

# Full wwPDB X-ray Structure Validation Report (i)

#### Feb 3, 2024 – 09:44 PM EST

PDB ID	:	1N38
Title	:	reovirus polymerase lambda3 elongation complex with one phosphodiester
		bond formed
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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 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	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:  $X\text{-}RAY \, DIFFRACTION$ 

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 <sub>free</sub>	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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	Qu	Quality of chain							
				100%							
1	В	2	50%	50	0%						
			17%								
2	С	6	33%	50%	17%						
			2%								
3	А	1267	64%		33% •						

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	А	1291	Х	-	-	-
6	CH1	А	1294	-	-	-	Х



## 2 Entry composition (i)

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	В	9	Total	С	Ν	Ο	Р	0	0	0
I D	D	2	43	19	8	14	2	0		

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

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

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

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

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

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

• Molecule 5 is 3'-DEOXY-URIDINE 5'-TRIPHOSPHATE (three-letter code: U3H) (formula:  $C_9H_{17}N_2O_{14}P_3$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
Б	5 1	1	Total	С	Ν	Ο	Р	0	0
D A	A	A 1	28	9	2	14	3	0	0

• Molecule 6 is 3'-DEOXY-CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CH1) (formula:  $C_9H_{16}N_3O_{13}P_3$ ).



Mol	Chain	Residues		At	oms		ZeroOcc	AltConf		
6	Λ	1	Total	С	Ν	Ο	Р	0	0	
0 A	1	28	9	3	13	3	0	0		
6	Λ	1	Total	С	Ν	Ο	Р	0	0	
0	6 A		28	9	3	13	3	0		



• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	2	$\begin{array}{cc} \text{Total} & \text{O} \\ 2 & 2 \end{array}$	0	0
7	С	2	Total O 2 2	0	0
7	А	261	Total O   261 261	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: 5'-R(P\*GP\*C)-3'



P501		100 <del>4</del>	V507	A508 I509	D512	T513	S514 ME1E	G516	L517	R518 N519	<b>q520</b>		R523 R524	P525	R526	S527 T528	M529	P530	L531 N530	V533	P534	0535 0536	<b>Q537</b>	V538	5539 4540	P541	H542	N554		T558	S559	G560 SE61	A562	V563	I564	K566	V567	1568 DECO	L570	G571	V572	P578	
N579 0580	<b>5581</b>	7997	D585	A591	S592	W595		2000 2600		M603	1606		V610	M620		V627	E630	S631	V632 V633	G634	V635	B630	P640	I641	264Z	0645	TC 10	1040 0649	H650	LOJI S652	K653	L654	F659		R662	D665		8668 5668	6003 G670	N671	G683	S684	
T685 A686	T687	2088 T689	E690	M698	M699 E700	T701	F702	W706	<mark>G7</mark> 07	V716		M7 20	T7 24	1725	Q7 26	R7 27 N7 28	Y729	V730	C731 0732		D735	M7 38	I739	1740	D/41 C740	T743	T7 44	6746	K747	V/ 40 N7 49	S750	E751	Q754	N755	D756 1.757		Y763	G764	E/ 00	D772	I773 A774	<u>Y775</u>	
D776 G777	T778	E780	Y781	L/82 K783	L784 Y785	F786	1787 5700	G789		R797 H798	P799		E804 R805		8809 8	U814	P815	A816	1817 1818	D819	<b>Q</b> 820	1821	V829		U834 U835	0836 0836	R837	1839	R840	L845	C846	C847	R851		T854 M855	I 856	G857	E858		G861	Y862 L863	<mark>Q864</mark>	
M867	W868	V878	K879	A880 F881	W886	-	W890	1031 M892	P893	T894	R907	P908	F A G A	V915		V920	R923		T926	L940	K941			M948	ROFA		K957	R960	A961	R964	E965	V966 P067	E968	<mark>0969</mark>	7977		0980		L984		R987	R990	
E994	<u>W995</u>	666D		11002 11003	H1004 N1005	P1006	P1007	V1012	P1013	F1022	A1023	A1024	11025 A1026	07014	E1029	M1034	D1035		M1039 R1040	A1041	R1042	R1043 H1044	S1045		L1052	R1062	M1063	E1065		L1073	R1074	11077		D1082	P1083 1.1084	1011	D1087	P1088	L1090		V1095	<b>Q1100</b>	
S1101 T1102		00111	T1109	M1112	L1129	R1130	95 1 1 3 C	DOTT	A1143	Q1144 1.1145	L1146	M1147	L.1150	Q1151		V1167 N1168		L1172	A1173 R1172	V1175	V1176	N1177	P1181	D1182	11183 W1184	M1185	S1186	M1192		K119/ K1198	L1199	L1200	1021	G1204	P1010	21211	M1215	G1216	M121/ L1218	R1219	R1223	-	
T1232	A1237	952TA	E1243	H1246	W1259		01262 51262	G1264	R1265	SER ALA	a la																																



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	70.72Å 85.21Å 248.47Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(A)	46.67 - 2.80	Depositor
Resolution (A)	46.67 - 2.49	EDS
% Data completeness	85.6 (46.67-2.80)	Depositor
(in resolution range)	85.7 (46.67 - 2.49)	EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.00 (at 2.48 \text{\AA})$	Xtriage
Refinement program	CNS	Depositor
P. P.	0.201 , $0.263$	Depositor
$n, n_{free}$	0.199 , $0.260$	DCC
$R_{free}$ test set	2767 reflections $(5.28%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	29.9	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	$0.35 \;,  35.7$	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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).

Mal	Chain	Bo	nd lengths	Bo	ond angles
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	В	1.37	1/47~(2.1%)	1.06	0/69
2	С	0.89	0/116	0.75	0/178
3	А	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	В	1275	G	OP3-P	-6.33	1.53	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
3	А	560	GLY	N-CA-C	-5.88	98.39	113.10
3	А	408	ILE	N-CA-C	-5.69	95.64	111.00
3	А	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	В	43	0	21	6	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes				
2	С	105	0	54	4	0				
3	А	9986	0	9903	392	0				
4	А	2	0	0	0	0				
5	А	28	0	11	0	0				
6	А	56	0	24	0	0				
7	А	261	0	0	10	0				
7	В	2	0	0	0	0				
7	С	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	Clash		
Atom-1	Atom-2	distance (Å)	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		



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	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:532:ASN:OD1	3:A:535:GLN:HG3	1.91	0.71
3:A:578:PRO:HB2	3:A:742:GLY:HA3	1.72	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:83:ARG:HG3	3:A:83:ARG:HH11	1.60	0.65
3:A:566:LYS:HD3	3:A:784:LEU:CD2	2.26	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:448:GLN:NE2	3:A:620:MET:H	1.94	0.64
3:A:779:ALA:HB3	3:A:786:PHE:HB2	1.79	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	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:457:THR:O	3:A:491:ILE:HG13	1.99	0.61
3:A:829:VAL:HG13	3:A:890:TRP:CE2	2.35	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:HD2	3:A:957:LYS:N	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:246:ASP:O	3:A:250:VAL:HG23	2.02	0.59
3:A:566:LYS:HD3	3:A:784:LEU:HD23	1.84	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:984:LEU:O	3:A:987:ARG:HB2	2.03	0.59
3:A:995:TRP:CZ2	3:A:1006:PRO:HG3	2.38	0.59
3:A:194:CYS:SG	3:A:206:PRO:HG2	2.43	0.58
3:A:379:ARG:HH12	3:A:387:GLN:NE2	2.00	0.58
3:A:538:VAL:HG13	3:A:651:LEU:HB2	1.85	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:38:THR:O	3:A:41:ASP:HB2	2.03	0.58
3:A:393:PRO:CG	3:A:592:SER:HA	2.34	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:579:ASN:OD1	3:A:741:ASP:HA	2.04	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:A:957:LYS:HE3	3:A:1026:ALA:HB2	1.87	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:294:CYS:SG	3:A:314:MET:HB3	2.44	0.56
3:A:595:TRP:CE2	3:A:600:SER:HB3	2.39	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: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:1145:LEU:HB3	3:A:1150:LEU:HD22	1.89	0.55
3:A:396:LYS:HD2	3:A:765:GLU:HB3	1.89	0.55
3:A:585:ASP:HB3	3:A:772:ASP:HB3	1.87	0.54
3:A:599:LEU:O	3:A:603:MET:HG2	2.07	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:14:GLU:C	3:A:20:THR:HG22	2.28	0.53
3:A:501:PRO:HD2	3:A:504:HIS:HD2	1.72	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



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	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:536:GLN:HA	3:A:536:GLN:HE21	1.74	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: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:15:SER:N	3:A:20:THR:HG22	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:1182:ASP:O	3:A:1185:MET:HG2	2.11	0.51
3:A:24:ASN:O	3:A:28:GLU:HG3	2.10	0.51
3:A:561:SER:O	3:A:562:ALA:HB3	2.11	0.51
3:A:47:ASP:HA	3:A:191:ARG:HH11	1.76	0.51
3:A:1029:GLU:OE1	3:A:1029:GLU:N	2.41	0.51
3:A:1065:GLU:H	3:A:1065:GLU:CD	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:201:LEU:HD13	3:A:217:LEU:HD11	1.94	0.49
3:A:1150:LEU:HD12	3:A:1150:LEU:N	2.27	0.49
3:A:21:ASP:OD1	3:A:879:LYS:HG2	2.12	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:749:ASN:ND2	3:A:751:GLU:HB3	2.21	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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:436:MET:C	3:A:436:MET:HE2	2.33	0.49
3:A:829:VAL:HG22	3:A:890:TRP:CD2	2.48	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:39:ARG:HH11	3:A:39:ARG:CG	2.26	0.48
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: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:HD12	3:A:740:ILE:N	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:436:MET:HE2	3:A:436:MET:O	2.14	0.48
3:A:582:ILE:HG21	3:A:757:LEU:HD22	1.95	0.48
3:A:815:PRO:HB2	3:A:953:ARG:O	2.13	0.48
3:A:1082:ASP:OD1	3:A:1084:LEU:HB2	2.14	0.48
3:A:805:ARG:HH11	3:A:805:ARG:HG2	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:473:ILE:HG21	3:A:507:VAL:HG11	1.95	0.47
3:A:1002:ILE:HD13	3:A:1136:ALA:HB2	1.95	0.47
3:A:149:ALA:HB1	3:A:150:PRO:CD	2.44	0.47
3:A:821:ILE:HG23	3:A:845:LEU:HD13	1.94	0.47
3:A:332:ARG:HG2	3:A:332:ARG:HH11	1.79	0.47
3:A:523:ARG:HG2	3:A:524:ARG:N	2.29	0.47
3:A:232:ASP:OD2	3:A:266:TYR:OH	2.25	0.47
3:A:279:GLN:NE2	3:A:283:HIS:HD2	2.12	0.47
3:A:76:ASP:OD2	3:A:80:ARG:HG3	2.15	0.47
3:A:863:LEU:HD11	3:A:1035:ASP:HB3	1.96	0.47
3:A:983:GLU:O	3:A:987:ARG:HG3	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:558:THR:O	3:A:559:SER:HB3	2.14	0.47
3:A:104:GLU:HG3	3:A:116:SER:CA	2.40	0.47
3:A:197:ILE:O	3:A:221:ARG:NH1	2.47	0.47



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:A:460:GLY:O	3:A:490:LYS:NZ	2.42	0.47	
3:A:531:LEU:HD12	3:A:684:SER:HA	1.97	0.47	
3:A:940:LEU:O	3:A:941:LYS:HB2	2.15	0.47	
3:A:957:LYS:HD3	3:A:1022:GLU:HA	1.95	0.47	
3:A:366:ARG:NH1	3:A:367:ASP:OD1	2.44	0.47	
3:A:410:GLU:H	3:A:649:GLN:HE21	1.53	0.47	
3:A:533:VAL:HB	3:A:534:PRO:HD3	1.97	0.47	
3:A:568:ILE:N	3:A:569:PRO:CD	2.78	0.47	
3:A:377:LEU:N	3:A:377:LEU:HD12	2.30	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: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:512:ASP:OD2	3:A:662:ARG:NH2	2.41	0.46	
3:A:554:ASN:HB2	7:A:1385:HOH:O	2.16	0.46	
3:A:437:ALA:HB2	3:A:610:VAL:HG22	1.98	0.46	
3:A:557:PRO:HG3	3:A:781:TYR:OH	2.15	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:523:ARG:HG2	3:A:523:ARG:HH11	1.81	0.46	
3:A:536:GLN:HE22	3:A:685:THR:H	1.63	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:603:MET:HE3	3:A:652:SER:OG	2.15	0.46	
3:A:436:MET:CE	3:A:437:ALA:HA	2.46	0.46	
3:A:541:PRO:HB2	3:A:648:ILE:HD11	1.98	0.46	
3:A:1012:VAL:HB	3:A:1013:PRO:HD3	1.97	0.46	
3:A:100:VAL:HG13	3:A:101:GLU:N	2.31	0.46	
3:A:513:THR:HG21	3:A:529:MET:HG2	1.98	0.46	
3:A:92:VAL:HG13	3:A:383:GLU:CG	2.45	0.46	
3:A:139:ILE:HD13	3:A:380:THR:HG22	1.98	0.46	
3:A:566:LYS:HD3	3:A:784:LEU:HD21	1.98	0.46	
3:A:606:ILE:O	3:A:610:VAL:HB	2.16	0.46	
3:A:863:LEU:HD21	3:A:1039:MET:HB2	1.98	0.46	
3:A:1112:MET:CE	3:A:1150:LEU:HD11	2.45	0.46	
3:A:700:GLU:HB2	3:A:725:ILE:HD13	1.96	0.45	
2:C:1284:A:N3	3:A:683:GLY:HA2	2.31	0.45	
3:A:516:GLY:HA3	3:A:528:ILE:HG22	1.97	0.45	
3:A:128:SER:O	3:A:132:ILE:HG12	2.15	0.45	
3:A:57:LEU:HD22	3:A:185:CYS:SG	2.56	0.45	
3:A:380:THR:HG23	7:A:1435:HOH:O	2.16	0.45	



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:A:15:SER:HA	3:A:20:THR:O	2.17	0.45
3:A:81:VAL:H	3:A:671:ASN:ND2	2.01	0.45
3:A:557:PRO:HG2	3:A:732:GLN:HB2	1.99	0.45
3:A:926:THR:CG2	3:A:1246:HIS:CD2	2.99	0.45
3:A:101:GLU:HG2	3:A:102:LEU:HG	1.99	0.45
3:A:814:TRP:O	3:A:816:ALA:N	2.50	0.45
3:A:815:PRO:HG2	3:A:1034:MET:HE3	1.96	0.45
3:A:743:THR:CG2	3:A:744:THR:N	2.79	0.45
3:A:169:ASP:HB3	3:A:172:LEU:HB2	1.99	0.44
3:A:886:TRP:HA	7:A:1442:HOH:O	2.17	0.44
3:A:69:HIS:CG	3:A:70:ASP:N	2.85	0.44
3:A:1007:PRO:HD2	3:A:1144:GLN:CD	2.37	0.44
3:A:944:GLN:CD	3:A:944:GLN:H	2.19	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: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:339:GLY:O	3:A:340:LEU:HD23	2.17	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: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:59:ILE:HA	3:A:60:PRO:HD3	1.89	0.44
3:A:381:PRO:HD2	3:A:665:ASP:OD1	2.17	0.44
3:A:523:ARG:NH1	3:A:524:ARG:O	2.50	0.44
3:A:855:MET:HE3	3:A:857:GLY:H	1.81	0.44
3:A:60:PRO:HA	3:A:61:PRO:HD3	1.89	0.43
3:A:194:CYS:SG	3:A:206:PRO:CG	3.06	0.43
3:A:539:SER:HA	3:A:651:LEU:HD22	2.00	0.43
3:A:421:ILE:HD12	3:A:421:ILE:HA	1.86	0.43
3:A:821:ILE:HD12	3:A:845:LEU:HD13	2.01	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:298:GLU:HB2	3:A:311:MET:CE	2.48	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: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:193:ILE:O	3:A:197:ILE:HG13	2.19	0.43



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
3:A:855:MET:SD	3:A:860:VAL:HG22	2.59	0.43	
3:A:27:PHE:CE1	3:A:847:CYS:HB2	2.53	0.43	
1:B:1275:G:O2'	3:A:561:SER:HB2	2.18	0.42	
1:B:1275:G:H21	3:A:560:GLY:CA	2.32	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:851:ARG:HH11	3:A:864:GLN:HE21	1.67	0.42	
3:A:1100:GLN:CG	3:A:1101:SER:N	2.81	0.42	
2:C:1285:G:O2'	2:C:1286:C:H5'	2.18	0.42	
3:A:78:LEU:HD23	3:A:78:LEU:HA	1.77	0.42	
3:A:146:GLN:NE2	3:A:804:GLU:HA	2.35	0.42	
3:A:286:TYR:C	3:A:288:SER:N	2.67	0.42	
3:A:404:TRP:O	3:A:415:LYS:HE3	2.19	0.42	
3:A:716:VAL:HG12	3:A:720:MET:CE	2.49	0.42	
3:A:907:ARG:CB	3:A:908:PRO:HD3	2.41	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:271:LEU:HD13	3:A:377:LEU:CD2	2.49	0.42	
3:A:366:ARG:NH2	7:A:1323:HOH:O	2.51	0.42	
3:A:523:ARG:HG3	7:A:1437:HOH:O	2.20	0.42	
3:A:564:ILE:HD13	3:A:1186:SER:HA	2.01	0.42	
3:A:1040:ARG:HG3	3:A:1043:ARG:NH2	2.35	0.42	
3:A:1102:THR:O	3:A:1106:PHE:HD2	2.03	0.42	
3:A:332:ARG:HG2	3:A:332:ARG:NH1	2.34	0.42	
3:A:632:VAL:HB	3:A:635:VAL:HB	2.01	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:201:LEU:HA	3:A:202:PRO:HD3	1.79	0.42	
3:A:381:PRO:HB3	3:A:515:MET:SD	2.60	0.42	
3:A:381:PRO:HG3	3:A:517:LEU:CD1	2.50	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:754:GLN:HE21	3:A:775:TYR:HD2	1.68	0.41	
3:A:1181:PRO:HD2	3:A:1184:TRP:CE3	2.55	0.41	
3:A:39:ARG:HE	3:A:208:LEU:HD22	1.85	0.41	
3:A:328:ASP:HA	3:A:348:ARG:CZ	2.50	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
3:A:520:GLN:NE2	3:A:526:ARG:NH1	2.67	0.41	
3:A:1262:GLN:HG2	3:A:1265:ARG:NH1	2.35	0.41	
3:A:6:LEU:O	3:A:10:GLY:N	2.51	0.41	
3:A:797:ARG:C	3:A:799:PRO:HD3	2.41	0.41	
3:A:393:PRO:HG3	3:A:591:ALA:O	2.20	0.41	
3:A:857:GLY:C	3:A:859:SER:H	2.21	0.41	
3:A:867:MET:HG3	3:A:868:TRP:N	2.35	0.41	
3:A:139:ILE:HD12	3:A:139:ILE:HA	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:706:TRP:O	3:A:707:GLY:C	2.59	0.41	
3:A:1052:LEU:HD13	3:A:1259:TRP:CG	2.56	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:1007:PRO:HD2	3:A:1144:GLN:HE22	1.82	0.41	
3:A:223:THR:CG2	3:A:224:SER:N	2.84	0.41	
3:A:270:ILE:HD12	3:A:373:SER:HB2	2.02	0.41	
3:A:471:TYR:CD1	3:A:471:TYR:C	2.94	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:778:THR:CG2	3:A:779:ALA:N	2.83	0.41	
3:A:322:ARG:NH1	3:A:325:PRO:O	2.42	0.41	
3:A:470:LEU:CD2	3:A:477:LEU:HD21	2.51	0.41	
3:A:39:ARG:CG	3:A:39:ARG:NH1	2.84	0.40	
3:A:205:ALA:HA	3:A:206:PRO:HD3	1.80	0.40	
3:A:797:ARG:HB3	7:A:1539:HOH:O	2.21	0.40	
3:A:855:MET:HE3	3:A:858:GLU:H	1.84	0.40	
3:A:92:VAL:HG13	3:A:383:GLU:HG3	2.03	0.40	
3:A:149:ALA:HB1	3:A:150:PRO:HD2	2.04	0.40	
3:A:178:ILE:HA	3:A:179:PRO:HD3	1.95	0.40	
3:A:279:GLN:HE21	3:A:283:HIS:CD2	2.30	0.40	
3:A:405:THR:HG23	3:A:413:ILE:O	2.21	0.40	
3:A:536:GLN:NE2	3:A:536:GLN:HA	2.36	0.40	
3:A:603:MET:HE1	3:A:651:LEU:HD23	2.03	0.40	
3:A:639:ARG:HA	3:A:640:PRO:HD3	1.85	0.40	
3:A:686:ALA:O	3:A:690:GLU:HB2	2.22	0.40	
3:A:1005:ASN:N	3:A:1006:PRO:CD	2.84	0.40	
3:A:134:THR:CG2	3:A:669:PRO:HG2	2.52	0.40	
3:A:564:ILE:HA	3:A:568:ILE:HG13	2.03	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 (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed Favoured Allowed		Outliers	Percentiles	
3	А	1262/1267~(100%)	1162~(92%)	84 (7%)	16 (1%)	12 36

All (16) Ramachandran outliers are listed below:

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

#### 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	nalysed Rotameric		Percentiles	
3	А	1081/1083~(100%)	1044 (97%)	37~(3%)	37	71

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

Mol	Chain	Res	Type		
3	А	35	SER		
3	А	37	PHE		
3	А	84	LYS		
3	А	107	GLU		
3	А	167	LEU		
3	А	187	LEU		
3	А	267	SER		
3	А	366	ARG		
3	А	387	GLN		
3	А	414	LEU		
3	А	431	LEU		
3	А	436	MET		
3	А	453	SER		
3	A	466	LEU		
3	А	471	TYR		
3	А	518	ARG		
3	А	536	GLN		
3	А	538	VAL		
3	А	735	ASP		
3	А	784	LEU		
3	А	809	SER		
3	А	845	LEU		
3	А	890	TRP		
3	А	894	THR		
3	А	909	LEU		
3	А	923	ARG		
3	А	980	GLN		
3	А	984	LEU		
3	А	990	ARG		
3	A	1045	SER		
3	А	1052	LEU		
3	A	1063	MET		
3	А	1065	GLU		
3	А	1077	LEU		
3	А	1151	GLN		
3	А	1176	VAL		
3	A	$12\overline{38}$	VAL		



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

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

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	В	0/2	-	-
2	С	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 (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 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).

Mal	Mol Type Chain Res		Tink	Bond lengths		Bond angles				
WIOI	Moi Type Cham Res	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2	
6	CH1	А	1294	-	24,29,29	1.22	4 (16%)	33,45,45	2.85	15 (45%)
5	U3H	А	1291	4	23,29,29	2.37	6 (26%)	27,45,45	<mark>3.14</mark>	14 (51%)
6	CH1	А	1295	-	24,29,29	1.11	1 (4%)	33,45,45	2.68	13 (39%)

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
6	CH1	А	1294	-	-	6/22/34/34	0/2/2/2
5	U3H	А	1291	4	1/1/9/12	7/22/47/47	0/2/2/2
6	CH1	А	1295	-	-	9/22/34/34	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
5	А	1291	U3H	C2-N1	6.28	1.63	1.46
5	А	1291	U3H	O2-C2	-5.16	1.23	1.40
5	А	1291	U3H	C2-N3	-4.48	1.39	1.46
5	А	1291	U3H	C4-N3	4.01	1.40	1.34
6	А	1294	CH1	C6-C5	2.68	1.41	1.35
6	А	1295	CH1	C6-C5	2.44	1.40	1.35
6	А	1294	CH1	C1'-N1	2.32	1.54	1.47
6	А	1294	CH1	PG-01G	2.18	1.57	1.50



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
6	А	1294	CH1	PB-O1B	2.12	1.58	1.50
5	А	1291	U3H	PB-O1B	2.08	1.58	1.50
5	А	1291	U3H	PG-01G	2.04	1.57	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	А	1291	U3H	O4'-C4'-C5'	7.82	122.37	109.52
6	А	1295	CH1	O3G-PG-O1G	-7.64	80.79	110.68
6	А	1294	CH1	O3G-PG-O1G	-7.36	81.88	110.68
6	А	1294	CH1	O3G-PG-O3B	-6.56	82.63	104.64
6	А	1295	CH1	O3G-PG-O3B	-6.39	83.19	104.64
5	А	1291	U3H	C5-C6-N1	6.08	131.60	124.65
5	А	1291	U3H	O3G-PG-O1G	-6.02	87.09	110.68
5	А	1291	U3H	O3G-PG-O3B	-5.60	85.85	104.64
6	А	1294	CH1	O3G-PG-O2G	-5.21	87.74	107.64
6	А	1294	CH1	O2-C2-N3	-5.20	113.88	122.33
6	А	1295	CH1	O3G-PG-O2G	-5.09	88.20	107.64
6	А	1295	CH1	O2-C2-N3	-4.97	114.25	122.33
6	А	1294	CH1	C3'-C4'-C5'	-4.29	104.65	113.11
5	А	1291	U3H	O3G-PG-O2G	-4.23	91.46	107.64
6	А	1294	CH1	O4'-C1'-C2'	-4.04	102.70	106.51
5	А	1291	U3H	O4'-C4'-C3'	3.99	110.21	105.07
5	А	1291	U3H	O4'-C1'-N1	3.87	115.25	108.83
6	А	1295	CH1	C3'-C4'-C5'	-3.21	106.77	113.11
6	А	1294	CH1	O4'-C4'-C5'	3.20	114.78	109.52
6	А	1294	CH1	PB-O3B-PG	-3.10	122.19	132.83
6	А	1294	CH1	C6-N1-C2	-3.08	115.16	120.49
5	А	1291	U3H	O2G-PG-O3B	3.00	114.70	104.64
6	А	1295	CH1	PB-O3A-PA	-2.97	122.65	132.83
5	А	1291	U3H	PB-O3A-PA	-2.93	122.77	132.83
6	А	1294	CH1	PB-O3A-PA	-2.90	122.86	132.83
6	А	1295	CH1	C6-N1-C2	-2.84	115.57	120.49
6	А	1295	CH1	O4'-C4'-C5'	2.83	114.18	109.52
6	А	1295	CH1	PB-O3B-PG	-2.76	123.34	132.83
5	А	1291	U3H	O4-C4-N3	-2.75	119.17	122.21
6	А	1294	CH1	O2G-PG-O3B	2.72	113.75	104.64
5	А	1291	U3H	PB-O3B-PG	-2.62	123.82	132.83
6	А	1295	CH1	O3B-PG-O1G	2.52	125.18	111.19
5	A	1291	U3H	O2G-PG-O1G	2.52	120.55	110.68
5	А	1291	U3H	O3B-PG-O1G	2.38	124.41	111.19
6	А	1294	CH1	N1-C2-N3	2.38	123.14	118.81



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	А	1295	CH1	O2G-PG-O3B	2.37	112.58	104.64
6	А	1295	CH1	N1-C2-N3	2.31	123.02	118.81
6	А	1294	CH1	O4'-C1'-N1	2.30	113.62	108.36
6	А	1294	CH1	O3B-PG-O1G	2.29	123.91	111.19
6	А	1294	CH1	O2G-PG-O1G	2.14	119.06	110.68
6	А	1295	CH1	O2G-PG-O1G	2.09	118.86	110.68
5	А	1291	U3H	C3'-C4'-C5'	-2.01	109.15	113.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	А	1291	U3H	C2

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	А	1291	U3H	C3'-C4'-C5'-O5'
5	А	1291	U3H	O4'-C4'-C5'-O5'
5	А	1291	U3H	C5'-O5'-PA-O3A
6	А	1294	CH1	C3'-C4'-C5'-O5'
6	А	1294	CH1	O4'-C4'-C5'-O5'
6	А	1294	CH1	C5'-O5'-PA-O1A
6	А	1294	CH1	C5'-O5'-PA-O2A
6	А	1295	CH1	C3'-C4'-C5'-O5'
6	А	1295	CH1	O4'-C4'-C5'-O5'
6	А	1295	CH1	C5'-O5'-PA-O3A
6	А	1294	CH1	C4'-C5'-O5'-PA
6	А	1295	CH1	PG-O3B-PB-O3A
5	А	1291	U3H	PB-O3A-PA-O1A
6	А	1295	CH1	PB-O3A-PA-O1A
5	А	1291	U3H	C5'-O5'-PA-O1A
5	А	1291	U3H	C5'-O5'-PA-O2A
6	А	1295	CH1	C5'-O5'-PA-O1A
6	А	1294	CH1	C5'-O5'-PA-O3A
6	А	1295	CH1	PG-O3B-PB-O1B
6	А	1295	CH1	PG-O3B-PB-O2B
6	А	1295	CH1	C5'-O5'-PA-O2A
5	А	1291	U3H	PB-O3B-PG-O1G

There are no ring outliers.

No monomer is involved in short contacts.



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 similar rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







#### 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

### 6.1 Protein, DNA and RNA chains (i)

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	< <b>RSRZ</b> >	#RSRZ>2	$OWAB(Å^2)$	$Q{<}0.9$
1	В	2/2~(100%)	4.61	2(100%) 0 0	96, 96, 96, 122	0
2	С	5/6~(83%)	1.22	1 (20%) 1 0	23, 41, 71, 74	0
3	А	1264/1267~(99%)	-0.33	24 (1%) 66 59	7, 21, 44, 85	0
All	All	1271/1275~(99%)	-0.32	27 (2%) 63 54	7, 21, 45, 122	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	А	2	SER	8.2
1	В	1275	G	6.0
3	А	858	GLU	5.2
2	С	1286	С	4.5
3	А	562	ALA	4.5
3	А	561	SER	4.2
3	А	856	ILE	4.1
3	А	744	THR	3.5
3	А	857	GLY	3.4
3	А	859	SER	3.4
3	А	563	VAL	3.4
3	А	633	VAL	3.2
1	В	1276	С	3.2
3	А	855	MET	3.2
3	А	746	GLY	2.9
3	А	565	GLU	2.9
3	А	564	ILE	2.7
3	А	559	SER	2.6
3	А	860	VAL	2.5
3	А	212	ALA	2.5
3	А	748	VAL	2.5
3	А	211	SER	2.3
3	А	961	ALA	2.3



Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	А	862	TYR	2.2
3	А	755	ASN	2.1
3	А	213	GLY	2.1
3	А	484	PRO	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 <sup>2</sup> )	Q<0.9
6	CH1	А	1294	28/28	0.47	0.58	98,112,132,132	0
5	U3H	А	1291	28/28	0.81	0.26	82,88,95,95	0
6	CH1	А	1295	28/28	0.86	0.22	48,61,74,75	0
4	MN	А	1301	1/1	0.94	0.07	63,63,63,63	0
4	MN	А	1302	1/1	0.96	0.12	39,39,39,39	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.













### 6.5 Other polymers (i)

There are no such residues in this entry.

