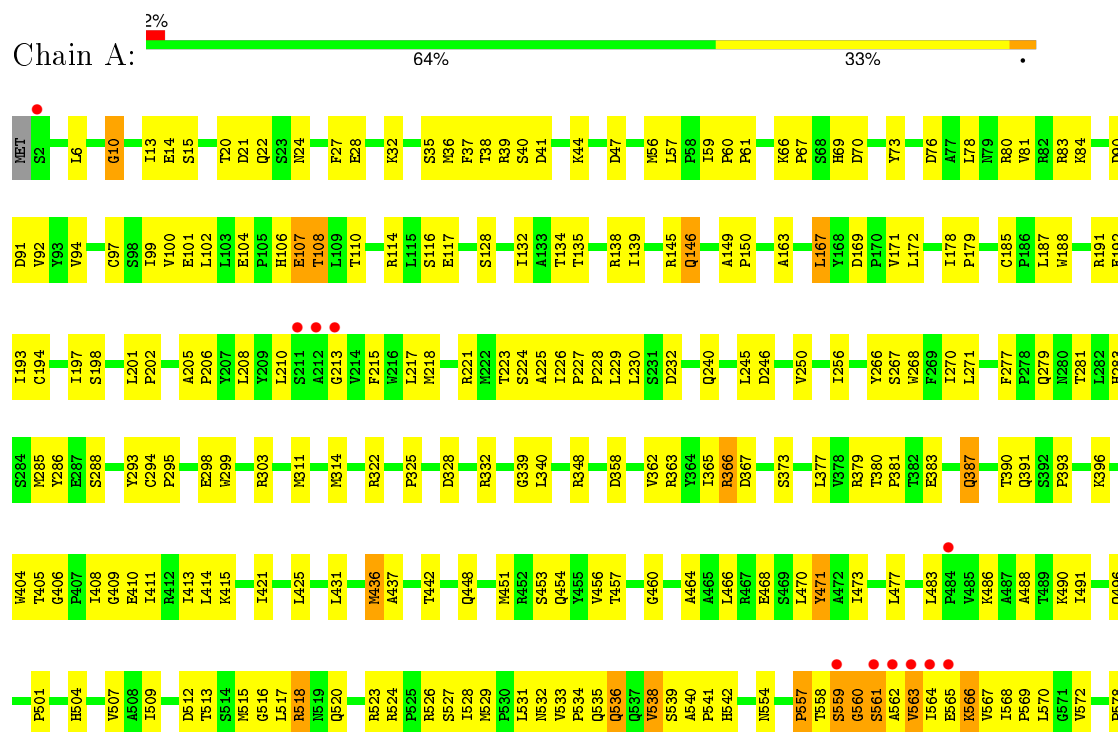
- Molecule 1: 5'-R(P*GP*C)-3'



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



- Molecule 3: Minor core protein lambda 3



T1232	S1101	E994	M867	D776	T685
A1237	T1102	E995	M868	G777	A686
V1238	F1106		M869	T778	T687
E1243	T1109	G999	V878	A779	S688
			K879	E780	T689
H1246	M1112	I1002	A880	Y781	E690
		I1003	F881	L782	
W1259	L1129	H1005	M886	L783	M698
	R1130	P1006		E784	M699
Q1262		P1007	M890	T785	E700
E1263	A1136		F891	F786	T701
G1264	A1143	P1012	M892	R787	F702
R1265	Q1144	P1013	F893	G788	L599
SER	L1145	E1022	T894	G789	S600
ALA	L1146	A1023	R907	Y798	M603
	M1147	I1024	P908	P799	
	L1150	A1025	L909	E804	T720
	Q1151	A1026	V915	R305	T724
		E1029		S809	T725
	V1167	M1034	V920		Q726
	M1168	D1035		E814	R727
	L1172	P915	R923	P915	N728
	A1173	M1039	T926	A816	E630
	R1174	R1040		I817	S631
	V1175	A1041	L940	L818	C731
	V1176	R1042	K941	D819	Q732
	M1177	R1043		E820	M633
		H1044	Q944	I821	M634
	P1181	S1045	M948	V829	V635
	D1182				R639
	T1183	L1052			P640
	W1184		R953	Q834	I641
	M1185	R1062		M835	S642
	S1186	M1063	K957	Q836	
		C1064		R837	Q645
	M1192	E1065	R960	M838	
			A961	I839	T648
	V1197	D1072		R940	G649
	K1198	L1073	R964	L845	T746
	L1199	R1074	E965	E946	L651
	L1200		V966	S750	M650
	P1201	L1077	R967	C947	L651
			E968		N748
	G1204	D1082	Q969	R851	N749
		P1083		T854	S652
	P1212	L1084	Y977	M855	M653
				I956	L654
	M1215	D1087	Q980	G957	
	G1216	P1088		R957	Y763
	W1217	F1089	E983	E858	G764
	L1218	L1090	L984	S959	E765
	R1219			V960	G670
		V1095	R987	G861	M671
	R1223			Y962	D772
				L863	I773
				S634	A774
				R900	Y775
					S682

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.72Å 85.21Å 248.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.67 – 2.80 46.67 – 2.49	Depositor EDS
% Data completeness (in resolution range)	85.6 (46.67-2.80) 85.7 (46.67-2.49)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.48Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.201 , 0.263 0.200 , 0.262	Depositor DCC
R_{free} test set	1973 reflections (6.03%)	DCC
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 52409 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10485	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, 0.375 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, MN, U3H

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	1.37	1/47 (2.1%)	1.06	0/69
2	C	0.89	0/116	0.75	0/178
3	A	0.40	0/10239	0.63	3/13905 (0.0%)
All	All	0.41	1/10402 (0.0%)	0.63	3/14152 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1275	G	OP3-P	-6.33	1.53	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	560	GLY	N-CA-C	-5.88	98.39	113.10
3	A	408	ILE	N-CA-C	-5.69	95.64	111.00
3	A	566	LYS	N-CA-C	-5.69	95.64	111.00

There are no chirality outliers.

There are no planarity outliers.

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	B	43	0	21	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	105	0	54	4	0
3	A	9986	0	9903	392	0
4	A	2	0	0	0	0
5	A	28	0	11	0	0
6	A	56	0	24	0	0
7	A	261	0	0	10	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
All	All	10485	0	10013	394	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 19.

All (394) 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:410:GLU:H	3:A:649:GLN:NE2	1.49	1.09
3:A:561:SER:HB3	3:A:566:LYS:HE3	1.34	1.07
3:A:223:THR:HG22	3:A:225:ALA:H	1.21	1.03
3:A:1005:ASN:HD21	3:A:1263:GLU:HB3	1.27	0.99
3:A:410:GLU:H	3:A:649:GLN:HE22	1.07	0.96
3:A:724:THR:HG22	3:A:726:GLN:H	1.31	0.95
3:A:563:VAL:O	3:A:564:ILE:HG22	1.69	0.92
3:A:557:PRO:HD2	3:A:731:CYS:O	1.74	0.86
3:A:81:VAL:H	3:A:671:ASN:HD21	1.22	0.85
3:A:561:SER:CB	3:A:566:LYS:HE3	2.06	0.85
3:A:78:LEU:HD12	3:A:80:ARG:NH2	1.91	0.85
3:A:363:ARG:HH22	3:A:834:GLN:HE22	1.24	0.85
3:A:743:THR:HG22	3:A:744:THR:H	1.41	0.83
3:A:104:GLU:HG3	3:A:116:SER:HA	1.60	0.83
3:A:749:ASN:HD21	3:A:751:GLU:HB3	1.45	0.81
3:A:1109:THR:HG22	3:A:1168:ASN:HD21	1.46	0.81
3:A:406:GLY:HA3	3:A:630:GLU:O	1.81	0.81
3:A:856:ILE:HB	3:A:859:SER:HB2	1.63	0.80
3:A:907:ARG:HB3	3:A:908:PRO:HD3	1.65	0.78
3:A:22:GLN:NE2	3:A:878:VAL:H	1.81	0.77
3:A:94:VAL:HG22	3:A:139:ILE:HG23	1.67	0.77
1:B:1275:G:N2	3:A:560:GLY:HA3	2.00	0.76
3:A:1004:HIS:C	3:A:1006:PRO:HD3	2.06	0.76
3:A:410:GLU:N	3:A:649:GLN:HE22	1.84	0.74
3:A:957:LYS:O	3:A:960:ARG:HG3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:410:GLU:N	3:A:649:GLN:NE2	2.33	0.72
3:A:1005:ASN:HB2	3:A:1130:ARG:HH22	1.54	0.72
3:A:566:LYS:HE2	3:A:782:LEU:O	1.88	0.72
3:A:1005:ASN:ND2	3:A:1263:GLU:HB3	2.03	0.72
3:A:814:TRP:HB3	3:A:815:PRO:HD3	1.72	0.71
3:A:146:GLN:HE22	3:A:805:ARG:H	1.37	0.71
3:A:578:PRO:HB2	3:A:742:GLY:HA3	1.72	0.71
3:A:532:ASN:OD1	3:A:535:GLN:HG3	1.91	0.71
3:A:564:ILE:HG12	3:A:1185:MET:O	1.90	0.71
3:A:564:ILE:HG21	3:A:1185:MET:HB3	1.71	0.71
3:A:1072:ASP:OD1	3:A:1074:ARG:HD3	1.91	0.71
3:A:22:GLN:HE21	3:A:878:VAL:H	1.39	0.70
3:A:167:LEU:HD23	3:A:837:ARG:HD2	1.72	0.70
3:A:393:PRO:HG3	3:A:592:SER:HA	1.73	0.69
3:A:815:PRO:HG2	3:A:1034:MET:CE	2.21	0.69
3:A:92:VAL:CG1	3:A:383:GLU:HB3	2.22	0.69
3:A:926:THR:HG21	3:A:1246:HIS:CG	2.28	0.69
3:A:540:ALA:HB3	3:A:541:PRO:HD3	1.74	0.69
3:A:572:VAL:HG13	3:A:789:GLY:O	1.93	0.68
3:A:570:LEU:HD21	3:A:730:VAL:HG21	1.74	0.68
3:A:193:ILE:HD13	3:A:229:LEU:HD21	1.75	0.68
3:A:56:MET:HG2	3:A:188:TRP:CE2	2.28	0.68
3:A:582:ILE:HG21	3:A:757:LEU:CD2	2.24	0.67
3:A:81:VAL:HG13	3:A:132:ILE:HD13	1.76	0.67
3:A:724:THR:HG22	3:A:726:GLN:N	2.07	0.67
3:A:582:ILE:HG21	3:A:757:LEU:HD21	1.77	0.67
3:A:776:ASP:OD1	3:A:778:THR:HB	1.94	0.67
3:A:915:VAL:HG13	3:A:920:VAL:HG22	1.77	0.66
3:A:743:THR:HG22	3:A:744:THR:N	2.10	0.66
3:A:279:GLN:HE21	3:A:283:HIS:HD2	1.43	0.66
3:A:114:ARG:HB2	3:A:215:PHE:CE1	2.31	0.66
3:A:227:PRO:HB2	3:A:228:PRO:HD3	1.76	0.66
3:A:171:VAL:HG11	3:A:1090:LEU:HD11	1.77	0.65
3:A:299:TRP:CD2	3:A:303:ARG:HG2	2.32	0.65
3:A:566:LYS:HD3	3:A:784:LEU:CD2	2.26	0.65
3:A:83:ARG:HG3	3:A:83:ARG:HH11	1.60	0.65
3:A:1064:CYS:HB3	3:A:1065:GLU:OE2	1.96	0.65
3:A:66:LYS:HB3	3:A:97:CYS:HA	1.78	0.64
3:A:90:ASP:O	3:A:92:VAL:N	2.29	0.64
3:A:779:ALA:HB3	3:A:786:PHE:HB2	1.79	0.64
3:A:448:GLN:NE2	3:A:620:MET:H	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:92:VAL:HG11	3:A:383:GLU:HB3	1.79	0.63
3:A:1201:PRO:HB2	3:A:1204:GLY:O	1.98	0.63
3:A:425:LEU:HB2	3:A:698:MET:HE1	1.81	0.63
3:A:855:MET:O	3:A:856:ILE:HD13	1.98	0.63
3:A:39:ARG:HH11	3:A:39:ARG:HG2	1.64	0.62
3:A:13:ILE:HD13	3:A:163:ALA:HB3	1.81	0.62
3:A:829:VAL:HG13	3:A:890:TRP:CE2	2.35	0.61
3:A:457:THR:O	3:A:491:ILE:HG13	1.99	0.61
3:A:281:THR:O	3:A:285:MET:HG2	2.00	0.61
3:A:819:ASP:OD1	3:A:953:ARG:NH1	2.35	0.60
3:A:1087:ASP:HB3	3:A:1088:PRO:HD3	1.83	0.60
3:A:1007:PRO:HD2	3:A:1144:GLN:NE2	2.15	0.60
3:A:104:GLU:CG	3:A:116:SER:HA	2.31	0.60
3:A:114:ARG:HB2	3:A:215:PHE:HE1	1.67	0.60
3:A:268:TRP:HB2	7:A:1352:HOH:O	2.01	0.60
3:A:536:GLN:NE2	3:A:685:THR:HG23	2.16	0.60
3:A:957:LYS:N	3:A:957:LYS:HD2	2.17	0.60
3:A:1176:VAL:O	3:A:1176:VAL:HG13	2.01	0.60
3:A:477:LEU:HB3	3:A:496:GLN:HB3	1.84	0.59
3:A:566:LYS:HD3	3:A:784:LEU:HD23	1.84	0.59
3:A:246:ASP:O	3:A:250:VAL:HG23	2.02	0.59
2:C:1286:C:OP1	3:A:454:GLN:HG3	2.03	0.59
3:A:451:MET:HA	3:A:451:MET:CE	2.32	0.59
3:A:855:MET:CE	3:A:858:GLU:H	2.16	0.59
3:A:995:TRP:CZ2	3:A:1006:PRO:HG3	2.38	0.59
3:A:984:LEU:O	3:A:987:ARG:HB2	2.03	0.59
3:A:538:VAL:HG13	3:A:651:LEU:HB2	1.85	0.58
3:A:379:ARG:HH12	3:A:387:GLN:NE2	2.00	0.58
3:A:194:CYS:SG	3:A:206:PRO:HG2	2.43	0.58
3:A:363:ARG:HH22	3:A:834:GLN:NE2	1.98	0.58
3:A:1219:ARG:O	3:A:1223:ARG:HG3	2.03	0.58
3:A:815:PRO:HG2	3:A:1034:MET:HE1	1.83	0.58
3:A:393:PRO:CG	3:A:592:SER:HA	2.34	0.58
3:A:38:THR:O	3:A:41:ASP:HB2	2.03	0.58
3:A:520:GLN:NE2	3:A:523:ARG:HD3	2.18	0.58
3:A:892:MET:HB2	3:A:1232:THR:HG23	1.86	0.58
3:A:542:HIS:NE2	3:A:690:GLU:HG3	2.19	0.58
3:A:293:TYR:CZ	3:A:1074:ARG:NH2	2.71	0.58
3:A:1112:MET:HE1	3:A:1150:LEU:HD11	1.85	0.58
3:A:1062:ARG:HG3	3:A:1243:GLU:HB2	1.86	0.57
3:A:957:LYS:HE3	3:A:1026:ALA:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:579:ASN:OD1	3:A:741:ASP:HA	2.04	0.57
2:C:1284:A:C5	3:A:528:ILE:HG12	2.39	0.57
3:A:595:TRP:HA	3:A:599:LEU:HB2	1.86	0.57
3:A:83:ARG:HG3	3:A:83:ARG:NH1	2.18	0.57
3:A:964:ARG:O	3:A:968:GLU:HG3	2.05	0.57
3:A:542:HIS:NE2	3:A:690:GLU:CG	2.68	0.57
3:A:990:ARG:HH11	3:A:994:GLU:CG	2.18	0.57
1:B:1275:G:O2'	3:A:561:SER:CB	2.53	0.56
3:A:595:TRP:CE2	3:A:600:SER:HB3	2.39	0.56
3:A:294:CYS:SG	3:A:314:MET:HB3	2.44	0.56
3:A:1112:MET:HE3	3:A:1150:LEU:HD21	1.87	0.56
3:A:107:GLU:O	3:A:108:THR:CB	2.53	0.56
3:A:456:VAL:HG21	3:A:977:TYR:CE2	2.41	0.56
3:A:1005:ASN:N	3:A:1006:PRO:HD3	2.19	0.56
3:A:926:THR:HG23	3:A:1246:HIS:CD2	2.41	0.56
3:A:814:TRP:O	3:A:817:ILE:HG22	2.05	0.55
3:A:1212:PRO:HB2	3:A:1215:MET:HB2	1.87	0.55
3:A:517:LEU:HD23	3:A:527:SER:HA	1.88	0.55
3:A:81:VAL:N	3:A:671:ASN:HD21	1.99	0.55
3:A:957:LYS:HE2	3:A:1024:ALA:O	2.07	0.55
3:A:167:LEU:HD21	3:A:840:ARG:CZ	2.36	0.55
3:A:1145:LEU:HB3	3:A:1150:LEU:HD22	1.89	0.55
3:A:40:SER:O	3:A:44:LYS:HG3	2.06	0.55
3:A:138:ARG:NH1	3:A:669:PRO:HG3	2.22	0.55
3:A:396:LYS:HD2	3:A:765:GLU:HB3	1.89	0.55
3:A:599:LEU:O	3:A:603:MET:HG2	2.07	0.54
3:A:585:ASP:HB3	3:A:772:ASP:HB3	1.87	0.54
3:A:784:LEU:HD12	3:A:786:PHE:CZ	2.42	0.54
3:A:1082:ASP:HB2	3:A:1083:PRO:CD	2.38	0.54
3:A:835:TRP:O	3:A:839:ILE:HG13	2.06	0.54
3:A:411:ILE:C	3:A:411:ILE:HD12	2.28	0.54
3:A:295:PRO:HD2	3:A:789:GLY:HA3	1.90	0.54
3:A:501:PRO:HD2	3:A:504:HIS:HD2	1.72	0.53
3:A:14:GLU:C	3:A:20:THR:HG22	2.28	0.53
3:A:1062:ARG:HD2	3:A:1243:GLU:OE2	2.08	0.53
3:A:76:ASP:OD2	3:A:80:ARG:NH1	2.40	0.53
3:A:565:GLU:OE1	3:A:565:GLU:HA	2.07	0.53
3:A:285:MET:HG3	3:A:365:ILE:HD11	1.90	0.53
3:A:114:ARG:HG3	3:A:114:ARG:HH11	1.74	0.53
3:A:1172:LEU:HD21	3:A:1217:TRP:HA	1.89	0.53
3:A:188:TRP:CZ2	3:A:192:GLU:HG3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:855:MET:HE1	3:A:858:GLU:H	1.74	0.53
3:A:965:GLU:O	3:A:969:GLN:HG3	2.08	0.53
3:A:464:ALA:O	3:A:468:GLU:HG2	2.09	0.52
3:A:210:LEU:HB2	3:A:213:GLY:O	2.10	0.52
1:B:1275:G:H5'	7:A:1539:HOH:O	2.08	0.52
3:A:32:LYS:O	3:A:36:MET:HG3	2.10	0.52
3:A:564:ILE:HG13	3:A:1102:THR:HG23	1.92	0.52
3:A:757:LEU:HD22	3:A:773:ILE:HG21	1.92	0.52
3:A:536:GLN:HA	3:A:536:GLN:HE21	1.74	0.52
3:A:135:THR:OG1	3:A:668:SER:HA	2.10	0.52
3:A:881:PHE:O	3:A:909:LEU:HD12	2.10	0.52
3:A:529:MET:O	3:A:683:GLY:HA3	2.10	0.52
3:A:784:LEU:HB3	3:A:786:PHE:CE2	2.46	0.51
3:A:73:TYR:HB2	3:A:132:ILE:HG23	1.92	0.51
3:A:829:VAL:HG13	3:A:890:TRP:NE1	2.26	0.51
3:A:409:GLY:HA3	3:A:627:VAL:HG21	1.92	0.51
3:A:926:THR:CG2	3:A:1246:HIS:CG	2.93	0.51
3:A:15:SER:N	3:A:20:THR:HG22	2.26	0.51
3:A:1182:ASP:O	3:A:1185:MET:HG2	2.11	0.51
3:A:561:SER:O	3:A:562:ALA:HB3	2.11	0.51
3:A:24:ASN:O	3:A:28:GLU:HG3	2.10	0.51
3:A:47:ASP:HA	3:A:191:ARG:HH11	1.76	0.51
3:A:1029:GLU:N	3:A:1029:GLU:OE1	2.41	0.51
3:A:1065:GLU:CD	3:A:1065:GLU:H	2.12	0.50
3:A:581:SER:HA	3:A:738:MET:O	2.12	0.50
3:A:854:THR:HG21	3:A:863:LEU:HG	1.92	0.50
3:A:814:TRP:O	3:A:815:PRO:C	2.48	0.50
3:A:990:ARG:HH11	3:A:994:GLU:HG3	1.77	0.50
3:A:457:THR:C	3:A:491:ILE:HG13	2.32	0.50
3:A:948:MET:HE1	3:A:1042:ARG:HG3	1.94	0.50
3:A:94:VAL:HG22	3:A:139:ILE:CG2	2.38	0.50
3:A:486:LYS:HE2	3:A:488:ALA:HB3	1.93	0.50
3:A:294:CYS:HB2	3:A:788:PHE:O	2.12	0.49
3:A:146:GLN:NE2	3:A:805:ARG:H	2.09	0.49
3:A:1150:LEU:HD12	3:A:1150:LEU:N	2.27	0.49
3:A:201:LEU:HD13	3:A:217:LEU:HD11	1.94	0.49
3:A:749:ASN:ND2	3:A:751:GLU:HB3	2.21	0.49
3:A:83:ARG:HG2	3:A:92:VAL:HA	1.93	0.49
3:A:509:ILE:HD13	3:A:538:VAL:HG21	1.94	0.49
3:A:542:HIS:HE2	3:A:690:GLU:CG	2.25	0.49
3:A:21:ASP:OD1	3:A:879:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:743:THR:CG2	3:A:744:THR:H	2.19	0.49
1:B:1275:G:H21	3:A:560:GLY:HA3	1.75	0.49
3:A:829:VAL:HG22	3:A:890:TRP:CD2	2.48	0.49
3:A:436:MET:C	3:A:436:MET:HE2	2.33	0.49
3:A:856:ILE:HB	3:A:859:SER:CB	2.39	0.49
3:A:990:ARG:NH1	3:A:994:GLU:CG	2.75	0.49
3:A:198:SER:HA	3:A:217:LEU:HD21	1.95	0.49
3:A:80:ARG:HA	3:A:671:ASN:ND2	2.28	0.48
3:A:145:ARG:O	3:A:805:ARG:HD2	2.13	0.48
3:A:299:TRP:CE2	3:A:303:ARG:HG2	2.49	0.48
3:A:39:ARG:CG	3:A:39:ARG:HH11	2.26	0.48
3:A:1095:VAL:HG23	3:A:1237:ALA:HB2	1.94	0.48
3:A:999:GLY:HA2	3:A:1002:ILE:HD12	1.96	0.48
3:A:409:GLY:HA3	3:A:649:GLN:NE2	2.29	0.48
3:A:740:ILE:N	3:A:740:ILE:HD12	2.29	0.48
3:A:107:GLU:O	3:A:108:THR:HB	2.13	0.48
3:A:1052:LEU:HD22	3:A:1259:TRP:CE2	2.48	0.48
3:A:654:LEU:HD21	3:A:659:PHE:CE1	2.49	0.48
3:A:815:PRO:HB2	3:A:953:ARG:O	2.13	0.48
3:A:582:ILE:HG21	3:A:757:LEU:HD22	1.95	0.48
3:A:1082:ASP:OD1	3:A:1084:LEU:HB2	2.14	0.48
3:A:436:MET:O	3:A:436:MET:HE2	2.14	0.48
3:A:805:ARG:HG2	3:A:805:ARG:HH11	1.79	0.48
3:A:524:ARG:HG2	3:A:524:ARG:HH11	1.78	0.48
3:A:1143:ALA:O	3:A:1147:MET:HG3	2.14	0.48
3:A:1002:ILE:HD13	3:A:1136:ALA:HB2	1.95	0.47
3:A:473:ILE:HG21	3:A:507:VAL:HG11	1.95	0.47
3:A:821:ILE:HG23	3:A:845:LEU:HD13	1.94	0.47
3:A:149:ALA:HB1	3:A:150:PRO:CD	2.44	0.47
3:A:523:ARG:HG2	3:A:524:ARG:N	2.29	0.47
3:A:332:ARG:HH11	3:A:332:ARG:HG2	1.79	0.47
3:A:279:GLN:NE2	3:A:283:HIS:HD2	2.12	0.47
3:A:232:ASP:OD2	3:A:266:TYR:OH	2.25	0.47
3:A:76:ASP:OD2	3:A:80:ARG:HG3	2.15	0.47
3:A:983:GLU:O	3:A:987:ARG:HG3	2.14	0.47
3:A:863:LEU:HD11	3:A:1035:ASP:HB3	1.96	0.47
3:A:558:THR:O	3:A:559:SER:HB3	2.14	0.47
3:A:256:ILE:HD12	3:A:277:PHE:CE2	2.50	0.47
3:A:358:ASP:O	3:A:362:VAL:HG22	2.14	0.47
3:A:104:GLU:HG3	3:A:116:SER:CA	2.40	0.47
3:A:957:LYS:HD3	3:A:1022:GLU:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:197:ILE:O	3:A:221:ARG:NH1	2.47	0.47
3:A:460:GLY:O	3:A:490:LYS:NZ	2.42	0.47
3:A:940:LEU:O	3:A:941:LYS:HB2	2.15	0.47
3:A:531:LEU:HD12	3:A:684:SER:HA	1.97	0.47
3:A:410:GLU:H	3:A:649:GLN:HE21	1.53	0.47
3:A:568:ILE:N	3:A:569:PRO:CD	2.78	0.47
3:A:366:ARG:NH1	3:A:367:ASP:OD1	2.44	0.47
3:A:533:VAL:HB	3:A:534:PRO:HD3	1.97	0.47
3:A:603:MET:HE3	3:A:648:ILE:HG23	1.96	0.47
3:A:1192:MET:O	3:A:1197:VAL:HG23	2.15	0.47
3:A:377:LEU:N	3:A:377:LEU:HD12	2.30	0.47
3:A:240:GLN:HA	3:A:245:LEU:HB2	1.97	0.47
3:A:1199:LEU:HD12	3:A:1219:ARG:HD3	1.97	0.46
3:A:554:ASN:HB2	7:A:1385:HOH:O	2.16	0.46
3:A:512:ASP:OD2	3:A:662:ARG:NH2	2.41	0.46
3:A:557:PRO:HG3	3:A:781:TYR:OH	2.15	0.46
3:A:437:ALA:HB2	3:A:610:VAL:HG22	1.98	0.46
3:A:567:VAL:HG12	3:A:567:VAL:O	2.15	0.46
3:A:67:PRO:O	3:A:97:CYS:HB3	2.16	0.46
3:A:536:GLN:HE22	3:A:685:THR:H	1.63	0.46
3:A:523:ARG:HG2	3:A:523:ARG:HH11	1.81	0.46
3:A:603:MET:HE3	3:A:652:SER:OG	2.15	0.46
3:A:114:ARG:HG3	3:A:114:ARG:NH1	2.30	0.46
3:A:390:THR:HG22	3:A:391:GLN:N	2.30	0.46
3:A:541:PRO:HB2	3:A:648:ILE:HD11	1.98	0.46
3:A:436:MET:CE	3:A:437:ALA:HA	2.46	0.46
3:A:1012:VAL:HB	3:A:1013:PRO:HD3	1.97	0.46
3:A:513:THR:HG21	3:A:529:MET:HG2	1.98	0.46
3:A:100:VAL:HG13	3:A:101:GLU:N	2.31	0.46
3:A:566:LYS:HD3	3:A:784:LEU:HD21	1.98	0.46
3:A:139:ILE:HD13	3:A:380:THR:HG22	1.98	0.46
3:A:92:VAL:HG13	3:A:383:GLU:CG	2.45	0.46
3:A:1112:MET:CE	3:A:1150:LEU:HD11	2.45	0.46
3:A:863:LEU:HD21	3:A:1039:MET:HB2	1.98	0.46
3:A:606:ILE:O	3:A:610:VAL:HB	2.16	0.46
3:A:700:GLU:HB2	3:A:725:ILE:HD13	1.96	0.45
3:A:516:GLY:HA3	3:A:528:ILE:HG22	1.97	0.45
2:C:1284:A:N3	3:A:683:GLY:HA2	2.31	0.45
3:A:128:SER:O	3:A:132:ILE:HG12	2.15	0.45
3:A:380:THR:HG23	7:A:1435:HOH:O	2.16	0.45
3:A:57:LEU:HD22	3:A:185:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:15:SER:HA	3:A:20:THR:O	2.17	0.45
3:A:557:PRO:HG2	3:A:732:GLN:HB2	1.99	0.45
3:A:81:VAL:H	3:A:671:ASN:ND2	2.01	0.45
3:A:926:THR:CG2	3:A:1246:HIS:CD2	2.99	0.45
3:A:815:PRO:HG2	3:A:1034:MET:HE3	1.96	0.45
3:A:814:TRP:O	3:A:816:ALA:N	2.50	0.45
3:A:101:GLU:HG2	3:A:102:LEU:HG	1.99	0.45
3:A:743:THR:CG2	3:A:744:THR:N	2.79	0.45
3:A:886:TRP:HA	7:A:1442:HOH:O	2.17	0.44
3:A:169:ASP:HB3	3:A:172:LEU:HB2	1.99	0.44
3:A:1007:PRO:HD2	3:A:1144:GLN:CD	2.37	0.44
3:A:69:HIS:CG	3:A:70:ASP:N	2.85	0.44
3:A:990:ARG:NH1	3:A:994:GLU:CD	2.70	0.44
3:A:1177:ASN:ND2	3:A:1259:TRP:HH2	2.14	0.44
3:A:944:GLN:CD	3:A:944:GLN:H	2.19	0.44
3:A:560:GLY:O	3:A:561:SER:OG	2.29	0.44
3:A:580:GLN:OE1	3:A:747:LYS:HB2	2.17	0.44
3:A:104:GLU:CD	3:A:117:GLU:H	2.21	0.44
3:A:948:MET:HE2	3:A:1042:ARG:HA	2.00	0.44
3:A:724:THR:H	3:A:728:ASN:HD22	1.65	0.44
3:A:1109:THR:HG22	3:A:1168:ASN:ND2	2.23	0.44
3:A:396:LYS:HB2	3:A:765:GLU:O	2.17	0.44
3:A:483:LEU:HD21	3:A:967:ARG:HA	1.99	0.44
3:A:339:GLY:O	3:A:340:LEU:HD23	2.17	0.44
3:A:381:PRO:HD2	3:A:665:ASP:OD1	2.17	0.44
3:A:59:ILE:HA	3:A:60:PRO:HD3	1.89	0.44
3:A:855:MET:HE3	3:A:857:GLY:H	1.81	0.44
3:A:523:ARG:NH1	3:A:524:ARG:O	2.50	0.44
3:A:194:CYS:SG	3:A:206:PRO:CG	3.06	0.43
3:A:60:PRO:HA	3:A:61:PRO:HD3	1.89	0.43
3:A:539:SER:HA	3:A:651:LEU:HD22	2.00	0.43
3:A:829:VAL:HG22	3:A:890:TRP:CE3	2.53	0.43
3:A:1082:ASP:HB2	3:A:1083:PRO:HD2	1.99	0.43
3:A:821:ILE:HD12	3:A:845:LEU:HD13	2.01	0.43
3:A:421:ILE:HD12	3:A:421:ILE:HA	1.86	0.43
3:A:501:PRO:HD2	3:A:504:HIS:CD2	2.53	0.43
3:A:836:GLN:NE2	3:A:886:TRP:CD1	2.87	0.43
3:A:298:GLU:HB2	3:A:311:MET:CE	2.48	0.43
3:A:1063:MET:HG2	3:A:1238:VAL:HG11	2.00	0.43
3:A:863:LEU:HD11	3:A:1035:ASP:CB	2.48	0.43
3:A:855:MET:SD	3:A:860:VAL:HG22	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:193:ILE:O	3:A:197:ILE:HG13	2.19	0.43
3:A:27:PHE:CE1	3:A:847:CYS:HB2	2.53	0.43
1:B:1275:G:H21	3:A:560:GLY:CA	2.32	0.42
1:B:1275:G:O2'	3:A:561:SER:HB2	2.18	0.42
3:A:13:ILE:HD13	3:A:163:ALA:CB	2.47	0.42
3:A:1129:LEU:HD21	3:A:1167:VAL:HG21	2.01	0.42
3:A:223:THR:HG22	3:A:224:SER:N	2.34	0.42
3:A:688:SER:HA	7:A:1567:HOH:O	2.18	0.42
3:A:1100:GLN:CG	3:A:1101:SER:N	2.81	0.42
3:A:851:ARG:HH11	3:A:864:GLN:HE21	1.67	0.42
3:A:78:LEU:HD23	3:A:78:LEU:HA	1.77	0.42
2:C:1285:G:O2'	2:C:1286:C:H5'	2.18	0.42
3:A:907:ARG:CB	3:A:908:PRO:HD3	2.41	0.42
3:A:146:GLN:NE2	3:A:804:GLU:HA	2.35	0.42
3:A:404:TRP:O	3:A:415:LYS:HE3	2.19	0.42
3:A:286:TYR:C	3:A:288:SER:N	2.67	0.42
3:A:716:VAL:HG12	3:A:720:MET:CE	2.49	0.42
3:A:1174:ARG:HB2	7:A:1335:HOH:O	2.17	0.42
3:A:245:LEU:CD2	3:A:367:ASP:HA	2.50	0.42
3:A:518:ARG:HG2	3:A:804:GLU:OE2	2.20	0.42
3:A:995:TRP:HZ2	3:A:1006:PRO:HG3	1.84	0.42
3:A:1102:THR:O	3:A:1106:PHE:HD2	2.03	0.42
3:A:564:ILE:HD13	3:A:1186:SER:HA	2.01	0.42
3:A:523:ARG:HG3	7:A:1437:HOH:O	2.20	0.42
3:A:366:ARG:NH2	7:A:1323:HOH:O	2.51	0.42
3:A:271:LEU:HD13	3:A:377:LEU:CD2	2.49	0.42
3:A:1040:ARG:HG3	3:A:1043:ARG:NH2	2.35	0.42
3:A:814:TRP:CE3	3:A:815:PRO:HG3	2.55	0.42
3:A:814:TRP:CB	3:A:815:PRO:HD3	2.45	0.42
3:A:814:TRP:CG	3:A:815:PRO:N	2.84	0.42
3:A:332:ARG:NH1	3:A:332:ARG:HG2	2.34	0.42
3:A:632:VAL:HB	3:A:635:VAL:HB	2.01	0.42
3:A:381:PRO:HG3	3:A:517:LEU:CD1	2.50	0.42
3:A:381:PRO:HB3	3:A:515:MET:SD	2.60	0.42
3:A:201:LEU:HA	3:A:202:PRO:HD3	1.79	0.42
3:A:836:GLN:HG2	3:A:886:TRP:CE3	2.54	0.42
3:A:436:MET:CE	3:A:442:THR:HG21	2.50	0.41
3:A:1181:PRO:HD2	3:A:1184:TRP:CE3	2.55	0.41
3:A:754:GLN:HE21	3:A:775:TYR:HD2	1.68	0.41
3:A:39:ARG:HE	3:A:208:LEU:HD22	1.85	0.41
3:A:520:GLN:NE2	3:A:526:ARG:NH1	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:328:ASP:HA	3:A:348:ARG:CZ	2.50	0.41
3:A:1262:GLN:HG2	3:A:1265:ARG:NH1	2.35	0.41
3:A:797:ARG:C	3:A:799:PRO:HD3	2.41	0.41
3:A:6:LEU:O	3:A:10:GLY:N	2.51	0.41
3:A:857:GLY:C	3:A:859:SER:H	2.21	0.41
3:A:393:PRO:HG3	3:A:591:ALA:O	2.20	0.41
3:A:867:MET:HG3	3:A:868:TRP:N	2.35	0.41
3:A:139:ILE:HA	3:A:139:ILE:HD12	1.91	0.41
3:A:167:LEU:CD2	3:A:837:ARG:HD2	2.47	0.41
3:A:702:PHE:HB2	3:A:763:TYR:CE2	2.55	0.41
3:A:1052:LEU:HD13	3:A:1259:TRP:CG	2.56	0.41
3:A:706:TRP:O	3:A:707:GLY:C	2.59	0.41
3:A:1007:PRO:HD2	3:A:1144:GLN:HE22	1.82	0.41
3:A:106:HIS:CE1	3:A:108:THR:HB	2.55	0.41
3:A:226:ILE:O	3:A:230:LEU:HG	2.21	0.41
3:A:778:THR:CG2	3:A:779:ALA:N	2.83	0.41
3:A:223:THR:CG2	3:A:224:SER:N	2.84	0.41
3:A:603:MET:CE	3:A:648:ILE:HG23	2.51	0.41
3:A:642:SER:OG	3:A:645:GLN:HG3	2.21	0.41
3:A:471:TYR:CD1	3:A:471:TYR:C	2.94	0.41
3:A:270:ILE:HD12	3:A:373:SER:HB2	2.02	0.41
3:A:470:LEU:CD2	3:A:477:LEU:HD21	2.51	0.41
3:A:322:ARG:NH1	3:A:325:PRO:O	2.42	0.41
3:A:797:ARG:HB3	7:A:1539:HOH:O	2.21	0.40
3:A:39:ARG:NH1	3:A:39:ARG:CG	2.84	0.40
3:A:205:ALA:HA	3:A:206:PRO:HD3	1.80	0.40
3:A:855:MET:HE3	3:A:858:GLU:H	1.84	0.40
3:A:1005:ASN:N	3:A:1006:PRO:CD	2.84	0.40
3:A:92:VAL:HG13	3:A:383:GLU:HG3	2.03	0.40
3:A:603:MET:HE1	3:A:651:LEU:HD23	2.03	0.40
3:A:279:GLN:HE21	3:A:283:HIS:CD2	2.30	0.40
3:A:536:GLN:HA	3:A:536:GLN:NE2	2.36	0.40
3:A:686:ALA:O	3:A:690:GLU:HB2	2.22	0.40
3:A:149:ALA:HB1	3:A:150:PRO:HD2	2.04	0.40
3:A:639:ARG:HA	3:A:640:PRO:HD3	1.85	0.40
3:A:405:THR:HG23	3:A:413:ILE:O	2.21	0.40
3:A:178:ILE:HA	3:A:179:PRO:HD3	1.95	0.40
3:A:564:ILE:HA	3:A:568:ILE:HG13	2.03	0.40
3:A:134:THR:CG2	3:A:669:PRO:HG2	2.52	0.40
3:A:783:LYS:HD2	3:A:797:ARG:NE	2.37	0.40
3:A:854:THR:HG21	3:A:863:LEU:CD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	1262/1267 (100%)	1162 (92%)	84 (7%)	16 (1%)	15	44

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	91	ASP
3	A	108	THR
3	A	561	SER
3	A	563	VAL
3	A	814	TRP
3	A	687	THR
3	A	110	THR
3	A	559	SER
3	A	10	GLY
3	A	146	GLN
3	A	557	PRO
3	A	815	PRO
3	A	218	MET
3	A	635	VAL
3	A	1005	ASN
3	A	99	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	1081/1083 (100%)	1044 (97%)	37 (3%)	44 78

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

Mol	Chain	Res	Type
3	A	35	SER
3	A	37	PHE
3	A	84	LYS
3	A	107	GLU
3	A	167	LEU
3	A	187	LEU
3	A	267	SER
3	A	366	ARG
3	A	387	GLN
3	A	414	LEU
3	A	431	LEU
3	A	436	MET
3	A	453	SER
3	A	466	LEU
3	A	471	TYR
3	A	518	ARG
3	A	536	GLN
3	A	538	VAL
3	A	735	ASP
3	A	784	LEU
3	A	809	SER
3	A	845	LEU
3	A	890	TRP
3	A	894	THR
3	A	909	LEU
3	A	923	ARG
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	1151	GLN
3	A	1176	VAL
3	A	1238	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	22	GLN
3	A	121	ASN
3	A	146	GLN
3	A	283	HIS
3	A	296	ASN
3	A	387	GLN
3	A	448	GLN
3	A	474	ASN
3	A	504	HIS
3	A	520	GLN
3	A	536	GLN
3	A	649	GLN
3	A	664	ASN
3	A	671	ASN
3	A	675	HIS
3	A	728	ASN
3	A	749	ASN
3	A	754	GLN
3	A	834	GLN
3	A	864	GLN
3	A	980	GLN
3	A	1004	HIS
3	A	1005	ASN
3	A	1165	GLN
3	A	1246	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	0/2	-	-
2	C	4/6 (66%)	0	0
All	All	4/8 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	U3H	A	1291	4	24,29,29	2.79	4 (16%)	24,45,45	3.33	14 (58%)
6	CH1	A	1294	-	21,29,29	1.17	0	27,45,45	3.07	11 (40%)
6	CH1	A	1295	-	21,29,29	1.08	1 (4%)	27,45,45	2.97	11 (40%)

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	U3H	A	1291	4	1/1/9/12	0/22/47/47	0/2/2/2
6	CH1	A	1294	-	-	0/18/34/34	0/2/2/2
6	CH1	A	1295	-	-	0/18/34/34	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1291	U3H	O2-C2	-9.46	1.23	1.40
5	A	1291	U3H	C2-N3	-4.21	1.39	1.46
6	A	1295	CH1	C6-N1	2.31	1.39	1.35
5	A	1291	U3H	C4-N3	3.96	1.40	1.34
5	A	1291	U3H	C2-N1	6.14	1.63	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1295	CH1	O3G-PG-O1G	-9.25	80.79	110.58
6	A	1294	CH1	O3G-PG-O1G	-8.91	81.88	110.58
5	A	1291	U3H	O3G-PG-O1G	-7.30	87.09	110.58
6	A	1294	CH1	C3'-C4'-C5'	-5.16	104.65	113.91
6	A	1294	CH1	O3G-PG-O2G	-5.16	87.74	107.38
6	A	1295	CH1	O3G-PG-O2G	-5.04	88.20	107.38
6	A	1294	CH1	O3G-PG-O3B	-4.95	82.63	105.09
6	A	1295	CH1	O3G-PG-O3B	-4.83	83.19	105.09
5	A	1291	U3H	O3G-PG-O3B	-4.24	85.85	105.09
5	A	1291	U3H	O3G-PG-O2G	-4.18	91.46	107.38
6	A	1295	CH1	C3'-C4'-C5'	-3.98	106.77	113.91
6	A	1294	CH1	C6-N1-C2	-3.78	115.16	121.28
5	A	1291	U3H	O4-C4-N3	-3.68	119.17	121.97
6	A	1295	CH1	PB-O3A-PA	-3.59	122.65	132.73
5	A	1291	U3H	PB-O3A-PA	-3.55	122.77	132.73
6	A	1295	CH1	C6-N1-C2	-3.52	115.57	121.28
6	A	1294	CH1	PB-O3A-PA	-3.51	122.86	132.73
6	A	1294	CH1	PB-O3B-PG	-3.13	122.19	132.67
6	A	1295	CH1	PB-O3B-PG	-2.78	123.34	132.67
5	A	1291	U3H	C3'-C4'-C5'	-2.65	109.15	113.91
5	A	1291	U3H	PB-O3B-PG	-2.64	123.82	132.67
5	A	1291	U3H	O2G-PG-O3B	2.12	114.70	105.09
6	A	1295	CH1	O4'-C1'-N1	2.18	112.69	108.08
5	A	1291	U3H	O2A-PA-O3A	2.25	115.30	105.09
5	A	1291	U3H	O2B-PB-O3B	2.30	115.55	105.09
6	A	1295	CH1	O2G-PG-O1G	2.57	118.86	110.58
6	A	1294	CH1	O4'-C1'-N1	2.63	113.62	108.08
6	A	1294	CH1	O2G-PG-O1G	2.63	119.06	110.58
5	A	1291	U3H	O2G-PG-O1G	3.10	120.55	110.58
6	A	1295	CH1	O4'-C4'-C5'	3.14	114.18	109.54
6	A	1295	CH1	C2-N3-C4	3.55	120.61	115.61
6	A	1294	CH1	O4'-C4'-C5'	3.55	114.78	109.54
6	A	1294	CH1	C2-N3-C4	3.72	120.86	115.61
5	A	1291	U3H	O4'-C4'-C3'	3.78	110.21	105.04
5	A	1291	U3H	C1'-N1-C6	4.37	133.97	120.37
5	A	1291	U3H	O4'-C4'-C5'	8.69	122.37	109.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1291	U3H	C2

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	2/2 (100%)	4.70	2 (100%) 0 0	96, 96, 96, 122	0
2	C	5/6 (83%)	1.14	1 (20%) 1 1	23, 41, 71, 74	0
3	A	1264/1267 (99%)	-0.33	25 (1%) 68 58	7, 21, 44, 85	0
All	All	1271/1275 (99%)	-0.31	28 (2%) 65 54	7, 21, 45, 122	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	2	SER	8.4
1	B	1275	G	6.1
3	A	858	GLU	5.3
2	C	1286	C	4.6
3	A	562	ALA	4.5
3	A	561	SER	4.3
3	A	856	ILE	4.2
3	A	744	THR	3.6
3	A	859	SER	3.5
3	A	857	GLY	3.5
3	A	563	VAL	3.4
1	B	1276	C	3.3
3	A	855	MET	3.3
3	A	633	VAL	3.2
3	A	565	GLU	3.0
3	A	746	GLY	2.9
3	A	564	ILE	2.7
3	A	559	SER	2.7
3	A	860	VAL	2.6
3	A	748	VAL	2.5
3	A	212	ALA	2.5
3	A	211	SER	2.4
3	A	961	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	755	ASN	2.2
3	A	862	TYR	2.2
3	A	484	PRO	2.2
3	A	213	GLY	2.1
3	A	968	GLU	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, 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	LLDF	B-factors(Å ²)	Q<0.9
6	CH1	A	1294	28/28	0.47	0.58	3.90	98,112,132,132	0
5	U3H	A	1291	28/28	0.81	0.26	1.26	82,88,95,95	0
6	CH1	A	1295	28/28	0.86	0.22	-0.30	48,61,74,75	0
4	MN	A	1301	1/1	0.94	0.07	-2.31	63,63,63,63	0
4	MN	A	1302	1/1	0.96	0.12	-	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.