

Full wwPDB X-ray Structure Validation Report (i)

Feb 5, 2024 – 06:23 AM EST

PDB ID	:	1SL0
Title	:	Ternary 3' complex of T7 DNA polymerase with a DNA primer/template
		containing a disordered cis-syn thymine dimer on the template and an incoming nucleotide
Authors	:	Li, Y.; Dutta, S.; Doublie, S.; Bdour, H.M.; Taylor, J.S.; Ellenberger, T.
Deposited on	:	2004-03-05
Resolution	:	3.20 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 3.20 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.



Matria	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	Р	21		43%	10%	48%	_	
1	Q	21	5%	43%	5%	48%	_	
2	Т	25	28%	12%		60%	_	
2	U	25	24%	16%		60%		



Mol	Chain	Length	Quality of chain						
3	А	698	^{2%} 46%	43%	5% 6%				
3	С	698	3% 47%	42%	6% 6%				
4	В	108	40%	52%	6% •				
4	D	108	43%	48%	6% •				

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
6	DAD	А	4004	Х	-	-	-
6	DAD	С	4005	Х	-	-	-



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11904 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 DNA chain called 5'-D(*CP*GP*AP*AP*AP*AP*CP*GP*AP*CP*GP*G P*CP*CP*AP*GP*TP*GP*CP*CP*(2DT))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	11	Total	С	Ν	0	Р	0	0	0
1	1	11	224	106	41	66	11	0	0	0
1	0	11	Total	С	Ν	0	Р	0	0	0
	Q	11	224	106	41	66	11	0	U	U

• Molecule 2 is a DNA chain called 5'-D(*CP*CP*CP*(TTD)P*AP*GP*GP*CP*AP*CP*T P*GP*GP*CP*GP*TP*CP*GP*TP*TP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Т	10	Total	С	Ν	Ο	Р	0	0	0
	T	10	207	97	41	59	10	0	0	0
0	II	10	Total	С	Ν	Ο	Р	0	0	0
	U	10	207	97	41	59	10	0	0	0

• Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	А	658	Total	С	Ν	Ο	\mathbf{S}	0	0	0
0		000	4782	3042	831	889	20	Ŭ	Ŭ	0
9	C	659	Total	С	Ν	0	\mathbf{S}	0	0	0
3		000	4772	3031	830	891	20	0	0	U

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	?	-	LYS	deletion	UNP P00581
А	?	-	ARG	deletion	UNP P00581
А	?	-	PHE	deletion	UNP P00581
А	?	-	GLY	deletion	UNP P00581
А	?	-	SER	deletion	UNP P00581
А	?	-	HIS	deletion	UNP P00581



Chain	Residue	Modelled	Actual	Comment	Reference
С	?	-	LYS	deletion	UNP P00581
С	?	-	ARG	deletion	UNP P00581
С	?	-	PHE	deletion	UNP P00581
С	?	-	GLY	deletion	UNP P00581
С	?	-	SER	deletion	UNP P00581
С	?	-	HIS	deletion	UNP P00581

• Molecule 4 is a protein called Thioredoxin 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
4	В	105	Total	С	Ν	0	S	0	0	0
-		100	716	461	118	135	2	0		Ū
4	П	105	Total	С	Ν	Ο	\mathbf{S}	0	0	0
4	D	105	712	456	119	135	2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Mg 1 1	0	0
5	С	1	Total Mg 1 1	0	0

• Molecule 6 is 2',3'-DIDEOXYADENOSINE-5'-TRIPHOSPHATE (three-letter code: DAD) (formula: $C_{10}H_{16}N_5O_{11}P_3$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
6	Δ	1	Total	С	Ν	Ο	Р	0	0
0	A	1	29	10	5	11	3	0	0
6	C	1	Total	С	Ν	0	Р	0	0
0			29	10	5	11	3	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'-D(*CP*GP*AP*AP*AP*AP*CP*GP*AP*CP*GP*GP*CP*CP*CP*AP*GP*TP*G P*CP*CP*(2DT))-3'

Chain P:	43%	10%	48%	
DC DG DA DA DA DA DG C12 C12	C13 A15 A15 C14 C14 C16 C16 C19 C20 C20 C20			
• Molecule 1: 5'- P*CP*CP*(2DT	-D(*CP*GP*AP*. '))-3'	AP*AP*AP*CF	P*GP*AP*Cl	P*GP*GP*CP*CP*AP*GP*
Chain Q: 5%	43%	5%	48%	
DC DA DA DA DA DA DC DC DC C11 C12	C13 C14 A15 G16 G16 G18 C19 C20 T21			
• Molecule 2: 5'- TP*CP*GP*TP	-D(*CP*CP*CP* *TP*TP*TP*CP	(TTD)P*AP*G *G)-3'	P*GP*CP*A	AP*CP*TP*GP*GP*CP*CP
Chain T:	28% 12%		60%	
DC DC DC C C C C C C C C C C C C C C C	DT DC DT DT DT DC DC			
• Molecule 2: 5'- TP*CP*GP*TP	-D(*CP*CP*CP* *TP*TP*TP*CP [;]	(TTD)P*AP*G *G)-3'	P*GP*CP*A	AP*CP*TP*GP*GP*CP*CP
Chain U:	24% 16%		60%	
DC DC CS CS CS CS CS CS CS CS CS CS CS CS CS	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0			
• Molecule 3: DI	NA polymerase			
Chain A:	46%		43%	5% 6%
M1 12 67 88 88 112 112 813 814 814 814 814 814	K17 F18 118 123 123 125 128 128 128 128 128 128 128 128 128 128	R35 P36 P36 P36 P36 P37 P36 P36 P36 P36 P36 P36 P36 P36 P36 P36	654 155 165 165 165 165 165 165 165	K63 1664 1665 1665 170 170 171 171 172 173 177 173 173









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	54.27Å 105.47Å 213.93Å	Deperitor
a, b, c, α , β , γ	90.00° 91.57° 90.00°	Depositor
$\mathbf{B}_{\mathrm{ascolution}}(\hat{\lambda})$	50.00 - 3.20	Depositor
Resolution (A)	39.63 - 3.20	EDS
% Data completeness	99.3 (50.00-3.20)	Depositor
(in resolution range)	91.7(39.63-3.20)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	$5.37 (at 3.18 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
B B.	0.282 , 0.351	Depositor
II, II, <i>free</i>	0.260 , 0.326	DCC
R_{free} test set	1987 reflections (5.01%)	wwPDB-VP
Wilson B-factor $(Å^2)$	87.3	Xtriage
Anisotropy	0.771	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.28, 56.9	EDS
L-test for twinning ²	$< L >=0.52, < L^2>=0.35$	Xtriage
Estimated twinning fraction	0.136 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11904	wwPDB-VP
Average B, all atoms $(Å^2)$	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.38% 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: DAD, MG, 2DT

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		
MOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	Р	0.73	0/229	0.84	0/351	
1	Q	0.54	0/229	0.86	0/351	
2	Т	0.67	0/232	0.82	0/356	
2	U	0.54	0/232	0.74	0/356	
3	А	0.46	0/4899	0.68	1/6701~(0.0%)	
3	С	0.42	0/4887	0.66	0/6685	
4	В	0.39	0/730	0.65	0/1006	
4	D	0.38	0/725	0.63	0/998	
All	All	0.45	0/12163	0.68	1/16804~(0.0%)	

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Р	0	2
1	Q	0	1
3	А	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	181	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
3	А	409	TYR	Sidechain
1	Р	17	DT	Sidechain
1	Р	19	DC	Sidechain
1	Q	20	DC	Sidechain

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	Р	224	0	124	18	0
1	Q	224	0	124	17	0
2	Т	207	0	112	5	0
2	U	207	0	112	6	0
3	А	4782	0	4271	326	0
3	С	4772	0	4237	333	0
4	В	716	0	647	76	0
4	D	712	0	647	73	0
5	А	1	0	0	0	0
5	С	1	0	0	0	0
6	А	29	0	12	0	0
6	С	29	0	12	0	0
All	All	11904	0	10298	818	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 37.

All (818) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
3:C:391:MET:HE1	3:C:392:ILE:HD13	1.38	1.02
3:C:131:ARG:HH11	3:C:131:ARG:HA	1.21	1.01
3:A:131:ARG:HA	3:A:131:ARG:HH11	1.21	1.00
3:A:164:ASN:HD21	3:A:167:MET:H	1.12	0.97
3:C:126:GLU:HG2	3:C:127:ALA:H	1.26	0.96
3:C:525:ILE:HG23	3:C:526:TYR:H	1.35	0.92
4:B:39:ALA:HB3	4:B:40:PRO:HD3	1.51	0.89
3:C:131:ARG:HA	3:C:131:ARG:NH1	1.86	0.89



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:A:164:ASN:C	3:A:164:ASN:HD22	1.74	0.89
3:C:253:LEU:O	3:C:257:LEU:HG	1.71	0.89
3:C:35:ARG:HB3	3:C:36:PRO:HD2	1.53	0.87
3:C:440:ILE:HB	3:C:452:ARG:NH1	1.89	0.87
3:A:274:PHE:O	3:A:283:LEU:HD12	1.74	0.86
3:A:164:ASN:ND2	3:A:167:MET:H	1.71	0.86
4:B:41:ILE:O	4:B:45:ILE:HG12	1.76	0.85
3:A:154:TYR:OH	3:A:159:GLU:HG2	1.76	0.84
3:C:274:PHE:HA	3:C:289:ILE:HD11	1.59	0.84
3:C:404:LYS:HA	3:C:409:TYR:HE2	1.42	0.84
3:C:3:VAL:HG12	3:C:175:VAL:HG13	1.61	0.83
3:C:346:LEU:HD13	3:C:372:VAL:HG11	1.61	0.82
3:A:91:THR:HB	3:A:181:LEU:HD13	1.60	0.81
4:D:23:ILE:HD13	4:D:54:THR:HB	1.61	0.81
3:C:521:ALA:CB	3:C:521:ALA:N	2.43	0.81
1:Q:14:DC:H5	2:U:13:DG:H22	1.28	0.80
3:C:325:PRO:O	4:D:92:GLY:HA2	1.82	0.80
3:C:517:THR:HG23	3:C:520:ASN:HB2	1.63	0.80
3:C:363:VAL:O	3:C:368:VAL:HG11	1.80	0.80
4:D:23:ILE:CD1	4:D:54:THR:HB	2.12	0.80
3:C:521:ALA:CB	3:C:521:ALA:C	2.50	0.80
3:C:597:ASP:OD2	3:C:599:ARG:HD2	1.82	0.78
3:C:484:LEU:O	3:C:488:MET:HG2	1.81	0.78
3:A:569:ILE:HD11	3:A:613:LEU:HD22	1.66	0.78
3:C:59:HIS:ND1	3:C:91:THR:HG23	1.99	0.78
3:C:633:LEU:HD11	3:C:669:VAL:HG13	1.66	0.77
4:D:32:CYS:HB2	4:D:75:ILE:HD11	1.65	0.77
3:C:440:ILE:HB	3:C:452:ARG:HH11	1.47	0.76
3:C:68:ALA:O	3:C:72:LEU:HG	1.86	0.76
3:A:404:LYS:HA	3:A:409:TYR:HE2	1.51	0.76
3:A:131:ARG:HA	3:A:131:ARG:NH1	2.01	0.75
3:A:126:GLU:HG2	3:A:127:ALA:H	1.51	0.75
3:C:525:ILE:HG23	3:C:526:TYR:N	2.02	0.75
3:C:267:PRO:HA	3:C:329:VAL:HG12	1.68	0.75
4:D:41:ILE:O	4:D:45:ILE:HG12	1.87	0.75
1:Q:12:DG:H1'	1:Q:13:DC:H5'	1.69	0.74
4:B:14:THR:HA	4:B:18:LYS:HE3	1.70	0.74
3:C:676:ALA:O	3:C:680:VAL:HG23	1.88	0.74
3:A:525:ILE:HG23	3:A:526:TYR:N	2.03	0.74
3:A:355:LYS:O	3:A:363:VAL:HG23	1.89	0.73
1:P:16:DG:H1'	1:P:17:DT:H5"	1.70	0.73



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:B:38:ILE:CD1	4:B:78:LEU:HD11	2.19	0.73
4:D:67:ALA:HB3	4:D:68:PRO:HD3	1.70	0.72
4:D:4:ILE:HD11	4:D:43:ASP:HA	1.70	0.72
3:A:84:PRO:HG2	3:A:87:ASN:OD1	1.90	0.72
4:B:12:PHE:O	4:B:16:VAL:HG12	1.90	0.72
3:C:516:PRO:HG2	3:C:517:THR:H	1.54	0.72
3:A:190:HIS:CG	3:A:600:LYS:HE3	2.24	0.72
1:Q:16:DG:H1'	1:Q:17:DT:H5"	1.72	0.71
4:D:8:THR:HG22	4:D:11:SER:HB3	1.72	0.71
3:A:513:ALA:HB2	3:A:555:PHE:HB2	1.72	0.71
3:C:126:GLU:HG2	3:C:127:ALA:N	2.04	0.71
3:A:329:VAL:HG11	4:B:75:ILE:HD11	1.73	0.71
3:A:173:GLN:O	3:A:176:VAL:HG22	1.91	0.71
3:C:521:ALA:N	3:C:521:ALA:C	2.45	0.70
4:B:16:VAL:HG21	4:B:25:VAL:HG21	1.74	0.70
4:D:8:THR:HG23	4:D:11:SER:H	1.56	0.70
3:A:319:GLU:HB3	3:A:320:TYR:CE2	2.27	0.70
3:A:364:VAL:HG12	3:A:364:VAL:O	1.90	0.70
4:B:53:LEU:HD13	4:B:107:LEU:HD13	1.73	0.70
3:A:363:VAL:O	3:A:368:VAL:HG21	1.91	0.69
3:A:487:PHE:O	3:A:565:LEU:HD11	1.92	0.69
3:C:670:ILE:HG23	3:C:694:GLY:HA3	1.73	0.69
4:D:80:LEU:O	4:D:87:ALA:HB3	1.93	0.69
3:A:173:GLN:NE2	3:A:176:VAL:HG21	2.07	0.69
3:A:456:GLY:HA2	3:A:471:GLN:OE1	1.92	0.69
3:C:45:ALA:O	3:C:48:ALA:HB3	1.93	0.69
3:C:173:GLN:O	3:C:176:VAL:HG22	1.93	0.69
3:A:393:GLN:HE21	3:A:393:GLN:HA	1.58	0.69
3:C:186:LEU:HA	3:C:192:PHE:CD2	2.27	0.69
3:A:15:VAL:HG22	3:A:72:LEU:HD21	1.74	0.69
3:A:276:HIS:HB3	3:A:279:THR:HB	1.74	0.69
3:C:342:ILE:O	3:C:346:LEU:HB2	1.93	0.69
3:C:640:HIS:CD2	3:C:647:ALA:HA	2.28	0.69
3:C:59:HIS:HA	3:C:91:THR:HG23	1.75	0.69
1:P:19:DC:H5'	1:P:19:DC:H6	1.57	0.68
3:A:425:ALA:O	3:A:426:VAL:HB	1.93	0.68
3:A:626:ILE:CG2	3:A:656:ILE:HG21	2.24	0.68
3:C:61:GLY:O	3:C:66:VAL:HG23	1.93	0.68
3:A:338:SER:O	3:A:342:ILE:HG13	1.92	0.68
3:A:392:ILE:O	3:A:396:ILE:HG13	1.93	0.68
3:A:628:LYS:HD2	3:A:632:MET:HG3	1.76	0.68



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:C:57:VAL:HG22	3:C:89:ILE:HB	1.75	0.68
3:A:482:ARG:NH1	3:A:689:LEU:O	2.26	0.68
3:A:464:ILE:HG13	3:A:465:THR:H	1.57	0.68
3:A:209:GLU:OE2	3:C:490:ARG:NH1	2.27	0.68
3:C:670:ILE:CG2	3:C:694:GLY:HA3	2.24	0.68
3:A:670:ILE:HG23	3:A:694:GLY:HA3	1.76	0.68
3:C:169:ASP:O	3:C:172:VAL:HG12	1.92	0.68
1:P:11:DG:H2"	1:P:12:DG:C8	2.28	0.68
3:C:660:CYS:SG	3:C:666:ALA:HA	2.34	0.67
3:A:205:THR:O	3:A:209:GLU:HB2	1.94	0.67
3:C:425:ALA:O	3:C:426:VAL:HG13	1.95	0.67
3:A:127:ALA:O	3:A:131:ARG:HB2	1.94	0.67
4:D:8:THR:HG22	4:D:11:SER:CB	2.25	0.67
3:A:547:ARG:O	3:A:551:LEU:HG	1.94	0.67
3:A:525:ILE:CG2	3:A:526:TYR:N	2.57	0.67
3:C:316:ASP:C	3:C:318:ARG:H	1.97	0.67
4:B:14:THR:HG22	4:B:18:LYS:NZ	2.10	0.67
3:C:22:VAL:HG21	3:C:172:VAL:HA	1.76	0.67
3:C:440:ILE:O	3:C:452:ARG:NH1	2.28	0.67
3:A:24:TYR:HE1	3:A:29:ALA:HA	1.59	0.66
3:A:164:ASN:C	3:A:164:ASN:ND2	2.49	0.66
3:A:474:ILE:HD12	3:A:474:ILE:N	2.10	0.66
3:C:234:PHE:CZ	3:C:239:ILE:HG13	2.30	0.66
3:C:462:ASP:OD2	3:C:465:THR:HG23	1.95	0.66
3:C:546:GLU:HG3	3:C:547:ARG:N	2.08	0.66
1:P:12:DG:H1'	1:P:13:DC:H5'	1.78	0.66
3:C:292:PRO:HB2	3:C:294:VAL:HG21	1.76	0.66
4:B:80:LEU:O	4:B:87:ALA:HB3	1.96	0.66
4:D:16:VAL:HG21	4:D:25:VAL:CG2	2.25	0.66
3:A:250:ARG:NH1	3:A:396:ILE:HD13	2.10	0.65
3:A:24:TYR:CE1	3:A:29:ALA:HA	2.30	0.65
3:A:250:ARG:HH12	3:A:396:ILE:HG21	1.61	0.65
3:C:57:VAL:HG22	3:C:89:ILE:CG2	2.26	0.65
3:A:186:LEU:HA	3:A:192:PHE:CD2	2.32	0.65
3:C:144:LYS:HE3	3:C:154:TYR:CD2	2.32	0.65
3:C:326:TYR:HB2	4:D:91:VAL:HG12	1.77	0.65
3:C:592:TRP:CD2	3:C:600:LYS:HG3	2.32	0.65
3:C:665:ILE:O	3:C:669:VAL:HG23	1.96	0.65
3:A:316:ASP:C	3:A:318:ARG:H	2.00	0.65
3:C:265:TYR:CE1	4:D:68:PRO:HG3	2.31	0.65
3:C:22:VAL:HG21	3:C:172:VAL:N	2.12	0.65



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:617:ALA:O	3:C:621:ILE:HD12	1.97	0.65
3:C:426:VAL:HG23	3:C:427:THR:HG23	1.78	0.64
3:A:404:LYS:HA	3:A:409:TYR:CE2	2.31	0.64
3:A:442:GLY:O	3:A:448:GLY:HA3	1.97	0.64
3:C:22:VAL:HG23	3:C:171:ASN:CG	2.18	0.64
4:B:95:SER:OG	4:B:98:GLN:HG3	1.98	0.64
3:A:488:MET:HB3	3:A:565:LEU:HD22	1.80	0.64
4:D:58:LEU:HD11	4:D:63:ASN:HB2	1.80	0.64
3:A:279:THR:HG22	3:A:280:GLY:N	2.14	0.63
3:A:357:THR:N	3:A:361:ALA:O	2.31	0.63
3:C:24:TYR:CG	3:C:31:TYR:HE2	2.15	0.63
3:C:593:ILE:HG22	3:C:594:LYS:N	2.14	0.63
3:A:525:ILE:CG2	3:A:526:TYR:H	2.12	0.63
3:A:562:ILE:HD12	3:A:562:ILE:H	1.63	0.63
3:A:617:ALA:O	3:A:621:ILE:HG13	1.99	0.63
4:B:14:THR:HG22	4:B:18:LYS:HZ2	1.63	0.63
3:A:19:HIS:O	3:A:36:PRO:HG3	2.00	0.62
4:D:59:ASN:OD1	4:D:62:GLN:N	2.25	0.62
1:Q:13:DC:H42	2:U:14:DG:H1	1.48	0.62
3:A:373:ARG:CD	3:A:380:GLN:HE22	2.12	0.62
3:A:660:CYS:SG	3:A:666:ALA:HA	2.39	0.62
3:A:489:ALA:C	3:A:491:PHE:H	2.03	0.62
3:C:442:GLY:O	3:C:448:GLY:HA3	2.00	0.62
4:B:12:PHE:CE2	4:B:16:VAL:HG11	2.35	0.62
3:C:624:LEU:HD12	3:C:680:VAL:HG22	1.81	0.62
1:P:11:DG:H2"	1:P:12:DG:H8	1.65	0.61
4:B:4:ILE:HD12	4:B:4:ILE:N	2.15	0.61
3:C:513:ALA:HB2	3:C:555:PHE:HB2	1.82	0.61
4:B:16:VAL:HG21	4:B:25:VAL:CG2	2.30	0.61
3:C:391:MET:HE1	3:C:392:ILE:HA	1.82	0.61
3:A:626:ILE:HG22	3:A:656:ILE:HG21	1.82	0.61
3:C:246:LEU:HD21	3:C:447:TYR:CE1	2.36	0.61
3:A:12:LEU:O	3:A:15:VAL:HG12	2.01	0.61
4:D:75:ILE:HA	4:D:77:THR:H	1.65	0.61
3:C:59:HIS:HA	3:C:91:THR:CG2	2.31	0.61
4:D:16:VAL:HG21	4:D:25:VAL:HG22	1.83	0.61
3:A:223:LEU:O	3:A:226:LYS:HB3	2.01	0.61
3:C:353:PRO:HB2	3:C:356:TYR:CZ	2.36	0.61
3:A:45:ALA:O	3:A:48:ALA:HB3	2.01	0.61
3:A:236:THR:HG22	3:A:240:GLU:OE1	2.01	0.61
3:A:35:ARG:HB3	3:A:36:PRO:CD	2.31	0.61



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:404:LYS:HA	3:C:409:TYR:CE2	2.30	0.61
4:D:95:SER:HB2	4:D:98:GLN:HG3	1.83	0.60
3:A:373:ARG:HD3	3:A:380:GLN:HE22	1.66	0.60
4:D:37:MET:O	4:D:40:PRO:HD2	2.01	0.60
3:C:425:ALA:O	3:C:426:VAL:HG22	2.01	0.60
3:A:473:GLY:C	3:A:474:ILE:HD12	2.21	0.60
3:A:488:MET:HA	3:A:565:LEU:CD1	2.31	0.60
3:A:628:LYS:HD2	3:A:632:MET:SD	2.41	0.60
4:D:58:LEU:HD12	4:D:63:ASN:HD22	1.67	0.60
3:A:9:ASN:OD1	3:A:17:LYS:N	2.34	0.60
3:A:139:TYR:OH	3:A:167:MET:HB2	2.02	0.60
3:C:357:THR:N	3:C:361:ALA:O	2.33	0.60
3:A:429:ARG:NH1	3:A:653:HIS:CE1	2.69	0.60
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.83	0.60
3:C:624:LEU:HD13	3:C:624:LEU:O	2.01	0.60
3:A:276:HIS:HD2	3:A:278:ARG:H	1.50	0.59
3:A:319:GLU:HB3	3:A:320:TYR:CD2	2.37	0.59
3:C:24:TYR:HB2	3:C:31:TYR:CE2	2.36	0.59
3:C:265:TYR:OH	4:D:68:PRO:HG3	2.03	0.59
3:C:562:ILE:HD12	3:C:562:ILE:H	1.67	0.59
3:A:429:ARG:HD2	3:A:653:HIS:ND1	2.15	0.59
4:B:75:ILE:HA	4:B:77:THR:H	1.68	0.59
3:A:7:GLU:O	3:A:19:HIS:HB2	2.01	0.59
3:C:279:THR:HG22	3:C:280:GLY:N	2.17	0.59
3:C:382:ALA:O	3:C:386:ILE:HG13	2.01	0.59
3:A:43:LEU:HD22	3:A:81:PHE:CD1	2.38	0.59
3:C:22:VAL:HG21	3:C:172:VAL:CA	2.31	0.59
3:C:223:LEU:HD21	3:C:648:TYR:CE2	2.37	0.59
4:D:7:LEU:HD21	4:D:56:ALA:HB1	1.84	0.59
3:A:458:GLU:CD	3:A:698:PRO:HB2	2.23	0.59
3:A:490:ARG:HD2	3:C:196:ILE:HG12	1.85	0.59
3:C:242:LEU:HD11	3:C:447:TYR:HD1	1.67	0.59
3:C:289:ILE:HG21	4:D:34:PRO:HG2	1.85	0.59
3:A:223:LEU:O	3:A:223:LEU:HD12	2.02	0.59
3:C:572:THR:HG22	3:C:572:THR:O	2.02	0.59
3:A:525:ILE:C	3:A:527:GLY:H	2.06	0.58
3:A:446:PRO:C	3:A:447:TYR:HD2	2.05	0.58
3:C:274:PHE:HA	3:C:289:ILE:CD1	2.33	0.58
3:A:488:MET:HA	3:A:565:LEU:HD13	1.85	0.58
3:C:207:TRP:HZ3	3:C:214:VAL:HG12	1.67	0.58
3:C:489:ALA:C	3:C:491:PHE:H	2.05	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:436:ASN:ND2	3:A:439:GLN:HG2	2.18	0.58
3:C:205:THR:HG23	3:C:209:GLU:HG3	1.85	0.58
3:C:521:ALA:O	3:C:525:ILE:HG22	2.03	0.58
4:D:4:ILE:CD1	4:D:43:ASP:HA	2.33	0.58
3:A:15:VAL:O	3:A:71:LYS:NZ	2.34	0.58
3:C:425:ALA:HB2	3:C:429:ARG:O	2.03	0.58
3:C:39:PHE:HD2	3:C:77:LEU:HD11	1.68	0.58
3:C:223:LEU:HD21	3:C:648:TYR:HE2	1.67	0.58
3:A:23:ILE:O	3:A:31:TYR:HA	2.04	0.58
4:B:29:ALA:HB1	4:B:31:TRP:NE1	2.18	0.58
3:C:65:ASP:O	3:C:69:LEU:HG	2.03	0.57
4:D:67:ALA:O	4:D:69:LYS:N	2.37	0.57
4:D:102:PHE:O	4:D:106:ASN:ND2	2.34	0.57
3:A:633:LEU:HD21	3:A:669:VAL:HA	1.86	0.57
3:C:91:THR:OG1	3:C:181:LEU:HD12	2.05	0.57
3:A:22:VAL:HG23	3:A:171:ASN:CG	2.25	0.57
3:A:135:MET:HG3	3:A:135:MET:O	2.03	0.57
3:A:516:PRO:HG2	3:A:517:THR:H	1.69	0.57
3:C:128:TRP:HB2	3:C:181:LEU:HD23	1.86	0.57
3:C:525:ILE:CG2	3:C:526:TYR:H	2.13	0.57
1:Q:19:DC:H6	1:Q:19:DC:H5'	1.68	0.57
3:A:342:ILE:O	3:A:346:LEU:HB2	2.05	0.57
4:B:13:ASP:OD1	4:B:18:LYS:HE2	2.05	0.57
3:A:2:ILE:HD13	3:A:49:GLU:HG3	1.86	0.57
3:A:236:THR:HG22	3:A:240:GLU:CD	2.25	0.57
4:B:58:LEU:HD23	4:B:59:ASN:O	2.05	0.57
4:B:75:ILE:HA	4:B:77:THR:N	2.20	0.57
3:C:487:PHE:HB3	3:C:565:LEU:HD11	1.86	0.57
3:A:249:ARG:HD2	3:A:249:ARG:O	2.04	0.56
3:C:525:ILE:C	3:C:527:GLY:H	2.08	0.56
3:A:372:VAL:O	3:A:373:ARG:HD3	2.05	0.56
3:C:371:GLY:O	3:C:373:ARG:HG2	2.05	0.56
3:A:474:ILE:HG21	3:A:673:ALA:HB1	1.87	0.56
3:C:182:LEU:HD12	3:C:182:LEU:O	2.05	0.56
4:D:75:ILE:HA	4:D:77:THR:N	2.20	0.56
3:C:57:VAL:HG22	3:C:89:ILE:CB	2.35	0.56
3:A:250:ARG:NH1	3:A:396:ILE:CD1	2.69	0.56
3:C:128:TRP:HA	3:C:131:ARG:HB2	1.88	0.56
3:A:203:TYR:CE1	3:A:204:THR:HG23	2.41	0.56
3:A:61:GLY:O	3:A:66:VAL:HB	2.05	0.56
3:C:22:VAL:HG23	3:C:171:ASN:OD1	2.06	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:23:ILE:O	3:C:31:TYR:HA	2.06	0.56
3:C:281:LYS:HG3	3:C:282:PRO:HD2	1.88	0.56
3:A:198:PHE:C	3:A:200:ASP:H	2.10	0.55
4:B:39:ALA:CB	4:B:40:PRO:HD3	2.32	0.55
3:A:195:GLU:HG3	3:C:572:THR:OG1	2.06	0.55
3:C:198:PHE:C	3:C:200:ASP:H	2.09	0.55
3:A:329:VAL:CG1	4:B:75:ILE:HD11	2.37	0.55
3:C:505:ILE:HG23	3:C:506:HIS:N	2.21	0.55
3:C:528:PHE:C	3:C:528:PHE:CD2	2.79	0.55
3:C:7:GLU:O	3:C:19:HIS:HB2	2.06	0.55
3:C:365:ASP:OD1	3:C:367:GLU:HB3	2.07	0.55
3:A:181:LEU:HD22	3:A:185:LEU:HD11	1.87	0.55
3:A:235:ASP:OD2	3:A:238:ALA:HB2	2.06	0.55
4:B:67:ALA:O	4:B:69:LYS:N	2.39	0.55
3:A:171:ASN:O	3:A:174:ASP:HB2	2.06	0.55
3:A:597:ASP:OD2	3:A:599:ARG:HD2	2.06	0.55
3:C:205:THR:O	3:C:209:GLU:HB2	2.07	0.55
3:A:276:HIS:CD2	3:A:277:PRO:HD2	2.41	0.55
3:C:478:GLY:O	3:C:482:ARG:HG3	2.07	0.55
4:B:4:ILE:HD12	4:B:4:ILE:H	1.72	0.55
3:C:181:LEU:HD13	3:C:185:LEU:HG	1.89	0.55
3:A:213:ALA:HB2	3:A:597:ASP:OD1	2.07	0.54
3:A:525:ILE:O	3:A:527:GLY:N	2.40	0.54
3:A:670:ILE:CG2	3:A:694:GLY:HA3	2.36	0.54
4:B:95:SER:N	4:B:98:GLN:HB2	2.22	0.54
3:C:445:SER:O	3:C:448:GLY:N	2.34	0.54
4:B:23:ILE:HA	4:B:54:THR:O	2.06	0.54
3:C:60:ASN:OD1	3:C:60:ASN:O	2.26	0.54
1:P:20:DC:H3'	1:P:21:2DT:H73	1.89	0.54
3:A:144:LYS:O	3:A:148:GLU:N	2.40	0.54
3:A:443:VAL:HA	3:A:448:GLY:O	2.06	0.54
3:A:699:ASN:OD1	3:A:701:ALA:HB3	2.08	0.54
4:D:79:LEU:HD23	4:D:86:VAL:CG2	2.38	0.54
4:D:38:ILE:HD11	4:D:78:LEU:HD11	1.90	0.54
3:C:105:THR:HG22	3:C:110:LEU:O	2.08	0.54
3:C:346:LEU:CD1	3:C:372:VAL:HG11	2.33	0.54
4:B:70:TYR:CZ	4:B:81:PHE:HZ	2.24	0.54
3:C:236:THR:O	3:C:240:GLU:HG3	2.08	0.54
3:A:28:THR:HG22	3:A:30:GLU:HB2	1.88	0.54
3:C:2:ILE:HD11	3:C:49:GLU:CD	2.28	0.54
4:D:23:ILE:HA	4:D:54:THR:O	2.06	0.54



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:T:9:DC:H4'	3:A:432:HIS:O	2.08	0.54
3:A:593:ILE:CG2	3:A:594:LYS:N	2.71	0.54
3:A:622:CYS:O	3:A:626:ILE:HG12	2.08	0.54
3:C:224:LEU:HD12	3:C:422:PRO:HB3	1.90	0.54
3:C:228:GLU:O	3:C:417:HIS:HD2	1.90	0.54
4:D:79:LEU:HG	4:D:89:THR:HG22	1.89	0.54
4:B:41:ILE:HG23	4:B:96:LYS:HA	1.90	0.53
4:B:53:LEU:HD13	4:B:107:LEU:CD1	2.38	0.53
3:C:264:TRP:CZ3	3:C:345:LYS:HE2	2.43	0.53
4:D:13:ASP:O	4:D:17:LEU:HB2	2.08	0.53
3:A:145:ARG:O	3:A:147:LEU:N	2.42	0.53
3:A:393:GLN:HE21	3:A:393:GLN:CA	2.22	0.53
3:A:628:LYS:CD	3:A:632:MET:HG3	2.37	0.53
3:C:525:ILE:O	3:C:527:GLY:N	2.42	0.53
3:A:624:LEU:HD22	3:A:684:TRP:CH2	2.43	0.53
3:C:207:TRP:HA	3:C:207:TRP:CE3	2.42	0.53
4:B:16:VAL:HG13	4:B:17:LEU:N	2.23	0.53
3:C:145:ARG:O	3:C:147:LEU:N	2.41	0.53
4:D:72:ILE:CD1	4:D:77:THR:HG21	2.38	0.53
4:D:78:LEU:C	4:D:79:LEU:HD12	2.27	0.53
3:C:592:TRP:CE3	3:C:600:LYS:HG3	2.44	0.53
1:P:21:2DT:OP2	1:P:21:2DT:H6	2.08	0.53
3:A:628:LYS:HD2	3:A:632:MET:CG	2.38	0.53
3:C:506:HIS:HA	3:C:509:ASN:HD22	1.73	0.53
2:U:8:DG:H4'	3:C:431:THR:HG22	1.91	0.53
3:A:182:LEU:O	3:A:186:LEU:HG	2.09	0.53
3:A:474:ILE:N	3:A:474:ILE:CD1	2.72	0.53
4:B:78:LEU:C	4:B:79:LEU:HD12	2.29	0.53
3:C:250:ARG:HH11	3:C:393:GLN:CD	2.12	0.53
4:B:19:ALA:C	4:B:21:GLY:H	2.12	0.53
3:C:62:HIS:HB2	3:C:90:ASP:OD2	2.09	0.53
3:C:159:GLU:HG2	3:C:160:TRP:CD1	2.43	0.53
3:C:435:PRO:O	3:C:437:LEU:HD12	2.09	0.53
4:D:19:ALA:C	4:D:21:GLY:H	2.11	0.53
3:A:2:ILE:HG22	3:A:25:ASP:HA	1.91	0.53
3:A:364:VAL:HA	3:A:368:VAL:HG21	1.90	0.53
3:A:698:PRO:HG2	3:A:702:ILE:HD12	1.91	0.53
4:B:35:CYS:SG	4:B:75:ILE:HB	2.49	0.53
3:C:353:PRO:O	3:C:356:TYR:HE1	1.91	0.53
3:A:223:LEU:HD12	3:A:223:LEU:C	2.30	0.52
3:A:232:PHE:CE1	3:A:455:PHE:HB3	2.44	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:378:GLU:O	3:A:381:ALA:HB3	2.08	0.52
1:P:16:DG:H2"	1:P:17:DT:C5'	2.39	0.52
1:Q:21:2DT:OP2	1:Q:21:2DT:H6	2.10	0.52
3:A:423:ASN:O	3:A:425:ALA:N	2.43	0.52
3:A:446:PRO:C	3:A:447:TYR:CD2	2.83	0.52
3:C:276:HIS:HB3	3:C:279:THR:HB	1.90	0.52
3:A:158:MET:HA	3:A:161:TRP:CD1	2.44	0.52
3:A:250:ARG:NH1	3:A:396:ILE:HG21	2.25	0.52
4:B:39:ALA:HB3	4:B:40:PRO:CD	2.33	0.52
3:A:343:GLN:O	3:A:347:GLN:HB2	2.10	0.52
3:C:55:LEU:HD21	3:C:203:TYR:HA	1.90	0.52
3:A:65:ASP:O	3:A:69:LEU:HG	2.08	0.52
3:A:267:PRO:HD3	4:B:31:TRP:CZ3	2.44	0.52
3:C:265:TYR:HE1	4:D:68:PRO:HG3	1.74	0.52
3:C:395:ARG:HH11	3:C:395:ARG:HG2	1.74	0.52
3:C:15:VAL:HG22	3:C:72:LEU:HD21	1.91	0.52
3:C:49:GLU:OE1	3:C:52:ARG:HD2	2.10	0.52
3:A:233:PRO:HB2	3:A:456:GLY:O	2.10	0.52
3:A:321:VAL:CG1	4:B:98:GLN:NE2	2.73	0.52
4:B:82:LYS:O	4:B:83:ASN:HB2	2.09	0.52
3:C:264:TRP:CE3	3:C:345:LYS:HE2	2.44	0.52
3:C:326:TYR:CB	4:D:91:VAL:HG12	2.40	0.52
3:C:421:ASN:OD1	3:C:423:ASN:N	2.36	0.52
1:P:12:DG:H2"	1:P:13:DC:O5'	2.10	0.52
3:A:447:TYR:CD2	3:A:447:TYR:N	2.77	0.52
3:C:76:GLN:O	3:C:77:LEU:HD23	2.10	0.52
4:D:95:SER:N	4:D:98:GLN:HB2	2.25	0.52
3:A:158:MET:HA	3:A:161:TRP:CE2	2.45	0.51
3:A:317:THR:HG22	3:A:317:THR:O	2.11	0.51
3:A:569:ILE:HD11	3:A:613:LEU:CD2	2.37	0.51
3:C:145:ARG:C	3:C:147:LEU:H	2.13	0.51
4:D:32:CYS:HB3	4:D:35:CYS:HB2	1.91	0.51
3:C:233:PRO:HB2	3:C:456:GLY:O	2.10	0.51
3:C:443:VAL:HA	3:C:448:GLY:O	2.10	0.51
3:A:366:ASP:OD2	3:A:387:LYS:HE3	2.09	0.51
3:C:223:LEU:O	3:C:226:LYS:HB3	2.11	0.51
3:A:478:GLY:O	3:A:482:ARG:HG3	2.10	0.51
3:A:597:ASP:OD2	3:A:599:ARG:NH1	2.40	0.51
3:A:35:ARG:O	3:A:38:ASP:N	2.43	0.51
3:C:3:VAL:HG12	3:C:3:VAL:O	2.10	0.51
3:C:213:ALA:HB2	3:C:597:ASP:OD1	2.11	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:Q:16:DG:H2"	1:Q:17:DT:C5'	2.41	0.51
3:A:234:PHE:CE2	3:A:239:ILE:HG13	2.46	0.51
3:C:336:PRO:O	3:C:342:ILE:HD11	2.11	0.51
4:D:9:ASP:OD2	4:D:63:ASN:HA	2.11	0.51
4:D:16:VAL:HG13	4:D:17:LEU:N	2.26	0.51
3:A:198:PHE:HB3	3:A:206:PHE:HD2	1.76	0.51
3:A:505:ILE:HG23	3:A:506:HIS:N	2.26	0.51
3:C:144:LYS:O	3:C:148:GLU:N	2.44	0.51
3:A:624:LEU:HD23	3:A:680:VAL:HG13	1.93	0.50
3:C:64:TYR:CD2	3:C:65:ASP:N	2.79	0.50
3:C:440:ILE:CB	3:C:452:ARG:HH11	2.22	0.50
3:C:35:ARG:HG3	3:C:35:ARG:HH11	1.76	0.50
3:C:246:LEU:CD2	3:C:447:TYR:CE1	2.94	0.50
3:C:410:VAL:HG23	3:C:410:VAL:O	2.10	0.50
3:A:243:TYR:CD1	3:A:243:TYR:O	2.64	0.50
3:A:392:ILE:HG22	3:A:396:ILE:HD11	1.93	0.50
3:C:5:ASP:OD2	3:C:171:ASN:ND2	2.44	0.50
4:D:72:ILE:HD12	4:D:77:THR:HG21	1.92	0.50
3:A:357:THR:O	3:A:359:LYS:N	2.42	0.50
4:B:45:ILE:O	4:B:49:TYR:HB2	2.12	0.50
4:D:31:TRP:NE1	4:D:61:ASP:OD2	2.43	0.50
4:D:23:ILE:HD12	4:D:54:THR:HB	1.93	0.50
3:A:145:ARG:C	3:A:147:LEU:H	2.14	0.50
3:C:2:ILE:HG22	3:C:3:VAL:N	2.26	0.50
3:C:8:ALA:HB3	3:C:64:TYR:OH	2.11	0.50
3:C:234:PHE:CE1	3:C:239:ILE:HG13	2.46	0.50
3:A:24:TYR:HA	3:A:30:GLU:O	2.11	0.50
3:C:24:TYR:CG	3:C:31:TYR:CE2	2.99	0.50
3:C:633:LEU:HD21	3:C:669:VAL:HA	1.94	0.50
3:A:321:VAL:HG11	4:B:98:GLN:NE2	2.27	0.50
3:C:253:LEU:HD11	3:C:388:GLU:HG2	1.92	0.50
2:U:9:DC:H4'	3:C:432:HIS:O	2.12	0.49
3:A:13:GLU:H	3:A:13:GLU:CD	2.15	0.49
3:A:349:ALA:HB3	3:A:374:VAL:HG11	1.93	0.49
4:D:38:ILE:CD1	4:D:78:LEU:HD11	2.41	0.49
4:B:11:SER:O	4:B:15:ASP:HB2	2.11	0.49
1:P:11:DG:C2'	1:P:12:DG:C8	2.96	0.49
3:A:250:ARG:HH11	3:A:396:ILE:CD1	2.25	0.49
3:C:234:PHE:CD2	3:C:410:VAL:HG12	2.48	0.49
3:C:421:ASN:HB3	3:C:431:THR:OG1	2.12	0.49
3:A:336:PRO:HB2	3:A:389:TYR:CD1	2.47	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:C:1:MET:C	3:C:2:ILE:HG13	2.33	0.49
3:A:267:PRO:HB3	4:B:31:TRP:HZ3	1.78	0.49
3:A:490:ARG:CG	3:A:490:ARG:O	2.61	0.49
3:C:207:TRP:HA	3:C:207:TRP:HE3	1.78	0.49
3:C:563:ALA:O	3:C:567:GLU:OE1	2.30	0.49
2:T:8:DG:H4'	3:A:431:THR:HG22	1.95	0.49
3:A:336:PRO:HB2	3:A:389:TYR:CE1	2.48	0.49
3:A:445:SER:O	3:A:448:GLY:N	2.33	0.49
4:B:3:LYS:CB	4:B:4:ILE:HD12	2.43	0.49
4:B:103:LEU:O	4:B:106:ASN:N	2.42	0.49
3:C:84:PRO:HG2	3:C:87:ASN:OD1	2.13	0.49
3:C:265:TYR:CZ	4:D:68:PRO:HG3	2.48	0.48
3:C:316:ASP:C	3:C:318:ARG:N	2.65	0.48
3:A:22:VAL:HG12	3:A:23:ILE:N	2.29	0.48
3:A:392:ILE:HG22	3:A:396:ILE:CD1	2.43	0.48
3:A:392:ILE:CG2	3:A:396:ILE:HD11	2.43	0.48
3:A:525:ILE:C	3:A:527:GLY:N	2.66	0.48
3:A:592:TRP:HE3	3:A:593:ILE:O	1.96	0.48
3:A:640:HIS:CD2	3:A:647:ALA:HA	2.48	0.48
3:C:357:THR:O	3:C:359:LYS:N	2.43	0.48
4:B:77:THR:HG22	4:B:79:LEU:CD1	2.43	0.48
3:C:6:ILE:HG22	3:C:42:TYR:OH	2.14	0.48
4:D:16:VAL:CG1	4:D:17:LEU:N	2.76	0.48
3:A:371:GLY:O	3:A:373:ARG:HG2	2.13	0.48
3:C:163:PHE:CD1	3:C:164:ASN:N	2.81	0.48
1:P:16:DG:C1'	1:P:17:DT:H5"	2.42	0.48
1:P:20:DC:H42	2:T:6:DA:H61	1.62	0.48
3:A:22:VAL:HG21	3:A:172:VAL:N	2.28	0.48
3:A:355:LYS:C	3:A:363:VAL:HG23	2.34	0.48
3:A:597:ASP:OD1	3:A:597:ASP:C	2.51	0.48
3:C:127:ALA:O	3:C:131:ARG:HB2	2.12	0.48
3:A:421:ASN:O	3:A:430:ALA:HB1	2.13	0.48
3:A:469:TRP:CE3	3:A:660:CYS:C	2.87	0.48
3:C:203:TYR:CD1	3:C:204:THR:N	2.81	0.48
3:A:329:VAL:HG11	4:B:31:TRP:HH2	1.78	0.48
3:C:2:ILE:HG23	3:C:25:ASP:HA	1.94	0.48
3:C:35:ARG:O	3:C:38:ASP:N	2.45	0.48
3:C:423:ASN:O	3:C:425:ALA:N	2.47	0.48
3:C:55:LEU:HD22	3:C:89:ILE:CD1	2.44	0.48
3:C:660:CYS:SG	3:C:669:VAL:HG21	2.54	0.48
1:Q:18:DG:C4	1:Q:19:DC:C5	3.02	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:276:HIS:CB	3:A:279:THR:HB	2.43	0.48
3:A:346:LEU:HD11	3:A:383:ILE:HG12	1.96	0.48
3:A:676:ALA:O	3:A:679:TRP:HB3	2.14	0.48
3:C:155:VAL:O	3:C:157:GLY:N	2.47	0.48
3:A:59:HIS:CD2	3:A:132:LEU:HD13	2.50	0.47
3:A:59:HIS:O	3:A:60:ASN:HB3	2.14	0.47
3:A:235:ASP:O	3:A:236:THR:C	2.51	0.47
3:C:206:PHE:O	3:C:210:SER:OG	2.21	0.47
3:C:320:TYR:CE1	4:D:91:VAL:HB	2.49	0.47
3:C:365:ASP:OD1	3:C:368:VAL:HG12	2.13	0.47
3:A:12:LEU:HD13	3:A:68:ALA:HB2	1.97	0.47
3:C:176:VAL:HG23	3:C:177:VAL:N	2.29	0.47
1:Q:12:DG:H2"	1:Q:13:DC:O5'	2.14	0.47
3:A:425:ALA:O	3:A:426:VAL:CB	2.61	0.47
3:A:678:ARG:HG2	3:A:678:ARG:HH11	1.79	0.47
3:C:97:LEU:O	3:C:97:LEU:HG	2.14	0.47
3:C:525:ILE:C	3:C:527:GLY:N	2.68	0.47
3:C:624:LEU:HD11	3:C:679:TRP:HZ3	1.78	0.47
4:D:12:PHE:O	4:D:16:VAL:HG12	2.14	0.47
3:A:139:TYR:CE1	3:A:167:MET:HA	2.50	0.47
3:A:351:TRP:O	3:A:353:PRO:HD3	2.14	0.47
3:C:2:ILE:HG22	3:C:3:VAL:H	1.78	0.47
3:C:421:ASN:O	3:C:430:ALA:HB1	2.14	0.47
3:C:633:LEU:CD1	3:C:669:VAL:HG13	2.42	0.47
1:P:16:DG:C2'	1:P:17:DT:H5"	2.44	0.47
1:Q:13:DC:N4	2:U:14:DG:H1	2.10	0.47
3:A:246:LEU:HD21	3:A:447:TYR:CE1	2.49	0.47
3:A:489:ALA:C	3:A:491:PHE:N	2.66	0.47
3:C:24:TYR:HA	3:C:30:GLU:O	2.14	0.47
3:C:223:LEU:HD11	3:C:648:TYR:CD2	2.49	0.47
3:A:49:GLU:OE2	3:A:54:GLY:HA3	2.14	0.47
3:A:191:TYR:CD2	3:A:211:LEU:HD23	2.50	0.47
3:A:347:GLN:OE1	3:A:353:PRO:HG2	2.15	0.47
3:A:415:LYS:HE3	3:A:642:TRP:NE1	2.28	0.47
4:B:27:PHE:CD1	4:B:27:PHE:N	2.82	0.47
3:C:224:LEU:O	3:C:228:GLU:HG3	2.14	0.47
3:C:253:LEU:CD1	3:C:388:GLU:HG2	2.44	0.47
3:C:389:TYR:CD1	3:C:389:TYR:C	2.87	0.47
4:D:103:LEU:O	4:D:106:ASN:N	2.42	0.47
1:P:20:DC:N4	2:T:6:DA:H61	2.12	0.47
3:C:22:VAL:HG12	3:C:23:ILE:N	2.30	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:190:HIS:NE2	3:A:600:LYS:HG3	2.30	0.47
3:A:698:PRO:CG	3:A:702:ILE:HD12	2.45	0.47
4:B:42:LEU:HA	4:B:45:ILE:CG1	2.44	0.47
3:C:235:ASP:O	3:C:236:THR:C	2.52	0.47
4:D:59:ASN:OD1	4:D:61:ASP:N	2.46	0.47
3:A:252:GLU:O	3:A:253:LEU:C	2.53	0.47
3:A:356:TYR:HA	3:A:362:PRO:HA	1.97	0.47
3:A:216:ILE:CD1	3:A:624:LEU:HD13	2.45	0.46
3:C:479:LEU:HD11	3:C:621:ILE:HG21	1.96	0.46
3:C:625:TRP:CZ2	3:C:692:THR:HG21	2.50	0.46
1:Q:16:DG:C1'	1:Q:17:DT:H5"	2.44	0.46
3:C:3:VAL:CG1	3:C:175:VAL:HG13	2.40	0.46
3:C:392:ILE:O	3:C:396:ILE:HG13	2.15	0.46
3:C:517:THR:HG23	3:C:520:ASN:CB	2.40	0.46
3:A:353:PRO:O	3:A:356:TYR:HE1	1.98	0.46
3:A:642:TRP:HA	3:A:642:TRP:CE3	2.51	0.46
3:C:343:GLN:OE1	3:C:343:GLN:C	2.54	0.46
3:A:316:ASP:C	3:A:318:ARG:N	2.68	0.46
3:A:2:ILE:CD1	3:A:49:GLU:HG3	2.45	0.46
3:A:321:VAL:HG12	3:A:322:ALA:N	2.31	0.46
3:A:389:TYR:CD1	3:A:389:TYR:C	2.88	0.46
3:A:569:ILE:O	3:A:572:THR:N	2.47	0.46
3:C:21:GLY:HA3	3:C:42:TYR:CE1	2.51	0.46
3:C:24:TYR:HB2	3:C:31:TYR:HE2	1.79	0.46
3:A:155:VAL:O	3:A:157:GLY:N	2.49	0.46
3:A:462:ASP:OD2	3:A:463:GLY:N	2.49	0.46
3:C:252:GLU:O	3:C:253:LEU:C	2.53	0.46
3:C:336:PRO:HB2	3:C:389:TYR:CD1	2.50	0.46
3:C:353:PRO:O	3:C:356:TYR:CE1	2.69	0.46
3:A:91:THR:O	3:A:95:SER:HB2	2.16	0.46
3:A:267:PRO:HB3	4:B:31:TRP:CZ3	2.51	0.46
3:A:445:SER:O	3:A:446:PRO:C	2.52	0.46
3:A:666:ALA:O	3:A:670:ILE:HG13	2.16	0.46
3:A:458:GLU:OE2	3:A:699:ASN:ND2	2.46	0.46
4:B:42:LEU:HA	4:B:45:ILE:HG13	1.98	0.46
3:C:327:THR:O	4:D:74:GLY:HA2	2.16	0.46
3:A:66:VAL:HG12	3:A:67:PRO:N	2.29	0.46
3:A:376:ASP:HB3	3:A:379:LYS:HD2	1.97	0.46
3:A:570:GLN:O	3:A:574:VAL:HG23	2.15	0.46
3:C:57:VAL:HG22	3:C:89:ILE:HG21	1.98	0.46
3:C:364:VAL:HG12	3:C:364:VAL:O	2.15	0.46



	A + O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:D:27:PHE:N	4:D:27:PHE:CD1	2.83	0.46
1:P:20:DC:H42	2:T:6:DA:N6	2.13	0.46
3:A:22:VAL:HG21	3:A:172:VAL:HA	1.97	0.46
3:A:257:LEU:O	3:A:259:GLU:N	2.49	0.46
3:A:395:ARG:HG2	3:A:395:ARG:HH11	1.81	0.46
3:C:8:ALA:HB1	3:C:15:VAL:CG2	2.46	0.46
3:C:139:TYR:HB2	3:C:170:TYR:CD1	2.50	0.46
3:C:321:VAL:CG1	3:C:322:ALA:N	2.80	0.46
1:P:13:DC:H2"	1:P:14:DC:OP2	2.16	0.45
3:A:292:PRO:HB2	3:A:294:VAL:HG21	1.97	0.45
4:B:38:ILE:HG12	4:B:38:ILE:O	2.17	0.45
3:C:321:VAL:HG12	3:C:322:ALA:O	2.16	0.45
3:C:524:PHE:O	3:C:524:PHE:CD1	2.69	0.45
1:P:14:DC:H2"	1:P:15:DA:O5'	2.16	0.45
4:B:65:GLY:O	4:B:68:PRO:HG2	2.16	0.45
3:C:39:PHE:CD2	3:C:77:LEU:HD11	2.48	0.45
1:Q:16:DG:C2'	1:Q:17:DT:H5"	2.46	0.45
3:A:126:GLU:HG2	3:A:127:ALA:N	2.26	0.45
3:A:602:HIS:CG	3:A:603:VAL:N	2.85	0.45
3:A:608:ALA:O	3:A:609:ALA:C	2.55	0.45
3:C:445:SER:O	3:C:446:PRO:C	2.54	0.45
4:D:77:THR:HG22	4:D:79:LEU:CD1	2.47	0.45
3:A:620:LEU:H	3:A:620:LEU:HG	1.57	0.45
3:C:155:VAL:O	3:C:156:ASP:C	2.55	0.45
3:C:489:ALA:C	3:C:491:PHE:N	2.69	0.45
3:A:279:THR:HG22	3:A:281:LYS:H	1.80	0.45
3:A:373:ARG:HD3	3:A:380:GLN:NE2	2.30	0.45
3:A:391:MET:CE	3:A:392:ILE:HD13	2.46	0.45
4:B:22:ALA:HB3	4:B:53:LEU:HD12	1.99	0.45
3:C:150:GLN:CD	3:C:150:GLN:N	2.69	0.45
3:C:415:LYS:HE2	3:C:642:TRP:NE1	2.32	0.45
4:D:8:THR:HG22	4:D:11:SER:OG	2.17	0.45
3:A:158:MET:HA	3:A:161:TRP:NE1	2.32	0.45
3:A:177:VAL:O	3:A:180:ALA:HB3	2.16	0.45
3:A:368:VAL:HG23	3:A:369:LEU:N	2.31	0.45
3:C:22:VAL:HG11	3:C:172:VAL:HA	1.97	0.45
3:C:171:ASN:O	3:C:174:ASP:HB2	2.16	0.45
3:C:443:VAL:HG12	3:C:449:GLU:HA	1.98	0.45
3:C:608:ALA:O	3:C:609:ALA:C	2.55	0.45
3:A:183:GLU:O	3:A:185:LEU:N	2.49	0.45
4:B:12:PHE:CZ	4:B:16:VAL:HG11	2.52	0.45



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
4:B:67:ALA:N	4:B:68:PRO:HD2	2.32	0.45	
3:C:446:PRO:C	3:C:447:TYR:HD2	2.20	0.45	
3:C:2:ILE:HD11	3:C:49:GLU:HB2	1.98	0.45	
3:C:55:LEU:HD11	3:C:206:PHE:HB2	1.98	0.45	
3:C:284:PRO:HG2	3:C:285:LYS:H	1.82	0.45	
3:C:286:TYR:HA	3:C:287:PRO:HD3	1.84	0.45	
3:A:163:PHE:CG	3:A:164:ASN:N	2.84	0.45	
3:A:165:GLU:O	3:A:166:GLU:C	2.56	0.45	
3:A:668:VAL:O	3:A:672:THR:N	2.45	0.45	
4:B:59:ASN:OD1	4:B:61:ASP:N	2.32	0.45	
4:B:94:LEU:N	4:B:94:LEU:HD23	2.32	0.45	
3:C:188:ASP:OD1	3:C:191:TYR:HD1	1.99	0.45	
3:C:504:ASP:OD2	3:C:507:THR:HG23	2.17	0.45	
3:A:267:PRO:HA	3:A:329:VAL:HG12	1.99	0.45	
3:C:23:ILE:HD11	3:C:46:LEU:HD21	1.99	0.45	
3:C:384:ASP:HA	3:C:387:LYS:HD3	1.99	0.45	
4:B:13:ASP:O	4:B:17:LEU:HB2	2.16	0.44	
3:A:395:ARG:HG2	3:A:395:ARG:NH1	2.32	0.44	
3:C:59:HIS:O	3:C:60:ASN:HB3	2.18	0.44	
3:C:246:LEU:HD21	3:C:447:TYR:CD1	2.52	0.44	
3:A:560:PRO:O	3:A:564:ALA:N	2.49	0.44	
3:A:592:TRP:HE3	3:A:593:ILE:C	2.20	0.44	
3:C:57:VAL:HG21	3:C:182:LEU:HD22	1.99	0.44	
3:C:59:HIS:ND1	3:C:91:THR:CG2	2.77	0.44	
3:C:593:ILE:CG2	3:C:594:LYS:N	2.81	0.44	
3:A:155:VAL:O	3:A:156:ASP:C	2.56	0.44	
4:B:29:ALA:HB1	4:B:31:TRP:CD1	2.52	0.44	
3:C:19:HIS:O	3:C:36:PRO:HD3	2.17	0.44	
3:C:257:LEU:C	3:C:259:GLU:N	2.70	0.44	
3:C:513:ALA:HB2	3:C:524:PHE:HE2	1.82	0.44	
3:A:166:GLU:O	3:A:169:ASP:HB2	2.18	0.44	
3:A:506:HIS:HA	3:A:509:ASN:ND2	2.33	0.44	
3:A:560:PRO:O	3:A:563:ALA:HB3	2.18	0.44	
3:A:666:ALA:O	3:A:670:ILE:CG1	2.66	0.44	
3:C:321:VAL:HG12	3:C:322:ALA:N	2.31	0.44	
1:Q:16:DG:C6	1:Q:17:DT:C4	3.05	0.44	
4:B:95:SER:H	4:B:98:GLN:HB2	1.82	0.44	
3:C:96:ARG:HG3	3:C:96:ARG:HH11	1.82	0.44	
3:C:596:LEU:HD13	3:C:621:ILE:HG13	2.00	0.44	
1:Q:14:DC:H2"	1:Q:15:DA:O5'	2.18	0.44	
3:A:176:VAL:HG23	3:A:177:VAL:N	2.32	0.44	



	o uo pugo	Interatomic	Clash
Atom-1 Atom-2		distance (Å)	overlap (Å)
3:A:421:ASN:HB3	3:A:431:THR:OG1	2.17	0.44
3:C:12:LEU:HD21	3:C:229:ARG:HD3	2.00	0.44
3:C:668:VAL:O	3:C:672:THR:N	2.45	0.44
4:D:59:ASN:OD1	4:D:59:ASN:C	2.55	0.44
3:A:155:VAL:HG11	3:A:161:TRP:HH2	1.82	0.44
3:A:198:PHE:HB3	3:A:206:PHE:CD2	2.53	0.44
3:A:257:LEU:C	3:A:259:GLU:N	2.70	0.44
3:A:483:CYS:O	3:A:487:PHE:HD2	2.00	0.44
3:A:630:GLU:O	3:A:634:VAL:HG23	2.18	0.44
4:B:38:ILE:HD12	4:B:78:LEU:HD11	1.98	0.44
3:C:128:TRP:HA	3:C:128:TRP:CE3	2.53	0.44
3:C:276:HIS:CB	3:C:279:THR:HB	2.47	0.44
3:C:356:TYR:HA	3:C:362:PRO:HA	2.00	0.44
3:C:569:ILE:HG21	3:C:609:ALA:HB1	2.00	0.44
3:C:640:HIS:NE2	3:C:647:ALA:HA	2.32	0.44
3:C:640:HIS:HD2	3:C:641:GLY:N	2.16	0.44
3:C:666:ALA:O	3:C:670:ILE:HG13	2.17	0.44
3:A:24:TYR:CD1	3:A:31:TYR:CE1	3.06	0.43
3:A:138:GLU:O	3:A:142:ASP:HB2	2.18	0.43
3:A:205:THR:HG23	3:A:209:GLU:HG3	2.00	0.43
3:A:250:ARG:HH11	3:A:396:ILE:HD12	1.80	0.43
3:C:43:LEU:HB3	3:C:79:ARG:NH1	2.32	0.43
3:C:49:GLU:OE1	3:C:49:GLU:HA	2.17	0.43
3:C:198:PHE:C	3:C:200:ASP:N	2.71	0.43
3:A:327:THR:CB	4:B:32:CYS:HG	2.26	0.43
3:C:3:VAL:HG22	3:C:57:VAL:HB	2.01	0.43
3:C:624:LEU:HD12	3:C:680:VAL:HG13	2.00	0.43
4:B:30:GLU:O	4:B:30:GLU:HG3	2.18	0.43
3:C:232:PHE:CE1	3:C:455:PHE:HB3	2.53	0.43
3:C:395:ARG:HG2	3:C:395:ARG:NH1	2.34	0.43
3:C:447:TYR:N	3:C:447:TYR:CD2	2.85	0.43
3:A:436:ASN:ND2	3:A:439:GLN:CG	2.80	0.43
3:A:590:ARG:C	3:A:592:TRP:H	2.22	0.43
4:B:14:THR:CG2	4:B:18:LYS:NZ	2.80	0.43
4:B:28:TRP:O	4:B:60:ILE:HG12	2.19	0.43
3:C:76:GLN:C	3:C:77:LEU:HD23	2.38	0.43
3:C:219:ARG:HB2	3:C:627:ILE:HD13	2.00	0.43
3:A:22:VAL:HG21	3:A:172:VAL:CA	2.47	0.43
3:A:329:VAL:HG11	4:B:31:TRP:CH2	2.53	0.43
3:A:505:ILE:HG23	3:A:506:HIS:H	1.83	0.43
4:B:19:ALA:O	4:B:21:GLY:N	2.45	0.43



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:8:ALA:HB1	3:C:15:VAL:HG23	2.00	0.43
3:C:263:SER:CB	3:C:331:HIS:NE2	2.81	0.43
4:D:19:ALA:O	4:D:21:GLY:N	2.45	0.43
1:Q:19:DC:H5'	1:Q:19:DC:C6	2.52	0.43
3:A:616:SER:O	3:A:619:ALA:HB3	2.19	0.43
3:C:128:TRP:CE3	3:C:128:TRP:CA	3.02	0.43
4:D:104:ASP:C	4:D:106:ASN:H	2.22	0.43
3:A:58:PHE:HB3	3:A:61:GLY:HA3	2.01	0.43
3:A:510:GLN:HE22	3:A:518:ARG:HB2	1.84	0.43
3:A:640:HIS:HB2	3:A:646:PHE:CZ	2.54	0.43
3:C:676:ALA:O	3:C:679:TRP:HB3	2.18	0.43
1:Q:20:DC:H2"	3:C:438:ALA:O	2.19	0.43
3:A:368:VAL:O	3:A:372:VAL:HG23	2.19	0.43
3:C:6:ILE:HG22	3:C:42:TYR:CZ	2.54	0.43
3:C:317:THR:HG22	3:C:317:THR:O	2.19	0.43
3:C:596:LEU:HD12	3:C:617:ALA:HA	2.00	0.43
3:A:252:GLU:O	3:A:254:LEU:N	2.52	0.43
3:A:676:ALA:O	3:A:680:VAL:HG23	2.19	0.43
4:B:27:PHE:CE2	4:B:67:ALA:HA	2.54	0.43
4:B:95:SER:C	4:B:97:GLY:N	2.72	0.43
3:C:43:LEU:HD13	3:C:81:PHE:CD1	2.53	0.43
3:A:490:ARG:HH11	3:C:196:ILE:HG12	1.82	0.43
4:B:27:PHE:HD1	4:B:27:PHE:H	1.67	0.43
3:C:35:ARG:HB3	3:C:36:PRO:CD	2.38	0.43
3:C:35:ARG:HG3	3:C:35:ARG:NH1	2.34	0.43
3:C:182:LEU:HD11	3:C:186:LEU:HD11	2.01	0.43
3:C:252:GLU:O	3:C:254:LEU:N	2.51	0.43
3:A:562:ILE:O	3:A:566:ARG:HG3	2.18	0.42
3:C:165:GLU:O	3:C:166:GLU:C	2.58	0.42
3:C:193:PRO:HA	3:C:194:PRO:HD3	1.89	0.42
4:D:32:CYS:SG	4:D:75:ILE:HG13	2.59	0.42
1:Q:13:DC:H2"	1:Q:14:DC:OP2	2.19	0.42
3:A:23:ILE:HG22	3:A:24:TYR:N	2.33	0.42
3:A:64:TYR:O	3:A:65:ASP:C	2.57	0.42
3:A:79:ARG:HG2	3:A:80:GLU:N	2.34	0.42
3:A:364:VAL:HA	3:A:368:VAL:CG2	2.49	0.42
3:C:249:ARG:O	3:C:253:LEU:HG	2.19	0.42
4:D:12:PHE:CZ	4:D:16:VAL:HG11	2.54	0.42
3:C:24:TYR:HB2	3:C:31:TYR:CD2	2.53	0.42
3:C:64:TYR:O	3:C:67:PRO:HD2	2.20	0.42
3:C:560:PRO:O	3:C:564:ALA:N	2.52	0.42



	ti a	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:C:569:ILE:HG22	3:C:570:GLN:N	2.33	0.42	
3:C:63:LYS:HE2	3:C:228:GLU:OE2	2.19	0.42	
3:C:257:LEU:O	3:C:259:GLU:N	2.53	0.42	
3:C:325:PRO:O	4:D:92:GLY:CA	2.59	0.42	
3:C:418:GLY:HA3	3:C:437:LEU:HD13	2.02	0.42	
3:C:516:PRO:CG	3:C:517:THR:H	2.28	0.42	
3:C:621:ILE:HD11	3:C:686:PHE:CE1	2.54	0.42	
3:A:391:MET:SD	3:A:446:PRO:HB2	2.59	0.42	
4:D:95:SER:H	4:D:98:GLN:HB2	1.83	0.42	
4:B:46:ALA:HA	4:B:55:VAL:HG21	2.01	0.42	
3:C:423:ASN:HB3	3:C:424:GLY:H	1.59	0.42	
3:A:190:HIS:CD2	3:A:600:LYS:HG3	2.55	0.42	
3:A:206:PHE:HE1	3:A:207:TRP:CZ3	2.36	0.42	
4:B:27:PHE:HE2	4:B:67:ALA:HA	1.84	0.42	
3:C:155:VAL:O	3:C:158:MET:HG2	2.20	0.42	
3:C:436:ASN:HB3	3:C:439:GLN:OE1	2.19	0.42	
4:D:94:LEU:H	4:D:94:LEU:HG	1.64	0.42	
3:A:175:VAL:O	3:A:178:THR:HB	2.19	0.42	
3:A:198:PHE:C	3:A:200:ASP:N	2.73	0.42	
3:A:281:LYS:HA	3:A:282:PRO:HD3	1.91	0.42	
3:A:284:PRO:HG2	3:A:285:LYS:H	1.84	0.42	
3:C:263:SER:O	3:C:264:TRP:HB3	2.20	0.42	
3:C:590:ARG:C	3:C:592:TRP:H	2.23	0.42	
4:D:95:SER:C	4:D:97:GLY:N	2.73	0.42	
1:P:18:DG:C4	1:P:19:DC:C5	3.07	0.42	
3:C:246:LEU:C	3:C:248:ALA:N	2.72	0.42	
3:A:158:MET:HB3	3:A:161:TRP:CZ2	2.55	0.42	
3:A:569:ILE:O	3:A:570:GLN:C	2.58	0.42	
4:B:16:VAL:HG23	4:B:23:ILE:HB	2.02	0.42	
4:B:104:ASP:C	4:B:106:ASN:H	2.24	0.42	
3:C:233:PRO:CG	3:C:460:HIS:HB2	2.50	0.42	
4:B:19:ALA:HB1	4:B:23:ILE:HD11	2.02	0.41	
3:C:158:MET:HB3	3:C:161:TRP:CZ3	2.55	0.41	
3:C:663:GLU:O	3:C:666:ALA:HB3	2.20	0.41	
3:A:334:PHE:CE1	3:A:345:LYS:HG3	2.55	0.41	
3:A:388:GLU:O	3:A:392:ILE:HG12	2.19	0.41	
3:C:128:TRP:HA	3:C:128:TRP:HE3	1.85	0.41	
3:C:513:ALA:O	3:C:515:LEU:N	2.53	0.41	
3:A:216:ILE:HD11	3:A:624:LEU:HD13	2.02	0.41	
3:A:257:LEU:O	3:A:260:THR:N	2.52	0.41	
3:A:638:LEU:HA	3:A:645:ASP:OD2	2.20	0.41	



	,	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:C:368:VAL:O	3:C:372:VAL:HG23	2.20	0.41	
3:C:628:LYS:O	3:C:632:MET:HG3	2.20	0.41	
3:A:193:PRO:HA	3:A:194:PRO:HD3	1.91	0.41	
4:B:95:SER:OG	4:B:98:GLN:N	2.44	0.41	
4:D:36:LYS:O	4:D:36:LYS:HG2	2.20	0.41	
3:A:234:PHE:CZ	3:A:239:ILE:HG13	2.54	0.41	
3:A:506:HIS:HB2	3:A:518:ARG:HE	1.86	0.41	
3:C:55:LEU:HD22	3:C:89:ILE:HD11	2.01	0.41	
3:A:1:MET:HA	3:A:55:LEU:O	2.21	0.41	
3:A:369:LEU:HB3	3:A:387:LYS:HD3	2.02	0.41	
3:A:488:MET:HA	3:A:565:LEU:HD11	2.00	0.41	
3:C:57:VAL:CG2	3:C:89:ILE:HB	2.48	0.41	
3:C:343:GLN:HG3	3:C:362:PRO:HG2	2.01	0.41	
3:C:509:ASN:O	3:C:512:ALA:HB3	2.20	0.41	
4:D:58:LEU:CD1	4:D:63:ASN:HD22	2.32	0.41	
2:U:8:DG:C6	2:U:9:DC:N4	2.88	0.41	
3:A:232:PHE:CE2	3:A:650:ALA:HB2	2.56	0.41	
3:A:349:ALA:CB	3:A:374:VAL:HG11	2.50	0.41	
3:A:517:THR:HG23	3:A:520:ASN:CB	2.51	0.41	
3:C:252:GLU:O	3:C:255:ARG:N	2.54	0.41	
3:C:292:PRO:HB2	3:C:294:VAL:CG2	2.47	0.41	
3:A:246:LEU:C	3:A:248:ALA:N	2.74	0.41	
3:A:665:ILE:O	3:A:669:VAL:HG23	2.21	0.41	
3:C:418:GLY:HA3	3:C:437:LEU:CD1	2.51	0.41	
3:C:436:ASN:CG	3:C:439:GLN:HG2	2.41	0.41	
3:A:31:TYR:CE2	3:A:176:VAL:HG12	2.56	0.41	
3:A:168:MET:O	3:A:172:VAL:HG23	2.21	0.41	
3:A:279:THR:CG2	3:A:280:GLY:N	2.80	0.41	
3:A:390:LEU:O	3:A:393:GLN:HB2	2.20	0.41	
3:A:429:ARG:HH11	3:A:653:HIS:CE1	2.38	0.41	
3:A:527:GLY:O	3:A:528:PHE:CB	2.67	0.41	
3:A:663:GLU:O	3:A:666:ALA:HB3	2.21	0.41	
4:B:79:LEU:HD12	4:B:79:LEU:N	2.35	0.41	
3:C:186:LEU:HD23	3:C:192:PHE:CE2	2.56	0.41	
3:C:366:ASP:OD1	3:C:387:LYS:NZ	2.53	0.41	
3:C:425:ALA:C	3:C:426:VAL:HG22	2.41	0.41	
3:C:624:LEU:HD22	3:C:624:LEU:HA	1.85	0.41	
4:D:27:PHE:CE2	4:D:67:ALA:HA	2.56	0.41	
4:D:9:ASP:OD1	4:D:66:THR:N	2.50	0.41	
4:D:27:PHE:HD1	4:D:27:PHE:H	1.68	0.41	
3:A:376:ASP:HA	3:A:377:PRO:HD2	1.87	0.40	



A + a = 1	A + ama 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:38:ASP:O	3:C:41:ALA:HB3	2.21	0.40
3:C:392:ILE:HD13	3:C:392:ILE:HA	1.86	0.40
3:A:22:VAL:HG23	3:A:171:ASN:OD1	2.20	0.40
3:A:43:LEU:HD13	3:A:79:ARG:HD2	2.02	0.40
3:A:145:ARG:C	3:A:147:LEU:N	2.74	0.40
3:A:181:LEU:O	3:A:182:LEU:C	2.60	0.40
3:A:286:TYR:HA	3:A:287:PRO:HD3	1.87	0.40
3:A:366:ASP:CG	3:A:387:LYS:HE3	2.42	0.40
3:A:688:CYS:O	3:A:689:LEU:C	2.60	0.40
3:C:155:VAL:HB	3:C:158:MET:SD	2.61	0.40
3:A:252:GLU:O	3:A:255:ARG:N	2.55	0.40
3:A:470:VAL:CG1	3:A:666:ALA:HB2	2.52	0.40
3:A:667:GLN:HA	3:A:670:ILE:HG13	2.03	0.40
3:C:24:TYR:CB	3:C:31:TYR:HE2	2.34	0.40
3:C:257:LEU:O	3:C:258:THR:C	2.59	0.40
3:C:316:ASP:O	3:C:318:ARG:N	2.54	0.40
4:D:38:ILE:O	4:D:41:ILE:HB	2.21	0.40
3:A:7:GLU:OE1	3:A:7:GLU:HA	2.22	0.40
3:A:257:LEU:O	3:A:258:THR:C	2.60	0.40
3:A:464:ILE:HG13	3:A:465:THR:N	2.32	0.40
3:C:49:GLU:HG3	3:C:54:GLY:HA3	2.02	0.40
3:C:145:ARG:C	3:C:147:LEU:N	2.74	0.40
3:C:436:ASN:C	3:C:436:ASN:OD1	2.60	0.40
3:C:524:PHE:CD1	3:C:524:PHE:C	2.93	0.40
4:D:80:LEU:O	4:D:87:ALA:CB	2.66	0.40
3:A:68:ALA:O	3:A:72:LEU:HG	2.22	0.40
3:A:432:HIS:O	3:A:433:ALA:HB2	2.21	0.40
3:A:678:ARG:HH11	3:A:678:ARG:CG	2.33	0.40
3:C:85:ARG:NH2	3:C:215:ASP:OD2	2.54	0.40
3:C:569:ILE:O	3:C:572:THR:N	2.48	0.40
4:D:24:LEU:O	4:D:24:LEU:HG	2.21	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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perc	entiles
3	А	646/698~(93%)	513 (79%)	111 (17%)	22 (3%)	3	24
3	С	645/698~(92%)	505~(78%)	117 (18%)	23~(4%)	3	23
4	В	103/108~(95%)	76 (74%)	23~(22%)	4 (4%)	3	22
4	D	103/108~(95%)	77~(75%)	21 (20%)	5(5%)	2	17
All	All	1497/1612~(93%)	1171 (78%)	272 (18%)	54 (4%)	3	23

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

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	А	156	ASP
3	А	279	THR
3	А	359	LYS
3	А	426	VAL
3	А	543	ALA
3	А	573	LEU
3	С	156	ASP
3	С	279	THR
3	С	359	LYS
3	С	426	VAL
3	С	543	ALA
3	А	75	LEU
3	А	102	LEU
3	А	146	MET
3	А	344	LYS
3	А	424	GLY
3	А	495	GLU
3	А	516	PRO
3	А	526	TYR
4	В	13	ASP
4	В	69	LYS
3	С	102	LEU
3	С	146	MET
3	С	424	GLY
3	С	495	GLU
3	С	514	GLU
3	С	516	PRO
3	С	526	TYR
3	С	573	LEU
4	D	13	ASP



Mol	Chain	Res	Type
4	D	69	LYS
3	А	126	GLU
3	А	184	LYS
3	С	184	LYS
3	С	344	LYS
3	С	596	LEU
3	А	209	GLU
3	А	514	GLU
3	С	126	GLU
3	С	209	GLU
3	С	253	LEU
4	D	76	PRO
3	А	86	GLU
4	В	7	LEU
3	С	75	LEU
3	С	263	SER
3	С	544	GLY
4	D	7	LEU
3	А	253	LEU
3	A	544	GLY
3	А	653	HIS
3	С	653	HIS
4	D	68	PRO
4	В	76	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	А	430/579~(74%)	397~(92%)	33 (8%)	13 44
3	С	427/579~(74%)	388 (91%)	39~(9%)	9 34
4	В	62/87~(71%)	58 (94%)	4 (6%)	17 51
4	D	62/87~(71%)	58 (94%)	4 (6%)	17 51
All	All	981/1332 (74%)	901 (92%)	80 (8%)	11 41



All ((80)	residues	with a	non-rotameric	sidechain	are listed	below:
-------	------	----------	--------	---------------	-----------	------------	--------

Mol	Chain	Res	Type
3	А	14	SER
3	А	62	HIS
3	А	75	LEU
3	А	131	ARG
3	А	135	MET
3	А	159	GLU
3	А	164	ASN
3	А	171	ASN
3	А	174	ASP
3	А	181	LEU
3	А	204	THR
3	А	232	PHE
3	А	258	THR
3	А	271	THR
3	А	283	LEU
3	А	294	VAL
3	А	337	SER
3	А	343	GLN
3	А	347	GLN
3	А	363	VAL
3	А	375	ASP
3	А	393	GLN
3	А	403	ASP
3	А	410	VAL
3	А	413	ASP
3	А	445	SER
3	А	450	GLN
3	А	464	ILE
3	А	465	THR
3	А	528	PHE
3	А	597	ASP
3	А	670	ILE
3	А	678	ARG
4	В	15	ASP
4	В	55	VAL
4	В	61	ASP
4	В	75	ILE
3	С	5	ASP
3	С	62	HIS
3	С	85	ARG
3	С	91	THR
3	С	105	THR



Mol	Chain	Res	Type
3	С	128	TRP
3	С	131	ARG
3	С	150	GLN
3	С	169	ASP
3	С	171	ASN
3	С	174	ASP
3	С	197	ASP
3	С	232	PHE
3	С	244	VAL
3	С	259	GLU
3	С	291	THR
3	С	343	GLN
3	С	346	LEU
3	С	368	VAL
3	С	391	MET
3	С	393	GLN
3	С	403	ASP
3	С	423	ASN
3	С	443	VAL
3	С	452	ARG
3	С	465	THR
3	С	480	GLU
3	С	490	ARG
3	С	519	ASP
3	С	520	ASN
3	С	528	PHE
3	С	546	GLU
3	С	611	ASN
3	С	638	LEU
3	С	652	VAL
3	С	662	THR
3	С	678	ARG
3	С	686	PHE
3	С	698	PRO
4	D	35	CYS
4	D	50	GLN
4	D	59	ASN
4	D	61	ASP

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



Mol	Chain	Res	Type
3	А	150	GLN
3	А	164	ASN
3	А	171	ASN
3	А	173	GLN
3	А	266	GLN
3	А	276	HIS
3	А	343	GLN
3	А	380	GLN
3	А	393	GLN
3	А	423	ASN
3	А	509	ASN
3	А	510	GLN
3	А	611	ASN
3	А	683	HIS
3	С	60	ASN
3	С	276	HIS
3	С	417	HIS
3	С	509	ASN
3	С	510	GLN
3	С	611	ASN
3	С	657	GLN
4	D	50	GLN
4	D	63	ΔSN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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).

Mal	Turne	Chain	Dec	Tiple	Bo	ond leng	$_{\rm sths}$	B	ond ang	les
INIOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2DT	Q	21	2,1	17,20,21	0.41	0	22,28,31	0.47	0
1	2DT	Р	21	2,1	17,20,21	0.51	0	22,28,31	0.52	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	2DT	Q	21	2,1	-	1/7/18/19	0/2/2/2
1	2DT	Р	21	2,1	-	1/7/18/19	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Р	21	2DT	O4'-C4'-C5'-O5'
1	Q	21	2DT	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	Q	21	2DT	1	0
1	Р	21	2DT	2	0

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	Turne	no Chain Bos	Tink	Bo	Bond lengths			Bond angles		
IVIOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	DAD	А	4004	-	25,31,31	0.72	0	26,48,48	1.09	2 (7%)
6	DAD	С	4005	-	25,31,31	0.72	0	26,48,48	1.10	3 (11%)

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	DAD	А	4004	-	2/2/5/5	2/18/31/31	0/3/3/3
6	DAD	С	4005	-	2/2/5/5	7/18/31/31	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	С	4005	DAD	C5-C6-N6	2.33	123.89	120.35
6	С	4005	DAD	O2G-PG-O1G	2.28	119.61	110.68
6	А	4004	DAD	O2G-PG-O1G	2.27	119.55	110.68
6	С	4005	DAD	C2'-C1'-N9	2.24	116.69	112.48
6	А	4004	DAD	C5-C6-N6	2.19	123.67	120.35

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	А	4004	DAD	C1'
6	А	4004	DAD	C4'
6	С	4005	DAD	C1'
6	С	4005	DAD	C4'

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	С	4005	DAD	C5'-O5'-PA-O1A
6	С	4005	DAD	C5'-O5'-PA-O2A
6	С	4005	DAD	PA-O3A-PB-O1B
6	С	4005	DAD	PB-O3A-PA-O1A
6	С	4005	DAD	PA-O3A-PB-O2B
6	С	4005	DAD	PB-O3A-PA-O2A
6	А	4004	DAD	PB-O3B-PG-O2G



Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	С	4005	DAD	C5'-O5'-PA-O3A
6	А	4004	DAD	PB-O3A-PA-O2A

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 sufficient must be 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	Р	10/21~(47%)	-0.17	0 100 100	53, 64, 118, 140	0
1	Q	10/21~(47%)	-0.38	0 100 100	70, 95, 153, 171	0
2	Т	10/25~(40%)	-0.03	0 100 100	43, 56, 91, 100	0
2	U	10/25~(40%)	-0.35	0 100 100	65, 95, 116, 139	0
3	А	658/698~(94%)	0.02	14 (2%) 63 49	23,65,125,182	0
3	С	658/698~(94%)	-0.04	22 (3%) 46 30	35, 76, 130, 198	0
4	В	105/108~(97%)	-0.10	0 100 100	48, 80, 127, 163	0
4	D	$10\overline{5/108}~(97\%)$	-0.13	2(1%) 66 53	$53, \overline{92, 122, 155}$	0
All	All	1566/1704~(91%)	-0.03	38 (2%) 59 44	23, 74, 130, 198	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	А	124	ALA	12.5
3	А	112	SER	12.3
3	А	113	GLY	10.8
3	А	114	LYS	7.7
3	С	275	CYS	7.5
3	А	125	LEU	5.6
3	С	126	GLU	4.5
3	А	107	MET	3.6
3	С	282	PRO	3.6
3	А	216	ILE	3.4
3	С	77	LEU	3.0
3	С	406	TRP	3.0
3	А	325	PRO	2.9
3	С	125	LEU	2.8
4	D	19	ALA	2.8
3	C	597	ASP	2.7



Mol	Chain	Res	Type	RSRZ
3	С	280	GLY	2.6
3	С	56	ILE	2.6
3	А	108	GLY	2.5
3	А	115	LEU	2.5
3	С	396	ILE	2.5
3	С	213	ALA	2.5
3	А	126	GLU	2.5
3	С	55	LEU	2.5
3	А	111	ARG	2.4
3	С	292	PRO	2.4
3	С	603	VAL	2.4
3	А	117	GLY	2.3
3	С	416	ILE	2.3
3	С	1	MET	2.3
3	А	603	VAL	2.3
3	С	182	LEU	2.2
4	D	70	TYR	2.2
3	С	599	ARG	2.1
3	С	294	VAL	2.1
3	С	87	ASN	2.1
3	С	81	PHE	2.0
3	С	167	MET	2.1

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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
1	2DT	Q	21	19/20	0.89	0.20	70,70,70,70	0
1	2DT	Р	21	19/20	0.95	0.21	70,70,70,70	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(Å ²)	Q<0.9
6	DAD	С	4005	29/29	0.74	0.18	132,132,188,188	0
6	DAD	А	4004	29/29	0.77	0.20	131,131,207,207	0
5	MG	С	4004	1/1	0.88	0.45	70,70,70,70	0
5	MG	А	4003	1/1	0.89	0.42	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.

