

Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 04:36 pm GMT

PDB ID	:	1GL7
Title	:	Plasmid coupling protein TrwB in complex with the non-hydrolisable ATP-
		analogue ADPNP.
Authors	:	Gomis-Ruth, F.X.; Moncalian, G.; De La cruz, F.; Coll, M.
Deposited on	:	2001-08-28
Resolution	:	3.00 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
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 3.00 Å.

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



Motria	Whole archive	Similar resolution		
wietric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
Clashscore	141614	2416 (3.00-3.00)		
Ramachandran outliers	138981	2333 (3.00-3.00)		
Sidechain outliers	138945	2336 (3.00-3.00)		

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain					
1	А	437	50%	39%	5% 6%			
1	В	437	54%	37%	• 5%			
1	D	437	57%	34%	5% 5%			
1	Е	437	51%	39%	5% 5%			
1	F	437	55%	35%	• 5%			
1	G	437	51%	39%	• 6%			



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19892 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	411	Total	С	Ν	0	\mathbf{S}	0	0	0
1	Л	411	3233	2046	577	600	10	0	0	0
1	В	417	Total	С	Ν	0	S	0	0	0
1	D	417	3276	2072	587	607	10	0	0	0
1	Л	417	Total	С	Ν	0	S	0	0	0
1	D	417	3273	2069	587	607	10		0	0
1	F	414	Total	С	Ν	0	S	0	0	0
1	Ľ	414	3254	2059	581	604	10	0	0	U
1	F	413	Total	С	Ν	0	S	0	0	0
1	Ľ	415	3240	2050	579	601	10	0	0	0
1	С	419	Total	С	Ν	0	\mathbf{S}	0	0	0
	G	412	3237	2048	578	601	10	0	0	0

• Molecule 1 is a protein called CONJUGAL TRANSFER PROTEIN TRWB.

• Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).





Fage 4 Full wwPDB A-ray Structure validation Report									eport		
Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf		
0	٨	1	Total	С	Ν	Ο	Р	0	0		
Z	A	1	31	10	6	12	3	0	0		
ი	D	1	Total	С	Ν	Ο	Р	0	0		
Z		1	31	10	6	12	3		0		
0	П	1	Total	С	Ν	Ο	Р	0	0		
Z	D	1	31	10	6	12	3	0	0		
ე	F	1	Total	С	Ν	Ο	Р	0	0		
Z	Ľ	1	31	10	6	12	3	0	0		
0	Б	F	F	1	Total	С	Ν	Ο	Р	0	0
	1	31	10	6	12	3	0	0			
0	С	0 1	Total	С	Ν	Ο	Р	0	0		
2	G	L	31	10	6	12	3	0	U		

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Cl 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	30	Total O 30 30	0	0
4	В	29	TotalO2929	0	0
4	D	39	Total O 39 39	0	0
4	Е	53	$\begin{array}{cc} \text{Total} & \text{O} \\ 53 & 53 \end{array}$	0	0
4	F	23	Total O 23 23	0	0
4	G	18	Total O 18 18	0	0

B



 $1 \mathrm{GL7}$

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. 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. 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.

Note EDS was not executed.



• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB





• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB









4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 31 2 1	Depositor	
Cell constants	152.70Å 152.70Å 252.10Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	50.00 - 3.00	Depositor	
% Data completeness	100.0 (50.00-3.00)	Depositor	
(in resolution range)	100.0 (00.00 0.00)	Depositor	
R_{merge}	0.11	Depositor	
R _{sym}	(Not available)	Depositor	
Refinement program	CNS 1.0	Depositor	
R, R_{free}	0.219 , 0.265	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	19892	wwPDB-VP	
Average B, all atoms $(Å^2)$	64.0	wwPDB-VP	



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: CL, ANP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.47	0/3297	0.68	0/4457	
1	В	0.46	0/3340	0.68	1/4514~(0.0%)	
1	D	0.47	0/3337	0.69	1/4509~(0.0%)	
1	Е	0.47	0/3318	0.70	0/4485	
1	F	0.46	0/3304	0.69	0/4466	
1	G	0.47	0/3301	0.68	0/4462	
All	All	0.47	0/19897	0.69	2/26893~(0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	В	157	VAL	N-CA-C	-5.51	96.12	111.00
1	D	157	VAL	N-CA-C	-5.14	97.11	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3233	0	3261	169	0
1	В	3276	0	3308	165	1
1	D	3273	0	3302	157	1



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Е	3254	0	3283	185	0
1	F	3240	0	3270	172	0
1	G	3237	0	3264	180	0
2	А	31	0	13	1	0
2	В	31	0	13	2	0
2	D	31	0	13	1	0
2	Ε	31	0	13	2	0
2	F	31	0	13	2	0
2	G	31	0	13	1	0
3	А	1	0	0	0	0
4	А	30	0	0	1	0
4	В	29	0	0	1	0
4	D	39	0	0	3	0
4	Ε	53	0	0	3	0
4	F	23	0	0	0	0
4	G	18	0	0	0	0
All	All	19892	0	19766	989	1

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 25.

All (989) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:367:LEU:HD13	1:B:403:LEU:HD11	1.36	1.05
1:D:413:LEU:HD23	1:D:475:ALA:HB2	1.37	1.03
1:F:463:MET:HB2	1:F:466:GLU:HG3	1.43	1.01
1:B:503:VAL:O	1:B:504:GLU:HB2	1.63	0.98
1:G:154:MET:HE3	1:G:156:ILE:HD11	1.44	0.98
1:F:105:GLU:H	1:F:109:GLN:NE2	1.60	0.98
1:G:94:VAL:HG21	1:G:98:LYS:HG2	1.46	0.97
1:F:105:GLU:H	1:F:109:GLN:HE22	1.02	0.97
1:B:372:THR:HG22	1:B:373:LYS:HG3	1.47	0.94
1:B:180:GLN:HE21	1:B:504:GLU:HG3	1.33	0.92
1:B:74:VAL:HB	1:B:84:PHE:O	1.70	0.92
1:D:463:MET:HB2	1:D:466:GLU:HG3	1.51	0.91
1:B:92:ARG:HB3	1:B:92:ARG:NH2	1.86	0.90
1:E:413:LEU:HD23	1:E:475:ALA:HB2	1.53	0.90
1:A:190:GLU:OE1	1:A:302:ARG:HG3	1.72	0.90
1:E:94:VAL:HG21	1:E:98:LYS:HG2	1.51	0.88
1:A:131:ALA:HB2	1:A:415:GLY:HA2	1.55	0.88



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:384:GLY:O	1:A:385:LEU:HD13	1.74	0.88
1:E:94:VAL:CG2	1:E:98:LYS:HG2	2.03	0.87
1:G:177:PRO:HB3	1:G:294:MET:HG2	1.57	0.87
1:G:463:MET:HB2	1:G:466:GLU:HG3	1.57	0.87
1:E:131:ALA:HB2	1:E:415:GLY:HA2	1.55	0.86
1:F:199:ARG:HE	1:F:338:THR:CG2	1.89	0.86
1:A:463:MET:HB2	1:A:466:GLU:HG3	1.56	0.85
1:E:199:ARG:HE	1:E:338:THR:CG2	1.91	0.84
1:G:432:GLU:HG2	1:G:460:ARG:HD3	1.60	0.82
1:F:199:ARG:HE	1:F:338:THR:HG22	1.44	0.82
1:G:94:VAL:CG2	1:G:98:LYS:HG2	2.09	0.82
1:D:180:GLN:NE2	1:D:505:GLY:HA2	1.95	0.82
1:E:107:ALA:HB3	1:E:119:ARG:HD2	1.61	0.81
1:F:498:ARG:O	1:F:499:GLN:HG3	1.80	0.81
1:E:169:ARG:HH11	1:E:169:ARG:HA	1.45	0.81
1:E:327:PRO:HG2	4:E:2039:HOH:O	1.80	0.81
1:B:384:GLY:O	1:B:385:LEU:HD13	1.81	0.81
1:E:169:ARG:HH11	1:E:169:ARG:CA	1.94	0.80
1:B:169:ARG:HH11	1:B:171:LYS:HD3	1.45	0.80
1:F:456:ARG:HG2	1:F:456:ARG:HH11	1.46	0.79
1:E:498:ARG:O	1:E:499:GLN:HG3	1.83	0.79
1:B:92:ARG:HB3	1:B:92:ARG:HH21	1.44	0.78
1:D:246:THR:O	1:D:281:ARG:HD2	1.82	0.78
1:E:463:MET:HB2	1:E:466:GLU:HG3	1.66	0.78
1:F:384:GLY:O	1:F:385:LEU:HD13	1.84	0.78
1:B:318:ARG:HH21	1:B:321:MET:CE	1.96	0.77
1:A:145:TYR:CZ	1:A:149:LEU:HD11	2.20	0.77
1:G:290:GLU:HB3	1:G:328:LEU:HD12	1.65	0.77
1:A:98:LYS:O	1:A:102:MET:HG3	1.85	0.77
1:B:318:ARG:HH21	1:B:321:MET:HE3	1.50	0.77
1:G:222:LEU:HA	1:G:225:ARG:NH1	2.00	0.76
1:E:304:TRP:CH2	1:E:313:LEU:HB2	2.21	0.76
1:E:169:ARG:HB2	1:E:172:ASP:OD2	1.86	0.76
1:G:169:ARG:HH11	1:G:171:LYS:HD3	1.50	0.75
1:E:84:PHE:HA	1:E:437:ARG:HG3	1.68	0.75
1:D:386:GLN:HB2	4:D:2028:HOH:O	1.87	0.75
1:F:413:LEU:HD23	1:F:475:ALA:HB2	1.68	0.75
1:B:463:MET:HB2	1:B:466:GLU:HG3	1.68	0.75
1:E:413:LEU:CD2	1:E:475:ALA:HB2	2.17	0.75
1:G:154:MET:HB3	1:G:352:TRP:HB2	1.69	0.74
1:D:199:ARG:HE	1:D:338:THR:HG22	1.52	0.74



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:331:ALA:O	1:D:335:VAL:HG23	1.87	0.74
1:A:166:LYS:HE2	1:A:497:ASN:ND2	2.03	0.74
1:D:180:GLN:HE21	1:D:505:GLY:HA2	1.52	0.74
1:A:166:LYS:HE2	1:A:497:ASN:HD21	1.51	0.73
1:F:358:LEU:HD11	1:F:367:LEU:HD11	1.71	0.73
1:B:180:GLN:HE21	1:B:504:GLU:CG	2.00	0.73
1:B:413:LEU:HD23	1:B:475:ALA:HB2	1.71	0.73
1:B:498:ARG:O	1:B:499:GLN:HG3	1.89	0.73
1:D:94:VAL:CG2	1:D:98:LYS:HG2	2.20	0.72
1:G:279:SER:O	1:G:283:VAL:HG23	1.90	0.72
1:F:331:ALA:O	1:F:335:VAL:HG23	1.90	0.71
1:F:488:VAL:HG13	1:F:489:PRO:HD2	1.72	0.71
1:F:379:LEU:HD23	1:F:380:ARG:N	2.05	0.71
1:E:199:ARG:HE	1:E:338:THR:HG22	1.56	0.71
1:A:328:LEU:O	1:A:331:ALA:HB3	1.90	0.71
1:G:498:ARG:O	1:G:499:GLN:HG3	1.90	0.71
1:A:358:LEU:HB3	1:A:385:LEU:HD11	1.72	0.71
1:F:356:ASP:OD2	1:F:357:GLU:N	2.24	0.71
1:F:346:GLU:OE2	1:F:346:GLU:HA	1.91	0.71
1:F:473:LEU:HD11	1:F:492:ILE:HD11	1.73	0.70
1:A:352:TRP:CZ2	1:A:380:ARG:HD3	2.25	0.70
1:E:497:ASN:N	1:E:497:ASN:HD22	1.90	0.69
1:A:352:TRP:CE2	1:A:380:ARG:HD3	2.26	0.69
1:A:456:ARG:HD2	1:A:456:ARG:N	2.07	0.69
1:E:384:GLY:O	1:E:385:LEU:HD13	1.92	0.69
1:E:456:ARG:HH21	1:E:456:ARG:HG3	1.57	0.69
1:E:154:MET:HB3	1:E:352:TRP:HB2	1.75	0.69
1:E:169:ARG:HH11	1:E:169:ARG:CG	2.05	0.69
1:F:184:GLY:HA3	1:F:297:GLY:HA3	1.73	0.69
1:G:246:THR:O	1:G:281:ARG:HD2	1.93	0.68
1:F:456:ARG:HG2	1:F:456:ARG:NH1	2.08	0.68
1:B:94:VAL:CG2	1:B:98:LYS:HE3	2.24	0.68
1:B:259:GLU:HA	1:B:264:GLU:HG3	1.75	0.67
1:D:184:GLY:HA3	1:D:297:GLY:HA3	1.75	0.67
1:D:482:ASN:C	1:D:482:ASN:HD22	1.96	0.67
1:A:222:LEU:HA	1:A:225:ARG:NH1	2.09	0.67
1:E:177:PRO:HB3	1:E:294:MET:HG2	1.76	0.67
1:F:345:GLU:N	1:F:345:GLU:OE1	2.28	0.67
1:A:158:ASP:OD2	1:A:161:GLY:HA2	1.95	0.67
1:A:93:ILE:HG13	1:A:485:ILE:HG13	1.78	0.66
1:E:169:ARG:NH1	1:E:170:ASP:H	1.91	0.66



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:82:ALA:O	1:B:437:ARG:NH1	2.28	0.66
1:B:131:ALA:HB2	1:B:415:GLY:HA2	1.78	0.66
1:B:488:VAL:HG13	1:B:489:PRO:HD2	1.78	0.66
1:F:379:LEU:HD23	1:F:380:ARG:H	1.60	0.66
1:G:105:GLU:HB2	1:G:109:GLN:NE2	2.11	0.66
1:E:169:ARG:HA	1:E:169:ARG:NH1	2.09	0.66
1:A:179:ASP:O	1:A:182:THR:HG22	1.96	0.66
1:B:432:GLU:HG2	1:B:460:ARG:HD3	1.77	0.66
1:E:246:THR:O	1:E:281:ARG:HD2	1.95	0.66
1:B:367:LEU:CD1	1:B:403:LEU:HD11	2.20	0.66
1:D:169:ARG:NH1	1:D:171:LYS:HD3	2.11	0.66
1:A:156:ILE:HG22	1:A:158:ASP:HB2	1.77	0.65
1:A:301:ILE:O	1:A:305:LEU:HG	1.97	0.65
1:A:497:ASN:N	1:A:497:ASN:HD22	1.93	0.65
1:D:238:SER:HB3	1:D:241:GLU:CG	2.26	0.65
1:E:169:ARG:NH1	1:E:169:ARG:HG2	2.11	0.65
1:D:255:ARG:HH21	1:D:255:ARG:HG3	1.62	0.65
1:F:471:PRO:HG2	1:F:474:THR:OG1	1.96	0.65
1:D:498:ARG:O	1:D:499:GLN:HG3	1.96	0.65
1:A:89:ARG:HD2	1:A:434:GLU:OE1	1.96	0.65
1:E:126:LEU:HD11	1:E:411:VAL:HG23	1.79	0.65
1:G:136:LYS:O	1:G:140:LEU:HD13	1.97	0.65
1:D:130:GLY:HA3	1:D:413:LEU:HB2	1.79	0.65
1:D:177:PRO:HG2	1:D:178:TYR:CD1	2.31	0.65
1:E:246:THR:C	1:E:281:ARG:HH11	1.98	0.65
1:A:367:LEU:HD13	1:A:403:LEU:HD11	1.79	0.64
1:D:384:GLY:O	1:D:385:LEU:HD13	1.97	0.64
1:D:410:LEU:HD12	1:D:411:VAL:H	1.61	0.64
1:F:154:MET:HB3	1:F:352:TRP:HB2	1.79	0.64
1:F:318:ARG:HH21	1:F:318:ARG:HB3	1.60	0.64
1:B:145:TYR:CZ	1:B:149:LEU:HD11	2.32	0.64
1:G:177:PRO:HD3	1:G:294:MET:HE3	1.79	0.64
1:E:156:ILE:HG22	1:E:158:ASP:HB2	1.79	0.64
1:F:318:ARG:HB3	1:F:318:ARG:NH2	2.13	0.64
1:A:159:PRO:HG3	1:A:317:TRP:CH2	2.33	0.64
1:E:184:GLY:HA3	1:E:297:GLY:HA3	1.79	0.64
1:A:479:PHE:O	1:G:417:ARG:NH1	2.31	0.64
1:B:346:GLU:OE2	1:B:346:GLU:HA	1.97	0.64
1:D:367:LEU:HD13	1:D:403:LEU:HD11	1.79	0.64
1:E:436:GLU:HG2	1:E:454:LEU:HD13	1.80	0.64
1:F:94:VAL:HG21	1:F:98:LYS:HG2	1.77	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:158:ASP:O	1:G:316:THR:HA	1.98	0.64
1:E:199:ARG:HE	1:E:338:THR:HG21	1.60	0.63
1:F:83:PRO:O	1:F:437:ARG:HD3	1.99	0.63
1:F:328:LEU:O	1:F:331:ALA:HB3	1.98	0.63
1:A:169:ARG:HH12	1:A:171:LYS:HD3	1.63	0.63
1:D:482:ASN:C	1:D:483:ARG:HG2	2.19	0.63
1:F:497:ASN:N	1:F:497:ASN:HD22	1.96	0.63
1:G:190:GLU:OE1	1:G:302:ARG:HG3	1.98	0.63
1:G:435:VAL:HG12	1:G:436:GLU:N	2.14	0.63
1:B:76:GLN:C	1:B:78:GLU:H	2.02	0.63
1:G:124:ARG:HB3	1:G:408:ARG:CG	2.29	0.63
1:A:306:GLU:O	1:A:308:PRO:HD3	1.99	0.63
1:B:313:LEU:HD23	1:B:314:PHE:N	2.14	0.63
1:G:159:PRO:HG3	1:G:317:TRP:CH2	2.33	0.63
1:A:432:GLU:HG2	1:A:460:ARG:HD3	1.80	0.63
1:B:428:LEU:O	1:B:428:LEU:HD23	1.99	0.62
1:D:199:ARG:HE	1:D:338:THR:CG2	2.11	0.62
1:E:166:LYS:HD2	1:E:495:PHE:HB2	1.81	0.62
1:G:380:ARG:HH21	1:G:380:ARG:HG3	1.64	0.62
1:A:154:MET:HB3	1:A:352:TRP:HB2	1.80	0.62
1:F:351:LEU:HD23	1:F:352:TRP:H	1.64	0.62
1:F:256:GLY:O	1:F:259:GLU:HG3	2.00	0.62
1:G:127:LEU:HD11	1:G:385:LEU:CD2	2.28	0.62
1:B:259:GLU:HA	1:B:264:GLU:CG	2.29	0.62
1:B:410:LEU:HD12	1:B:411:VAL:H	1.64	0.62
1:D:238:SER:HB3	1:D:241:GLU:HG3	1.80	0.62
1:F:131:ALA:HB2	1:F:415:GLY:HA2	1.82	0.62
1:F:152:ASP:OD1	1:F:350:ARG:NH2	2.33	0.62
1:G:154:MET:HA	1:G:351:LEU:CD2	2.29	0.62
1:G:177:PRO:HG2	1:G:178:TYR:CD1	2.34	0.62
1:F:246:THR:O	1:F:281:ARG:HD2	1.99	0.62
1:A:230:LYS:HG2	1:A:257:PHE:CZ	2.35	0.62
1:G:353:LEU:HD13	1:G:355:ILE:HD11	1.81	0.62
1:G:488:VAL:HG13	1:G:489:PRO:HD2	1.81	0.62
1:B:159:PRO:HG3	1:B:317:TRP:CH2	2.35	0.61
1:B:410:LEU:HD12	1:B:411:VAL:N	2.15	0.61
1:D:94:VAL:HG21	1:D:98:LYS:HG2	1.81	0.61
1:F:463:MET:SD	1:G:89:ARG:HD3	2.39	0.61
1:G:497:ASN:N	1:G:497:ASN:HD22	1.97	0.61
1:D:103:THR:OG1	1:D:116:PRO:HG2	2.01	0.61
1:G:124:ARG:HB3	1:G:408:ARG:HB2	1.81	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:433:HIS:HD2	1:B:433:HIS:O	1.83	0.61
1:G:207:ARG:HB2	1:G:363:LYS:HD3	1.83	0.61
2:B:701:ANP:PG	1:D:375:ARG:HE	2.24	0.61
1:E:328:LEU:O	1:E:331:ALA:HB3	2.01	0.61
1:B:124:ARG:HB3	1:B:408:ARG:HB2	1.82	0.61
1:B:417:ARG:NH1	1:D:479:PHE:O	2.33	0.61
1:G:461:VAL:HG11	1:G:485:ILE:HD11	1.82	0.61
1:G:222:LEU:HD23	1:G:267:PHE:CE1	2.35	0.61
1:A:420:PRO:HB2	1:B:428:LEU:HD22	1.82	0.61
1:E:94:VAL:HG22	1:E:98:LYS:HG2	1.83	0.61
1:D:131:ALA:HB2	1:D:415:GLY:HA2	1.82	0.61
1:E:463:MET:SD	1:F:89:ARG:HD3	2.41	0.61
1:G:131:ALA:HB2	1:G:415:GLY:HA2	1.83	0.61
1:G:435:VAL:CG1	1:G:436:GLU:N	2.63	0.61
1:E:85:LYS:HD3	1:E:454:LEU:HD11	1.83	0.60
1:E:130:GLY:HA3	1:E:413:LEU:HB2	1.82	0.60
1:F:86:ARG:HD3	1:F:436:GLU:OE1	2.01	0.60
1:F:127:LEU:HD11	1:F:385:LEU:HD22	1.83	0.60
1:A:433:HIS:HD2	1:A:433:HIS:O	1.84	0.60
1:D:94:VAL:HG22	1:D:98:LYS:HG2	1.83	0.60
1:D:372:THR:HG22	1:D:373:LYS:HG3	1.82	0.60
1:E:470:LEU:HD23	1:E:471:PRO:HD2	1.83	0.60
1:A:95:SER:OG	1:A:98:LYS:HB2	2.01	0.60
1:B:130:GLY:HA3	1:B:413:LEU:HB2	1.83	0.60
1:F:139:LEU:HD23	1:F:139:LEU:O	2.01	0.60
1:B:367:LEU:HD22	1:B:371:LEU:HG	1.84	0.60
1:E:432:GLU:HG2	1:E:460:ARG:HD3	1.84	0.60
1:G:103:THR:OG1	1:G:116:PRO:HG2	2.02	0.60
1:G:322:GLY:N	1:G:323:PRO:HD2	2.17	0.60
1:E:190:GLU:OE1	1:E:302:ARG:HG3	2.02	0.59
1:A:177:PRO:HB3	1:A:294:MET:HG2	1.83	0.59
1:B:126:LEU:HD11	1:B:411:VAL:HG23	1.84	0.59
1:F:380:ARG:HH21	1:F:380:ARG:HG3	1.67	0.59
1:G:180:GLN:HE21	1:G:505:GLY:HA2	1.66	0.59
1:D:84:PHE:HB3	1:D:437:ARG:HG3	1.84	0.59
1:F:410:LEU:HD12	1:F:411:VAL:H	1.66	0.59
1:F:252:ASP:O	1:F:255:ARG:HB2	2.02	0.59
1:A:410:LEU:HD12	1:A:411:VAL:H	1.66	0.59
1:B:322:GLY:N	1:B:323:PRO:HD2	2.17	0.59
1:E:169:ARG:HH11	1:E:169:ARG:CB	2.16	0.59
1:F:154:MET:HA	1:F:351:LEU:HD23	1.84	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:193:ASN:O	1:F:196:ASP:HB2	2.01	0.59
1:F:351:LEU:HD23	1:F:352:TRP:N	2.18	0.59
1:G:158:ASP:HB3	1:G:316:THR:HG22	1.85	0.59
1:G:180:GLN:NE2	1:G:505:GLY:HA2	2.16	0.59
1:E:135:GLY:HA2	2:E:701:ANP:O1A	2.02	0.59
1:F:199:ARG:HE	1:F:338:THR:HG21	1.67	0.59
1:A:139:LEU:HB2	1:A:490:LEU:HD11	1.85	0.59
1:E:455:GLU:O	1:E:455:GLU:HG3	2.04	0.58
1:A:246:THR:O	1:A:281:ARG:HD2	2.03	0.58
1:F:139:LEU:HD23	1:F:139:LEU:C	2.23	0.58
1:F:255:ARG:HH21	1:F:255:ARG:HG3	1.69	0.58
1:B:98:LYS:O	1:B:102:MET:HG3	2.02	0.58
1:B:169:ARG:NH1	1:B:171:LYS:HD3	2.17	0.58
1:B:225:ARG:O	1:B:229:LYS:HB2	2.04	0.58
1:A:177:PRO:HD3	1:A:294:MET:HE3	1.85	0.58
1:B:184:GLY:HA3	1:B:297:GLY:HA3	1.84	0.58
1:E:136:LYS:O	1:E:140:LEU:HD13	2.04	0.58
1:A:83:PRO:HB3	4:A:2009:HOH:O	2.04	0.58
1:D:145:TYR:CZ	1:D:149:LEU:HD11	2.39	0.58
1:G:199:ARG:HE	1:G:338:THR:CG2	2.16	0.58
1:F:145:TYR:CZ	1:F:149:LEU:HD11	2.39	0.58
1:D:463:MET:SD	1:E:89:ARG:HD3	2.43	0.58
1:E:179:ASP:O	1:E:182:THR:HG22	2.03	0.58
1:G:379:LEU:CD2	1:G:380:ARG:N	2.67	0.58
1:G:105:GLU:HB2	1:G:109:GLN:CD	2.25	0.57
1:G:328:LEU:O	1:G:331:ALA:HB3	2.04	0.57
1:A:139:LEU:C	1:A:139:LEU:HD23	2.25	0.57
1:F:177:PRO:HG2	1:F:178:TYR:CD1	2.39	0.57
1:G:184:GLY:HA3	1:G:297:GLY:HA3	1.86	0.57
1:D:164:LEU:HA	1:D:314:PHE:CE2	2.39	0.57
1:D:184:GLY:HA3	1:D:297:GLY:CA	2.35	0.57
1:E:169:ARG:HD3	1:E:171:LYS:HG2	1.87	0.57
1:D:410:LEU:HD12	1:D:411:VAL:N	2.19	0.57
1:E:456:ARG:HG3	1:E:456:ARG:NH2	2.20	0.57
1:F:105:GLU:N	1:F:109:GLN:HE22	1.86	0.57
1:F:353:LEU:HD22	1:F:355:ILE:CG1	2.33	0.57
1:G:160:ASN:HD21	1:G:319:GLU:CD	2.07	0.57
1:D:127:LEU:HD11	1:D:385:LEU:HD22	1.87	0.57
1:A:103:THR:OG1	1:A:116:PRO:HG2	2.05	0.57
1:B:380:ARG:HH21	1:B:380:ARG:HG3	1.69	0.57
1:A:255:ARG:HH21	1:A:255:ARG:HG3	1.69	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan (Å)
1.B.180.GLN.HB3	1·B·503·VAL·HG12	1.87	0.57
1:A:84:PHE:CD1	1:A:84:PHE:N	2.72	0.57
1.B.356.ASP.OD2	1.B:357.GLU:N	2.38	0.57
$1 \cdot D \cdot 304 \cdot TBP \cdot CH2$	1.D.313.LEU.HB2	2.30	0.57
1:G:154:MET:HA	1:G:351:LEU:HD23	1.85	0.57
1.A.338.THR.O	$1 \cdot A \cdot 341 \cdot LEU \cdot HB2$	2.05	0.57
1:G:175:LEU:HD12	1:G:313:LEU:HD21	1.85	0.57
$1 \cdot \text{F} \cdot 145 \cdot \text{TYR} \cdot \text{CE1}$	$1 \cdot \text{F} \cdot 149 \cdot \text{LEU} \cdot \text{HD} 21$	2 40	0.56
1:F:432:GLU:HG2	1:F:460:ARG:HD3	1.87	0.56
1:G:98:LYS:O	1:G:102:MET:HG3	2.05	0.56
1:B:246:THB:O	1:B:281:ABG:HD2	2.06	0.56
1:D:346:GLU:OE2	1:D:346:GLU:HA	2.04	0.56
1:D:433:HIS:HD2	1:D:433:HIS:O	1.88	0.56
1:E:169:ARG:HH11	1:E:169:ARG:HG2	1.67	0.56
1.E.249:ALA:O	1·E·281·ABG·NH2	2.28	0.56
1.E.430.LEU.HD23	1.E.462.VAL:HG21	1.20	0.56
1:G:158:ASP:OD2	1.G·161·GLY·HA2	2.04	0.56
1:E:322:GLY:N	1:E:323:PRO:HD2	2.20	0.56
1:F:145:TYB:O	1:F:149:LEU:HG	2.05	0.56
1:D:372:THR:HG22	1:D:373:LYS:CG	2.36	0.56
1:F:105:GLU:OE2	1:F:118:PRO:HA	2.06	0.56
1:A:127:LEU:HD11	1:A:385:LEU:CD2	2.36	0.56
1:D:292:VAL:C	1:D:294:MET:H	2.09	0.56
1:D:482:ASN:C	1:D:482:ASN:ND2	2.59	0.56
1:E:318:ARG:HH21	1:E:321:MET:CE	2.18	0.56
1:G:207:ARG:CB	1:G:363:LYS:HD3	2.35	0.56
1:D:159:PRO:HG3	1:D:317:TRP:CH2	2.41	0.56
1:E:198:GLN:HG2	4:E:2021:HOH:O	2.05	0.56
1:G:331:ALA:O	1:G:335:VAL:HG23	2.06	0.56
1:A:113:ALA:HA	1:A:490:LEU:HD23	1.88	0.56
1:A:252:ASP:N	1:A:252:ASP:OD2	2.37	0.56
1:F:322:GLY:N	1:F:323:PRO:HD2	2.21	0.56
1:A:326:ARG:N	1:A:327:PRO:HD2	2.20	0.56
1:A:358:LEU:HB3	1:A:385:LEU:CD1	2.36	0.56
1:D:139:LEU:HB2	1:D:490:LEU:HD11	1.87	0.56
1:A:154:MET:CE	1:A:156:ILE:HD11	2.35	0.55
1:B:326:ARG:N	1:B:327:PRO:HD2	2.21	0.55
1:B:419:ASP:HB2	1:D:405:ALA:HB2	1.88	0.55
1:D:154:MET:HB3	1:D:352:TRP:HB2	1.88	0.55
1:D:169:ARG:HH11	1:D:171:LYS:HD3	1.70	0.55
1:A:334:ASP:O	1:A:337:CYS:HB2	2.05	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:136:LYS:O	1:D:140:LEU:HD13	2.06	0.55
1:D:177:PRO:HG2	1:D:178:TYR:HD1	1.71	0.55
1:E:420:PRO:HA	1:E:423:ASN:HD22	1.71	0.55
1:F:410:LEU:HD12	1:F:411:VAL:N	2.21	0.55
1:G:345:GLU:HA	1:G:345:GLU:OE1	2.07	0.55
1:F:124:ARG:HB3	1:F:408:ARG:CG	2.36	0.55
1:B:169:ARG:HG3	1:B:498:ARG:NH2	2.22	0.55
1:E:333:VAL:HG21	1:E:361:LEU:CD1	2.37	0.55
1:G:379:LEU:HD23	1:G:380:ARG:N	2.22	0.55
1:D:344:PRO:O	1:D:349:ARG:NH2	2.39	0.55
1:F:502:PHE:CE2	1:F:504:GLU:HB2	2.42	0.55
1:G:96:GLY:O	1:G:100:LYS:HG3	2.07	0.55
1:A:177:PRO:HG2	1:A:178:TYR:CD1	2.41	0.55
1:A:356:ASP:OD2	1:A:357:GLU:N	2.39	0.55
1:B:331:ALA:O	1:B:335:VAL:HG23	2.07	0.55
1:E:199:ARG:NE	1:E:338:THR:HG22	2.20	0.55
1:F:177:PRO:HB3	1:F:294:MET:HG2	1.88	0.55
1:G:294:MET:SD	1:G:295:PRO:HD2	2.47	0.55
1:D:469:ASN:O	1:E:482:ASN:HB2	2.07	0.55
1:F:292:VAL:C	1:F:294:MET:H	2.10	0.55
1:G:94:VAL:HG21	1:G:98:LYS:CG	2.30	0.55
1:D:281:ARG:HH21	1:E:265:SER:HB3	1.73	0.54
1:D:352:TRP:CZ2	1:D:380:ARG:HD3	2.41	0.54
1:G:258:LEU:O	1:G:261:THR:OG1	2.15	0.54
1:D:287:LYS:C	1:D:289:PRO:HD2	2.28	0.54
1:E:380:ARG:HH21	1:E:380:ARG:HG3	1.71	0.54
1:A:420:PRO:CB	1:B:428:LEU:HD22	2.36	0.54
1:B:199:ARG:HE	1:B:338:THR:CG2	2.20	0.54
1:D:414:GLY:HA2	1:D:467:ILE:HG23	1.89	0.54
1:E:333:VAL:HG21	1:E:361:LEU:HD13	1.89	0.54
1:G:252:ASP:OD2	1:G:252:ASP:N	2.41	0.54
1:A:346:GLU:OE2	1:A:346:GLU:HA	2.08	0.54
1:D:152:ASP:OD1	1:D:350:ARG:NH2	2.40	0.54
1:E:199:ARG:NE	1:E:338:THR:CG2	2.67	0.54
1:F:159:PRO:HG3	1:F:317:TRP:CH2	2.43	0.54
1:G:244:HIS:HA	1:G:248:ILE:CG1	2.38	0.54
1:G:321:MET:C	1:G:323:PRO:HD2	2.27	0.54
1:G:433:HIS:C	1:G:433:HIS:CD2	2.81	0.54
1:A:410:LEU:HD12	1:A:411:VAL:N	2.23	0.54
1:B:160:ASN:HD21	1:B:319:GLU:HG3	1.73	0.54
1:B:419:ASP:HB2	1:D:405:ALA:CB	2.37	0.54



	is as page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:157:VAL:O	1:A:159:PRO:HD3	2.08	0.54
1:D:76:GLN:O	1:D:78:GLU:HG2	2.08	0.54
1:E:84:PHE:HA	1:E:437:ARG:CG	2.37	0.54
1:A:145:TYR:CE2	1:A:149:LEU:HD11	2.42	0.54
1:A:322:GLY:N	1:A:323:PRO:HD2	2.23	0.54
1:D:124:ARG:HB3	1:D:408:ARG:HB2	1.90	0.54
1:D:239:MET:CE	1:D:291:HIS:HB3	2.38	0.54
1:E:98:LYS:HD2	1:E:101:ARG:HH21	1.73	0.54
1:B:463:MET:SD	1:D:89:ARG:HD3	2.48	0.54
1:F:94:VAL:HG22	1:F:95:SER:H	1.72	0.54
1:B:181:ARG:NH1	1:B:500:PRO:HG2	2.23	0.53
1:E:304:TRP:CZ2	1:E:313:LEU:HB2	2.42	0.53
1:F:199:ARG:NE	1:F:338:THR:HG22	2.20	0.53
1:G:177:PRO:HG2	1:G:178:TYR:HD1	1.73	0.53
1:D:124:ARG:HB3	1:D:408:ARG:CG	2.38	0.53
1:D:126:LEU:HD11	1:D:411:VAL:HG23	1.89	0.53
1:E:84:PHE:CA	1:E:437:ARG:HG3	2.38	0.53
1:A:203:SER:O	1:A:331:ALA:HA	2.09	0.53
1:F:98:LYS:HD3	1:F:101:ARG:HH11	1.73	0.53
1:F:333:VAL:HG21	1:F:361:LEU:HD13	1.89	0.53
1:G:139:LEU:HD22	1:G:140:LEU:HD12	1.90	0.53
1:D:281:ARG:NH2	1:E:265:SER:HB3	2.22	0.53
1:G:334:ASP:O	1:G:337:CYS:HB2	2.09	0.53
1:G:395:TYR:HB3	1:G:399:GLU:HB3	1.89	0.53
1:A:158:ASP:O	1:A:316:THR:HA	2.08	0.53
1:D:82:ALA:O	1:D:437:ARG:NH1	2.42	0.53
1:D:433:HIS:NE2	1:D:459:GLU:HG3	2.24	0.53
1:E:367:LEU:HD13	1:E:403:LEU:HD11	1.91	0.53
1:G:106:LYS:N	1:G:106:LYS:HE3	2.23	0.53
1:G:157:VAL:O	1:G:159:PRO:HD3	2.08	0.53
1:G:238:SER:HB3	1:G:241:GLU:HB2	1.89	0.53
1:G:433:HIS:HD2	1:G:433:HIS:O	1.91	0.53
1:D:255:ARG:HG3	1:D:255:ARG:NH2	2.24	0.53
1:A:94:VAL:HG22	1:A:98:LYS:HB3	1.90	0.53
1:A:175:LEU:HG	1:A:313:LEU:HD21	1.89	0.53
1:A:428:LEU:HG	1:A:460:ARG:NH2	2.23	0.53
1:B:435:VAL:CG1	1:B:436:GLU:N	2.72	0.53
1:D:358:LEU:HB3	1:D:385:LEU:HD11	1.90	0.53
1:E:127:LEU:HD11	1:E:385:LEU:HD22	1.88	0.53
1:G:430:LEU:HD23	1:G:462:VAL:HB	1.89	0.53
1:B:177:PRO:HG2	1:B:178:TYR:CD1	2.43	0.53



	lo ao pagoni	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:96:GLY:O	1:D:100:LYS:HG3	2.08	0.53
1:D:497:ASN:N	1:D:497:ASN:HD22	2.05	0.53
1:F:88:LEU:HB2	1:F:434:GLU:O	2.08	0.53
1:G:456:ARG:HB2	1:G:456:ARG:CZ	2.33	0.53
1:A:124:ARG:HB3	1:A:408:ARG:CG	2.39	0.53
1:A:159:PRO:HG2	1:A:356:ASP:OD1	2.09	0.53
1:E:83:PRO:O	1:E:437:ARG:HD3	2.09	0.53
1:E:139:LEU:HD23	1:E:139:LEU:C	2.30	0.53
1:B:318:ARG:NH2	1:B:321:MET:HE3	2.22	0.53
1:D:367:LEU:HD22	1:D:371:LEU:HG	1.90	0.53
1:G:84:PHE:N	1:G:84:PHE:CD1	2.77	0.53
1:G:139:LEU:C	1:G:139:LEU:HD23	2.30	0.53
1:G:410:LEU:HD12	1:G:411:VAL:H	1.72	0.53
1:D:322:GLY:N	1:D:323:PRO:HD2	2.24	0.52
1:G:379:LEU:HD23	1:G:380:ARG:H	1.74	0.52
1:A:259:GLU:HA	1:A:264:GLU:CG	2.39	0.52
1:A:259:GLU:HA	1:A:264:GLU:HG3	1.91	0.52
1:D:252:ASP:HB3	4:D:2018:HOH:O	2.09	0.52
1:F:176:ASN:O	1:F:182:THR:HB	2.09	0.52
1:G:130:GLY:HA3	1:G:413:LEU:HB2	1.91	0.52
1:A:432:GLU:CG	1:A:460:ARG:HD3	2.39	0.52
1:G:84:PHE:CB	1:G:435:VAL:HG11	2.39	0.52
1:B:260:GLY:H	1:B:264:GLU:CD	2.13	0.52
1:E:456:ARG:H	1:E:456:ARG:HD3	1.75	0.52
1:A:136:LYS:O	1:A:140:LEU:HD13	2.09	0.52
1:A:433:HIS:NE2	1:A:459:GLU:HG3	2.25	0.52
1:E:384:GLY:O	1:E:385:LEU:CD1	2.58	0.52
1:A:207:ARG:HB2	1:A:363:LYS:HB3	1.92	0.52
1:E:105:GLU:OE2	1:E:118:PRO:HA	2.10	0.52
1:F:154:MET:HA	1:F:351:LEU:CD2	2.39	0.52
1:F:222:LEU:HD13	1:F:225:ARG:HH12	1.74	0.52
1:A:184:GLY:HA3	1:A:297:GLY:HA3	1.90	0.52
1:B:214:GLU:O	1:B:217:ALA:HB3	2.09	0.52
1:E:261:THR:O	1:E:264:GLU:HB2	2.10	0.52
1:B:166:LYS:HD2	1:B:495:PHE:HB2	1.92	0.52
1:B:304:TRP:CZ2	1:B:313:LEU:HB2	2.45	0.52
1:A:164:LEU:HA	1:A:314:PHE:CE2	2.45	0.52
1:B:166:LYS:O	1:B:498:ARG:HG2	2.10	0.52
1:B:180:GLN:NE2	1:B:504:GLU:CG	2.71	0.52
1:B:203:SER:O	1:B:331:ALA:HA	2.10	0.52
1:E:356:ASP:OD2	1:E:357:GLU:N	2.42	0.52



	is as page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:353:LEU:CD1	1:G:355:ILE:HD11	2.40	0.52
1:F:340:ILE:CD1	1:F:341:LEU:HD13	2.40	0.51
1:G:352:TRP:CZ2	1:G:380:ARG:HD3	2.44	0.51
1:D:159:PRO:HG3	1:D:317:TRP:CZ2	2.46	0.51
1:D:252:ASP:O	1:D:255:ARG:HB2	2.09	0.51
1:E:488:VAL:HG13	1:E:489:PRO:HD2	1.92	0.51
1:A:92:ARG:HG3	1:A:484:PRO:HB3	1.92	0.51
1:D:313:LEU:HD23	1:D:314:PHE:N	2.25	0.51
1:E:457:VAL:HG12	1:E:458:ARG:N	2.25	0.51
1:F:433:HIS:HD2	1:F:433:HIS:O	1.93	0.51
1:G:181:ARG:CZ	1:G:503:VAL:HG23	2.40	0.51
1:G:244:HIS:HA	1:G:248:ILE:HG12	1.93	0.51
1:G:432:GLU:CG	1:G:460:ARG:HD3	2.35	0.51
1:B:154:MET:HB3	1:B:352:TRP:HB2	1.93	0.51
1:B:318:ARG:NH2	1:B:321:MET:CE	2.70	0.51
1:D:84:PHE:CB	1:D:437:ARG:HG3	2.40	0.51
1:D:152:ASP:OD1	1:D:350:ARG:HD2	2.11	0.51
1:G:84:PHE:CD2	1:G:435:VAL:HG13	2.45	0.51
1:E:156:ILE:O	1:E:158:ASP:N	2.43	0.51
1:F:94:VAL:CG2	1:F:98:LYS:HG2	2.39	0.51
1:F:139:LEU:HB2	1:F:490:LEU:HD11	1.92	0.51
1:G:128:VAL:O	1:G:384:GLY:HA2	2.10	0.51
1:A:199:ARG:HD3	1:A:200:TYR:CE1	2.46	0.51
1:E:184:GLY:HA3	1:E:297:GLY:CA	2.40	0.51
1:F:313:LEU:HD23	1:F:314:PHE:N	2.25	0.51
1:G:315:ILE:HG23	1:G:332:TRP:CE3	2.45	0.51
1:G:169:ARG:NH1	1:G:171:LYS:HD3	2.23	0.51
1:B:413:LEU:CD2	1:B:475:ALA:HB2	2.40	0.51
1:D:272:GLU:OE2	1:D:272:GLU:HA	2.11	0.51
1:G:173:ILE:HD12	1:G:183:LYS:HE3	1.93	0.51
1:B:249:ALA:O	1:B:281:ARG:NH2	2.28	0.51
1:E:124:ARG:HB3	1:E:408:ARG:HB2	1.93	0.51
1:E:226:GLU:HG3	1:E:263:ALA:HB2	1.91	0.51
1:E:252:ASP:OD2	1:E:252:ASP:N	2.45	0.51
1:F:338:THR:O	1:F:341:LEU:HB2	2.11	0.51
1:G:338:THR:O	1:G:341:LEU:HB2	2.11	0.51
1:A:105:GLU:HB2	1:A:109:GLN:CD	2.31	0.50
1:A:180:GLN:HB2	1:A:503:VAL:HG12	1.93	0.50
1:G:124:ARG:HB3	1:G:408:ARG:CB	2.41	0.50
1:A:84:PHE:HA	1:A:437:ARG:HG3	1.92	0.50
1:D:488:VAL:HG13	1:D:489:PRO:HD2	1.94	0.50



	to do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:154:MET:HE3	1:E:156:ILE:HD11	1.92	0.50
1:F:105:GLU:N	1:F:109:GLN:NE2	2.44	0.50
1:F:177:PRO:HA	1:F:294:MET:HE1	1.92	0.50
1:F:334:ASP:OD1	1:F:366:SER:OG	2.28	0.50
1:G:219:TYR:HB3	1:G:280:ALA:HB2	1.93	0.50
1:A:154:MET:HE3	1:A:156:ILE:HD11	1.93	0.50
1:B:433:HIS:C	1:B:433:HIS:CD2	2.85	0.50
1:F:352:TRP:CZ2	1:F:380:ARG:HD3	2.46	0.50
1:G:124:ARG:HB3	1:G:408:ARG:HG3	1.94	0.50
1:B:139:LEU:C	1:B:139:LEU:HD23	2.31	0.50
1:E:258:LEU:O	1:E:261:THR:OG1	2.25	0.50
1:F:435:VAL:CG1	1:F:436:GLU:N	2.74	0.50
1:A:200:TYR:O	1:A:204:VAL:HG23	2.11	0.50
1:A:456:ARG:CZ	1:G:437:ARG:HD3	2.42	0.50
1:E:287:LYS:C	1:E:289:PRO:HD2	2.31	0.50
1:E:352:TRP:HB3	1:E:354:PHE:CE2	2.46	0.50
1:B:259:GLU:HA	1:B:264:GLU:CD	2.31	0.50
1:D:417:ARG:NH1	1:E:479:PHE:O	2.38	0.50
1:G:251:PHE:CZ	1:G:277:LEU:HD13	2.47	0.50
1:A:265:SER:HB3	1:G:281:ARG:NH2	2.27	0.50
1:A:426:MET:CE	1:A:426:MET:HA	2.42	0.50
1:E:180:GLN:NE2	1:E:504:GLU:HG3	2.26	0.50
1:F:340:ILE:HD11	1:F:341:LEU:HD13	1.94	0.50
1:A:290:GLU:HG3	1:A:325:LEU:HD23	1.94	0.49
1:E:158:ASP:O	1:E:316:THR:HA	2.12	0.49
1:F:340:ILE:HD12	1:F:341:LEU:N	2.27	0.49
1:A:166:LYS:CE	1:A:497:ASN:ND2	2.75	0.49
1:A:249:ALA:O	1:A:281:ARG:NH2	2.37	0.49
1:B:76:GLN:C	1:B:78:GLU:N	2.63	0.49
1:B:292:VAL:C	1:B:294:MET:H	2.15	0.49
1:B:328:LEU:O	1:B:331:ALA:HB3	2.12	0.49
1:A:379:LEU:HD23	1:A:380:ARG:H	1.77	0.49
1:F:94:VAL:HG21	1:F:98:LYS:CG	2.41	0.49
1:F:337:CYS:HB3	1:F:366:SER:HB2	1.94	0.49
1:F:435:VAL:HG13	1:F:436:GLU:N	2.28	0.49
1:G:497:ASN:N	1:G:497:ASN:ND2	2.61	0.49
1:B:198:GLN:HA	1:B:198:GLN:OE1	2.12	0.49
1:D:428:LEU:O	1:D:428:LEU:HD23	2.12	0.49
1:E:106:LYS:HD3	1:E:106:LYS:N	2.27	0.49
1:F:130:GLY:HA3	1:F:413:LEU:HB2	1.95	0.49
1:G:351:LEU:HD23	1:G:352:TRP:H	1.78	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:139:LEU:C	1:D:139:LEU:HD23	2.33	0.49
1:G:222:LEU:HD12	1:G:225:ARG:NH1	2.27	0.49
1:A:169:ARG:NH1	1:A:171:LYS:HD3	2.27	0.49
1:D:156:ILE:HG22	1:D:158:ASP:HB2	1.94	0.49
1:G:225:ARG:O	1:G:229:LYS:HB2	2.13	0.49
1:F:378:GLY:O	1:F:380:ARG:NH2	2.46	0.49
1:F:379:LEU:CD2	1:F:380:ARG:N	2.75	0.49
1:A:345:GLU:H	1:A:345:GLU:CD	2.15	0.49
1:B:199:ARG:HE	1:B:338:THR:HG22	1.77	0.49
1:E:98:LYS:HD2	1:E:101:ARG:NH2	2.28	0.49
1:E:313:LEU:HD23	1:E:314:PHE:N	2.28	0.49
1:G:154:MET:CE	1:G:156:ILE:HD11	2.30	0.49
1:B:145:TYR:CE1	1:B:149:LEU:HD21	2.48	0.49
1:B:180:GLN:NE2	1:B:504:GLU:HG3	2.15	0.49
1:A:127:LEU:HD11	1:A:385:LEU:HD22	1.95	0.49
1:A:498:ARG:O	1:A:499:GLN:HG3	2.13	0.49
1:B:226:GLU:OE1	1:B:261:THR:HB	2.13	0.49
1:F:223:LEU:HD23	1:F:284:LEU:CD2	2.43	0.49
1:A:197:TRP:NE1	1:A:229:LYS:HG3	2.28	0.48
1:A:241:GLU:HA	1:A:241:GLU:OE1	2.12	0.48
1:A:292:VAL:C	1:A:294:MET:H	2.16	0.48
1:D:352:TRP:CE2	1:D:380:ARG:HD3	2.47	0.48
1:F:488:VAL:CG1	1:F:489:PRO:HD2	2.41	0.48
1:G:175:LEU:CD1	1:G:313:LEU:HD21	2.43	0.48
1:G:457:VAL:HG12	1:G:459:GLU:HG2	1.94	0.48
1:A:433:HIS:CD2	1:A:433:HIS:C	2.86	0.48
1:E:456:ARG:NH2	1:E:456:ARG:CG	2.75	0.48
1:F:437:ARG:HH21	1:G:456:ARG:HH11	1.61	0.48
1:G:157:VAL:HG21	1:G:355:ILE:HG23	1.95	0.48
1:G:326:ARG:N	1:G:327:PRO:HD2	2.28	0.48
1:B:196:ASP:OD1	1:B:199:ARG:HD3	2.12	0.48
1:B:248:ILE:O	1:D:265:SER:OG	2.27	0.48
1:B:318:ARG:HH21	1:B:321:MET:HE2	1.74	0.48
1:F:184:GLY:HA3	1:F:297:GLY:CA	2.41	0.48
1:F:326:ARG:HB3	1:F:327:PRO:CD	2.42	0.48
1:G:473:LEU:HD11	1:G:492:ILE:HD11	1.95	0.48
1:A:148:LEU:HD21	1:A:154:MET:SD	2.54	0.48
1:A:199:ARG:HE	1:A:338:THR:CG2	2.26	0.48
1:A:238:SER:HB3	1:A:241:GLU:HB2	1.94	0.48
1:B:180:GLN:HB2	1:B:504:GLU:HG3	1.94	0.48
1:B:287:LYS:C	1:B:289:PRO:HD2	2.34	0.48



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:179:ASP:O	1:D:182:THR:HG22	2.13	0.48
1:A:118:PRO:HB3	1:A:483:ARG:NH2	2.28	0.48
1:A:214:GLU:O	1:A:217:ALA:HB3	2.13	0.48
1:E:154:MET:CE	1:E:156:ILE:HD11	2.43	0.48
1:G:301:ILE:O	1:G:305:LEU:HG	2.13	0.48
1:G:325:LEU:O	1:G:329:ILE:HG13	2.13	0.48
1:G:380:ARG:HG3	1:G:380:ARG:NH2	2.28	0.48
1:B:94:VAL:HG21	1:B:98:LYS:HE3	1.94	0.48
1:D:288:LEU:O	1:D:289:PRO:C	2.51	0.48
1:D:433:HIS:O	1:D:433:HIS:CD2	2.67	0.48
1:A:130:GLY:HA3	1:A:413:LEU:HB2	1.95	0.48
1:A:488:VAL:HG13	1:A:489:PRO:HD2	1.95	0.48
1:E:430:LEU:HD23	1:E:462:VAL:CG2	2.43	0.48
1:F:185:TRP:CZ2	1:F:187:PHE:HA	2.49	0.48
1:A:175:LEU:CD1	1:A:313:LEU:HD21	2.44	0.48
1:E:104:ARG:NH1	1:E:104:ARG:HG3	2.28	0.48
1:E:203:SER:O	1:E:331:ALA:HA	2.13	0.48
1:F:89:ARG:HD2	1:F:434:GLU:OE1	2.14	0.48
1:G:88:LEU:HB2	1:G:434:GLU:O	2.14	0.48
1:G:252:ASP:O	1:G:255:ARG:HB2	2.14	0.48
1:B:238:SER:HB3	1:B:241:GLU:HB2	1.96	0.48
1:G:378:GLY:O	1:G:380:ARG:NH2	2.47	0.48
1:D:456:ARG:HD2	1:D:456:ARG:N	2.29	0.47
1:E:225:ARG:O	1:E:229:LYS:HB2	2.13	0.47
1:A:435:VAL:CG1	1:A:436:GLU:N	2.77	0.47
1:B:158:ASP:OD2	1:B:161:GLY:HA2	2.14	0.47
1:B:433:HIS:O	1:B:433:HIS:CD2	2.64	0.47
1:D:288:LEU:O	1:D:291:HIS:HB2	2.14	0.47
1:D:375:ARG:HG2	1:D:375:ARG:HH21	1.78	0.47
1:F:124:ARG:HB3	1:F:408:ARG:HB2	1.95	0.47
1:B:255:ARG:HH21	1:B:255:ARG:HG3	1.79	0.47
1:D:418:THR:OG1	1:E:405:ALA:HA	2.14	0.47
1:F:255:ARG:HG3	1:F:255:ARG:NH2	2.28	0.47
1:A:251:PHE:CZ	1:A:277:LEU:HD13	2.48	0.47
1:B:84:PHE:CB	1:B:435:VAL:HG11	2.45	0.47
1:F:290:GLU:HG3	1:F:325:LEU:HD23	1.95	0.47
1:A:84:PHE:HE2	1:A:87:PHE:HB2	1.80	0.47
1:A:124:ARG:HB3	1:A:408:ARG:HG3	1.95	0.47
1:A:245:TRP:HA	1:A:245:TRP:CE3	2.49	0.47
1:B:352:TRP:CZ2	1:B:380:ARG:HD3	2.50	0.47
1:D:225:ARG:O	1:D:229:LYS:HB2	2.14	0.47



	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:139:LEU:C	1:F:139:LEU:CD2	2.82	0.47
1:F:173:ILE:HG22	1:F:174:ILE:N	2.30	0.47
1:D:419:ASP:HB2	1:E:405:ALA:CB	2.45	0.47
1:E:301:ILE:HD12	1:E:335:VAL:HG11	1.97	0.47
1:F:337:CYS:CB	1:F:366:SER:HB2	2.45	0.47
1:G:179:ASP:O	1:G:182:THR:HG22	2.14	0.47
1:A:105:GLU:HB2	1:A:109:GLN:NE2	2.30	0.47
1:A:223:LEU:HD23	1:A:284:LEU:HD22	1.97	0.47
1:B:144:ALA:O	1:B:148:LEU:HG	2.15	0.47
1:D:215:GLU:HG2	1:D:219:TYR:CE1	2.49	0.47
1:D:328:LEU:O	1:D:331:ALA:HB3	2.15	0.47
1:G:99:LEU:HD13	1:G:484:PRO:HG2	1.97	0.47
1:G:127:LEU:HD12	1:G:127:LEU:HA	1.67	0.47
1:E:259:GLU:HA	1:E:264:GLU:HG3	1.96	0.47
1:A:279:SER:O	1:A:283:VAL:HG23	2.15	0.46
1:B:133:GLY:N	2:B:701:ANP:O1B	2.41	0.46
1:E:107:ALA:HB3	1:E:119:ARG:CD	2.37	0.46
1:E:334:ASP:O	1:E:337:CYS:HB2	2.15	0.46
1:E:497:ASN:N	1:E:497:ASN:ND2	2.61	0.46
1:F:340:ILE:HD12	1:F:341:LEU:CD1	2.46	0.46
1:G:346:GLU:HB3	1:G:349:ARG:NH1	2.31	0.46
1:A:433:HIS:O	1:A:433:HIS:CD2	2.66	0.46
1:B:130:GLY:O	1:B:136:LYS:NZ	2.48	0.46
1:B:145:TYR:CE1	1:B:149:LEU:HD11	2.51	0.46
1:B:497:ASN:N	1:B:497:ASN:HD22	2.13	0.46
1:F:184:GLY:CA	1:F:297:GLY:HA3	2.43	0.46
1:F:200:TYR:O	1:F:204:VAL:HG23	2.15	0.46
1:F:417:ARG:NH1	1:G:479:PHE:O	2.47	0.46
1:A:469:ASN:O	1:B:482:ASN:HB2	2.15	0.46
1:B:353:LEU:HD22	1:B:355:ILE:HG13	1.98	0.46
1:E:346:GLU:HA	1:E:346:GLU:OE2	2.15	0.46
1:G:106:LYS:HE3	1:G:106:LYS:H	1.79	0.46
1:A:196:ASP:O	1:A:200:TYR:HD1	1.99	0.46
1:A:497:ASN:ND2	1:A:497:ASN:N	2.63	0.46
1:B:416:SER:HB2	1:D:408:ARG:HD2	1.98	0.46
1:D:433:HIS:CD2	1:D:433:HIS:C	2.88	0.46
1:E:318:ARG:HH21	1:E:321:MET:HE2	1.80	0.46
1:F:118:PRO:HB3	1:F:483:ARG:NH2	2.30	0.46
1:F:318:ARG:HD3	1:F:502:PHE:CE2	2.50	0.46
1:G:214:GLU:O	1:G:217:ALA:HB3	2.15	0.46
1:A:325:LEU:C	1:A:327:PRO:HD2	2.35	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:492:ILE:HG22	1:A:492:ILE:O	2.15	0.46
1:D:154:MET:CB	1:D:352:TRP:HB2	2.45	0.46
1:A:113:ALA:HA	1:A:490:LEU:CD2	2.46	0.46
1:F:78:GLU:HG2	1:F:95:SER:HB3	1.97	0.46
1:G:437:ARG:HG2	1:G:438:ASP:H	1.80	0.46
1:A:298:ASP:OD2	1:A:298:ASP:N	2.42	0.46
1:E:85:LYS:HD2	1:E:454:LEU:HD21	1.97	0.46
1:F:503:VAL:HG12	1:F:503:VAL:O	2.15	0.46
1:A:304:TRP:CZ2	1:A:313:LEU:HB2	2.51	0.46
1:D:111:THR:OG1	1:D:146:THR:HG21	2.15	0.46
1:D:184:GLY:HA3	1:D:297:GLY:N	2.30	0.46
1:G:323:PRO:HG2	1:G:324:ALA:H	1.81	0.46
1:A:198:GLN:OE1	1:A:198:GLN:HA	2.16	0.46
1:D:105:GLU:HB2	1:D:109:GLN:NE2	2.31	0.46
1:D:413:LEU:CD2	1:D:475:ALA:HB2	2.27	0.46
1:E:366:SER:HA	4:E:2041:HOH:O	2.15	0.46
1:B:420:PRO:HB2	1:D:428:LEU:HD22	1.98	0.45
1:G:315:ILE:HG23	1:G:332:TRP:HE3	1.81	0.45
1:D:292:VAL:C	1:D:294:MET:N	2.70	0.45
1:E:435:VAL:CG1	1:E:436:GLU:N	2.80	0.45
1:G:127:LEU:HD12	1:G:383:ALA:O	2.16	0.45
1:A:154:MET:HE2	1:A:156:ILE:HD11	1.98	0.45
1:D:166:LYS:O	1:D:498:ARG:HG2	2.16	0.45
1:E:131:ALA:CB	1:E:415:GLY:HA2	2.37	0.45
1:E:414:GLY:HA2	1:E:467:ILE:HG23	1.97	0.45
1:F:128:VAL:O	1:F:384:GLY:HA2	2.16	0.45
1:G:288:LEU:O	1:G:291:HIS:HB2	2.17	0.45
1:G:413:LEU:HD23	1:G:475:ALA:HB2	1.97	0.45
1:A:156:ILE:O	1:A:158:ASP:N	2.50	0.45
1:B:189:ASN:ND2	1:B:298:ASP:HA	2.31	0.45
1:E:118:PRO:HB3	1:E:483:ARG:NH2	2.31	0.45
1:E:184:GLY:HA3	1:E:296:ASP:C	2.37	0.45
1:E:338:THR:O	1:E:341:LEU:HB2	2.16	0.45
1:F:226:GLU:OE1	1:F:261:THR:HB	2.17	0.45
1:F:288:LEU:HA	1:F:288:LEU:HD23	1.72	0.45
1:G:471:PRO:HG2	1:G:474:THR:OG1	2.16	0.45
1:A:156:ILE:CG2	1:A:158:ASP:HB2	2.47	0.45
1:D:391:LEU:HD21	1:D:403:LEU:HD23	1.98	0.45
1:F:124:ARG:HB3	1:F:408:ARG:HG3	1.98	0.45
1:F:358:LEU:HB2	1:F:383:ALA:HB1	1.98	0.45
1:F:433:HIS:C	1:F:433:HIS:CD2	2.90	0.45



	,	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:288:LEU:O	1:G:289:PRO:C	2.54	0.45
1:G:290:GLU:HG3	1:G:325:LEU:HD23	1.97	0.45
1:D:437:ARG:NH2	1:E:456:ARG:NH2	2.65	0.45
1:E:158:ASP:OD2	1:E:161:GLY:HA2	2.17	0.45
1:B:304:TRP:CH2	1:B:313:LEU:HB2	2.52	0.45
1:B:372:THR:HG22	1:B:373:LYS:CG	2.32	0.45
1:F:419:ASP:HB2	1:G:405:ALA:HB2	1.98	0.45
1:G:430:LEU:HD23	1:G:462:VAL:CG2	2.47	0.45
1:G:435:VAL:CG1	1:G:436:GLU:H	2.30	0.45
1:A:99:LEU:HD22	1:A:486:ALA:HB3	1.98	0.45
1:B:315:ILE:HG23	1:B:332:TRP:CE3	2.52	0.45
1:D:304:TRP:CZ2	1:D:313:LEU:HB2	2.51	0.45
1:F:222:LEU:HD13	1:F:225:ARG:NH1	2.32	0.45
1:F:288:LEU:O	1:F:289:PRO:C	2.55	0.45
1:F:367:LEU:HD13	1:F:403:LEU:HD11	1.98	0.45
1:A:337:CYS:HB3	1:A:366:SER:HB2	1.99	0.45
1:A:227:THR:HG22	1:A:242:LEU:HD12	1.99	0.45
1:B:175:LEU:HB3	1:B:332:TRP:CZ3	2.52	0.45
1:D:106:LYS:H	1:D:106:LYS:HG2	1.32	0.45
1:D:133:GLY:N	2:D:701:ANP:O1B	2.34	0.45
1:E:180:GLN:HE21	1:E:504:GLU:CG	2.30	0.45
1:F:340:ILE:CD1	1:F:341:LEU:CD1	2.95	0.45
1:A:207:ARG:CB	1:A:363:LYS:HD3	2.47	0.44
1:B:180:GLN:CB	1:B:503:VAL:HG12	2.46	0.44
1:D:105:GLU:OE2	1:D:118:PRO:HA	2.18	0.44
1:F:133:GLY:N	2:F:701:ANP:O1B	2.41	0.44
1:F:236:THR:O	1:F:238:SER:N	2.45	0.44
1:A:354:PHE:CD1	1:A:382:VAL:HB	2.53	0.44
1:B:349:ARG:HD2	1:B:377:ALA:O	2.17	0.44
1:B:488:VAL:CG1	1:B:489:PRO:HD2	2.47	0.44
1:D:158:ASP:O	1:D:316:THR:HA	2.18	0.44
1:D:180:GLN:CB	1:D:503:VAL:HG12	2.47	0.44
1:E:164:LEU:HD21	1:E:174:ILE:HD11	2.00	0.44
1:F:177:PRO:HB3	1:F:294:MET:HE2	1.98	0.44
1:G:318:ARG:HH21	1:G:321:MET:HE1	1.83	0.44
1:A:212:GLU:O	1:A:215:GLU:HB3	2.16	0.44
1:B:157:VAL:O	1:B:159:PRO:HD3	2.17	0.44
1:F:166:LYS:HE2	1:F:497:ASN:HD21	1.81	0.44
1:F:497:ASN:N	1:F:497:ASN:ND2	2.65	0.44
1:G:473:LEU:HB3	1:G:490:LEU:O	2.17	0.44
1:B:103:THR:OG1	1:B:116:PRO:HG2	2.17	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:299:PHE:CD1	1:B:299:PHE:C	2.91	0.44
1:B:332:TRP:O	1:B:335:VAL:HB	2.17	0.44
1:F:306:GLU:O	1:F:308:PRO:HD3	2.17	0.44
1:G:154:MET:CB	1:G:352:TRP:HB2	2.44	0.44
1:B:134:THR:HG21	1:B:414:GLY:O	2.17	0.44
1:B:154:MET:HA	1:B:351:LEU:CD2	2.47	0.44
1:D:124:ARG:HB3	1:D:408:ARG:HG3	1.99	0.44
1:D:419:ASP:HB2	1:E:405:ALA:HB2	1.98	0.44
1:E:108:LYS:O	1:E:119:ARG:NH1	2.50	0.44
1:E:288:LEU:N	1:E:289:PRO:CD	2.81	0.44
1:F:206:PRO:HG3	1:F:362:GLU:OE2	2.17	0.44
1:F:356:ASP:CG	1:F:357:GLU:N	2.70	0.44
1:F:456:ARG:NH1	1:F:456:ARG:CG	2.75	0.44
1:A:131:ALA:CB	1:A:415:GLY:HA2	2.39	0.44
1:B:92:ARG:HB3	1:B:92:ARG:CZ	2.45	0.44
1:E:343:LEU:HB3	1:E:349:ARG:NH2	2.33	0.44
1:F:353:LEU:HD22	1:F:355:ILE:HG12	1.98	0.44
1:A:345:GLU:OE1	1:A:345:GLU:N	2.39	0.44
1:B:158:ASP:O	1:B:316:THR:HA	2.18	0.44
1:B:184:GLY:HA3	1:B:297:GLY:CA	2.48	0.44
1:B:420:PRO:CB	1:D:428:LEU:HD22	2.47	0.44
1:D:148:LEU:HD21	1:D:154:MET:SD	2.57	0.44
1:D:340:ILE:HD12	1:D:341:LEU:HD12	1.99	0.44
1:E:392:ASP:OD1	1:E:404:ARG:NH2	2.36	0.44
1:F:433:HIS:O	1:F:433:HIS:CD2	2.71	0.44
1:G:426:MET:HA	1:G:426:MET:CE	2.48	0.44
1:G:430:LEU:HD23	1:G:462:VAL:CB	2.47	0.44
1:G:436:GLU:HA	1:G:455:GLU:O	2.17	0.44
1:B:84:PHE:CG	1:B:435:VAL:HG11	2.52	0.44
1:B:134:THR:HA	1:B:472:ASP:OD1	2.18	0.44
1:D:200:TYR:O	1:D:204:VAL:HG23	2.18	0.44
1:E:192:ARG:HG3	1:E:302:ARG:NH1	2.33	0.44
1:E:199:ARG:HH21	1:E:338:THR:HG22	1.83	0.44
1:F:287:LYS:C	1:F:289:PRO:HD2	2.38	0.44
1:G:234:ILE:O	1:G:236:THR:HG23	2.18	0.44
1:A:89:ARG:HD3	1:G:463:MET:SD	2.58	0.44
1:A:288:LEU:O	1:A:289:PRO:C	2.55	0.44
1:A:290:GLU:HB3	1:A:328:LEU:HD12	1.99	0.44
1:B:325:LEU:C	1:B:327:PRO:HD2	2.39	0.44
1:D:89:ARG:HD2	1:D:434:GLU:OE1	2.17	0.44
1:D:181:ARG:NH1	1:D:500:PRO:HG2	2.32	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:384:GLY:O	1:D:385:LEU:CD1	2.64	0.44
1:F:135:GLY:HA2	2:F:701:ANP:O1A	2.17	0.44
1:G:326:ARG:NH1	1:G:361:LEU:O	2.50	0.44
1:A:118:PRO:CB	1:A:483:ARG:NH2	2.81	0.43
1:B:164:LEU:HA	1:B:314:PHE:CE2	2.53	0.43
1:B:177:PRO:HG2	1:B:178:TYR:CE1	2.53	0.43
1:D:338:THR:O	1:D:341:LEU:HB2	2.18	0.43
1:D:497:ASN:N	1:D:497:ASN:ND2	2.65	0.43
1:F:419:ASP:HB2	1:G:405:ALA:CB	2.48	0.43
1:F:433:HIS:NE2	1:F:459:GLU:HG3	2.33	0.43
1:G:217:ALA:O	1:G:221:ARG:HG3	2.18	0.43
1:G:233:LEU:HD23	1:G:233:LEU:HA	1.85	0.43
1:A:304:TRP:CH2	1:A:313:LEU:HB2	2.53	0.43
1:D:292:VAL:O	1:D:294:MET:N	2.51	0.43
1:E:139:LEU:HD23	1:E:139:LEU:O	2.18	0.43
1:E:180:GLN:HB2	1:E:504:GLU:HB3	2.00	0.43
1:E:308:PRO:C	1:E:310:GLY:H	2.20	0.43
1:E:427:SER:CB	1:E:464:PRO:HG3	2.48	0.43
1:F:222:LEU:HA	1:F:225:ARG:CZ	2.48	0.43
1:G:159:PRO:HG2	1:G:356:ASP:OD1	2.19	0.43
1:A:126:LEU:HD11	1:A:411:VAL:HG23	1.99	0.43
1:A:417:ARG:NH1	1:B:479:PHE:O	2.51	0.43
1:B:491:GLU:O	1:B:491:GLU:HG3	2.18	0.43
1:D:328:LEU:HD22	1:D:332:TRP:CE2	2.53	0.43
1:E:279:SER:O	1:E:283:VAL:HG23	2.18	0.43
1:G:259:GLU:HA	1:G:264:GLU:HG3	2.00	0.43
1:A:173:ILE:HG23	1:A:183:LYS:HG3	2.01	0.43
1:A:420:PRO:HB2	1:B:428:LEU:CD2	2.47	0.43
1:B:288:LEU:O	1:B:289:PRO:C	2.56	0.43
1:B:325:LEU:O	1:B:326:ARG:C	2.57	0.43
1:B:388:THR:HG23	1:B:422:THR:HG23	1.99	0.43
1:G:379:LEU:HD22	1:G:380:ARG:N	2.33	0.43
1:A:315:ILE:HG23	1:A:332:TRP:CE3	2.54	0.43
1:E:139:LEU:HD22	1:E:140:LEU:HD12	2.01	0.43
1:G:199:ARG:NH2	1:G:339:SER:HA	2.34	0.43
1:A:177:PRO:CD	1:A:294:MET:HE3	2.48	0.43
1:B:145:TYR:O	1:B:148:LEU:HB2	2.19	0.43
1:B:288:LEU:N	1:B:289:PRO:CD	2.82	0.43
1:E:419:ASP:O	1:E:423:ASN:ND2	2.52	0.43
1:G:178:TYR:CD1	1:G:178:TYR:N	2.85	0.43
1:A:379:LEU:CD2	1:A:380:ARG:N	2.82	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:317:TRP:HB2	1:D:325:LEU:HD12	2.01	0.43
1:E:214:GLU:O	1:E:217:ALA:HB3	2.18	0.43
1:E:367:LEU:HD22	1:E:371:LEU:HG	2.01	0.43
1:E:400:ALA:O	1:E:404:ARG:HG3	2.17	0.43
1:F:159:PRO:HG2	1:F:356:ASP:OD1	2.19	0.43
1:F:294:MET:SD	1:F:295:PRO:HD2	2.58	0.43
1:G:192:ARG:HG3	1:G:302:ARG:NH1	2.33	0.43
1:B:469:ASN:O	1:D:482:ASN:HB2	2.18	0.43
1:D:184:GLY:CA	1:D:297:GLY:HA3	2.46	0.43
1:D:432:GLU:OE1	1:D:458:ARG:HD2	2.19	0.43
1:E:139:LEU:C	1:E:139:LEU:CD2	2.87	0.43
1:E:176:ASN:O	1:E:182:THR:HB	2.19	0.43
1:E:355:ILE:O	1:E:356:ASP:C	2.57	0.43
1:G:197:TRP:NE1	1:G:229:LYS:HG3	2.34	0.43
1:A:158:ASP:HA	1:A:159:PRO:HD3	1.81	0.43
1:E:105:GLU:HB2	1:E:109:GLN:NE2	2.34	0.43
1:B:169:ARG:NH2	1:B:169:ARG:HB2	2.33	0.43
1:B:241:GLU:OE1	1:B:241:GLU:HA	2.19	0.43
1:E:318:ARG:HD2	1:E:502:PHE:CE2	2.54	0.43
1:A:320:ASP:OD2	1:A:321:MET:HG3	2.19	0.42
1:D:259:GLU:HA	1:D:264:GLU:HG3	2.00	0.42
1:D:358:LEU:HB3	1:D:385:LEU:CD1	2.47	0.42
1:E:184:GLY:HA3	1:E:297:GLY:N	2.34	0.42
1:E:318:ARG:NH2	1:E:321:MET:CE	2.82	0.42
1:G:318:ARG:HH21	1:G:321:MET:CE	2.31	0.42
1:G:498:ARG:O	1:G:499:GLN:CG	2.64	0.42
1:B:154:MET:HA	1:B:351:LEU:HD23	2.00	0.42
1:F:126:LEU:HD12	1:F:409:SER:O	2.19	0.42
1:F:353:LEU:HD22	1:F:355:ILE:HG13	2.02	0.42
1:F:379:LEU:HD22	1:F:381:VAL:HG23	1.99	0.42
1:F:437:ARG:NH2	1:G:456:ARG:HH11	2.16	0.42
1:G:84:PHE:CD2	1:G:435:VAL:CG1	3.03	0.42
1:B:246:THR:O	1:B:281:ARG:CD	2.67	0.42
1:E:138:VAL:HG21	1:E:473:LEU:HD21	2.01	0.42
1:F:199:ARG:HG3	1:F:338:THR:HG21	2.00	0.42
1:F:333:VAL:HG21	1:F:361:LEU:CD1	2.50	0.42
1:G:430:LEU:HD23	1:G:462:VAL:HG21	2.01	0.42
1:A:227:THR:CG2	1:A:242:LEU:HD12	2.49	0.42
1:B:345:GLU:HA	1:B:345:GLU:OE1	2.19	0.42
1:D:166:LYS:HD2	1:D:495:PHE:HB2	2.02	0.42
1:E:104:ARG:HG3	1:E:104:ARG:HH11	1.83	0.42



	t i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:82:ALA:O	1:F:437:ARG:NH1	2.53	0.42
1:A:326:ARG:NH1	1:A:361:LEU:O	2.52	0.42
1:A:375:ARG:NH1	2:G:701:ANP:O3G	2.53	0.42
1:B:363:LYS:HG3	1:B:395:TYR:CD2	2.55	0.42
1:E:113:ALA:HA	1:E:490:LEU:HD23	2.01	0.42
1:E:414:GLY:HA2	1:E:467:ILE:CG2	2.50	0.42
1:E:435:VAL:HG13	1:E:436:GLU:N	2.35	0.42
1:F:357:GLU:OE2	1:F:357:GLU:HA	2.19	0.42
1:A:419:ASP:HB2	1:B:405:ALA:CB	2.50	0.42
1:A:430:LEU:HD12	1:A:430:LEU:HA	1.64	0.42
1:D:202:LEU:HD13	1:D:221:ARG:NE	2.35	0.42
1:E:84:PHE:CB	1:E:437:ARG:HG3	2.49	0.42
1:E:154:MET:HA	1:E:351:LEU:CD2	2.49	0.42
1:F:184:GLY:HA2	1:F:295:PRO:O	2.19	0.42
1:G:294:MET:HA	1:G:295:PRO:HD3	1.84	0.42
1:B:173:ILE:HG22	1:B:174:ILE:N	2.35	0.42
1:D:83:PRO:O	1:D:437:ARG:HD3	2.18	0.42
1:E:156:ILE:HG21	1:E:163:MET:HG3	2.02	0.42
1:E:158:ASP:HA	1:E:159:PRO:HD3	1.85	0.42
1:E:246:THR:HB	1:E:284:LEU:HD23	2.01	0.42
1:E:372:THR:HG22	1:E:373:LYS:HG3	2.01	0.42
1:G:119:ARG:HA	1:G:122:GLU:OE2	2.20	0.42
1:G:184:GLY:HA3	1:G:297:GLY:CA	2.50	0.42
1:G:203:SER:OG	1:G:334:ASP:OD1	2.30	0.42
1:A:173:ILE:HG22	1:A:174:ILE:N	2.33	0.42
1:B:89:ARG:HD2	1:B:434:GLU:OE1	2.20	0.42
1:B:117:MET:HG3	1:B:479:PHE:CE1	2.54	0.42
1:E:352:TRP:CZ2	1:E:380:ARG:HD3	2.54	0.42
1:A:250:THR:OG1	1:A:253:ASP:OD2	2.31	0.42
1:B:283:VAL:O	1:B:286:ASP:HB2	2.20	0.42
1:G:358:LEU:HB2	1:G:383:ALA:HB1	2.02	0.42
1:B:180:GLN:HB2	1:B:504:GLU:CG	2.49	0.42
1:B:205:VAL:O	1:B:205:VAL:HG12	2.19	0.42
1:B:435:VAL:HG13	1:B:436:GLU:N	2.35	0.42
1:D:435:VAL:CG1	1:D:436:GLU:N	2.82	0.42
1:D:498:ARG:O	1:D:499:GLN:CG	2.67	0.42
1:E:181:ARG:NH1	1:E:500:PRO:HG2	2.35	0.42
1:E:241:GLU:O	1:E:244:HIS:HB3	2.19	0.42
1:E:417:ARG:NH1	1:F:479:PHE:O	2.53	0.42
1:F:222:LEU:CD1	1:F:225:ARG:NH1	2.83	0.42
1:F:292:VAL:C	1:F:294:MET:N	2.73	0.42



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:G:203:SER:O	1:G:331:ALA:HA	2.20	0.42	
1:G:304:TRP:CZ2	1:G:313:LEU:HB2	2.55	0.42	
1:B:117:MET:HE2	1:B:121:ALA:CB	2.50	0.41	
1:E:168:GLY:HA3	1:E:499:GLN:NE2	2.35	0.41	
1:E:169:ARG:NH1	1:E:170:ASP:N	2.64	0.41	
1:G:437:ARG:CG	1:G:438:ASP:H	2.33	0.41	
1:B:318:ARG:HD2	1:B:502:PHE:CE2	2.55	0.41	
1:D:212:GLU:HB2	4:D:2014:HOH:O	2.19	0.41	
1:E:340:ILE:C	1:E:340:ILE:HD12	2.40	0.41	
1:D:133:GLY:HA3	1:E:124:ARG:NH1	2.36	0.41	
1:E:498:ARG:O	1:E:499:GLN:CG	2.63	0.41	
1:F:351:LEU:CD2	1:F:352:TRP:N	2.82	0.41	
1:G:437:ARG:N	1:G:455:GLU:O	2.38	0.41	
1:A:184:GLY:HA3	1:A:297:GLY:CA	2.50	0.41	
1:B:159:PRO:HG2	1:B:356:ASP:OD1	2.20	0.41	
1:D:117:MET:HA	1:D:118:PRO:HD3	1.86	0.41	
1:D:503:VAL:HG12	1:D:503:VAL:O	2.20	0.41	
1:E:251:PHE:CZ	1:E:277:LEU:HB3	2.56	0.41	
1:E:267:PHE:HB3	1:E:277:LEU:HG	2.03	0.41	
1:F:84:PHE:CB	1:F:435:VAL:HG11	2.50	0.41	
1:F:380:ARG:HG3	1:F:380:ARG:NH2	2.35	0.41	
1:G:251:PHE:CE1	1:G:277:LEU:HD13	2.56	0.41	
1:G:369:ASP:O	1:G:373:LYS:N	2.49	0.41	
1:D:180:GLN:HB2	1:D:503:VAL:HG12	2.01	0.41	
1:A:433:HIS:CD2	1:A:459:GLU:HG3	2.56	0.41	
1:B:117:MET:HA	1:B:118:PRO:HD3	1.93	0.41	
1:D:290:GLU:HG3	1:D:325:LEU:HD23	2.02	0.41	
1:E:233:LEU:HA	1:E:233:LEU:HD23	1.78	0.41	
1:E:284:LEU:HB3	1:E:288:LEU:HD12	2.01	0.41	
1:F:103:THR:OG1	1:F:116:PRO:HG2	2.20	0.41	
1:F:279:SER:O	1:F:283:VAL:HG23	2.21	0.41	
1:A:236:THR:O	1:A:238:SER:N	2.48	0.41	
1:A:426:MET:HA	1:A:426:MET:HE2	2.02	0.41	
1:B:84:PHE:CD1	1:B:84:PHE:N	2.88	0.41	
1:B:128:VAL:O	1:B:384:GLY:HA2	2.20	0.41	
1:F:284:LEU:HD12	1:F:284:LEU:HA	1.83	0.41	
1:G:199:ARG:HE	1:G:338:THR:HG21	1.85	0.41	
1:G:199:ARG:HE	1:G:338:THR:HG22	1.84	0.41	
1:G:199:ARG:NE	1:G:338:THR:HG22	2.36	0.41	
1:A:225:ARG:HG3	1:A:226:GLU:N	2.36	0.41	
1:D:236:THR:O	1:D:238:SER:N	2.49	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:D:243:PHE:CD1	1:D:243:PHE:C	2.93	0.41	
1:D:252:ASP:N	1:D:252:ASP:OD2	2.54	0.41	
1:F:179:ASP:O	1:F:182:THR:HG22	2.21	0.41	
1:F:252:ASP:N	1:F:252:ASP:OD2	2.52	0.41	
1:A:135:GLY:HA2	2:A:701:ANP:O1A	2.21	0.41	
1:B:318:ARG:NH2	1:B:321:MET:HE2	2.34	0.41	
1:D:143:LEU:HD23	1:D:143:LEU:HA	1.89	0.41	
1:D:227:THR:CG2	1:D:242:LEU:HD12	2.50	0.41	
1:E:76:GLN:HB3	1:E:77:GLY:H	1.68	0.41	
1:E:117:MET:HA	1:E:118:PRO:HD3	1.90	0.41	
1:E:233:LEU:C	1:E:235:GLY:H	2.24	0.41	
1:E:288:LEU:O	1:E:289:PRO:C	2.59	0.41	
1:E:413:LEU:HD23	1:E:413:LEU:HA	1.93	0.41	
1:F:154:MET:HE3	1:F:156:ILE:HD11	2.03	0.41	
1:F:177:PRO:CA	1:F:294:MET:HE1	2.51	0.41	
1:F:225:ARG:O	1:F:229:LYS:HB2	2.20	0.41	
1:F:288:LEU:O	1:F:291:HIS:HB2	2.21	0.41	
1:G:332:TRP:O	1:G:336:VAL:HG23	2.20	0.41	
1:G:340:ILE:C	1:G:340:ILE:HD12	2.41	0.41	
1:A:82:ALA:O	1:A:437:ARG:NH2	2.54	0.41	
1:A:229:LYS:O	1:A:232:ALA:HB3	2.21	0.41	
1:A:482:ASN:C	1:A:483:ARG:HG2	2.41	0.41	
1:D:124:ARG:HB3	1:D:408:ARG:CB	2.50	0.41	
1:E:113:ALA:HA	1:E:490:LEU:CD2	2.51	0.41	
1:E:457:VAL:CG1	1:E:458:ARG:N	2.84	0.41	
1:E:492:ILE:HD13	2:E:701:ANP:N3	2.36	0.41	
1:F:200:TYR:OH	1:F:302:ARG:HD2	2.22	0.41	
1:F:494:GLN:HA	1:F:494:GLN:NE2	2.36	0.41	
1:G:308:PRO:C	1:G:310:GLY:H	2.22	0.41	
1:G:504:GLU:OE1	1:G:504:GLU:HA	2.21	0.41	
1:B:343:LEU:HD23	1:B:343:LEU:HA	1.87	0.40	
1:B:345:GLU:OE2	1:B:376:LYS:HE2	2.21	0.40	
1:B:351:LEU:HD23	1:B:352:TRP:H	1.86	0.40	
1:E:403:LEU:HD12	1:E:403:LEU:HA	1.91	0.40	
1:F:437:ARG:HH21	1:G:456:ARG:HD2	1.86	0.40	
1:G:175:LEU:CD1	1:G:313:LEU:HD11	2.51	0.40	
1:A:127:LEU:HD12	1:A:127:LEU:HA	1.87	0.40	
1:A:199:ARG:HH21	1:A:338:THR:C	2.24	0.40	
1:A:358:LEU:HB2	1:A:383:ALA:HB1	2.03	0.40	
1:B:259:GLU:HB3	4:B:2010:HOH:O	2.21	0.40	
1:B:352:TRP:CE2	1:B:380:ARG:HD3	2.56	0.40	



A 4 amo 1		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:380:ARG:HG3	1:B:380:ARG:NH2	2.35	0.40
1:D:215:GLU:O	1:D:218:SER:OG	2.27	0.40
1:E:267:PHE:CG	1:E:277:LEU:HG	2.56	0.40
1:F:202:LEU:HD13	1:F:221:ARG:CD	2.51	0.40
1:F:294:MET:HA	1:F:295:PRO:HD3	1.96	0.40
1:G:144:ALA:HB1	1:G:154:MET:CE	2.51	0.40
1:A:304:TRP:CE3	1:A:305:LEU:HD23	2.57	0.40
1:D:202:LEU:HD13	1:D:202:LEU:HA	1.82	0.40
1:D:437:ARG:NH2	1:E:456:ARG:HH22	2.19	0.40
1:E:127:LEU:O	1:E:410:LEU:HD12	2.22	0.40
1:F:299:PHE:CD1	1:F:299:PHE:C	2.93	0.40
1:F:494:GLN:HA	1:F:494:GLN:HE21	1.87	0.40
1:G:157:VAL:CG2	1:G:355:ILE:HA	2.52	0.40
1:A:94:VAL:HG22	1:A:98:LYS:CB	2.51	0.40
1:B:99:LEU:HD23	1:B:486:ALA:HB3	2.03	0.40
1:B:246:THR:HB	1:B:284:LEU:HD23	2.04	0.40
1:D:164:LEU:HD21	1:D:174:ILE:HD11	2.03	0.40
1:D:288:LEU:O	1:D:291:HIS:N	2.54	0.40
1:E:154:MET:HA	1:E:351:LEU:HD23	2.04	0.40
1:E:217:ALA:O	1:E:221:ARG:HG3	2.22	0.40
1:F:292:VAL:O	1:F:294:MET:N	2.54	0.40
1:G:82:ALA:HA	1:G:83:PRO:HD3	2.00	0.40
1:A:137:SER:O	1:A:138:VAL:C	2.59	0.40
1:A:427:SER:OG	1:A:460:ARG:NH1	2.53	0.40
1:B:103:THR:HB	1:B:116:PRO:O	2.22	0.40
1:E:432:GLU:CG	1:E:460:ARG:HD3	2.50	0.40
1:E:503:VAL:O	1:E:504:GLU:HB3	2.22	0.40
1:F:110:VAL:O	1:F:116:PRO:HA	2.22	0.40
1:G:145:TYR:CZ	1:G:149:LEU:HD11	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LYS:NZ	$1:D:241:GLU:OE1[4_456]$	2.08	0.12



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	407/437~(93%)	367~(90%)	36 (9%)	4 (1%)	15	53
1	В	413/437~(94%)	369~(89%)	39 (9%)	5(1%)	13	48
1	D	413/437~(94%)	373 (90%)	36 (9%)	4 (1%)	15	53
1	Е	410/437~(94%)	373 (91%)	34 (8%)	3 (1%)	22	60
1	F	409/437~(94%)	371 (91%)	32 (8%)	6(2%)	10	42
1	G	408/437~(93%)	369 (90%)	35 (9%)	4 (1%)	15	53
All	All	2460/2622~(94%)	2222 (90%)	212 (9%)	26 (1%)	14	50

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	289	PRO
1	F	293	THR
1	В	125	HIS
1	В	189	ASN
1	D	289	PRO
1	D	293	THR
1	D	480	ALA
1	G	189	ASN
1	G	289	PRO
1	А	189	ASN
1	А	293	THR
1	В	293	THR
1	Е	125	HIS
1	А	206	PRO
1	А	499	GLN
1	D	499	GLN
1	Е	289	PRO
1	F	107	ALA
1	F	189	ASN
1	F	503	VAL



Continued from previous page...

Mol	Chain	Res	Type
1	G	125	HIS
1	F	499	GLN
1	G	234	ILE
1	В	289	PRO
1	В	75	GLY
1	Е	234	ILE

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Per	ce	entiles
1	А	344/364~(94%)	315~(92%)	29 (8%)	1	1	38
1	В	348/364~(96%)	316 (91%)	32 (9%)	Ģ)	34
1	D	347/364~(95%)	314 (90%)	33 (10%)	8	3	32
1	Е	346/364~(95%)	315 (91%)	31 (9%)	Ģ)	35
1	F	344/364~(94%)	313 (91%)	31 (9%)	Ģ)	35
1	G	344/364~(94%)	319~(93%)	25 (7%)	1	4	44
All	All	2073/2184 (95%)	1892 (91%)	181 (9%)	1	0	37

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	78	GLU
1	А	84	PHE
1	А	89	ARG
1	А	136	LYS
1	А	143	LEU
1	А	202	LEU
1	А	251	PHE
1	А	252	ASP
1	А	255	ARG
1	А	277	LEU
1	А	284	LEU
1	А	294	MET



Mol	Chain	Res	Type
1	А	313	LEU
1	А	328	LEU
1	А	338	THR
1	А	351	LEU
1	А	353	LEU
1	А	366	SER
1	А	367	LEU
1	А	379	LEU
1	А	385	LEU
1	А	399	GLU
1	А	416	SER
1	А	428	LEU
1	А	430	LEU
1	А	433	HIS
1	А	438	ASP
1	А	483	ARG
1	А	497	ASN
1	В	89	ARG
1	В	92	ARG
1	В	94	VAL
1	В	104	ARG
1	В	142	GLU
1	В	143	LEU
1	В	154	MET
1	В	169	ARG
1	В	202	LEU
1	В	233	LEU
1	В	251	PHE
1	В	252	ASP
1	В	254	LEU
1	В	277	LEU
1	В	294	MET
1	В	309	ASN
1	В	328	LEU
1	В	341	LEU
1	В	350	ARG
1	В	351	LEU
1	В	353	LEU
1	В	366	SER
1	В	367	LEU
1	В	372	THR
1	В	379	LEU



Mol	Chain	Res	Type
1	В	385	LEU
1	В	417	ARG
1	В	430	LEU
1	В	433	HIS
1	В	456	ARG
1	В	490	LEU
1	В	504	GLU
1	D	89	ARG
1	D	92	ARG
1	D	94	VAL
1	D	106	LYS
1	D	136	LYS
1	D	143	LEU
1	D	180	GLN
1	D	192	ARG
1	D	202	LEU
1	D	212	GLU
1	D	233	LEU
1	D	251	PHE
1	D	277	LEU
1	D	284	LEU
1	D	289	PRO
1	D	294	MET
1	D	313	LEU
1	D	328	LEU
1	D	350	ARG
1	D	351	LEU
1	D	353	LEU
1	D	366	SER
1	D	367	LEU
1	D	372	THR
1	D	379	LEU
1	D	385	LEU
1	D	399	GLU
1	D	409	SER
1	D	430	LEU
1	D	433	HIS
1	D	482	ASN
1	D	483	ARG
1	D	490	LEU
1	E	76	GLN
1	E	89	ARG



Mol	Chain	Res	Type
1	Е	106	LYS
1	Е	143	LEU
1	Е	169	ARG
1	Е	202	LEU
1	Е	210	THR
1	Е	240	ARG
1	Е	251	PHE
1	Е	252	ASP
1	Е	254	LEU
1	Е	255	ARG
1	Е	277	LEU
1	Е	294	MET
1	Е	296	ASP
1	E	313	LEU
1	Е	328	LEU
1	Е	341	LEU
1	Е	345	GLU
1	Е	351	LEU
1	Е	353	LEU
1	Е	367	LEU
1	Ε	379	LEU
1	Е	385	LEU
1	Ε	399	GLU
1	Е	428	LEU
1	Ε	430	LEU
1	Ε	433	HIS
1	Е	456	ARG
1	Ε	497	ASN
1	Ε	498	ARG
1	F	89	ARG
1	F	92	ARG
1	F	132	THR
1	F	136	LYS
1	F	143	LEU
1	F	180	GLN
1	F	194	ASP
1	F	202	LEU
1	F	233	LEU
1	F	251	PHE
1	F	277	LEU
1	F	284	LEU
1	F	289	PRO



Mol	Chain	Res	Type
1	F	294	MET
1	F	313	LEU
1	F	328	LEU
1	F	341	LEU
1	F	345	GLU
1	F	351	LEU
1	F	366	SER
1	F	367	LEU
1	F	375	ARG
1	F	379	LEU
1	F	385	LEU
1	F	399	GLU
1	F	428	LEU
1	F	430	LEU
1	F	433	HIS
1	F	456	ARG
1	F	490	LEU
1	F	497	ASN
1	G	84	PHE
1	G	89	ARG
1	G	106	LYS
1	G	126	LEU
1	G	136	LYS
1	G	143	LEU
1	G	202	LEU
1	G	251	PHE
1	G	252	ASP
1	G	277	LEU
1	G	284	LEU
1	G	289	PRO
1	G	294	MET
1	G	313	LEU
1	G	351	LEU
1	G	353	LEU
1	G	367	LEU
1	G	379	LEU
1	G	399	GLU
1	G	428	LEU
1	G	430	LEU
1	G	433	HIS
1	G	438	ASP
1	G	456	ARG



 $Continued \ from \ previous \ page...$

Mol	Chain	Res	Type
1	G	490	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	160	ASN
1	А	180	GLN
1	А	433	HIS
1	А	497	ASN
1	А	499	GLN
1	В	129	ASN
1	В	180	GLN
1	В	401	GLN
1	В	423	ASN
1	В	433	HIS
1	В	494	GLN
1	В	497	ASN
1	В	499	GLN
1	D	160	ASN
1	D	180	GLN
1	D	423	ASN
1	D	433	HIS
1	D	482	ASN
1	D	494	GLN
1	D	497	ASN
1	D	499	GLN
1	Е	76	GLN
1	Е	180	GLN
1	Е	423	ASN
1	E	433	HIS
1	E	494	GLN
1	Е	497	ASN
1	E	499	GLN
1	F	109	GLN
1	F	129	ASN
1	F	423	ASN
1	F	433	HIS
1	F	494	GLN
1	F	497	ASN
1	F	499	GLN
1	G	180	GLN
1	G	423	ASN



Continued from previous page...

Mol	Chain	Res	Type
1	G	433	HIS
1	G	497	ASN
1	G	499	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	Chain	Dec	Tink	B	ond leng	gths	B	ond ang	les
MOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ANP	А	701	-	29,33,33	2.03	11 (37%)	31,52,52	2.16	6 (19%)
2	ANP	В	701	-	29,33,33	2.03	11 (37%)	31,52,52	2.20	6 (19%)
2	ANP	D	701	-	29,33,33	2.07	12 (41%)	31,52,52	2.15	8 (25%)
2	ANP	F	701	-	29,33,33	1.97	10 (34%)	31,52,52	2.22	7 (22%)
2	ANP	Е	701	-	29,33,33	2.03	11 (37%)	31,52,52	2.19	6 (19%)
2	ANP	G	701	-	29,33,33	1.97	11 (37%)	31,52,52	2.19	6 (19%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	А	701	-	-	1/14/38/38	0/3/3/3
2	ANP	В	701	-	-	1/14/38/38	0/3/3/3
2	ANP	D	701	-	-	1/14/38/38	0/3/3/3
2	ANP	F	701	-	-	1/14/38/38	0/3/3/3
2	ANP	E	701	-	-	3/14/38/38	0/3/3/3
2	ANP	G	701	-	-	1/14/38/38	0/3/3/3

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	D	701	ANP	PG-N3B	5.39	1.77	1.63
2	А	701	ANP	PG-N3B	5.13	1.76	1.63
2	В	701	ANP	PG-N3B	5.07	1.76	1.63
2	Е	701	ANP	PG-N3B	5.04	1.76	1.63
2	F	701	ANP	PG-N3B	4.80	1.75	1.63
2	G	701	ANP	PG-N3B	4.41	1.74	1.63
2	F	701	ANP	PB-O3A	3.28	1.63	1.59
2	G	701	ANP	PB-O3A	3.11	1.63	1.59
2	G	701	ANP	PG-O3G	-3.03	1.48	1.56
2	Е	701	ANP	PG-O3G	-3.02	1.48	1.56
2	Е	701	ANP	O4'-C4'	-2.95	1.38	1.45
2	А	701	ANP	O4'-C4'	-2.89	1.38	1.45
2	А	701	ANP	PG-O3G	-2.87	1.49	1.56
2	Е	701	ANP	PB-O2B	-2.82	1.49	1.56
2	А	701	ANP	PG-01G	2.82	1.50	1.46
2	Е	701	ANP	C5-N7	2.81	1.49	1.39
2	D	701	ANP	PB-N3B	2.80	1.70	1.63
2	D	701	ANP	O4'-C4'	-2.79	1.38	1.45
2	А	701	ANP	C5-N7	2.77	1.49	1.39
2	D	701	ANP	PG-O3G	-2.75	1.49	1.56
2	F	701	ANP	C5-N7	2.74	1.49	1.39
2	В	701	ANP	C2-N1	2.74	1.39	1.33
2	F	701	ANP	PG-O3G	-2.73	1.49	1.56
2	В	701	ANP	C5-N7	2.72	1.49	1.39
2	В	701	ANP	PG-01G	2.71	1.50	1.46
2	G	701	ANP	C6-N6	2.70	1.43	1.34
2	В	701	ANP	PG-O3G	-2.69	1.49	1.56
2	А	701	ANP	PB-N3B	2.68	1.70	1.63
2	D	701	ANP	C5-N7	2.68	1.49	1.39
2	В	701	ANP	PB-O3A	2.67	1.62	1.59
2	В	701	ANP	O4'-C4'	-2.67	1.39	1.45



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	701	ANP	C5-N7	2.66	1.49	1.39
2	Е	701	ANP	C6-N6	2.66	1.43	1.34
2	В	701	ANP	C6-N6	2.65	1.43	1.34
2	F	701	ANP	C6-N6	2.64	1.43	1.34
2	D	701	ANP	PG-O1G	2.64	1.50	1.46
2	G	701	ANP	C2-N1	2.64	1.38	1.33
2	D	701	ANP	C6-N6	2.63	1.43	1.34
2	D	701	ANP	C2-N1	2.61	1.38	1.33
2	А	701	ANP	C6-N6	2.59	1.43	1.34
2	Е	701	ANP	PB-N3B	2.57	1.70	1.63
2	В	701	ANP	PB-N3B	2.55	1.70	1.63
2	D	701	ANP	PB-O2B	-2.54	1.49	1.56
2	G	701	ANP	O4'-C4'	-2.52	1.39	1.45
2	В	701	ANP	PB-O2B	-2.52	1.50	1.56
2	Е	701	ANP	C2-N1	2.51	1.38	1.33
2	G	701	ANP	PB-O2B	-2.50	1.50	1.56
2	F	701	ANP	PG-O1G	2.48	1.50	1.46
2	А	701	ANP	PB-O2B	-2.47	1.50	1.56
2	А	701	ANP	C2-N1	2.45	1.38	1.33
2	F	701	ANP	O4'-C4'	-2.45	1.39	1.45
2	F	701	ANP	PB-O2B	-2.43	1.50	1.56
2	Е	701	ANP	PG-O1G	2.37	1.49	1.46
2	G	701	ANP	PG-O1G	2.37	1.49	1.46
2	F	701	ANP	C2-N1	2.35	1.38	1.33
2	Е	701	ANP	C2'-C1'	-2.33	1.50	1.53
2	А	701	ANP	C4-N3	2.27	1.38	1.35
2	D	701	ANP	PA-O5'	-2.19	1.50	1.59
2	F	701	ANP	PB-N3B	2.19	1.69	1.63
2	D	701	ANP	C2'-C1'	-2.18	1.50	1.53
2	А	701	ANP	PA-O5'	-2.12	1.50	1.59
2	В	701	ANP	PA-05'	-2.12	1.50	1.59
2	G	701	ANP	PB-N3B	2.09	1.68	1.63
2	Е	701	ANP	C4-N3	2.08	1.38	1.35
2	G	701	ANP	C4-N3	2.06	1.38	1.35
2	D	701	ANP	C4-N3	2.05	1.38	1.35

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	В	701	ANP	O1G-PG-N3B	-7.17	101.22	111.77
2	F	701	ANP	O1G-PG-N3B	-7.01	101.45	111.77
2	D	701	ANP	O1G-PG-N3B	-6.94	101.54	111.77



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	Е	701	ANP	O1G-PG-N3B	-6.92	101.58	111.77
2	G	701	ANP	O1G-PG-N3B	-6.88	101.64	111.77
2	А	701	ANP	O1G-PG-N3B	-6.56	102.11	111.77
2	Е	701	ANP	C5-C6-N6	6.27	129.89	120.35
2	F	701	ANP	C5-C6-N6	6.22	129.80	120.35
2	А	701	ANP	C5-C6-N6	6.13	129.67	120.35
2	G	701	ANP	C5-C6-N6	6.11	129.64	120.35
2	В	701	ANP	C5-C6-N6	6.07	129.57	120.35
2	D	701	ANP	C5-C6-N6	5.74	129.08	120.35
2	В	701	ANP	C5-C6-N1	-4.17	110.90	120.35
2	G	701	ANP	C5-C6-N1	-4.16	110.92	120.35
2	Е	701	ANP	C5-C6-N1	-4.14	110.97	120.35
2	D	701	ANP	C5-C6-N1	-4.10	111.06	120.35
2	А	701	ANP	C5-C6-N1	-4.05	111.17	120.35
2	F	701	ANP	C5-C6-N1	-4.02	111.24	120.35
2	G	701	ANP	O2B-PB-O1B	3.53	117.32	109.92
2	F	701	ANP	O2B-PB-O1B	3.51	117.28	109.92
2	Е	701	ANP	O2B-PB-O1B	3.46	117.18	109.92
2	В	701	ANP	O2B-PB-O1B	3.46	117.17	109.92
2	А	701	ANP	O2B-PB-O1B	3.44	117.13	109.92
2	D	701	ANP	O2B-PB-O1B	3.27	116.78	109.92
2	Ε	701	ANP	N3-C2-N1	3.13	133.57	128.68
2	G	701	ANP	N3-C2-N1	3.10	133.52	128.68
2	А	701	ANP	N3-C2-N1	3.09	133.51	128.68
2	F	701	ANP	N3-C2-N1	3.05	133.45	128.68
2	В	701	ANP	N3-C2-N1	3.03	133.42	128.68
2	D	701	ANP	N3-C2-N1	2.99	133.35	128.68
2	F	701	ANP	O4'-C4'-C5'	2.86	118.77	109.37
2	G	701	ANP	O4'-C4'-C5'	2.49	117.56	109.37
2	Е	701	ANP	O4'-C4'-C5'	2.42	117.33	109.37
2	В	701	ANP	O4'-C4'-C5'	2.42	117.32	109.37
2	А	701	ANP	O4'-C4'-C5'	2.30	116.93	109.37
2	F	701	ANP	O3A-PB-N3B	-2.27	100.29	106.59
2	D	701	ANP	O4'-C4'-C5'	2.27	116.83	109.37
2	D	701	ANP	O3A-PB-N3B	-2.15	100.63	106.59
2	D	701	ANP	O2G-PG-O1G	-2.08	108.23	113.45

Continued from previous page...

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms			
2	А	701	ANP	PG-N3B-PB-O1B			
	α i 1 i						



	v	1	1 0	
Mol	Chain	\mathbf{Res}	Type	Atoms
2	В	701	ANP	PG-N3B-PB-O1B
2	D	701	ANP	PG-N3B-PB-O1B
2	Е	701	ANP	PG-N3B-PB-O1B
2	F	701	ANP	PG-N3B-PB-O1B
2	G	701	ANP	PG-N3B-PB-O1B
2	Е	701	ANP	O4'-C4'-C5'-O5'
2	Е	701	ANP	C3'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	701	ANP	1	0
2	В	701	ANP	2	0
2	D	701	ANP	1	0
2	F	701	ANP	2	0
2	Е	701	ANP	2	0
2	G	701	ANP	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 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 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

