

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	2HNY
Title	:	Crystal Structure of E138K Mutant HIV-1 Reverse Transcriptase in Complex
		with Nevirapine
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Deposited on	:	2006-07-13
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

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
EDS	:	2.23.2
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)	:	2.23.2

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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Motria	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	$5231 \ (2.50-2.50)$
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	Quality of chain						
1	А	534	<u>4%</u> 62%	33% ••					
2	В	422	55%	38% • 5%					



2HNY

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7744 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	523	Total 4295	C 2784	N 711	O 792	S 8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual Comment		Reference
А	138	LYS	GLU	engineered mutation	UNP P04585
А	280	CSD	CYS	modified residue	UNP P04585

• Molecule 2 is a protein called Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	401	Total 3334	C 2177	N 551	O 599	${ m S} 7$	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	138	LYS	GLU	engineered mutation	UNP P04585

• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Mg 1 1	0	0

• Molecule 5 is 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3' -E][1,4]DIAZEPIN-6-ONE (three-letter code: NVP) (formula: $C_{15}H_{14}N_4O$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	Δ	1	Total	С	Ν	0	0	0
0	Л	1	20	15	4	1	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	51	$\begin{array}{cc} \text{Total} & \text{O} \\ 51 & 51 \end{array}$	0	0
6	В	28	TotalO2828	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: Reverse transcriptase/ribonuclease H

 \bullet Molecule 2: Reverse transcript ase/ribonuclease H







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	139.60Å 115.00Å 65.60Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	19.94 - 2.50	Depositor
Resolution (A)	19.94 - 2.50	EDS
% Data completeness	99.5 (19.94-2.50)	Depositor
(in resolution range)	99.5(19.94-2.50)	EDS
R_{merge}	0.10	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.26 (at 2.50 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
B B.	0.214 , 0.284	Depositor
II, II, <i>free</i>	0.200 , 0.203	DCC
R_{free} test set	1856 reflections (5.01%)	wwPDB-VP
Wilson B-factor $(Å^2)$	56.8	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, 56.7	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	0.96	EDS
Total number of atoms	7744	wwPDB-VP
Average B, all atoms $(Å^2)$	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities 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: PO4, NVP, CSD, MG

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	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.43	0/4401	0.63	0/5982
2	В	0.41	0/3431	0.64	0/4659
All	All	0.42	0/7832	0.63	0/10641

There are no bond length outliers.

There are no bond angle outliers.

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	А	4295	0	4338	167	0
2	В	3334	0	3366	169	0
3	А	15	0	0	0	0
4	А	1	0	0	0	0
5	А	20	0	14	0	0
6	А	51	0	0	7	0
6	В	28	0	0	1	0
All	All	7744	0	7718	327	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 21.



A 1 -		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:227:PHE:HB3	2:B:231:GLY:HA2	1.36	1.08
2:B:66:LYS:HD2	2:B:230:MET:HA	1.43	0.98
1:A:135:ILE:HD13	1:A:135:ILE:H	1.29	0.96
2:B:227:PHE:CB	2:B:231:GLY:HA2	1.99	0.91
1:A:33:ALA:O	1:A:37:ILE:HG12	1.71	0.90
1:A:6:GLU:HG2	6:A:1001:HOH:O	1.73	0.88
1:A:473:THR:HG23	1:A:476:LYS:HB2	1.56	0.88
1:A:113:ASP:HA	1:A:116:PHE:HD2	1.39	0.86
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.41	0.84
2:B:331:LYS:O	2:B:424:LYS:HE2	1.76	0.84
2:B:270:ILE:O	2:B:272:PRO:HD3	1.80	0.81
1:A:23:GLN:HE22	1:A:60:VAL:H	1.29	0.80
1:A:469:LEU:HD11	1:A:480:GLN:HG3	1.63	0.79
2:B:135:ILE:O	2:B:138:LYS:HG3	1.82	0.79
2:B:295:LEU:N	2:B:295:LEU:HD12	1.97	0.78
1:A:136:ASN:HB2	1:A:139:THR:HB	1.65	0.78
1:A:63:ILE:HD11	1:A:74:LEU:HD22	1.66	0.77
1:A:24:TRP:HZ2	1:A:61:PHE:HD2	1.31	0.76
2:B:66:LYS:CD	2:B:230:MET:HA	2.14	0.76
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.66	0.76
2:B:66:LYS:HB2	2:B:407:GLN:HE22	1.51	0.75
2:B:7:THR:HG22	2:B:119:PRO:HB2	1.69	0.74
2:B:40:GLU:HG3	2:B:44:GLU:OE2	1.90	0.71
2:B:194:GLU:OE2	2:B:195:ILE:HG12	1.91	0.71
2:B:206:ARG:HD2	2:B:227:PHE:CE1	2.27	0.70
2:B:305:GLU:O	2:B:309:ILE:HG13	1.92	0.70
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.74	0.70
1:A:308:GLU:OE1	1:A:311:LYS:HD2	1.92	0.69
2:B:164:MET:SD	2:B:167:ILE:HD11	2.33	0.69
1:A:31:ILE:HG21	1:A:135:ILE:HG23	1.74	0.69
1:A:131:THR:OG1	1:A:143:ARG:HG2	1.93	0.69
1:A:399:GLU:HG3	1:A:402:TRP:CE3	2.27	0.69
1:A:244:ILE:HD13	1:A:310:LEU:HD13	1.75	0.68
2:B:342:TYR:HB3	2:B:348:ASN:HD22	1.59	0.68
2:B:254:VAL:O	2:B:258:GLN:HG3	1.93	0.68
2:B:427:TYR:O	2:B:428:GLN:HB3	1.91	0.68
1:A:515:SER:HB2	6:A:1038:HOH:O	1.93	0.68
2:B:66:LYS:HB2	2:B:407:GLN:NE2	2.08	0.67
2:B:238:LYS:O	2:B:240:THR:HG23	1.93	0.67
1:A:46:LYS:HE3	1:A:116:PHE:HD1	1.60	0.67

All (327) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:30:LYS:HE3	1:A:71:TRP:CZ3	2.29	0.67
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.78	0.66
1:A:30:LYS:HE3	1:A:71:TRP:HZ3	1.60	0.66
1:A:24:TRP:HE1	1:A:61:PHE:HB3	1.61	0.66
2:B:168:LEU:O	2:B:172:ARG:HB2	1.95	0.66
2:B:238:LYS:HD2	2:B:238:LYS:N	2.11	0.65
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.77	0.65
2:B:295:LEU:HD12	2:B:295:LEU:H	1.59	0.65
2:B:319:TYR:OH	2:B:385:LYS:HD3	1.95	0.65
1:A:65:LYS:HD2	1:A:72:ARG:HD2	1.78	0.65
1:A:507:GLN:HE22	2:B:421:PRO:HB3	1.61	0.65
2:B:66:LYS:NZ	2:B:66:LYS:HB3	2.10	0.65
2:B:175:ASN:HD21	2:B:201:LYS:CE	2.10	0.65
1:A:61:PHE:CZ	1:A:74:LEU:HD23	2.32	0.64
1:A:498:ASP:HA	1:A:536:VAL:O	1.97	0.64
1:A:281:LYS:HE3	1:A:284:ARG:CZ	2.28	0.64
1:A:42:GLU:OE2	1:A:49:LYS:HG3	1.97	0.63
1:A:480:GLN:C	1:A:480:GLN:HE21	2.02	0.63
1:A:294:PRO:HA	6:A:1027:HOH:O	1.98	0.63
2:B:246:LEU:HD12	2:B:307:ARG:HG2	1.81	0.63
1:A:28:GLU:HG3	1:A:135:ILE:CG2	2.29	0.62
2:B:284:ARG:O	2:B:287:LYS:NZ	2.29	0.62
1:A:46:LYS:HE3	1:A:116:PHE:CD1	2.34	0.62
1:A:399:GLU:HG3	1:A:402:TRP:CZ3	2.35	0.62
1:A:24:TRP:CZ2	1:A:61:PHE:HD2	2.16	0.62
1:A:135:ILE:H	1:A:135:ILE:CD1	2.06	0.62
2:B:420:PRO:HG2	2:B:423:VAL:HG12	1.80	0.62
2:B:171:PHE:CE2	2:B:178:ILE:HD11	2.35	0.62
1:A:235:HIS:HB2	1:A:238:LYS:O	2.00	0.61
1:A:357:MET:HE1	1:A:512:GLN:HE21	1.65	0.61
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.36	0.61
2:B:104:LYS:O	2:B:235:HIS:HA	2.01	0.61
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.31	0.61
1:A:530:LYS:HA	6:A:1075:HOH:O	1.99	0.61
2:B:423:VAL:HG13	2:B:424:LYS:N	2.17	0.60
2:B:172:ARG:O	2:B:176:PRO:HG3	2.02	0.60
1:A:136:ASN:HB2	1:A:139:THR:CB	2.32	0.60
2:B:116:PHE:CE1	2:B:151:GLN:HG3	2.36	0.60
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.31	0.60
1:A:28:GLU:O	1:A:32:LYS:HD3	2.02	0.60
1:A:473:THR:HG23	1:A:476:LYS:CB	2.28	0.60



	A i a	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.99	0.60	
2:B:135:ILE:HB	2:B:138:LYS:HE2	1.82	0.60	
1:A:72:ARG:HH21	1:A:74:LEU:HD13	1.67	0.59	
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.84	0.59	
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.36	0.59	
1:A:28:GLU:OE1	1:A:31:ILE:HD12	2.02	0.59	
1:A:63:ILE:CD1	1:A:74:LEU:HD22	2.32	0.59	
2:B:116:PHE:HE1	2:B:151:GLN:HG3	1.68	0.59	
2:B:368:LEU:O	2:B:372:VAL:HG23	2.03	0.59	
1:A:255:ASN:ND2	1:A:289:LEU:HB3	2.17	0.59	
1:A:28:GLU:HG3	1:A:135:ILE:HG22	1.85	0.58	
2:B:171:PHE:HE2	2:B:178:ILE:HD11	1.68	0.58	
1:A:523:GLU:O	1:A:527:LYS:HG2	2.02	0.58	
1:A:516:GLU:O	1:A:520:GLN:HG3	2.02	0.58	
2:B:8:VAL:O	2:B:121:ASP:HB2	2.04	0.58	
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.84	0.58	
1:A:376:THR:HG23	1:A:386:THR:HG22	1.85	0.57	
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.87	0.57	
2:B:46:LYS:HZ3	2:B:116:PHE:HD2	1.51	0.57	
2:B:295:LEU:N	2:B:295:LEU:CD1	2.68	0.57	
1:A:357:MET:CE	1:A:512:GLN:HE21	2.16	0.57	
1:A:497:THR:O	1:A:535:TRP:HA	2.05	0.57	
2:B:164:MET:O	2:B:167:ILE:HG12	2.04	0.57	
1:A:150:PRO:HG2	1:A:153:TRP:HB2	1.87	0.57	
1:A:113:ASP:HA	1:A:116:PHE:CD2	2.30	0.56	
2:B:163:SER:O	2:B:167:ILE:HG23	2.05	0.56	
2:B:189:VAL:HG11	2:B:202:ILE:HD13	1.86	0.56	
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.86	0.56	
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.40	0.56	
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.71	0.56	
1:A:401:TRP:HA	1:A:404:GLU:HG2	1.88	0.56	
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.06	0.55	
1:A:356:ARG:HH21	1:A:358:ARG:HD2	1.71	0.55	
2:B:233:GLU:N	2:B:233:GLU:OE2	2.40	0.55	
1:A:356:ARG:NH2	6:A:1029:HOH:O	2.39	0.55	
1:A:255:ASN:O	1:A:259:LYS:HG3	2.06	0.55	
2:B:175:ASN:HD21	2:B:201:LYS:HE3	1.70	0.54	
1:A:35:VAL:HG22	1:A:132:ILE:HG21	1.88	0.54	
1:A:91:GLN:HE22	1:A:184:MET:H	1.55	0.54	
1:A:340:GLN:HG3	1:A:351:THR:HG22	1.88	0.54	
1:A:195:ILE:HG13	6:A:1022:HOH:O	2.05	0.54	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:90:VAL:HG12	1:A:91:GLN:HG2	1.89	0.54	
1:A:53:GLU:O	1:A:55:PRO:HD3	2.08	0.53	
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.08	0.53	
2:B:106:VAL:HG13	2:B:234:LEU:HB2	1.90	0.53	
1:A:76:ASP:OD2	1:A:78:ARG:HG3	2.08	0.53	
2:B:164:MET:HA	2:B:167:ILE:HG12	1.91	0.53	
1:A:254:VAL:O	1:A:258:GLN:HG3	2.09	0.53	
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.09	0.53	
2:B:227:PHE:CB	2:B:231:GLY:CA	2.82	0.52	
2:B:242:GLN:HG3	2:B:352:GLY:HA2	1.90	0.52	
1:A:65:LYS:O	1:A:67:ASP:N	2.42	0.52	
2:B:66:LYS:HD2	2:B:230:MET:CA	2.29	0.52	
2:B:169:GLU:N	2:B:170:PRO:HD2	2.24	0.52	
2:B:195:ILE:HD13	2:B:195:ILE:N	2.24	0.52	
1:A:503:LEU:O	1:A:507:GLN:HG3	2.10	0.52	
2:B:191:SER:OG	2:B:198:HIS:ND1	2.39	0.52	
1:A:23:GLN:HE22	1:A:60:VAL:HG12	1.74	0.52	
1:A:72:ARG:HH21	1:A:74:LEU:CD1	2.22	0.52	
1:A:131:THR:HG23	1:A:143:ARG:HG3	1.92	0.51	
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.92	0.51	
2:B:395:LYS:HG3	2:B:416:PHE:CE1	2.46	0.51	
1:A:434:ILE:HB	1:A:437:ALA:HB3	1.91	0.51	
2:B:159:ILE:HG22	2:B:159:ILE:O	2.09	0.51	
1:A:209:LEU:O	1:A:214:LEU:HB2	2.10	0.51	
2:B:257:ILE:HG22	2:B:283:LEU:HD11	1.93	0.51	
1:A:366:LYS:NZ	1:A:366:LYS:HB3	2.24	0.51	
1:A:20:LYS:HE2	1:A:55:PRO:HB2	1.93	0.51	
1:A:246:LEU:HD13	1:A:303:LEU:CD1	2.41	0.50	
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.45	0.50	
2:B:224:GLU:O	2:B:226:PRO:HD3	2.12	0.50	
1:A:363:ASN:HA	1:A:511:ASP:CG	2.31	0.50	
2:B:178:ILE:HG22	2:B:191:SER:HB3	1.93	0.50	
1:A:345:PRO:O	1:A:346:PHE:HB2	2.11	0.50	
2:B:66:LYS:CE	2:B:230:MET:H	2.24	0.50	
2:B:164:MET:HA	2:B:167:ILE:CD1	2.41	0.50	
2:B:66:LYS:HE3	2:B:230:MET:N	2.27	0.50	
1:A:37:ILE:O	1:A:41:MET:HG3	2.12	0.49	
1:A:23:GLN:NE2	1:A:60:VAL:HG12	2.26	0.49	
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.47	0.49	
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.40	0.49	
2:B:175:ASN:ND2	2:B:201:LYS:CE	2.76	0.49	



	loue page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.48	0.49
2:B:46:LYS:HD3	2:B:116:PHE:CD2	2.46	0.49
1:A:406:TRP:CZ3	1:A:407:GLN:HB2	2.47	0.49
2:B:66:LYS:HE3	2:B:230:MET:CA	2.42	0.49
1:A:72:ARG:NH2	1:A:74:LEU:HD13	2.28	0.49
1:A:368:LEU:O	1:A:372:VAL:HG23	2.13	0.48
1:A:480:GLN:O	1:A:483:TYR:HB3	2.13	0.48
1:A:90:VAL:HG12	1:A:91:GLN:N	2.27	0.48
2:B:150:PRO:HG2	2:B:153:TRP:HB2	1.96	0.48
1:A:417:VAL:O	1:A:417:VAL:HG13	2.12	0.48
2:B:372:VAL:HA	2:B:389:PHE:CE2	2.48	0.48
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.96	0.48
1:A:408:ALA:HA	2:B:364:ASP:OD1	2.14	0.48
1:A:228:LEU:HD23	1:A:233:GLU:HA	1.96	0.48
1:A:399:GLU:HG3	1:A:402:TRP:HE3	1.76	0.48
2:B:297:GLU:O	2:B:301:LEU:HG	2.12	0.48
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.48	0.48
1:A:469:LEU:CD1	1:A:480:GLN:HG3	2.38	0.48
2:B:66:LYS:CE	2:B:230:MET:HA	2.44	0.48
2:B:265:ASN:O	2:B:268:SER:HB3	2.13	0.48
2:B:395:LYS:O	2:B:399:GLU:HG2	2.14	0.48
1:A:225:PRO:HA	1:A:226:PRO:C	2.34	0.48
2:B:161:GLN:O	2:B:164:MET:HB3	2.13	0.48
1:A:535:TRP:CZ3	1:A:537:PRO:HD3	2.49	0.47
1:A:287:LYS:HG2	1:A:291:GLU:OE2	2.15	0.47
2:B:33:ALA:O	2:B:37:ILE:HG13	2.15	0.47
1:A:475:GLN:HB2	1:A:501:TYR:CD2	2.49	0.47
1:A:486:LEU:O	1:A:528:LYS:NZ	2.46	0.47
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.95	0.47
1:A:518:VAL:O	1:A:522:ILE:HG13	2.14	0.47
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.49	0.47
1:A:281:LYS:HE3	1:A:284:ARG:NH2	2.30	0.47
2:B:66:LYS:CD	2:B:230:MET:CA	2.92	0.47
2:B:242:GLN:HE22	2:B:353:LYS:HD3	1.80	0.47
2:B:242:GLN:OE1	2:B:353:LYS:HE2	2.14	0.47
2:B:242:GLN:HE21	2:B:242:GLN:HB3	1.53	0.47
1:A:35:VAL:O	1:A:39:THR:HB	2.15	0.47
1:A:31:ILE:O	1:A:35:VAL:HG23	2.15	0.47
1:A:332:GLN:O	1:A:332:GLN:HG2	2.14	0.47
2:B:194:GLU:O	2:B:198:HIS:N	2.45	0.47
2:B:170:PRO:HG3	2:B:208:HIS:CE1	2.50	0.47



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:B:164:MET:C	2:B:167:ILE:HG12	2.36	0.46	
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.50	0.46	
2:B:115:TYR:C	2:B:117:SER:H	2.18	0.46	
2:B:11:LYS:HE2	2:B:11:LYS:HB3	1.69	0.46	
2:B:46:LYS:NZ	2:B:116:PHE:HD2	2.14	0.46	
1:A:5:ILE:HG13	1:A:6:GLU:N	2.30	0.46	
2:B:211:ARG:HG3	2:B:211:ARG:HH11	1.79	0.46	
2:B:242:GLN:NE2	2:B:353:LYS:HD3	2.31	0.46	
1:A:139:THR:HA	1:A:140:PRO:HD3	1.81	0.46	
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.97	0.46	
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.50	0.46	
2:B:79:GLU:O	2:B:83:ARG:HG3	2.15	0.46	
1:A:57:ASN:HA	1:A:129:ALA:O	2.16	0.46	
1:A:406:TRP:HH2	2:B:418:ASN:OD1	1.99	0.46	
1:A:409:THR:O	2:B:364:ASP:HB2	2.16	0.46	
1:A:208:HIS:O	1:A:212:TRP:HD1	1.98	0.45	
1:A:391:LEU:C	1:A:417:VAL:HG12	2.36	0.45	
2:B:365:VAL:O	2:B:369:THR:HG23	2.16	0.45	
2:B:175:ASN:C	2:B:177:ASP:H	2.19	0.45	
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.51	0.45	
2:B:175:ASN:ND2	2:B:201:LYS:HE3	2.31	0.45	
2:B:178:ILE:HG22	2:B:191:SER:CB	2.46	0.45	
1:A:31:ILE:CG2	1:A:135:ILE:HG23	2.46	0.45	
2:B:66:LYS:HE3	2:B:230:MET:HA	1.99	0.45	
2:B:156:SER:N	2:B:157:PRO:HD2	2.31	0.45	
2:B:186:ASP:OD1	2:B:228:LEU:HD12	2.17	0.45	
2:B:295:LEU:H	2:B:295:LEU:CD1	2.25	0.45	
2:B:420:PRO:HG2	2:B:423:VAL:CG1	2.46	0.45	
1:A:507:GLN:NE2	2:B:421:PRO:HB3	2.27	0.45	
2:B:238:LYS:HD2	2:B:238:LYS:H	1.81	0.45	
1:A:376:THR:HG23	1:A:386:THR:CG2	2.47	0.45	
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.98	0.45	
2:B:427:TYR:O	2:B:428:GLN:CB	2.63	0.45	
1:A:8:VAL:HA	1:A:9:PRO:HD3	1.78	0.44	
1:A:58:THR:HG21	1:A:77:PHE:CD2	2.53	0.44	
1:A:108:VAL:HG12	1:A:227:PHE:CE1	2.52	0.44	
1:A:90:VAL:HG12	1:A:91:GLN:H	1.83	0.44	
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.53	0.44	
1:A:522:ILE:O	1:A:526:ILE:HG13	2.16	0.44	
2:B:423:VAL:CG1	2:B:424:LYS:N	2.79	0.44	
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.99	0.44	



		Interatomic	nic Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:275:LYS:HE2	1:A:332:GLN:NE2	2.33	0.44		
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.52	0.44		
2:B:241:VAL:O	2:B:243:PRO:HD3	2.18	0.44		
2:B:276:VAL:O	2:B:279:LEU:N	2.51	0.44		
1:A:100:LEU:O	1:A:318:TYR:HB3	2.16	0.44		
1:A:177:ASP:N	1:A:177:ASP:OD2	2.51	0.44		
2:B:171:PHE:HE2	2:B:178:ILE:CD1	2.29	0.44		
2:B:66:LYS:HE3	2:B:230:MET:H	1.83	0.44		
2:B:422:LEU:HB3	2:B:426:TRP:CH2	2.53	0.44		
2:B:350:LYS:HG2	2:B:351:THR:N	2.32	0.43		
1:A:182:GLN:HB3	6:A:1018:HOH:O	2.16	0.43		
1:A:357:MET:CE	1:A:512:GLN:NE2	2.81	0.43		
2:B:282:LEU:CD2	2:B:296:THR:HG23	2.48	0.43		
2:B:326:ILE:O	2:B:341:ILE:HA	2.18	0.43		
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.00	0.43		
2:B:195:ILE:HD13	2:B:195:ILE:H	1.82	0.43		
2:B:24:TRP:CG	2:B:25:PRO:HD2	2.53	0.43		
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.99	0.43		
2:B:376:THR:HB	2:B:410:TRP:CH2	2.54	0.43		
2:B:154:LYS:O	2:B:157:PRO:HD2	2.19	0.43		
2:B:116:PHE:CD1	2:B:116:PHE:N	2.87	0.43		
1:A:246:LEU:HD13	1:A:303:LEU:HD12	1.99	0.43		
2:B:380:ILE:O	2:B:384:GLY:N	2.51	0.43		
1:A:56:TYR:O	1:A:143:ARG:NH2	2.44	0.43		
1:A:390:LYS:HD3	1:A:415:GLU:HG2	2.00	0.43		
1:A:150:PRO:HG2	1:A:153:TRP:CB	2.48	0.43		
1:A:505:ILE:O	1:A:510:PRO:HD3	2.19	0.43		
1:A:10:VAL:HG11	1:A:153:TRP:HZ2	1.83	0.42		
2:B:112:GLY:HA3	2:B:151:GLN:HE21	1.83	0.42		
2:B:164:MET:CA	2:B:167:ILE:HG12	2.49	0.42		
1:A:434:ILE:HB	1:A:437:ALA:CB	2.49	0.42		
2:B:66:LYS:CD	2:B:230:MET:H	2.32	0.42		
2:B:96:HIS:HA	2:B:97:PRO:HD3	1.82	0.42		
2:B:27:THR:OG1	2:B:30:LYS:HG2	2.18	0.42		
2:B:345:PRO:C	2:B:347:LYS:H	2.21	0.42		
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.55	0.42		
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.53	0.42		
2:B:227:PHE:HB2	2:B:231:GLY:HA2	1.96	0.42		
1:A:457:TYR:CD1	1:A:457:TYR:C	2.93	0.42		
2:B:160:PHE:O	2:B:160:PHE:CD1	2.72	0.42		
2:B:195:ILE:H	2:B:195:ILE:CD1	2.33	0.42		



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:350:LYS:HE2	1:A:350:LYS:HB2	1.73	0.42	
2:B:164:MET:HA	2:B:167:ILE:HD11	2.01	0.42	
1:A:368:LEU:O	1:A:368:LEU:HD12	2.20	0.42	
1:A:343:GLN:HG3	1:A:349:LEU:HD11	2.01	0.42	
1:A:61:PHE:CD1	1:A:61:PHE:C	2.94	0.42	
1:A:244:ILE:O	1:A:244:ILE:HG23	2.20	0.42	
2:B:13:LYS:HB2	2:B:16:MET:SD	2.60	0.41	
2:B:306:ASN:O	2:B:310:LEU:HG	2.19	0.41	
2:B:260:LEU:O	2:B:264:LEU:HG	2.21	0.41	
1:A:210:LEU:HD12	1:A:210:LEU:HA	1.91	0.41	
1:A:475:GLN:HB2	1:A:501:TYR:CE2	2.56	0.41	
2:B:178:ILE:O	2:B:178:ILE:HG13	2.20	0.41	
2:B:201:LYS:HA	2:B:201:LYS:HD3	1.87	0.41	
1:A:398:TRP:NE1	1:A:411:ILE:HD12	2.35	0.41	
2:B:106:VAL:CG1	2:B:234:LEU:HB2	2.50	0.41	
2:B:210:LEU:HD12	2:B:224:GLU:CG	2.51	0.41	
1:A:78:ARG:O	1:A:82:LYS:HG3	2.20	0.41	
2:B:66:LYS:O	2:B:67:ASP:HB2	2.21	0.41	
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.56	0.41	
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.86	0.41	
1:A:516:GLU:O	1:A:517:LEU:C	2.58	0.41	
2:B:164:MET:HA	2:B:167:ILE:CG1	2.51	0.41	
1:A:208:HIS:O	1:A:212:TRP:CD1	2.73	0.41	
1:A:411:ILE:O	1:A:412:PRO:O	2.38	0.41	
2:B:328:GLU:O	2:B:339:TYR:HA	2.20	0.41	
1:A:113:ASP:HB3	1:A:116:PHE:HB2	2.02	0.41	
1:A:328:GLU:HG2	1:A:330:GLN:HE21	1.85	0.41	
2:B:175:ASN:N	2:B:176:PRO:HD3	2.35	0.41	
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.88	0.41	
2:B:366:LYS:HE2	2:B:370:GLU:OE1	2.22	0.40	
2:B:193:LEU:HD12	2:B:193:LEU:N	2.35	0.40	
1:A:358:ARG:HD3	1:A:370:GLU:CD	2.41	0.40	
2:B:116:PHE:N	2:B:116:PHE:HD1	2.19	0.40	
2:B:323:LYS:HD3	2:B:323:LYS:HA	1.75	0.40	
2:B:374:LYS:O	2:B:378:GLU:HG3	2.21	0.40	
1:A:435:VAL:HG22	2:B:290:THR:HG21	2.03	0.40	
1:A:480:GLN:HE22	1:A:484:LEU:HG	1.86	0.40	
2:B:211:ARG:HG3	2:B:211:ARG:NH1	2.36	0.40	
2:B:30:LYS:HG3	6:B:1041:HOH:O	2.20	0.40	
2:B:77:PHE:CE1	2:B:150:PRO:HB2	2.56	0.40	
2:B:257:ILE:CG2	2:B:283:LEU:HD11	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	Perce	entiles
1	А	518/534~(97%)	479 (92%)	34~(7%)	5 (1%)	15	28
2	В	393/422~(93%)	359~(91%)	32~(8%)	2~(0%)	29	48
All	All	911/956~(95%)	838~(92%)	66~(7%)	7(1%)	19	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	66	LYS
1	А	412	PRO
1	А	91	GLN
2	В	116	PHE
2	В	239	TRP
1	А	195	ILE
1	А	345	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	472/479~(98%)	451 (96%)	21 (4%)	28 52		
2	В	367/384~(96%)	354 (96%)	13~(4%)	36 62		
All	All	839/863~(97%)	805 (96%)	34 (4%)	30 55		



Mol	Chain	Res	Type
1	А	7	THR
1	А	24	TRP
1	А	28	GLU
1	А	39	THR
1	А	135	ILE
1	А	137	ASN
1	А	169	GLU
1	А	244	ILE
1	А	250	ASP
1	А	255	ASN
1	А	312	GLU
1	A	350	LYS
1	А	400	THR
1	А	402	TRP
1	А	443	ASP
1	А	459	THR
1	А	473	THR
1	А	477	THR
1	А	480	GLN
1	А	517	LEU
1	А	523	GLU
2	В	55	PRO
2	В	66	LYS
2	В	122	GLU
2	В	195	ILE
2	В	238	LYS
2	В	242	GLN
2	В	250	ASP
2	В	289	LEU
2	В	290	THR
2	В	295	LEU
2	В	303	LEU
2	В	374	LYS
2	В	414	TRP

All (34) residues with a non-rotameric sidechain are listed below:

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	23	GLN
1	А	91	GLN
1	А	151	GLN



Mol	Chain	Res	Type
1	А	222	GLN
1	А	255	ASN
1	А	265	ASN
1	А	278	GLN
1	А	332	GLN
1	А	336	GLN
1	А	428	GLN
1	А	475	GLN
1	А	480	GLN
1	А	507	GLN
1	А	509	GLN
1	А	512	GLN
1	А	520	GLN
2	В	147	ASN
2	В	151	GLN
2	В	175	ASN
2	В	269	GLN
2	В	278	GLN
2	В	348	ASN
2	В	407	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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		Dec	los Link	Bond lengths			Bond angles			
	Type	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	А	280	1	3,7,8	0.92	0	1,8,10	1.60	0

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
1	CSD	А	280	1	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	А	280	CSD	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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		Dog	Tinle	Bo	Bond lengths			Bond angles		
	туре	Unann	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
5	NVP	А	999	-	15,23,23	1.18	0	13,34,34	1.05	0	
3	PO4	А	1302	-	4,4,4	1.61	0	6,6,6	0.43	0	
3	PO4	А	1301	-	4,4,4	1.60	0	6,6,6	0.44	0	
3	PO4	А	1300	-	4,4,4	1.52	0	6,6,6	0.44	0	

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	NVP	А	999	-	-	0/0/6/6	0/3/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	<RSRZ $>$	#RSRZ>2		$OWAB(Å^2)$	Q<0.9	
1	А	522/534~(97%)	-0.05	24~(4%)	32	34	30, 57, 105, 150	0
2	В	401/422~(95%)	0.09	29~(7%)	15	16	30, 62, 123, 138	0
All	All	923/956~(96%)	0.01	53 (5%)	23	25	30, 58, 117, 150	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	88	TRP	7.4
2	В	230	MET	7.0
1	А	470	THR	6.2
2	В	232	TYR	5.2
2	В	421	PRO	5.0
1	А	66	LYS	5.0
1	А	65	LYS	4.8
1	А	67	ASP	4.8
1	А	68	SER	4.7
1	А	69	THR	4.6
1	А	469	LEU	4.6
2	В	173	LYS	4.3
1	А	468	THR	4.0
1	А	70	LYS	4.0
1	А	139	THR	3.9
1	А	72	ARG	3.6
2	В	67	ASP	3.5
1	А	91	GLN	3.4
2	В	66	LYS	3.2
2	В	102	LYS	3.2
2	В	189	VAL	3.2
2	В	212	TRP	3.2
2	В	210	LEU	3.0
2	В	65	LYS	2.9



Mol	Chain	\mathbf{Res}	Type	RSRZ	
2	В	224	GLU	2.9	
2	В	195	ILE	2.9	
1	А	52	PRO	2.8	
2	В	424	LYS	2.8	
2	В	237	ASP	2.6	
2	В	362	THR	2.6	
2	В	419	THR	2.5	
2	В	334	GLN	2.5	
1	А	53	GLU	2.5	
1	А	346	PHE	2.5	
1	А	467	VAL	2.4	
2	В	188	TYR	2.4	
1	А	130	PHE	2.4	
1	А	471	ASP	2.4	
2	В	223	LYS	2.3	
1	А	140	PRO	2.3	
1	А	64	LYS	2.3	
2	В	238	LYS	2.3	
2	В	166	LYS	2.2	
1	А	402	TRP	2.2	
2	В	240	THR	2.2	
1	А	491	LEU	2.2	
2	В	106	VAL	2.1	
2	В	95	PRO	2.1	
2	В	211	ARG	2.1	
2	В	104	LYS	2.1	
2	В	174	GLN	2.0	
1	А	495	ILE	2.0	
1	A	128	THR	2.0	

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
1	CSD	А	280	8/9	0.96	0.15	47,50,82,90	0



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	$B-factors(A^2)$	Q<0.9
3	PO4	А	1300	5/5	0.64	0.21	148,148,150,150	0
4	MG	А	1303	1/1	0.74	0.14	62,62,62,62	0
3	PO4	А	1302	5/5	0.82	0.24	147,150,150,150	0
3	PO4	А	1301	5/5	0.95	0.15	126,126,127,129	0
5	NVP	А	999	20/20	0.98	0.15	28,38,43,46	0

6.5 Other polymers (i)

There are no such residues in this entry.

