

Full wwPDB X-ray Structure Validation Report (i)

Feb 25, 2024 – 06:12 AM EST

PDB ID	:	5C53
Title	:	Probing the Structural and Molecular Basis of Nucleotide Selectivity by Hu-
		man Mitochondrial DNA Polymerase gamma
Authors	:	Sohl, C.D.; Szymanski, M.R.; Mislak, A.C.; Shumate, C.K.; Amiralaei, S.;
		Schinazi, R.F.; Anderson, K.S.; Yin, Y.W.
Deposited on	:	2015-06-19
Resolution	:	3.57 Å(reported)

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

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

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 3.57 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 $(#Entries, resolution range(Å))$					
Ba	13070/	$(77 \pm 1020, 1020$					
Itfree	100104	1020 (0.02-0.00)					
Clashscore	141614	1100(3.62-3.50)					
Ramachandran outliers	138981	1065 (3.62 - 3.50)					
Sidechain outliers	138945	1066 (3.62-3.50)					
RSRZ outliers	127900	1009 (3.64-3.48)					

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	v of chain	
1	А	1205	5%	56%	21% •	18%
2	В	903	31%	8% •	60%	
2	С	903	3% 	9% •	60%	
3	Т	26	12%	62%	3	8%



Mol	Chain	Length	Quality of chain		
4	Р	22	68%	27%	5%



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14634 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 DNA polymerase subunit gamma-1.

Mol	Chain	Residues		Α	toms		ZeroOcc	AltConf	Trace	
1	А	983	Total 7799	C 4966	N 1371	0 1413	S 49	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	?	-	GLN	deletion	UNP P54098
А	?	-	GLN	deletion	UNP P54098
А	?	-	GLN	deletion	UNP P54098
А	?	-	GLN	deletion	UNP P54098
А	?	-	GLN	deletion	UNP P54098
А	?	-	GLN	deletion	UNP P54098
А	?	-	GLN	deletion	UNP P54098
А	?	-	GLN	deletion	UNP P54098
А	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098

• Molecule 2 is a protein called Pol gamma B.

Mol	Chain	Residues		Atoms					AltConf	Trace
2	В	363	Total 2942	C 1885	N 520	O 521	S 16	0	0	0
2	С	358	Total 2883	C 1850	N 506	O 511	S 16	0	0	0

• Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf	Trace
3	Т	26	Total 529	C 251	N 93	O 159	Р 26	0	0	0

• Molecule 4 is a DNA chain called DNA (5'-D(*AP*AP*AP*AP*CP*GP*AP*GP*GP*GP*GP*



CP*CP*AP*GP*TP*GP*CP*CP*GP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Р	21	Total 433	C 205	N 89	0 119	Р 20	0	0	0

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	2	Total Mg 2 2	0	0

• Molecule 6 is [[(2 {S},5 {R})-5-(4-azanyl-5-fluoranyl-2-oxidanylidene-pyrimidin-1-yl)-1, $3^{1} {4}$ -oxathiolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (three-letter code: 4Y3) (formula: $C_8H_{15}FN_3O_{12}P_3S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	А	1	Total 28	C 8	F 1	N 3	O 12	Р 3	S 1	0	0

• Molecule 7 is 2',3'-DIDEOXYCYTIDINE-5'-MONOPHOSPHATE (three-letter code: DOC) (formula: $C_9H_{14}N_3O_6P$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
7	D	1	Total	С	Ν	0	Р	0	0
1	1	1	18	9	3	5	1	0	U



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: DNA polymerase subunit gamma-1





• Molecule 2: Pol gamma B





• Molecule 4: DNA (5'-D(*AP*AP*AP*AP*CP*GP*AP*GP*GP*GP*CP*CP*AP*GP*TP*GP *CP*CP*GP*TP*AP*C)-3')











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	217.45Å 217.45Å 163.59Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(Å)	48.91 - 3.57	Depositor
Resolution (A)	48.91 - 3.57	EDS
% Data completeness	99.0 (48.91-3.57)	Depositor
(in resolution range)	$85.1 \ (48.91 - 3.57)$	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.41 (at 3.57 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
D D .	0.300 , 0.338	Depositor
Λ, Λ_{free}	0.333 , 0.363	DCC
R_{free} test set	2000 reflections (4.24%)	wwPDB-VP
Wilson B-factor $(Å^2)$	135.3	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.26 , 7.5	EDS
L-test for $twinning^2$	$ L > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	14634	wwPDB-VP
Average B, all atoms $(Å^2)$	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.41% 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: MG, 4Y3, DOC

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	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.22	0/7999	0.43	1/10852~(0.0%)	
2	В	0.22	0/3015	0.39	0/4074	
2	С	0.23	0/2956	0.42	2/3997~(0.1%)	
3	Т	0.51	0/591	0.88	0/909	
4	Р	0.49	0/488	0.75	0/752	
All	All	0.25	0/15049	0.47	3/20584~(0.0%)	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	135	PRO	CA-N-CD	-8.64	99.41	111.50
2	С	96	HIS	C-N-CD	-7.46	104.20	120.60
1	А	752	LEU	C-N-CD	-6.44	106.44	120.60

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	7799	0	7692	184	0
2	В	2942	0	2937	44	0
2	С	2883	0	2858	64	0



\mathbf{Mol}	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes	
3	Т	529	0	291	10	0	
4	Р	433	0	234	6	0	
5	А	2	0	0	0	0	
6	А	28	0	11	4	0	
7	Р	18	0	12	1	0	
All	All	14634	0	14035	292	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 10.

All (292) 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 (\AA)	overlap (Å)
2:C:134:LYS:CD	2:C:135:PRO:HD3	1.82	1.08
2:C:135:PRO:HD2	2:C:136:GLY:H	1.11	1.06
2:C:134:LYS:HD2	2:C:135:PRO:CD	1.92	1.00
2:C:134:LYS:HD2	2:C:135:PRO:HD3	1.01	1.00
2:C:419:GLU:H	2:C:420:THR:HA	1.35	0.92
2:C:135:PRO:HD2	2:C:136:GLY:N	1.88	0.86
2:C:134:LYS:NZ	2:C:135:PRO:HD2	1.92	0.85
2:C:134:LYS:CD	2:C:135:PRO:CD	2.57	0.78
2:C:443:VAL:HG22	2:C:453:ILE:HD11	1.66	0.77
1:A:243:ASP:HB3	1:A:279:ARG:HE	1.49	0.77
2:C:135:PRO:CD	2:C:136:GLY:H	1.94	0.74
2:C:442:LEU:HB3	2:C:454:HIS:HB2	1.69	0.73
1:A:464:MET:HB2	1:A:589:PRO:HG2	1.71	0.73
1:A:487:ASP:OD2	1:A:601:LYS:NZ	2.22	0.72
1:A:849:THR:HG22	1:A:850:ILE:HD13	1.71	0.72
1:A:1068:ASP:HA	1:A:1085:PRO:HG2	1.72	0.71
2:C:134:LYS:HZ2	2:C:135:PRO:HD2	1.56	0.70
1:A:153:ALA:HB1	1:A:194:ALA:HB2	1.74	0.69
2:C:134:LYS:NZ	2:C:135:PRO:CD	2.55	0.69
1:A:938:THR:H	1:A:939:VAL:HA	1.61	0.66
1:A:533:CYS:SG	1:A:534:SER:N	2.69	0.65
1:A:1161:ARG:HE	1:A:1177:VAL:HG22	1.61	0.65
2:B:77:HIS:HE1	2:B:431:LYS:HG3	1.61	0.65
2:C:213:VAL:HG22	2:C:235:THR:HG22	1.77	0.65
1:A:856:GLU:OE1	1:A:859:TRP:N	2.26	0.65
2:B:197:LEU:HD22	2:B:202:LYS:HA	1.79	0.64
1:A:800:PHE:HB2	1:A:869:ARG:HE	1.63	0.64
1:A:896:LEU:HD21	1:A:931:LEU:HD23	1.79	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:83:LYS:HG2	2:C:84:GLN:HG2	1.79	0.64
2:C:134:LYS:HZ3	2:C:135:PRO:CD	2.11	0.63
1:A:230:GLU:OE2	1:A:386:ARG:NH1	2.32	0.62
1:A:1057:MET:SD	1:A:1057:MET:N	2.73	0.62
2:B:442:LEU:HB3	2:B:454:HIS:HB2	1.82	0.62
1:A:884:TYR:HA	1:A:1142:ARG:HA	1.80	0.62
1:A:850:ILE:HG22	3:T:6:DT:H4'	1.81	0.61
1:A:79:LEU:H	1:A:83:LEU:HG	1.65	0.61
2:C:135:PRO:CD	2:C:136:GLY:N	2.56	0.61
2:C:429:TYR:HE1	2:C:463:LYS:HZ3	1.47	0.60
1:A:963:GLU:HG3	1:A:981:LYS:HZ3	1.66	0.60
1:A:978:ALA:HA	1:A:981:LYS:HD2	1.83	0.60
1:A:502:LYS:HB3	1:A:503:VAL:HB	1.83	0.59
1:A:1142:ARG:NH1	1:A:1144:GLU:OE1	2.34	0.59
1:A:744:ILE:HG23	1:A:745:PRO:HD3	1.83	0.59
1:A:1069:ILE:O	1:A:1071:ARG:N	2.35	0.59
1:A:1108:TYR:OH	1:A:1161:ARG:NH1	2.34	0.59
1:A:743:ASP:N	1:A:743:ASP:OD1	2.36	0.59
2:B:75:ARG:NH1	2:B:84:GLN:OE1	2.35	0.59
1:A:134:ASN:ND2	1:A:1166:TYR:OH	2.32	0.59
1:A:938:THR:N	1:A:939:VAL:HA	2.16	0.59
1:A:463:LEU:HD21	1:A:594:LEU:HD23	1.84	0.58
2:C:219:PHE:HD1	2:C:229:LYS:HG2	1.69	0.58
1:A:107:LEU:O	1:A:112:LEU:N	2.36	0.57
1:A:208:CYS:SG	1:A:227:ARG:NH2	2.77	0.57
1:A:921:LEU:HD22	1:A:1174:PRO:HG2	1.86	0.57
2:C:197:LEU:HD12	2:C:202:LYS:HG2	1.86	0.57
1:A:831:TYR:H	1:A:832:ASP:HA	1.69	0.57
1:A:951:TYR:CD2	6:A:4003:4Y3:H7	2.40	0.57
2:B:363:ARG:HD3	2:B:364:LYS:H	1.70	0.56
2:B:428:LEU:HD13	2:B:428:LEU:H	1.70	0.56
1:A:887:VAL:HG22	1:A:1185:ILE:HG23	1.87	0.56
1:A:488:LEU:HD13	1:A:488:LEU:H	1.69	0.55
2:B:185:LEU:H	2:B:185:LEU:HD23	1.71	0.55
2:C:319:VAL:HA	2:C:322:LEU:HD13	1.88	0.55
1:A:1079:ILE:HG12	1:A:1099:TRP:CZ3	2.42	0.55
1:A:869:ARG:NH1	4:P:22:DT:OP1	2.41	0.54
2:B:104:VAL:HG23	2:B:107:ARG:HH21	1.72	0.54
1:A:1073:PRO:HA	1:A:1074:VAL:HG13	1.89	0.54
1:A:162:LEU:HG	1:A:401:TRP:CZ3	2.42	0.54
1:A:1096:ARG:HA	1:A:1099:TRP:HB3	1.88	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:278:CYS:SG	2:C:288:LYS:NZ	2.81	0.54
1:A:239:LEU:O	1:A:279:ARG:NH1	2.41	0.54
2:B:241:TRP:HB3	2:B:336:LEU:HB3	1.90	0.54
1:A:466:LEU:HB3	1:A:602:LEU:HD21	1.89	0.53
2:B:323:HIS:HB3	2:B:330:ASN:HB2	1.90	0.53
2:C:424:SER:HB3	2:C:427:GLN:HG2	1.90	0.53
1:A:861:THR:HG21	3:T:8:DC:H1'	1.91	0.52
2:B:262:TRP:HA	2:B:265:LYS:HE2	1.91	0.52
2:C:184:ASN:OD1	2:C:185:LEU:N	2.41	0.52
1:A:1089:GLN:N	1:A:1090:GLU:HA	2.24	0.52
1:A:911:HIS:NE2	1:A:1172:ASP:O	2.37	0.52
1:A:761:ASN:OD1	1:A:761:ASN:N	2.43	0.52
1:A:977:GLU:HB3	1:A:981:LYS:HZ2	1.74	0.52
1:A:549:LEU:HD11	2:B:468:ILE:HG21	1.92	0.52
1:A:353:VAL:HG13	1:A:355:SER:H	1.75	0.52
1:A:752:LEU:HB2	1:A:753:PRO:HA	1.90	0.52
1:A:834:GLU:HG3	2:B:328:ARG:HH21	1.75	0.52
1:A:895:GLU:CG	6:A:4003:4Y3:H4	2.23	0.52
2:C:419:GLU:N	2:C:420:THR:HA	2.07	0.52
1:A:196:VAL:HG22	1:A:215:ILE:HG12	1.93	0.51
2:B:83:LYS:HG2	2:B:85:GLN:H	1.74	0.51
1:A:866:ARG:HH21	1:A:869:ARG:HD2	1.75	0.51
1:A:562:ARG:HH11	1:A:563:PRO:HD2	1.74	0.51
1:A:622:TYR:HB2	1:A:770:PHE:HE2	1.75	0.51
1:A:93:GLU:HA	1:A:94:MET:HB2	1.93	0.51
1:A:212:ALA:HB3	1:A:223:TRP:HB3	1.92	0.51
1:A:296:SER:HB2	1:A:847:ALA:HB3	1.93	0.51
1:A:1061:LEU:HB3	1:A:1097:VAL:HG13	1.92	0.51
1:A:495:PHE:HB3	1:A:496:LYS:HB2	1.92	0.51
2:B:407:LEU:HD13	2:C:120:VAL:HG12	1.92	0.51
2:C:262:TRP:HA	2:C:265:LYS:HE2	1.93	0.51
1:A:299:MET:HG2	1:A:848:GLY:HA2	1.93	0.51
2:B:365:LYS:H	2:B:365:LYS:HD2	1.75	0.50
2:B:219:PHE:HA	2:B:229:LYS:N	2.27	0.50
2:C:444:THR:OG1	2:C:445:GLU:OE2	2.28	0.50
1:A:963:GLU:HG3	1:A:981:LYS:NZ	2.27	0.50
1:A:1200:PRO:O	1:A:1202:ASN:N	2.44	0.50
2:C:252:LEU:HD22	2:C:305:ASN:HB2	1.93	0.50
2:C:389:ARG:HD3	2:C:395:LEU:HD11	1.93	0.50
2:B:404:ASN:HA	2:B:407:LEU:HG	1.93	0.50
2:C:444:THR:OG1	2:C:445:GLU:N	2.44	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:262:GLN:HB2	1:A:263:GLU:HG2	1.94	0.49
2:B:393:LEU:HD12	2:B:394:GLU:HG2	1.93	0.49
2:C:134:LYS:HZ3	2:C:135:PRO:HD2	1.70	0.49
2:C:201:ASN:O	2:C:201:ASN:ND2	2.42	0.49
1:A:608:ASP:OD1	1:A:778:THR:OG1	2.29	0.49
1:A:750:PHE:HD1	1:A:751:LYS:HG2	1.76	0.49
2:C:134:LYS:CG	2:C:135:PRO:CD	2.91	0.49
1:A:1088:VAL:HG12	1:A:1090:GLU:HA	1.94	0.49
1:A:556:THR:HA	1:A:559:LEU:HD13	1.95	0.49
2:C:205:PRO:HB3	2:C:243:THR:HA	1.95	0.49
2:C:241:TRP:HD1	2:C:336:LEU:HD22	1.77	0.49
1:A:94:MET:HG3	1:A:1170:LEU:HD11	1.95	0.49
1:A:953:ARG:HG3	1:A:957:ALA:HB2	1.93	0.49
1:A:987:ALA:HB1	1:A:1056:GLU:HG2	1.95	0.49
1:A:1115:ALA:HB3	1:A:1156:THR:HG23	1.95	0.49
1:A:275:ARG:NH2	1:A:433:SER:O	2.42	0.49
2:B:441:VAL:HG23	2:B:453:ILE:HG13	1.94	0.48
1:A:856:GLU:H	1:A:860:LEU:HD12	1.78	0.48
1:A:1075:LEU:HD23	1:A:1075:LEU:H	1.78	0.48
2:C:436:SER:OG	2:C:458:ARG:NH1	2.46	0.48
1:A:1154:GLN:HG3	1:A:1218:LEU:HD21	1.95	0.48
2:B:457:SER:OG	2:B:460:THR:O	2.32	0.48
2:B:213:VAL:HA	2:B:235:THR:HA	1.95	0.48
2:C:134:LYS:HG3	2:C:135:PRO:HD2	1.96	0.48
2:B:384:ALA:HB2	2:B:437:ILE:HD13	1.94	0.48
2:C:105:GLU:O	2:C:109:ASN:ND2	2.43	0.48
1:A:825:VAL:HG13	1:A:882:PRO:HG2	1.95	0.48
1:A:869:ARG:HB2	1:A:872:SER:HB2	1.96	0.48
1:A:175:TRP:CD2	1:A:223:TRP:HB2	2.48	0.48
1:A:991:GLY:HA2	1:A:1052:GLY:HA2	1.96	0.48
1:A:616:GLU:HB2	1:A:617:ARG:HD3	1.96	0.48
1:A:1134:HIS:HD2	7:P:101:DOC:H1'	1.78	0.48
2:C:317:GLY:HA3	2:C:318:ASN:HA	1.58	0.48
1:A:803:ASN:HA	3:T:10:DG:H4'	1.95	0.47
1:A:849:THR:OG1	3:T:7:DA:OP1	2.23	0.47
1:A:887:VAL:HG13	1:A:1185:ILE:HG12	1.95	0.47
1:A:178:TYR:O	1:A:219:ALA:HB1	2.14	0.47
1:A:475:SER:HA	1:A:476:GLY:HA2	1.49	0.47
1:A:1183:VAL:HB	1:A:1214:GLN:HB3	1.96	0.47
1:A:1183:VAL:N	1:A:1214:GLN:O	2.47	0.47
1:A:611:PRO:HG3	1:A:652:ILE:HD13	1.97	0.47



	A t area D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:1090:GLU:O	1:A:1091:GLU:HG2	2.14	0.47
2:C:235:THR:OG1	2:C:343:ASP:OD1	2.29	0.47
1:A:272:SER:HB3	1:A:843:GLN:HA	1.97	0.46
1:A:804:ALA:O	1:A:808:ILE:HG12	2.14	0.46
1:A:642:SER:HA	1:A:643:ALA:HA	1.58	0.46
1:A:765:PRO:HA	1:A:766:PHE:HA	1.58	0.46
2:C:246:ARG:NH2	2:C:326:ASP:OD2	2.46	0.46
2:B:428:LEU:HA	2:B:431:LYS:HB3	1.96	0.46
1:A:593:SER:HB2	1:A:596:MET:HB2	1.97	0.46
1:A:939:VAL:HA	1:A:940:GLY:HA3	1.71	0.46
1:A:135:LEU:HD23	1:A:135:LEU:H	1.79	0.46
1:A:866:ARG:HE	1:A:869:ARG:HD2	1.79	0.46
1:A:977:GLU:HB3	1:A:981:LYS:NZ	2.31	0.46
4:P:14:DC:H2'	4:P:15:DA:C8	2.50	0.46
1:A:302:SER:HB2	1:A:1081:ARG:HD3	1.96	0.46
1:A:636:THR:OG1	1:A:637:GLY:N	2.49	0.46
1:A:888:GLY:HA3	1:A:1138:ARG:HD2	1.97	0.46
1:A:897:TRP:CD1	1:A:1177:VAL:HG21	2.50	0.46
2:B:193:TYR:OH	2:B:333:PRO:HG3	2.15	0.46
1:A:606:THR:HB	1:A:612:LEU:HD13	1.97	0.46
2:B:266:PHE:HA	2:B:375:HIS:CD2	2.51	0.46
2:B:197:LEU:HA	2:B:197:LEU:HD23	1.84	0.45
2:B:364:LYS:HB2	2:B:364:LYS:HE2	1.65	0.45
1:A:618:HIS:CD2	1:A:619:GLY:H	2.34	0.45
2:C:381:ILE:HG21	2:C:414:TRP:HB2	1.97	0.45
3:T:16:DG:H1	4:P:13:DC:H42	1.63	0.45
1:A:942:SER:HA	1:A:943:ARG:HA	1.58	0.45
2:B:278:CYS:SG	2:B:288:LYS:NZ	2.87	0.45
2:B:420:THR:HG23	2:B:421:MET:HG2	1.99	0.45
2:B:467:HIS:HB3	2:B:470:LYS:HB2	1.97	0.45
1:A:617:ARG:HB2	1:A:763:GLY:HA3	1.99	0.45
1:A:384:ASP:OD1	1:A:384:ASP:N	2.42	0.45
1:A:894:GLN:HG3	1:A:895:GLU:H	1.81	0.45
1:A:262:GLN:HA	1:A:263:GLU:HA	1.51	0.45
1:A:110:HIS:HB3	1:A:111:GLY:HA2	1.98	0.45
1:A:435:LEU:HD22	1:A:878:VAL:HG11	1.98	0.45
1:A:778:THR:HA	1:A:779:LEU:HA	1.61	0.45
2:B:244:PRO:HA	2:B:245:PRO:HD3	1.86	0.45
1:A:895:GLU:CD	6:A:4003:4Y3:H4	2.21	0.45
1:A:976:GLN:O	1:A:980:GLU:HG2	2.17	0.45
2:C:67:GLU:N	2:C:88:ARG:HH21	2.15	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1124:ALA:O	1:A:1148:ARG:NH2	2.44	0.44
2:C:389:ARG:HB3	2:C:395:LEU:HD11	1.98	0.44
1:A:268:GLY:HA2	1:A:403:THR:HG21	1.99	0.44
1:A:307:PHE:O	1:A:310:SER:OG	2.34	0.44
1:A:1214:GLN:HA	1:A:1215:GLY:HA3	1.58	0.44
2:C:293:PHE:HB3	2:C:295:TRP:H	1.82	0.44
1:A:372:GLU:HG3	1:A:375:GLU:H	1.82	0.44
1:A:612:LEU:HD12	1:A:612:LEU:HA	1.76	0.44
1:A:808:ILE:HD12	1:A:874:LEU:HG	1.99	0.44
2:B:454:HIS:ND1	2:B:463:LYS:HE3	2.33	0.44
1:A:162:LEU:HD22	1:A:163:PRO:HD2	1.99	0.44
1:A:582:ASP:HA	1:A:583:PRO:HD3	1.90	0.44
1:A:856:GLU:HA	1:A:857:PRO:HD3	1.85	0.44
2:B:421:MET:HA	2:B:422:GLN:HB3	1.99	0.44
2:C:239:LEU:HB3	2:C:338:VAL:HB	1.99	0.44
1:A:1133:ILE:HG12	1:A:1136:GLU:HB3	1.98	0.44
2:B:365:LYS:HG2	2:B:367:LEU:H	1.82	0.44
2:C:303:LEU:HD22	2:C:338:VAL:HG22	2.00	0.44
1:A:579:ARG:NH1	4:P:12:DG:OP1	2.51	0.44
1:A:267:VAL:HG12	1:A:292:LEU:HB3	1.98	0.44
1:A:1187:ARG:HH11	1:A:1209:ARG:HH12	1.66	0.44
1:A:536:GLU:HG3	2:C:257:ARG:HH12	1.82	0.43
1:A:773:LYS:HD2	1:A:773:LYS:HA	1.89	0.43
1:A:892:ASP:HA	1:A:893:SER:HA	1.66	0.43
1:A:566:LEU:HD13	1:A:566:LEU:H	1.81	0.43
1:A:856:GLU:N	1:A:860:LEU:HD12	2.33	0.43
1:A:973:LEU:HD21	1:A:976:GLN:HG3	1.99	0.43
1:A:505:LYS:HD3	1:A:505:LYS:HA	1.78	0.43
1:A:895:GLU:HG3	6:A:4003:4Y3:H4	1.81	0.43
1:A:1047:ARG:H	1:A:1047:ARG:HG3	1.64	0.43
1:A:831:TYR:N	1:A:832:ASP:HA	2.30	0.43
2:C:134:LYS:CE	2:C:135:PRO:HD3	2.47	0.43
2:C:419:GLU:OE2	2:C:422:GLN:HB2	2.18	0.43
3:T:9:DG:H2'	3:T:10:DG:C8	2.53	0.43
2:C:316:PRO:HA	2:C:317:GLY:HA2	1.57	0.43
2:C:134:LYS:HG3	2:C:135:PRO:CD	2.49	0.43
4:P:21:DG:H2'	4:P:22:DT:C6	2.53	0.43
1:A:1079:ILE:HG12	1:A:1099:TRP:CE3	2.54	0.43
1:A:1198:LYS:HB3	1:A:1198:LYS:HE3	1.81	0.43
2:B:418:LEU:HD22	2:C:204:LEU:HD12	1.99	0.43
3:T:17:DC:H42	4:P:12:DG:H1	1.67	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:1026:ARG:HD2	1:A:1026:ARG:O	2.20	0.42
1:A:498:LYS:HD3	3:T:23:DT:OP1	2.19	0.42
1:A:782:GLY:HA2	1:A:784:GLY:HA2	2.01	0.42
1:A:864:ASN:HB3	1:A:1191:LYS:HD3	2.01	0.42
1:A:1060:LYS:HE2	1:A:1064:ILE:HD11	2.01	0.42
2:C:205:PRO:HB3	2:C:244:PRO:HD3	2.01	0.42
1:A:155:ASN:O	1:A:159:GLN:HG2	2.20	0.42
1:A:963:GLU:HA	1:A:981:LYS:HE2	2.02	0.42
2:C:243:THR:HG1	2:C:251:TRP:HE3	1.64	0.42
1:A:206:GLY:HA3	1:A:207:THR:HA	1.82	0.42
1:A:299:MET:SD	1:A:849:THR:HG23	2.59	0.42
2:B:133:HIS:ND1	2:C:233:GLU:OE2	2.51	0.42
1:A:87:ILE:HD13	1:A:127:LEU:HD22	2.01	0.41
1:A:828:HIS:O	1:A:830:ASP:N	2.45	0.41
1:A:79:LEU:HD13	1:A:80:SER:H	1.84	0.41
1:A:176:THR:OG1	1:A:222:SER:OG	2.36	0.41
1:A:288:ARG:HE	1:A:288:ARG:HA	1.86	0.41
1:A:818:ARG:H	1:A:818:ARG:HE	1.68	0.41
1:A:298:HIS:HB2	1:A:410:GLN:HE22	1.85	0.41
1:A:371:LYS:HD2	1:A:371:LYS:HA	1.97	0.41
1:A:595:GLN:OE1	1:A:795:ASN:ND2	2.37	0.41
2:B:213:VAL:HG11	2:C:132:HIS:CE1	2.55	0.41
1:A:247:LEU:H	1:A:247:LEU:HD13	1.85	0.41
3:T:14:DT:H2"	3:T:15:DG:C8	2.55	0.41
1:A:78:MET:HA	1:A:79:LEU:HA	1.77	0.41
2:C:389:ARG:HG2	2:C:390:GLY:N	2.35	0.41
2:C:418:LEU:N	2:C:419:GLU:HA	2.36	0.41
1:A:499:LYS:H	1:A:499:LYS:HG3	1.59	0.41
1:A:850:ILE:HA	1:A:851:THR:HA	1.76	0.41
1:A:1074:VAL:HB	1:A:1167:LYS:HB3	2.01	0.41
2:B:439:PHE:HB3	2:B:455:LEU:HD11	2.03	0.41
3:T:6:DT:H2'	3:T:7:DA:O4'	2.20	0.41
1:A:851:THR:O	1:A:1106:VAL:HG21	2.21	0.41
1:A:864:ASN:O	1:A:872:SER:OG	2.38	0.41
1:A:1075:LEU:HB2	1:A:1076:GLY:HA3	2.02	0.41
2:B:79:LEU:HG	2:B:102:LEU:HB2	2.03	0.41
2:C:440:THR:OG1	2:C:456:ARG:HB3	2.20	0.41
1:A:749:PHE:HB2	1:A:750:PHE:H	1.60	0.41
1:A:1064:ILE:HG22	1:A:1071:ARG:HB3	2.03	0.41
2:C:264:ARG:HG3	2:C:270:PRO:HB3	2.02	0.41
1:A:211:LEU:HD12	1:A:377:PHE:HZ	1.86	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:SER:HB3	1:A:227:ARG:NH2	2.35	0.40
1:A:1213:PRO:O	1:A:1214:GLN:NE2	2.54	0.40
1:A:502:LYS:HA	1:A:503:VAL:HA	1.94	0.40
2:B:382:LYS:H	2:B:412:SER:HB2	1.86	0.40
2:C:293:PHE:N	2:C:294:PRO:HA	2.37	0.40
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.95	0.40
1:A:299:MET:HG3	1:A:849:THR:HG23	2.03	0.40
1:A:304:LEU:HD13	1:A:309:ARG:HG2	2.02	0.40
1:A:771:LEU:HD21	1:A:792:LEU:HB3	2.02	0.40
1:A:1157:ASN:ND2	1:A:1178:ALA:O	2.55	0.40
1:A:175:TRP:CE3	1:A:223:TRP:HB2	2.57	0.40
1:A:631:LEU:HB3	1:A:633:LYS:NZ	2.35	0.40
2:B:446:THR:O	2:B:450:ASN:ND2	2.53	0.40
1:A:151:LEU:HD21	1:A:424:LEU:HD11	2.04	0.40
1:A:1136:GLU:OE2	1:A:1138:ARG:NH1	2.55	0.40
2:B:290:TYR:HD1	2:B:299:LEU:HA	1.87	0.40
2:B:423:SER:OG	2:B:424:SER:N	2.54	0.40
2:C:244:PRO:HA	2:C:245:PRO:HD3	1.81	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	P	erce	entiles
1	А	969/1205~(80%)	835~(86%)	114 (12%)	20 (2%)		7	40
2	В	355/903~(39%)	326 (92%)	27 (8%)	2 (1%)		25	64
2	С	350/903~(39%)	325~(93%)	18 (5%)	7 (2%)		7	42
All	All	1674/3011~(56%)	1486 (89%)	159 (10%)	29 (2%)		9	45

All (29) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	752	LEU
1	А	1070	PRO
2	С	97	PRO
1	А	749	PHE
1	А	1177	VAL
2	С	98	GLY
2	С	423	SER
1	А	642	SER
1	А	767	ALA
1	А	1073	PRO
1	А	1080	SER
1	А	1134	HIS
2	С	316	PRO
2	С	319	VAL
2	С	391	PRO
1	А	95	PRO
1	А	610	PHE
1	А	618	HIS
1	А	811	GLN
1	А	927	ARG
1	А	1074	VAL
1	А	743	ASP
1	А	765	PRO
2	В	317	GLY
2	С	380	PRO
2	В	451	GLY
1	А	560	PRO
1	А	1043	VAL
1	А	1141	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	823/1017 (81%)	749~(91%)	74 (9%)	9 39		
2	В	325/791~(41%)	307~(94%)	18~(6%)	21 56		
2	С	316/791~(40%)	297~(94%)	19 (6%)	19 54		



Continued from previous page...

Mol	Chain	Analysed	Analysed Rotameric Outliers		Percentiles		
All	All	1464/2599~(56%)	1353~(92%)	111 (8%)	13 44		

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	79	LEU
1	А	101	ARG
1	А	118	VAL
1	А	130	LEU
1	А	133	ASP
1	А	195	LEU
1	А	197	PHE
1	А	201	VAL
1	А	227	ARG
1	А	236	THR
1	А	245	ILE
1	А	247	LEU
1	А	292	LEU
1	А	304	LEU
1	А	311	LEU
1	А	316	LYS
1	А	424	LEU
1	А	488	LEU
1	А	499	LYS
1	А	548	CYS
1	А	558	LEU
1	А	565	HIS
1	А	566	LEU
1	А	595	GLN
1	А	596	MET
1	A	613	HIS
1	А	617	ARG
1	А	636	THR
1	A	639	THR
1	А	640	LEU
1	A	655	LEU
1	А	743	ASP
1	A	744	ILE
1	А	748	TRP
1	A	751	LYS
1	А	761	ASN
1	A	768	LYS



Mol	Chain	Res	Type
1	А	774	MET
1	А	779	LEU
1	А	816	LEU
1	А	818	ARG
1	А	821	LEU
1	А	841	LEU
1	А	851	THR
1	А	927	ARG
1	А	941	ILE
1	А	964	ARG
1	А	970	ASN
1	А	973	LEU
1	А	977	GLU
1	А	1026	ARG
1	А	1027	LYS
1	А	1038	TRP
1	А	1043	VAL
1	А	1047	ARG
1	А	1057	MET
1	А	1069	ILE
1	А	1071	ARG
1	А	1074	VAL
1	А	1075	LEU
1	А	1081	ARG
1	А	1090	GLU
1	А	1099	TRP
1	А	1118	TRP
1	А	1120	PHE
1	А	1129	PHE
1	А	1133	ILE
1	А	1141	VAL
1	А	1190	ARG
1	А	1191	LYS
1	А	1197	CYS
1	А	1198	LYS
1	А	1210	TYR
1	А	1218	LEU
2	В	69	LEU
2	В	89	ASP
2	В	186	LEU
2	В	197	LEU
2	В	231	ILE



Mol	Chain	Res	Type
2	В	263	TRP
2	В	329	LYS
2	В	364	LYS
2	В	365	LYS
2	В	368	HIS
2	В	372	LEU
2	В	394	GLU
2	В	396	ARG
2	В	428	LEU
2	В	453	ILE
2	В	460	THR
2	В	461	THR
2	В	467	HIS
2	С	83	LYS
2	С	86	LEU
2	С	115	TRP
2	С	122	ARG
2	С	186	LEU
2	С	197	LEU
2	С	201	ASN
2	С	204	LEU
2	С	251	TRP
2	С	256	LEU
2	С	262	TRP
2	С	281	GLU
2	С	282	GLU
2	С	284	ARG
2	С	295	TRP
2	С	300	ILE
2	С	386	ASP
2	С	402	LEU
2	С	453	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	264	GLN
1	А	1134	HIS
2	С	96	HIS



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	Al Type Chain Res		Tiple	Bond lengths			Bond angles			
INIOI	of Type Chain Re	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
6	4Y3	А	4003	5	25,29,29	4.32	10 (40%)	35,45,45	1.80	7 (20%)
7	DOC	Р	101	4	16,19,20	0.42	0	20,26,29	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
6	4Y3	А	4003	5	-	5/22/31/31	0/2/2/2
7	DOC	Р	101	4	-	0/7/18/19	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	А	4003	4Y3	O2-C2	10.19	1.42	1.23



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
6	А	4003	4Y3	C2'-S	-10.06	1.51	1.81
6	А	4003	4Y3	O4'-C1'	8.80	1.62	1.42
6	А	4003	4Y3	C4'-S	-6.81	1.58	1.81
6	А	4003	4Y3	C2'- $C1$ '	-5.62	1.33	1.52
6	А	4003	4Y3	C6-C5	5.57	1.41	1.33
6	А	4003	4Y3	O4'-C4'	-4.99	1.29	1.44
6	А	4003	4Y3	C4-N4	4.59	1.46	1.34
6	А	4003	4Y3	C2-N1	-3.07	1.33	1.40
6	А	4003	4Y3	F-C5	-2.52	1.31	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	А	4003	4Y3	C2'-S-C4'	6.80	106.11	88.24
6	А	4003	4Y3	F-C5-C4	4.44	120.92	118.02
6	А	4003	4Y3	PB-O3A-PA	-2.79	123.25	132.83
6	А	4003	4Y3	PB-O3B-PG	-2.52	124.19	132.83
6	А	4003	4Y3	O2-C2-N3	-2.49	118.28	122.33
6	А	4003	4Y3	N1-C2-N3	2.24	122.88	118.81
6	А	4003	4Y3	C4'-O4'-C1'	-2.19	107.95	112.59

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
6	А	4003	4Y3	C5'-O5'-PA-O1A
6	А	4003	4Y3	C5'-O5'-PA-O2A
6	А	4003	4Y3	PA-O3A-PB-O2B
6	А	4003	4Y3	C5'-O5'-PA-O3A
6	А	4003	4Y3	PG-O3B-PB-O2B

All (5) torsion outliers are listed below:

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	А	4003	4Y3	4	0
7	Р	101	DOC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will



5C53

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	983/1205~(81%)	0.32	59 (6%) 21 13	44, 73, 91, 163	0
2	В	363/903~(40%)	0.21	8 (2%) 62 45	47, 65, 87, 101	0
2	С	358/903~(39%)	0.33	25 (6%) 16 10	54, 73, 86, 96	0
3	Т	26/26~(100%)	0.76	3(11%) 4 4	84, 107, 126, 131	0
4	Р	21/22~(95%)	0.17	0 100 100	92, 105, 127, 166	0
All	All	1751/3059~(57%)	0.30	95 (5%) 25 16	44, 72, 94, 166	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	745	PRO	11.1
1	А	630	ASN	9.6
1	А	746	GLY	9.1
1	А	747	CYS	8.0
1	А	632	ALA	7.0
2	С	282	GLU	5.8
1	А	501	LYS	5.8
1	А	631	LEU	5.5
1	А	744	ILE	5.0
2	С	228	VAL	4.9
1	А	500	ALA	4.5
1	А	509	THR	4.5
2	В	366	ASN	4.4
1	А	741	ASP	4.3
1	А	622	TYR	4.3
1	А	508	ALA	4.2
1	A	619	GLY	4.0
2	С	121	PHE	4.0
1	А	865	ALA	3.8
1	A	640	LEU	3.7



Mol	Chain	Res	Type	RSRZ
1	А	1202	ASN	3.6
1	А	1031	GLU	3.5
1	А	506	GLU	3.4
1	А	230	GLU	3.4
1	А	759	SER	3.4
1	А	1087	ALA	3.4
2	С	123	GLU	3.3
1	А	102	ARG	3.3
1	А	214	ALA	3.1
1	А	760	CYS	3.1
1	А	507	PRO	3.1
2	С	325	ARG	3.1
1	A	94	MET	3.0
1	А	1207	GLU	3.0
1	A	431	GLY	3.0
1	А	764	SER	2.9
2	С	421	MET	2.9
1	А	633	LYS	2.9
2	С	288	LYS	2.8
1	А	601	LYS	2.8
1	А	969	PHE	2.8
2	В	328	ARG	2.8
1	А	173	GLU	2.8
2	С	124	GLN	2.7
2	В	322	LEU	2.7
2	С	204	LEU	2.7
2	С	328	ARG	2.7
2	С	229	LYS	2.7
2	В	108	LYS	2.7
2	С	304	TRP	2.6
1	А	1213	PRO	2.6
2	C	137	PRO	2.6
2	С	388	GLY	2.6
1	A	893	SER	2.6
2	С	351	TYR	2.5
1	А	502	LYS	2.5
2	С	468	ILE	2.5
2	С	455	LEU	2.5
2	В	81	GLY	2.5
3	Т	25	DT	2.5
2	С	285	LYS	2.4
1	А	846	THR	2.4



Mol	Chain	Res	Type	RSRZ
1	А	1082	ALA	2.4
2	С	466	MET	2.4
2	С	122	ARG	2.4
1	А	1208	ARG	2.4
1	А	927	ARG	2.4
1	А	1076	GLY	2.3
1	А	342	ILE	2.3
1	А	832	ASP	2.3
1	А	1134	HIS	2.3
1	А	890	ASP	2.3
1	А	942	SER	2.3
2	В	391	PRO	2.2
1	А	348	LEU	2.2
2	С	203	ARG	2.2
2	С	219	PHE	2.2
2	В	109	ASN	2.2
2	В	393	LEU	2.2
3	Т	22	DG	2.2
2	С	387	VAL	2.2
2	С	236	GLU	2.2
1	А	1036	SER	2.2
1	А	1068	ASP	2.1
1	А	304	LEU	2.1
2	С	326	ASP	2.1
1	А	912	GLY	2.1
1	A	1131	ILE	2.1
1	А	122	ASP	2.1
1	A	892	ASP	2.1
1	A	1050	LYS	2.1
3	Т	21	DC	2.0
1	А	1132	SER	2.0
1	А	93	GLU	2.0
1	A	510	ALA	2.0

Continued from previous page...

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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
6	4Y3	А	4003	28/28	0.82	0.39	80,100,106,107	0
7	DOC	Р	101	18/19	0.84	0.35	91,94,98,99	0
5	MG	А	4002	1/1	0.88	0.34	60,60,60,60	0
5	MG	А	4001	1/1	0.94	0.20	70,70,70,70	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.

