

Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2021 – 01:05 PM BST

PDB ID	:	7NPJ
Title	:	Crystal structure of Mycobacterium tuberculosis ArgC in complex with 6-phe
		noxy-3-pyridinamine
Authors	:	Gupta, P.; Mendes, V.; Blundell, T.L.
Deposited on	:	2021-02-27
Resolution	:	2.81 Å(reported)

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

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

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

MolProbity	÷	4.02b-467
Mogul		1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
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)	:	2.20

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${igstyle {1.5cm} { m Similar resolution} \ (\#{ m Entries, resolution range(Å)})}$		
R_{free}	130704	3617(2.84-2.80)		
Clashscore	141614	4060 (2.84-2.80)		
Ramachandran outliers	138981	3978 (2.84 - 2.80)		
Sidechain outliers	138945	3980 (2.84-2.80)		
RSRZ outliers	127900	3552(2.84-2.80)		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain						
1	А	354	56%	37%	•••				
1	В	354	57%	37%	•••				
1	С	354	^{2%} 60%	34%	•••				
1	D	354	% 68%	27%	•••				
1	Е	354	<u>6%</u> 57%	36%	••				



Mol	Chain	Length	Quality of chain				
1	Б	254	14%				
	Г	504	62%	34%	• •		
			10%				
1	G	354	63%	32%	••		
			3%				
1	H	354	62%	33%	••		



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18617 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	Δ	244	Total	С	Ν	Ο	S	0	0	0
	A	044	2344	1492	403	444	5	0	0	0
1	р	244	Total	С	Ν	Ο	S	0	0	0
	D	344	2403	1518	434	446	5	0	0	0
1	C	244	Total	С	Ν	Ο	S	0	0	0
		344	2427	1538	424	460	5	0	0	0
1	р	244	Total	С	Ν	Ο	S	0	0	0
		344	2388	1512	418	453	5	0	0	0
1	Б	244	Total	С	Ν	Ο	S	0	0	0
L T		044	2324	1456	418	445	5	0	0	0
1	Б	244	Total	С	Ν	Ο	S	0	0	0
	Г	344	2212	1378	399	430	5	0	0	0
1	C	244	Total	С	Ν	Ο	S	0	0	0
	G	344	2231	1395	392	439	5	0	0	0
1	ц	244	Total	С	Ν	Ο	S	0	0	0
	11	044	2274	1438	404	427	5		U	U

• Molecule 1 is a protein called N-acetyl-gamma-glutamyl-phosphate reductase.

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-1	GLY	-	expression tag	UNP P9WPZ9
А	0	SER	-	expression tag	UNP P9WPZ9
В	-1	GLY	-	expression tag	UNP P9WPZ9
В	0	SER	-	expression tag	UNP P9WPZ9
С	-1	GLY	-	expression tag	UNP P9WPZ9
С	0	SER	-	expression tag	UNP P9WPZ9
D	-1	GLY	-	expression tag	UNP P9WPZ9
D	0	SER	-	expression tag	UNP P9WPZ9
Е	-1	GLY	-	expression tag	UNP P9WPZ9
E	0	SER	-	expression tag	UNP P9WPZ9
F	-1	GLY	-	expression tag	UNP P9WPZ9
F	0	SER	-	expression tag	UNP P9WPZ9
G	-1	GLY	-	expression tag	UNP P9WPZ9



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Chain	Residue	Modelled	Actual	Comment	Reference					
G	0	SER	-	expression tag	UNP P9WPZ9					
Н	-1	GLY	-	expression tag	UNP P9WPZ9					
Н	0	SER	-	expression tag	UNP P9WPZ9					

• Molecule 2 is 6-phenoxy-3-pyridinamine (three-letter code: UKK) (formula: $C_{11}H_{10}N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	В	1	Total	С	Ν	Ο	0	0
2 D		14	11	2	1			



Chain C:

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.



34%

• Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase

60%



• Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	84.34Å 132.81Å 122.82Å	Deperitor
a, b, c, α , β , γ	90.00° 90.12° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	69.59 - 2.81	Depositor
Resolution (A)	71.20 - 2.81	EDS
% Data completeness	99.6 (69.59-2.81)	Depositor
(in resolution range)	99.6 (71.20-2.81)	EDS
R _{merge}	0.13	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.39 (at 2.81 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
D D .	0.237 , 0.325	Depositor
Π, Π_{free}	0.257 , 0.326	DCC
R_{free} test set	3176 reflections $(4.82%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	77.6	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.30 , 73.7	EDS
L-test for twinning ²	$< L > = 0.46, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18617	wwPDB-VP
Average B, all atoms $(Å^2)$	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.04% 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.



 $^{^1 {\}rm Intensities}$ estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UKK

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		
	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.52	0/2399	0.73	0/3309	
1	В	0.54	0/2457	0.77	0/3375	
1	С	0.54	0/2483	0.74	0/3413	
1	D	0.47	0/2444	0.71	0/3363	
1	Е	0.46	0/2372	0.70	0/3263	
1	F	0.38	0/2260	0.65	0/3119	
1	G	0.38	0/2277	0.62	0/3145	
1	Н	0.46	0/2328	0.71	0/3212	
All	All	0.48	0/19020	0.71	0/26199	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2344	0	2215	115	0
1	В	2403	0	2330	96	0
1	С	2427	0	2362	90	0
1	D	2388	0	2287	72	0
1	Е	2324	0	2180	128	0



	J	1	1 5			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2212	0	1922	95	0
1	G	2231	0	2000	90	0
1	Н	2274	0	2061	102	0
2	В	14	0	0	1	0
All	All	18617	0	17357	731	0

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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 20.

All (731) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 9	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:140:LEU:HD12	1:A:141:PRO:CD	1.49	1.42
1:E:13:ALA:HB3	1:E:84:VAL:HG22	1.22	1.18
1:A:140:LEU:HD12	1:A:141:PRO:HD3	1.23	1.17
1:E:155:VAL:HG12	1:E:156:PRO:HD2	1.32	1.09
1:A:140:LEU:HD12	1:A:141:PRO:HD2	1.27	1.09
1:C:12:VAL:HG13	1:C:83:ALA:HB3	1.35	1.07
1:E:291:GLY:O	1:E:351:ALA:HB2	1.57	1.03
1:E:288:PRO:HD2	1:E:315:ILE:HD11	1.42	1.02
1:E:14:VAL:HG23	1:E:45:LEU:HA	1.44	0.99
1:F:108:ASP:O	1:F:155:VAL:HG23	1.61	0.99
1:A:14:VAL:HG23	1:A:17:ALA:HB2	1.47	0.96
1:A:157:GLY:HA3	1:A:219:HIS:CE1	2.02	0.95
1:A:140:LEU:CD1	1:A:141:PRO:CD	2.45	0.94
1:E:113:PHE:HB2	1:E:154:ALA:HB2	1.48	0.94
1:F:166:ALA:HB2	1:F:316:ALA:HB2	1.48	0.94
1:E:135:TYR:CZ	1:E:156:PRO:HB3	2.06	0.91
1:A:140:LEU:CD1	1:A:141:PRO:HD2	2.01	0.90
1:E:71:GLU:CB	1:E:72:PRO:HD2	2.01	0.90
1:G:46:THR:HG21	1:G:78:LEU:HD21	1.53	0.90
1:E:14:VAL:HG11	1:E:26:LEU:HD21	1.52	0.89
1:F:86:LEU:HB2	1:F:108:ASP:HA	1.54	0.87
1:C:92:HIS:HA	1:E:49:THR:HG22	1.56	0.87
1:E:113:PHE:HB3	1:E:133:TRP:H	1.39	0.85
1:E:13:ALA:CB	1:E:84:VAL:HG22	2.06	0.83
1:A:14:VAL:CG2	1:A:17:ALA:HB2	2.10	0.81
1:A:105:LEU:HD11	1:A:336:ALA:HB1	1.61	0.81
1:F:137:LEU:HD11	1:F:161:THR:HG23	1.64	0.80
1:C:228:ARG:HG3	1:C:235:VAL:HG22	1.64	0.80
1:B:158:CYS:HB2	1:B:250:ILE:HD11	1.63	0.79



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:H:322:VAL:HG23	1:H:323:LYS:H	1.46	0.78
1:B:115:LEU:HA	1:B:225:GLN:HE22	1.48	0.78
1:E:71:GLU:CB	1:E:72:PRO:CD	2.62	0.78
1:B:139:GLU:HG2	1:B:279:ILE:HD11	1.65	0.78
1:C:102:PRO:HA	1:C:152:ARG:HH22	1.49	0.77
1:A:105:LEU:HD11	1:A:336:ALA:CB	2.15	0.77
1:C:51:ALA:HB1	1:C:72:PRO:HD3	1.65	0.77
1:F:297:ASN:O	1:F:297:ASN:ND2	2.15	0.76
1:E:88:LEU:HD12	1:E:91:GLY:HA3	1.66	0.76
1:G:61:HIS:CE1	1:H:351:ALA:HB3	2.21	0.76
1:B:322:VAL:HG23	1:B:323:LYS:H	1.51	0.75
1:E:169:PRO:HB2	1:E:269:TYR:CE2	2.20	0.75
1:A:157:GLY:HA3	1:A:219:HIS:HE1	1.51	0.75
1:D:182:VAL:HG22	1:D:254:CYS:HB3	1.68	0.75
1:H:14:VAL:HG22	1:H:85:PHE:HB2	1.67	0.75
1:A:290:THR:HG23	1:D:208:ALA:O	1.86	0.75
1:A:98:GLN:O	1:A:99:GLN:HG3	1.88	0.74
1:C:12:VAL:HG13	1:C:83:ALA:CB	2.17	0.74
1:A:282:MET:HE3	1:A:288:PRO:HA	1.68	0.73
1:B:255:THR:HG22	1:B:313:VAL:HG12	1.68	0.73
1:A:32:HIS:HE1	1:A:343:ASP:HB3	1.53	0.73
1:H:144:ARG:HG3	1:H:335:LEU:HD21	1.71	0.73
1:E:209:ARG:HB3	1:H:289:ARG:HB3	1.71	0.73
1:A:199:LEU:HD23	1:A:199:LEU:O	1.88	0.72
1:A:105:LEU:CD1	1:A:336:ALA:HB1	2.19	0.72
1:B:140:LEU:HD12	1:B:141:PRO:HD2	1.72	0.72
1:F:294:ILE:O	1:F:350:VAL:HG23	1.90	0.71
1:D:109:CYS:HA	1:D:155:VAL:HB	1.71	0.71
1:E:117:ASP:HB3	1:E:120:VAL:HG22	1.72	0.71
1:F:262:LEU:HA	1:F:265:LEU:HD12	1.71	0.71
1:A:140:LEU:CD1	1:A:141:PRO:HD3	2.13	0.71
1:G:348:VAL:HG12	1:H:61:HIS:O	1.91	0.70
1:E:32:HIS:ND1	1:E:33:PRO:HD2	2.06	0.70
1:H:135:TYR:O	1:H:147:LEU:HD21	1.91	0.70
1:F:159:TYR:CB	1:F:160:PRO:HD3	2.21	0.70
1:E:125:TYR:HA	1:E:218:ARG:HH12	1.58	0.69
1:A:276:GLU:HG2	1:A:279:ILE:HG12	1.75	0.69
1:D:180:VAL:HG13	1:D:256:ALA:HB2	1.75	0.68
1:E:168:PHE:CG	1:E:169:PRO:HD3	2.28	0.68
1:G:137:LEU:HB2	1:G:156:PRO:HG2	1.75	0.68
1:E:12:VAL:HA	1:E:83:ALA:O	1.93	0.68



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:181:THR:HG21	1:D:181:THR:HG21	1.75	0.68
1:D:42:ILE:O	1:D:68:ARG:NH2	2.23	0.68
1:B:200:LEU:HD21	1:D:195:ALA:HA	1.75	0.68
1:A:143:ALA:HA	1:A:146:GLN:HG2	1.75	0.67
1:H:213:ILE:O	1:H:216:VAL:HG22	1.95	0.67
1:H:135:TYR:CZ	1:H:156:PRO:HB3	2.30	0.66
1:A:89:PRO:HA	1:A:110:GLY:HA2	1.77	0.66
1:E:10:THR:HB	1:E:39:ARG:O	1.95	0.65
1:F:185:VAL:HG11	1:G:185:VAL:HG11	1.77	0.65
1:H:201:GLY:HA2	1:H:204:VAL:HG22	1.78	0.65
1:C:136:GLY:O	1:C:138:PRO:HD3	1.95	0.65
1:C:59:HIS:HB3	1:C:62:LEU:HD12	1.76	0.65
1:A:161:THR:O	1:A:165:LEU:HD12	1.95	0.65
1:E:155:VAL:HG12	1:E:156:PRO:CD	2.19	0.65
1:G:250:ILE:HD11	1:G:320:ASN:HB3	1.77	0.65
1:C:278:PHE:CE1	1:C:297:ASN:HB3	2.31	0.65
1:G:321:LEU:HA	1:G:325:THR:HG22	1.79	0.65
1:E:65:LEU:HD12	1:E:65:LEU:N	2.12	0.64
1:H:228:ARG:HG2	1:H:235:VAL:HG11	1.79	0.64
1:A:157:GLY:CA	1:A:219:HIS:HE1	2.10	0.64
1:A:177:GLU:HG3	1:A:179:ALA:H	1.62	0.64
1:D:20:TYR:CE2	1:D:193:ARG:HG3	2.32	0.64
1:E:102:PRO:HA	1:E:152:ARG:HH22	1.61	0.64
1:B:115:LEU:HD13	1:B:120:VAL:HG23	1.79	0.64
1:E:113:PHE:HB2	1:E:154:ALA:CB	2.26	0.64
1:E:322:VAL:HG13	1:E:323:LYS:H	1.62	0.64
1:E:319:ASP:HB3	1:E:322:VAL:HG12	1.80	0.64
1:B:53:SER:HB2	1:B:58:HIS:HE1	1.62	0.63
1:F:108:ASP:C	1:F:155:VAL:HG23	2.18	0.63
1:H:105:LEU:HD21	1:H:107:ILE:HD11	1.80	0.63
1:G:352:PRO:HG3	1:H:20:TYR:CE1	2.34	0.63
1:A:13:ALA:HB2	1:A:81:HIS:CD2	2.34	0.63
1:E:109:CYS:HA	1:E:155:VAL:HG23	1.81	0.63
1:F:181:THR:HG23	1:F:238:SER:OG	1.99	0.63
1:C:133:TRP:CG	1:C:152:ARG:HB3	2.32	0.63
1:A:42:ILE:HD13	1:A:65:LEU:HD11	1.80	0.63
1:H:296:SER:HB2	1:H:348:VAL:O	1.98	0.63
1:A:170:ALA:HB2	1:A:269:TYR:HE1	1.63	0.63
1:A:74:GLU:O	1:A:78:LEU:HD12	1.99	0.62
1:F:290:THR:HB	1:G:208:ALA:H	1.64	0.62
1:D:211:TYR:CE1	1:D:241:PRO:HB2	2.35	0.62



	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:E:57:GLU:O	1:E:57:GLU:HG3	1.98	0.62
1:F:334:ASN:O	1:F:338:GLY:N	2.32	0.62
1:F:183:VAL:HG21	1:G:183:VAL:HG11	1.82	0.62
1:F:125:TYR:CZ	1:F:218:ARG:HB3	2.34	0.62
1:G:289:ARG:HD2	1:H:60:PRO:HG3	1.81	0.62
1:B:244:ILE:HD12	1:C:245:PRO:HD2	1.82	0.62
1:B:249:GLY:N	1:B:320:ASN:OD1	2.33	0.62
1:C:185:VAL:HG12	1:C:242:VAL:HB	1.82	0.62
1:E:171:LEU:HG	1:E:231:THR:OG1	2.00	0.62
1:G:352:PRO:CG	1:H:20:TYR:CD1	2.82	0.62
1:F:27:ARG:HA	1:F:62:LEU:HD21	1.82	0.62
1:A:213:ILE:HG22	1:A:240:THR:HG23	1.81	0.61
1:E:14:VAL:HG11	1:E:26:LEU:CD2	2.28	0.61
1:E:220:THR:HG22	1:E:239:PHE:HB3	1.81	0.61
1:A:53:SER:H	1:A:70:VAL:HG22	1.64	0.61
1:A:153:ILE:HD13	1:A:332:SER:HB3	1.81	0.61
1:D:183:VAL:HG22	1:D:240:THR:HB	1.83	0.61
1:A:35:TYR:CE2	1:A:42:ILE:HD12	2.36	0.61
1:G:61:HIS:ND1	1:H:351:ALA:HB3	2.15	0.61
1:B:138:PRO:HG2	1:B:331:GLN:HG2	1.82	0.61
1:G:352:PRO:HG2	1:H:20:TYR:CD1	2.34	0.61
1:E:159:TYR:HB2	1:E:160:PRO:HD3	1.83	0.60
1:H:59:HIS:HB3	1:H:61:HIS:CE1	2.36	0.60
1:B:158:CYS:HB2	1:B:250:ILE:CD1	2.30	0.60
1:F:213:ILE:HG21	1:G:315:ILE:HD11	1.83	0.60
1:F:188:THR:HG21	1:F:204:VAL:HG11	1.83	0.60
1:A:138:PRO:HG3	1:A:147:LEU:HD23	1.84	0.60
1:B:335:LEU:HD11	1:B:341:GLU:OE1	2.01	0.60
1:F:210:ALA:CB	1:G:315:ILE:HD13	2.32	0.60
1:D:167:LEU:HD11	1:D:254:CYS:HB3	1.84	0.60
1:A:11:LYS:H	1:A:82:ASP:HB2	1.67	0.59
1:H:134:PRO:HB2	1:H:147:LEU:HD13	1.83	0.59
1:G:61:HIS:ND1	1:H:351:ALA:CB	2.65	0.59
1:H:220:THR:HG22	1:H:239:PHE:HD2	1.67	0.59
1:C:188:THR:HG21	1:C:204:VAL:HG21	1.84	0.59
1:C:273:TYR:CG	1:C:279:ILE:HG21	2.38	0.59
1:E:224:ALA:HB1	1:E:228:ARG:HH12	1.67	0.59
1:F:158:CYS:HA	1:F:324:GLY:HA3	1.82	0.59
1:G:111:ALA:HA	1:G:114:ARG:HG3	1.84	0.59
1:A:32:HIS:CE1	1:A:343:ASP:HB3	2.36	0.59
1:C:22:GLY:HA2	1:C:25:ILE:HD12	1.83	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:152:ARG:HG3	1:D:152:ARG:HH11	1.68	0.59
1:A:112:ASP:HA	1:A:121:TRP:CZ3	2.38	0.59
1:H:255:THR:HA	1:H:312:PHE:O	2.03	0.58
1:E:170:ALA:HB2	1:E:269:TYR:CE1	2.38	0.58
1:E:288:PRO:HB3	1:E:300:HIS:CB	2.34	0.58
1:B:352:PRO:HB2	1:C:202:ALA:O	2.02	0.58
1:D:35:TYR:CE1	1:D:42:ILE:HD12	2.38	0.58
1:F:158:CYS:HA	1:F:324:GLY:CA	2.33	0.58
1:G:282:MET:HB3	1:G:286:GLN:O	2.03	0.58
1:A:282:MET:HE2	1:A:300:HIS:HB3	1.85	0.58
1:D:198:ASP:HB3	1:D:209:ARG:NH2	2.17	0.58
1:G:322:VAL:O	1:G:327:GLY:N	2.33	0.58
1:H:24:GLU:OE2	1:H:27:ARG:NH2	2.33	0.58
1:C:147:LEU:HD23	1:C:153:ILE:HG12	1.86	0.58
1:A:22:GLY:HA2	1:A:25:ILE:HD12	1.84	0.58
1:F:260:SER:OG	1:F:264:GLN:HB2	2.04	0.58
1:F:213:ILE:HG21	1:G:315:ILE:CD1	2.34	0.57
1:E:168:PHE:CD2	1:E:169:PRO:HD3	2.38	0.57
1:E:84:VAL:HB	1:E:106:ILE:HG22	1.86	0.57
1:G:61:HIS:CG	1:H:351:ALA:CB	2.88	0.57
1:H:17:ALA:HA	1:H:22:GLY:HA3	1.87	0.57
1:G:135:TYR:OH	1:G:156:PRO:HB3	2.04	0.57
1:A:63:THR:HA	1:A:66:ALA:HB2	1.84	0.57
1:E:73:THR:HG22	1:E:73:THR:O	2.04	0.57
1:B:107:ILE:HG12	1:B:153:ILE:HD12	1.87	0.57
1:B:220:THR:HG23	1:B:239:PHE:HB3	1.87	0.57
1:E:158:CYS:HB2	1:E:250:ILE:HD11	1.86	0.57
1:F:112:ASP:HA	1:F:121:TRP:CZ3	2.40	0.57
1:B:335:LEU:HD21	1:B:341:GLU:HB2	1.87	0.57
1:H:282:MET:HE2	1:H:300:HIS:HB3	1.86	0.57
1:B:282:MET:SD	1:B:300:HIS:HB3	2.44	0.57
1:C:282:MET:HG2	1:C:301:ILE:O	2.04	0.57
1:E:108:ASP:O	1:E:155:VAL:HG23	2.05	0.57
1:F:183:VAL:HG23	1:F:253:THR:HB	1.85	0.57
1:H:21:ALA:O	1:H:25:ILE:HG13	2.04	0.57
1:H:350:VAL:O	1:H:352:PRO:OXT	2.23	0.57
1:F:303:VAL:HB	1:F:312:PHE:HE1	1.69	0.56
1:H:94:ALA:HB3	1:H:113:PHE:HE2	1.70	0.56
1:B:293:VAL:HB	1:B:298:ALA:HB3	1.87	0.56
1:C:14:VAL:HG22	1:C:85:PHE:HB2	1.87	0.56
1:E:170:ALA:HB2	1:E:269:TYR:HE1	1.70	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:201:GLY:O	1:G:205:ILE:HG13	2.03	0.56
1:B:291:GLY:HA3	1:C:207:SER:HB2	1.88	0.56
1:D:253:THR:HA	1:D:315:ILE:HD13	1.87	0.56
1:H:200:LEU:O	1:H:204:VAL:HG13	2.05	0.56
1:C:133:TRP:CD2	1:C:152:ARG:HB3	2.40	0.56
1:C:147:LEU:O	1:C:150:THR:HG22	2.06	0.56
1:E:85:PHE:HE1	1:E:329:ALA:HB1	1.70	0.56
1:E:319:ASP:O	1:E:321:LEU:N	2.39	0.56
1:G:283:PRO:HD2	1:G:286:GLN:CB	2.36	0.56
1:G:348:VAL:CG1	1:H:62:LEU:HA	2.35	0.56
1:H:124:PHE:HB3	1:H:218:ARG:HG2	1.88	0.56
1:D:279:ILE:HD13	1:D:299:ALA:HB3	1.88	0.56
1:F:150:THR:HG22	1:F:152:ARG:H	1.71	0.56
1:F:162:ALA:HB2	1:F:318:ILE:HG12	1.87	0.56
1:H:16:GLY:HA3	1:H:88:LEU:HD13	1.88	0.56
1:H:153:ILE:HG21	1:H:332:SER:HB3	1.87	0.56
1:A:51:ALA:HA	1:A:70:VAL:HG23	1.89	0.55
1:A:182:VAL:HG22	1:A:254:CYS:SG	2.46	0.55
1:C:247:SER:CB	1:D:352:PRO:O	2.55	0.55
1:D:44:ALA:O	1:D:45:LEU:HD23	2.06	0.55
1:D:74:GLU:O	1:D:78:LEU:HD13	2.06	0.55
1:D:135:TYR:CZ	1:D:156:PRO:HB3	2.42	0.55
1:F:211:TYR:O	1:F:241:PRO:HG2	2.07	0.55
1:H:78:LEU:HD12	1:H:78:LEU:H	1.71	0.55
1:F:22:GLY:O	1:F:26:LEU:HG	2.05	0.55
1:E:55:LEU:HD23	1:E:65:LEU:O	2.06	0.55
1:G:352:PRO:CG	1:H:20:TYR:CE1	2.90	0.55
1:C:132:SER:O	1:C:132:SER:OG	2.25	0.55
1:D:118:ALA:HA	1:D:129:HIS:ND1	2.22	0.55
1:G:249:GLY:N	1:G:320:ASN:OD1	2.21	0.55
1:H:231:THR:HG23	1:H:233:ARG:H	1.71	0.55
1:B:115:LEU:HA	1:B:225:GLN:NE2	2.21	0.55
1:E:162:ALA:HB2	1:E:318:ILE:HD11	1.88	0.55
1:E:182:VAL:HG22	1:E:254:CYS:HB3	1.88	0.55
1:B:259:ARG:H	1:B:259:ARG:HD2	1.70	0.55
1:E:55:LEU:HB3	1:E:66:ALA:HA	1.89	0.55
1:E:100:LEU:HD12	1:E:101:SER:H	1.71	0.55
1:E:352:PRO:O	1:F:247:SER:CB	2.55	0.55
1:G:177:GLU:O	1:G:179:ALA:N	2.37	0.55
1:A:204:VAL:O	1:A:245:PRO:HG3	2.06	0.55
1:C:319:ASP:HB3	1:C:322:VAL:HB	1.89	0.55



A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:E:291:GLY:O	1:E:351:ALA:CB	2.45	0.55
1:G:61:HIS:CG	1:H:351:ALA:HB2	2.42	0.55
1:C:10:THR:HA	1:C:82:ASP:OD2	2.07	0.55
1:F:231:THR:HG22	1:F:233:ARG:H	1.71	0.55
1:G:24:GLU:CD	1:G:27:ARG:HE	2.10	0.54
1:A:147:LEU:O	1:A:149:GLY:N	2.40	0.54
1:B:326:ALA:O	1:B:329:ALA:N	2.39	0.54
1:E:288:PRO:HB3	1:E:300:HIS:HB3	1.90	0.54
1:F:322:VAL:HA	1:F:327:GLY:H	1.73	0.54
1:G:170:ALA:HB3	1:G:176:ILE:HD13	1.88	0.54
1:F:108:ASP:OD1	1:F:110:GLY:N	2.32	0.54
1:F:159:TYR:CB	1:F:160:PRO:CD	2.85	0.54
1:G:24:GLU:OE2	1:G:27:ARG:NE	2.29	0.54
1:B:199:LEU:O	1:D:201:GLY:N	2.40	0.54
1:G:291:GLY:O	1:G:351:ALA:HB2	2.08	0.54
1:B:12:VAL:HG12	1:B:41:ARG:O	2.08	0.54
1:H:107:ILE:HG12	1:H:153:ILE:HD12	1.90	0.54
1:H:178:PRO:HB2	1:H:235:VAL:HA	1.89	0.54
1:A:315:ILE:HD11	1:D:213:ILE:HD13	1.88	0.54
1:E:220:THR:HG22	1:E:239:PHE:CB	2.37	0.54
1:C:134:PRO:HD2	1:C:152:ARG:O	2.08	0.54
1:E:220:THR:OG1	1:E:221:PRO:HD3	2.07	0.54
1:F:185:VAL:HG12	1:F:242:VAL:HB	1.89	0.54
1:C:250:ILE:HG13	1:C:320:ASN:HB3	1.89	0.53
1:C:303:VAL:HG12	1:C:314:ALA:HA	1.90	0.53
1:H:273:TYR:CD2	1:H:279:ILE:HG21	2.42	0.53
1:B:180:VAL:HG23	1:B:237:VAL:HG22	1.90	0.53
1:H:112:ASP:HA	1:H:121:TRP:CH2	2.43	0.53
1:A:170:ALA:HB2	1:A:269:TYR:CE1	2.43	0.53
1:B:296:SER:O	1:B:322:VAL:HG21	2.08	0.53
1:D:59:HIS:HB3	1:D:61:HIS:CE1	2.43	0.53
1:H:30:LEU:HD21	1:H:65:LEU:HG	1.89	0.53
1:H:335:LEU:CD1	1:H:341:GLU:HB2	2.39	0.53
1:B:63:THR:OG1	1:B:64:PRO:HD3	2.08	0.53
1:C:121:TRP:NE1	1:C:128:SER:O	2.41	0.53
1:E:228:ARG:HH11	1:E:235:VAL:HB	1.73	0.53
1:F:17:ALA:O	1:F:59:HIS:NE2	2.42	0.53
1:F:256:ALA:O	1:F:312:PHE:N	2.36	0.53
1:E:125:TYR:HA	1:E:218:ARG:NH1	2.24	0.53
1:A:167:LEU:HD21	1:A:254:CYS:HB3	1.90	0.53
1:G:335:LEU:HD21	1:G:341:GLU:OE1	2.09	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:348:VAL:CG1	1:H:61:HIS:O	2.57	0.53
1:E:153:ILE:O	1:E:153:ILE:HG22	2.07	0.53
1:H:225:GLN:HG3	1:H:226:GLY:N	2.24	0.53
1:B:21:ALA:O	1:B:25:ILE:HG13	2.09	0.53
1:C:158:CYS:HB2	1:C:250:ILE:CD1	2.39	0.53
1:D:137:LEU:HD22	1:D:140:LEU:HG	1.91	0.53
1:A:117:ASP:OD1	1:A:118:ALA:N	2.42	0.52
1:B:160:PRO:HD3	1:B:219:HIS:ND1	2.25	0.52
1:A:52:GLY:H	1:A:70:VAL:HG23	1.74	0.52
1:A:312:PHE:CZ	1:A:314:ALA:HB2	2.43	0.52
1:B:288:PRO:HB3	1:B:300:HIS:HB2	1.90	0.52
1:B:26:LEU:HD11	1:B:45:LEU:HD13	1.90	0.52
1:B:322:VAL:HG23	1:B:323:LYS:N	2.20	0.52
1:E:288:PRO:HD2	1:E:315:ILE:CD1	2.28	0.52
1:E:266:ARG:NH2	1:E:284:GLU:HG3	2.24	0.52
1:E:312:PHE:CZ	1:E:314:ALA:HB2	2.45	0.52
1:H:73:THR:O	1:H:73:THR:OG1	2.24	0.52
1:F:203:GLU:OE2	1:H:20:TYR:OH	2.26	0.52
1:H:162:ALA:HB1	1:H:252:ALA:HB2	1.92	0.52
1:A:157:GLY:CA	1:A:219:HIS:CE1	2.82	0.52
1:A:122:GLU:OE2	1:A:129:HIS:HB2	2.09	0.52
1:B:15:ALA:HA	1:B:46:THR:OG1	2.09	0.52
1:C:139:GLU:HG2	1:C:279:ILE:HD13	1.91	0.51
1:E:138:PRO:O	1:E:144:ARG:HB2	2.10	0.51
1:A:290:THR:O	1:A:293:VAL:HG22	2.10	0.51
1:B:194:ALA:O	1:B:196:THR:HG23	2.11	0.51
1:F:16:GLY:HA2	1:F:47:ALA:HB2	1.92	0.51
1:F:182:VAL:HG12	1:F:254:CYS:HB3	1.92	0.51
1:A:244:ILE:O	1:A:246:ALA:N	2.42	0.51
1:D:325:THR:HG22	1:D:326:ALA:N	2.25	0.51
1:C:262:LEU:HD13	1:C:305:VAL:HG23	1.91	0.51
1:F:322:VAL:HG13	1:F:327:GLY:HA3	1.91	0.51
1:C:48:ALA:O	1:C:50:SER:N	2.43	0.51
1:D:253:THR:HG22	1:D:253:THR:O	2.10	0.51
1:G:183:VAL:O	1:G:253:THR:N	2.42	0.51
1:G:185:VAL:HG12	1:G:242:VAL:HB	1.92	0.51
1:C:147:LEU:CD2	1:C:153:ILE:HG12	2.40	0.51
1:C:159:TYR:HB2	1:C:160:PRO:HD3	1.92	0.51
1:F:183:VAL:HG21	1:G:183:VAL:HG21	1.91	0.51
1:A:282:MET:CE	1:A:288:PRO:HA	2.36	0.51
1:B:195:ALA:HA	1:D:200:LEU:HD21	1.91	0.51



	ous puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:261:PRO:HD2	1:B:264:GLN:HB2	1.93	0.51
1:B:105:LEU:HD22	1:B:337:LEU:HD21	1.93	0.51
1:B:340:PRO:O	1:B:343:ASP:HB2	2.10	0.51
1:D:41:ARG:HG3	1:D:41:ARG:HH11	1.74	0.51
1:G:323:LYS:O	1:G:328:ALA:HB2	2.11	0.51
1:A:97:ALA:HB1	1:A:133:TRP:HH2	1.76	0.51
1:C:282:MET:SD	1:C:300:HIS:HB3	2.51	0.51
1:C:335:LEU:HG	1:C:341:GLU:HG3	1.93	0.51
1:B:266:ARG:HD2	1:B:303:VAL:HG23	1.93	0.50
1:G:252:ALA:HB3	1:G:316:ALA:HB3	1.91	0.50
1:E:25:ILE:O	1:E:29:LEU:HG	2.12	0.50
1:C:92:HIS:ND1	1:C:92:HIS:N	2.59	0.50
1:A:59:HIS:CE1	1:A:193:ARG:NH1	2.80	0.50
1:A:160:PRO:HD2	1:A:219:HIS:ND1	2.26	0.50
1:B:102:PRO:O	1:B:152:ARG:NH1	2.44	0.50
1:F:102:PRO:HA	1:F:152:ARG:HH22	1.76	0.50
1:G:294:ILE:HA	1:G:319:ASP:HB2	1.94	0.50
1:B:151:ARG:O	1:B:152:ARG:HD3	2.12	0.50
1:C:89:PRO:HD2	1:C:92:HIS:CD2	2.47	0.50
1:B:21:ALA:HB3	1:B:87:ALA:HB1	1.93	0.50
1:C:253:THR:HA	1:C:315:ILE:HD13	1.93	0.50
1:D:185:VAL:HG22	1:D:251:LEU:HB3	1.93	0.50
1:F:231:THR:HG22	1:F:233:ARG:N	2.27	0.50
1:B:9:ALA:HA	1:B:39:ARG:O	2.11	0.50
1:B:170:ALA:O	1:B:176:ILE:HG12	2.11	0.50
1:C:323:LYS:NZ	1:C:331:GLN:OE1	2.43	0.50
1:E:85:PHE:O	1:E:86:LEU:HD23	2.11	0.50
1:E:250:ILE:HG13	1:E:320:ASN:HB3	1.93	0.50
1:F:209:ARG:HB2	1:G:289:ARG:HB3	1.94	0.50
1:A:124:PHE:CE2	1:A:221:PRO:HD3	2.47	0.49
1:C:158:CYS:HB2	1:C:250:ILE:HD11	1.91	0.49
1:E:64:PRO:HB2	1:E:65:LEU:HD12	1.92	0.49
1:E:155:VAL:CG1	1:E:156:PRO:HD2	2.23	0.49
1:G:42:ILE:HD13	1:G:65:LEU:HD11	1.93	0.49
1:H:46:THR:OG1	1:H:73:THR:HG22	2.11	0.49
1:H:133:TRP:HB2	1:H:154:ALA:HB2	1.94	0.49
1:A:135:TYR:OH	1:A:156:PRO:HB3	2.13	0.49
1:G:288:PRO:HD3	1:G:302:ALA:HB2	1.93	0.49
1:A:10:THR:O	1:A:40:LEU:HA	2.13	0.49
1:B:103:GLU:O	1:B:151:ARG:NH2	2.46	0.49
1:B:159:TYR:HB2	1:B:160:PRO:HD3	1.93	0.49



	lous puge	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap(Å)
1:F:282:MET:HG3	1:F:288:PBO:HG3	1.93	0.49
1:H:282:MET:CE	1:H:300:HIS:HB3	2.43	0.49
1:A:116:THR:HG22	1:A:132:SER:HB2	1.93	0.49
1:B:53:SER:CB	1:B:58:HIS:HE1	2.25	0.49
1:C:105:LEU:HD11	1:C:153:ILE:HD12	1.93	0.49
1:G:173:ALA:HB3	1:G:175:LEU:HD11	1.95	0.49
1:A:95:VAL:O	1:A:98:GLN:N	2.46	0.49
1:B:49:THR:O	1:B:49:THR:OG1	2.28	0.49
1:B:135:TYR:OH	1:B:156:PRO:HB3	2.13	0.49
1:F:333:MET:O	1:F:337:LEU:HD12	2.13	0.49
1:E:114:ARG:HD3	1:E:222:GLU:OE2	2.13	0.49
1:E:266:ARG:O	1:E:270:GLU:HG3	2.13	0.49
1:F:176:ILE:HA	1:F:258:THR:HA	1.95	0.49
1:G:182:VAL:HG13	1:G:254:CYS:SG	2.53	0.49
1:A:105:LEU:CD1	1:A:336:ALA:CB	2.83	0.48
1:A:109:CYS:HA	1:A:155:VAL:HB	1.95	0.48
1:A:137:LEU:O	1:A:139:GLU:N	2.44	0.48
1:A:148:ARG:HA	1:A:335:LEU:O	2.13	0.48
1:C:159:TYR:CG	1:C:239:PHE:HZ	2.31	0.48
1:E:14:VAL:CG2	1:E:45:LEU:HA	2.30	0.48
1:E:169:PRO:HB2	1:E:269:TYR:CZ	2.47	0.48
1:H:170:ALA:HB2	1:H:269:TYR:HE1	1.78	0.48
1:A:134:PRO:HD2	1:A:152:ARG:O	2.12	0.48
1:A:158:CYS:HB2	1:A:250:ILE:CD1	2.42	0.48
1:D:182:VAL:HG22	1:D:254:CYS:CB	2.42	0.48
1:E:34:ALA:HB1	1:E:39:ARG:HB2	1.94	0.48
1:E:61:HIS:HB2	1:F:349:GLY:HA3	1.95	0.48
1:E:348:VAL:HG23	1:E:348:VAL:O	2.12	0.48
1:F:331:GLN:HB2	1:F:345:LEU:HD11	1.95	0.48
1:A:115:LEU:HD12	1:A:121:TRP:HB2	1.93	0.48
1:D:278:PHE:N	1:D:278:PHE:CD1	2.81	0.48
1:H:217:HIS:O	1:H:220:THR:HG23	2.12	0.48
1:A:105:LEU:HD12	1:A:150:THR:O	2.13	0.48
1:F:257:ARG:HA	1:F:311:THR:HA	1.95	0.48
1:A:86:LEU:HB2	1:A:108:ASP:HA	1.94	0.48
1:B:251:LEU:HB2	1:B:290:THR:CG2	2.44	0.48
1:B:313:VAL:HG21	1:C:214:ALA:HB2	1.96	0.48
1:F:290:THR:CB	1:G:208:ALA:H	2.27	0.48
1:H:47:ALA:C	1:H:73:THR:HG23	2.34	0.48
1:F:210:ALA:HB3	1:G:315:ILE:HD13	1.96	0.48
1:H:135:TYR:OH	1:H:156:PRO:HB3	2.12	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:24:GLU:CD	1:B:248:ARG:HH22	2.17	0.48
1:A:195:ALA:HB2	1:C:197:THR:HG22	1.95	0.47
1:A:232:ASP:N	1:A:232:ASP:OD1	2.47	0.47
1:E:193:ARG:O	1:E:193:ARG:HG2	2.13	0.47
1:E:195:ALA:HA	1:G:200:LEU:HD21	1.96	0.47
1:D:269:TYR:O	1:D:273:TYR:HB2	2.14	0.47
1:D:289:ARG:HG3	1:D:292:ALA:H	1.78	0.47
1:E:150:THR:O	1:E:336:ALA:HB1	2.15	0.47
1:H:24:GLU:HG3	1:H:24:GLU:O	2.14	0.47
1:A:211:TYR:CE1	1:A:241:PRO:HB2	2.49	0.47
1:G:108:ASP:O	1:G:155:VAL:HG23	2.14	0.47
1:H:92:HIS:CG	1:H:92:HIS:O	2.67	0.47
1:H:144:ARG:CG	1:H:335:LEU:HD21	2.42	0.47
1:E:236:SER:HB3	1:H:309:ALA:HA	1.96	0.47
1:E:288:PRO:HD3	1:E:302:ALA:HB3	1.96	0.47
1:G:132:SER:O	1:G:133:TRP:CD1	2.68	0.47
1:B:213:ILE:HG22	1:B:240:THR:HG23	1.95	0.47
1:D:105:LEU:HD12	1:D:151:ARG:HA	1.96	0.47
1:F:251:LEU:HD12	1:F:316:ALA:O	2.14	0.47
1:G:34:ALA:O	1:G:40:LEU:N	2.47	0.47
1:B:330:VAL:HG13	1:B:333:MET:HE2	1.95	0.47
1:C:168:PHE:CD2	1:C:169:PRO:HD3	2.50	0.47
1:H:14:VAL:HG12	1:H:17:ALA:HB2	1.97	0.47
1:H:150:THR:OG1	1:H:151:ARG:N	2.47	0.47
1:A:191:ALA:HB3	1:A:199:LEU:HD11	1.96	0.47
1:C:96:LEU:HD22	1:C:96:LEU:HA	1.76	0.47
1:D:13:ALA:HB3	1:D:84:VAL:HG22	1.97	0.47
1:D:252:ALA:O	1:D:315:ILE:HA	2.15	0.47
1:D:322:VAL:O	1:D:327:GLY:N	2.47	0.47
1:H:141:PRO:C	1:H:143:ALA:H	2.18	0.47
1:A:183:VAL:HB	1:D:183:VAL:HG11	1.96	0.47
1:B:255:THR:HA	1:B:312:PHE:O	2.14	0.47
1:C:261:PRO:HD2	1:C:264:GLN:OE1	2.15	0.47
1:D:29:LEU:HA	1:D:32:HIS:HB2	1.97	0.47
1:F:26:LEU:HG	1:F:26:LEU:H	1.56	0.47
1:F:28:LEU:O	1:F:31:GLY:N	2.48	0.47
1:F:182:VAL:HA	1:F:253:THR:O	2.15	0.47
1:E:109:CYS:HA	1:E:155:VAL:CG2	2.43	0.47
1:A:73:THR:HG23	1:A:78:LEU:HD11	1.97	0.46
1:A:109:CYS:HB3	1:A:325:THR:HG23	1.97	0.46
1:B:228:ARG:HG2	1:B:235:VAL:HB	1.97	0.46



	Interstomic		Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:E:135:TYR:OH	1:E:156:PRO:HB3	2.13	0.46
1:E:322:VAL:HG13	1:E:323:LYS:N	2.29	0.46
1:H:138:PRO:HG2	1:H:331:GLN:HG2	1.96	0.46
1:A:24:GLU:HG2	1:A:321:LEU:HB3	1.96	0.46
1:A:77:VAL:O	1:A:81:HIS:HE1	1.97	0.46
1:D:213:ILE:O	1:D:216:VAL:HG22	2.15	0.46
1:D:350:VAL:HG12	1:D:350:VAL:O	2.15	0.46
1:G:166:ALA:HB1	1:G:314:ALA:HB1	1.98	0.46
1:A:112:ASP:HA	1:A:121:TRP:CH2	2.51	0.46
1:B:67:HIS:CD2	1:B:67:HIS:H	2.32	0.46
1:H:29:LEU:O	1:H:32:HIS:N	2.47	0.46
1:A:98:GLN:O	1:A:99:GLN:CG	2.61	0.46
1:A:167:LEU:HD21	1:A:254:CYS:CB	2.46	0.46
1:B:20:TYR:CZ	1:B:193:ARG:HG3	2.50	0.46
1:C:158:CYS:CB	1:C:250:ILE:HD11	2.45	0.46
1:E:193:ARG:NH2	1:G:203:GLU:OE1	2.48	0.46
1:E:296:SER:HB2	1:E:346:SER:O	2.15	0.46
1:H:220:THR:N	1:H:221:PRO:HD2	2.30	0.46
1:D:251:LEU:HB2	1:D:290:THR:CG2	2.45	0.46
1:E:221:PRO:HA	1:E:224:ALA:HB3	1.97	0.46
1:F:286:GLN:O	1:F:287:LEU:HD12	2.15	0.46
1:G:63:THR:OG1	1:G:64:PRO:HD3	2.15	0.46
1:G:162:ALA:HA	1:G:165:LEU:HD12	1.97	0.46
1:A:279:ILE:HD12	1:A:299:ALA:HB3	1.96	0.46
1:G:118:ALA:O	1:G:122:GLU:HG3	2.16	0.46
1:H:101:SER:HB3	1:H:104:THR:OG1	2.16	0.46
1:B:25:ILE:HG21	1:B:85:PHE:CD2	2.51	0.46
1:B:148:ARG:HA	1:B:335:LEU:O	2.16	0.46
1:E:346:SER:HB2	1:E:348:VAL:HG22	1.97	0.46
1:G:276:GLU:OE2	1:G:276:GLU:HA	2.15	0.46
1:B:61:HIS:CE1	1:B:62:LEU:HD21	2.51	0.46
1:B:251:LEU:HB2	1:B:290:THR:HG23	1.98	0.46
1:B:259:ARG:HD2	1:B:259:ARG:N	2.31	0.46
1:E:63:THR:N	1:E:64:PRO:HD2	2.30	0.46
1:G:13:ALA:HB2	1:G:81:HIS:CG	2.51	0.46
1:C:24:GLU:HA	1:C:24:GLU:OE1	2.15	0.46
1:F:86:LEU:N	1:F:107:ILE:O	2.31	0.46
1:H:92:HIS:O	1:H:92:HIS:ND1	2.49	0.46
1:H:94:ALA:HB3	1:H:113:PHE:CE2	2.50	0.46
1:C:178:PRO:HB2	1:C:235:VAL:HA	1.98	0.45
1:F:13:ALA:HA	1:F:44:ALA:O	2.17	0.45



	to do pago	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:G:228:ARG:HA	1:G:231:THR:HG22	1.98	0.45		
1:G:325:THR:HG23	1:G:326:ALA:N 2.31		0.45		
1:H:212:ASN:HB2	1:H:217:HIS:HD2	1.80	0.45		
1:A:251:LEU:HD22	1:D:208:ALA:O	2.15	0.45		
1:H:28:LEU:HD22	1:H:345:LEU:HD23	1.98	0.45		
1:H:215:GLY:C	1:H:217:HIS:H	2.19	0.45		
1:H:282:MET:HB2	1:H:302:ALA:HB2	1.99	0.45		
1:C:90:HIS:O	1:C:90:HIS:CG	2.70	0.45		
1:C:125:TYR:O	1:C:127:SER:N	2.50	0.45		
1:D:219:HIS:O	1:D:223:ILE:HD12	2.16	0.45		
1:H:322:VAL:HG23	1:H:323:LYS:N	2.24	0.45		
1:A:129:HIS:ND1	1:A:130:ALA:N	2.65	0.45		
1:A:343:ASP:O	1:A:345:LEU:HD12	2.17	0.45		
1:B:10:THR:HG22	1:B:82:ASP:OD2	2.17	0.45		
1:B:47:ALA:HB3	1:B:50:SER:HB3	1.98	0.45		
1:B:109:CYS:HA	1:B:155:VAL:HB	1.98	0.45		
1:B:266:ARG:HH22	1:B:284:GLU:HB2	1.81	0.45		
1:B:329:ALA:O	1:B:333:MET:HB2	2.17	0.45		
1:F:278:PHE:CZ	1:F:345:LEU:HD12	2.51	0.45		
1:C:188:THR:HG22	1:C:243:LEU:HD22	1.99	0.45		
1:D:147:LEU:HA	1:D:147:LEU:HD23	1.71	0.45		
1:A:252:ALA:O	1:A:315:ILE:HA	2.17	0.45		
1:B:223:ILE:HG22	1:B:227:LEU:HD12	1.99	0.45		
1:C:116:THR:HG23	1:C:225:GLN:NE2	2.31	0.45		
1:E:168:PHE:N	1:E:169:PRO:CD	2.79	0.45		
1:G:61:HIS:CG	1:H:351:ALA:HB3	2.50	0.45		
1:A:155:VAL:HA	1:A:156:PRO:HD3	1.83	0.45		
1:C:253:THR:HG23	1:C:315:ILE:CD1	2.47	0.45		
1:F:139:GLU:OE2	1:F:331:GLN:NE2	2.27	0.45		
1:F:164:LEU:N	1:F:164:LEU:HD23	2.30	0.45		
1:E:14:VAL:HG23	1:E:44:ALA:O	2.17	0.45		
1:F:290:THR:HB	1:G:207:SER:HA	1.98	0.45		
1:H:281:LEU:O	1:H:283:PRO:HD3	2.16	0.45		
1:B:175:LEU:HD22	1:B:260:SER:HB3	1.99	0.45		
1:C:177:GLU:HG2	1:C:257:ARG:O	2.17	0.45		
1:C:197:THR:HA	1:C:200:LEU:HG	1.99	0.45		
1:E:100:LEU:HD23	1:E:106:ILE:HG21	1.98	0.45		
1:E:135:TYR:CE2	1:E:156:PRO:HB3	2.51	0.45		
1:F:273:TYR:CD1	1:F:279:ILE:HG21	2.52	0.45		
1:H:168:PHE:CD2	1:H:169:PRO:HD3	2.52	0.45		
1:E:106:ILE:O	1:E:106:ILE:HG13	2.17	0.44		



	Interstomic		
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:F:303:VAL:HB	1:F:312:PHE:CE1	2.51	0.44
1:C:237:VAL:HG12	1:C:239:PHE:HB2	1.99	0.44
1:C:280:TYR:HB3	1:C:300:HIS:ND1	2.32	0.44
1:E:288:PRO:HB3	1:E:300:HIS:HB2	1.97	0.44
1:E:319:ASP:C	1:E:321:LEU:H	2.20	0.44
1:F:198:ASP:OD1	1:F:198:ASP:N	2.51	0.44
1:A:322:VAL:HG12	1:A:327:GLY:HA3	2.00	0.44
1:C:295:GLY:N	1:C:319:ASP:OD2	2.43	0.44
1:C:351:ALA:HA	1:C:352:PRO:HA	1.76	0.44
1:D:49:THR:O	1:D:50:SER:C	2.55	0.44
1:D:155:VAL:HG21	1:D:329:ALA:HB2	1.99	0.44
1:D:218:ARG:O	1:D:221:PRO:HD2	2.17	0.44
1:H:159:TYR:CG	1:H:239:PHE:HZ	2.35	0.44
1:H:326:ALA:O	1:H:329:ALA:HB3	2.18	0.44
1:G:306:ASP:OD2	1:G:309:ALA:N	2.45	0.44
1:C:322:VAL:HG12	1:C:323:LYS:N	2.33	0.44
1:E:158:CYS:HB2	1:E:250:ILE:CD1	2.47	0.44
1:G:88:LEU:N	1:G:88:LEU:HD23	2.33	0.44
1:C:109:CYS:HA	1:C:155:VAL:HB	1.99	0.44
1:C:120:VAL:HG23	1:C:121:TRP:H	1.83	0.44
1:C:273:TYR:CD1	1:C:279:ILE:HG21	2.53	0.44
1:H:86:LEU:HB2	1:H:108:ASP:OD1	2.18	0.44
1:B:10:THR:O	1:B:41:ARG:N	2.46	0.44
1:D:63:THR:N	1:D:64:PRO:CD	2.80	0.44
1:E:164:LEU:HD21	1:E:223:ILE:HA	1.99	0.44
1:E:182:VAL:HG22	1:E:254:CYS:CB	2.47	0.44
1:E:253:THR:HG22	1:E:315:ILE:CG2	2.47	0.44
1:F:132:SER:O	1:F:133:TRP:CD1	2.71	0.44
1:E:269:TYR:HH	1:E:312:PHE:HZ	1.66	0.44
1:H:109:CYS:O	1:H:114:ARG:NH2	2.51	0.44
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.89	0.44
1:B:112:ASP:HA	1:B:121:TRP:CH2	2.53	0.44
1:A:87:ALA:O	1:A:88:LEU:HG	2.18	0.43
1:E:63:THR:N	1:E:64:PRO:CD	2.81	0.43
1:E:85:PHE:CE1	1:E:329:ALA:HB1	2.52	0.43
1:G:297:ASN:OD1	1:G:327:GLY:HA3	2.18	0.43
1:A:309:ALA:HA	1:D:236:SER:HB2	2.00	0.43
2:B:401:UKK:C10	2:B:401:UKK:C06	2.95	0.43
1:C:90:HIS:ND1	1:C:90:HIS:C	2.71	0.43
1:D:344:GLY:O	1:D:345:LEU:HD23	2.18	0.43
1:E:125:TYR:CG	1:E:218:ARG:NH1	2.86	0.43



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:F:181:THR:O	1:F:254:CYS:HA	2.18	0.43	
1:A:202:ALA:O	1:D:352:PRO:HB2	2.18	0.43	
1:F:330:VAL:HA	1:F:333:MET:HB3	1.99	0.43	
1:H:351:ALA:HA	1:H:352:PRO:HA	1.82	0.43	
1:A:178:PRO:O	1:A:235:VAL:HA	2.19	0.43	
1:A:293:VAL:HG12	1:A:300:HIS:ND1	2.33	0.43	
1:C:88:LEU:HD23	1:C:92:HIS:HD2	1.83	0.43	
1:E:248:ARG:NH1	1:E:319:ASP:OD2	2.50	0.43	
1:A:52:GLY:N	1:A:70:VAL:O	2.52	0.43	
1:C:270:GLU:O	1:C:274:HIS:HB3	2.17	0.43	
1:D:78:LEU:HD23	1:D:84:VAL:HG11	2.01	0.43	
1:E:162:ALA:HB2	1:E:318:ILE:CD1	2.47	0.43	
1:F:61:HIS:O	1:F:63:THR:N	2.49	0.43	
1:G:227:LEU:HD23	1:G:227:LEU:HA	1.73	0.43	
1:C:334:ASN:ND2	1:C:340:PRO:O	2.52	0.43	
1:F:200:LEU:HD11	1:H:195:ALA:HA	1.99	0.43	
1:H:228:ARG:HG2	1:H:235:VAL:CG1	2.48	0.43	
1:A:282:MET:HE1	1:A:300:HIS:CD2	2.54	0.43	
1:C:168:PHE:CG	1:C:169:PRO:HD3	2.54	0.43	
1:D:189:SER:O	1:D:192:GLY:N	2.46	0.43	
1:F:222:GLU:HA	1:F:225:GLN:HB3	1.99	0.43	
1:G:148:ARG:HA	1:G:335:LEU:O	2.17	0.43	
1:B:29:LEU:HD22	1:B:40:LEU:HD21	2.00	0.43	
1:D:32:HIS:CG	1:D:33:PRO:HD2	2.53	0.43	
1:E:207:SER:O	1:E:245:PRO:HD3	2.18	0.43	
1:F:16:GLY:O	1:F:22:GLY:HA3	2.19	0.43	
1:F:179:ALA:HA	1:F:236:SER:OG	2.18	0.43	
1:F:214:ALA:HB1	1:G:306:ASP:N	2.34	0.43	
1:H:111:ALA:O	1:H:113:PHE:N	2.52	0.43	
1:A:32:HIS:ND1	1:A:33:PRO:HD2	2.34	0.43	
1:A:161:THR:HG21	1:A:323:LYS:O	2.18	0.43	
1:B:18:SER:HB2	1:B:58:HIS:CD2	2.54	0.43	
1:E:30:LEU:HD11	1:E:65:LEU:CD1	2.49	0.43	
1:F:238:SER:OG	1:F:238:SER:O	2.35	0.43	
1:G:166:ALA:O	1:G:167:LEU:HD23	2.19	0.43	
1:B:12:VAL:HG13	1:B:42:ILE:HA	2.00	0.43	
1:C:331:GLN:HG3	1:C:341:GLU:HG2	2.01	0.43	
1:E:200:LEU:HD21	1:G:195:ALA:HA	2.01	0.43	
1:E:266:ARG:HH22	1:E:284:GLU:HG3	1.84	0.43	
1:F:125:TYR:CE1	1:F:218:ARG:HB3	2.54	0.43	
1:G:165:LEU:HB3	1:G:301:ILE:HD11	2.00	0.43	



	Interstomic		
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:C:59:HIS:HB3	1:C:61:HIS:CE1	2.54	0.42
1:E:252:ALA:O	1:E:315:ILE:HA	2.18	0.42
1:H:20:TYR:CZ	1:H:193:ARG:HG3	2.53	0.42
1:A:40:LEU:HD23	1:A:41:ARG:N	2.34	0.42
1:A:160:PRO:HD3	1:A:219:HIS:HB3	2.00	0.42
1:A:211:TYR:CZ	1:A:241:PRO:HB2	2.53	0.42
1:C:46:THR:HA	1:C:71:GLU:O	2.19	0.42
1:D:135:TYR:OH	1:D:156:PRO:HB3	2.18	0.42
1:E:14:VAL:CG2	1:E:44:ALA:O	2.66	0.42
1:E:255:THR:HA	1:E:312:PHE:O	2.19	0.42
1:F:108:ASP:O	1:F:155:VAL:N	2.47	0.42
1:G:223:ILE:O	1:G:227:LEU:HB2	2.19	0.42
1:H:118:ALA:O	1:H:122:GLU:HG3	2.18	0.42
1:H:189:SER:C	1:H:191:ALA:H	2.22	0.42
1:A:165:LEU:HB3	1:A:301:ILE:HD11	2.00	0.42
1:B:273:TYR:HB3	1:B:279:ILE:HB	2.00	0.42
1:B:339:TRP:N	1:B:339:TRP:CD1	2.86	0.42
1:G:136:GLY:O	1:G:138:PRO:HD3	2.20	0.42
1:A:85:PHE:HE2	1:A:329:ALA:HB1	1.83	0.42
1:B:32:HIS:ND1	1:B:33:PRO:HD2	2.34	0.42
1:D:278:PHE:N	1:D:278:PHE:HD1	2.18	0.42
1:E:59:HIS:HB2	1:E:62:LEU:HD12	2.02	0.42
1:F:153:ILE:HD13	1:F:153:ILE:HA	1.86	0.42
1:F:253:THR:HG21	1:G:240:THR:HG21	2.01	0.42
1:G:24:GLU:O	1:G:28:LEU:HG	2.19	0.42
1:B:167:LEU:HD21	1:B:254:CYS:HB3	2.01	0.42
1:B:281:LEU:O	1:B:281:LEU:HG	2.20	0.42
1:E:21:ALA:HB3	1:E:87:ALA:HB1	2.00	0.42
1:G:262:LEU:HD11	1:G:266:ARG:NH1	2.35	0.42
1:B:334:ASN:ND2	1:B:341:GLU:O	2.46	0.42
1:E:151:ARG:O	1:E:152:ARG:HD3	2.19	0.42
1:E:319:ASP:C	1:E:321:LEU:N	2.73	0.42
1:F:210:ALA:CB	1:G:315:ILE:CD1	2.97	0.42
1:H:335:LEU:HD11	1:H:341:GLU:OE1	2.19	0.42
1:F:263:SER:OG	1:F:264:GLN:N	2.53	0.42
1:G:157:GLY:C	1:G:160:PRO:HD2	2.40	0.42
1:B:155:VAL:HG11	1:B:325:THR:O	2.20	0.42
1:F:152:ARG:HA	1:F:152:ARG:HD3	1.86	0.42
1:F:185:VAL:HG11	1:G:185:VAL:CG1	2.49	0.42
1:G:43:GLY:HA3	1:G:81:HIS:CD2	2.55	0.42
1:H:134:PRO:HD2	1:H:152:ARG:O	2.19	0.42



		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:C:40:LEU:HG	1:C:41:ARG:N	2.35	0.42	
1:E:55:LEU:HD12	1:E:55:LEU:HA	1.78	0.42	
1:F:273:TYR:HB3	1:F:281:LEU:HD11	2.02	0.42	
1:F:279:ILE:N	1:F:279:ILE:HD12	2.35	0.42	
1:G:280:TYR:C	1:G:281:LEU:HD23	2.40	0.42	
1:B:168:PHE:O	1:B:172:ALA:N	2.47	0.42	
1:C:250:ILE:CG1	1:C:320:ASN:HB3	2.50	0.42	
1:D:211:TYR:HE1	1:D:241:PRO:HB2	1.80	0.42	
1:G:290:THR:O	1:G:293:VAL:HG22	2.20	0.42	
1:C:89:PRO:HB2	1:C:92:HIS:CE1	2.55	0.41	
1:C:257:ARG:HE	1:C:257:ARG:HB3	1.68	0.41	
1:D:168:PHE:CD1	1:D:169:PRO:HD3	2.55	0.41	
1:H:74:GLU:O	1:H:76:ALA:N	2.52	0.41	
1:A:58:HIS:O	1:A:59:HIS:ND1	2.52	0.41	
1:C:211:TYR:O	1:C:241:PRO:HD2	2.21	0.41	
1:D:168:PHE:HE1	1:D:273:TYR:HH	1.67	0.41	
1:E:297:ASN:OD1	1:E:322:VAL:HG22	2.19	0.41	
1:F:340:PRO:HD2	1:F:343:ASP:OD2	2.19	0.41	
1:G:210:ALA:HB2	1:G:242:VAL:HG22	2.02	0.41	
1:H:155:VAL:HA	1:H:156:PRO:HD3	1.94	0.41	
1:B:181:THR:HG23	1:B:238:SER:HB3	2.03	0.41	
1:B:274:HIS:CG	1:B:275:ALA:N	2.89	0.41	
1:D:93:SER:O	1:D:96:LEU:N	2.50	0.41	
1:G:234:ASP:N	1:G:234:ASP:OD1	2.54	0.41	
1:B:183:VAL:HA	1:B:240:THR:O	2.21	0.41	
1:D:41:ARG:HG3	1:D:41:ARG:NH1	2.34	0.41	
1:E:18:SER:O	1:E:59:HIS:NE2	2.53	0.41	
1:F:25:ILE:HG23	1:F:29:LEU:HD13	2.03	0.41	
1:A:208:ALA:O	1:D:290:THR:HG23	2.20	0.41	
1:D:186:SER:HA	1:D:249:GLY:O	2.20	0.41	
1:A:160:PRO:CD	1:A:219:HIS:ND1	2.83	0.41	
1:B:117:ASP:O	1:B:120:VAL:HG22	2.21	0.41	
1:C:266:ARG:O	1:C:269:TYR:N	2.53	0.41	
1:D:95:VAL:O	1:D:99:GLN:HG3	2.20	0.41	
1:E:165:LEU:HD11	1:E:279:ILE:HD12	2.02	0.41	
1:F:17:ALA:O	1:F:59:HIS:CD2	2.73	0.41	
1:F:209:ARG:O	1:F:209:ARG:HG2	2.19	0.41	
1:H:118:ALA:HA	1:H:129:HIS:ND1	2.36	0.41	
1:B:330:VAL:HB	1:B:345:LEU:HD21	2.02	0.41	
1:C:26:LEU:O	1:C:30:LEU:HG	2.21	0.41	
1:D:250:ILE:HG13	1:D:320:ASN:HB3	2.03	0.41	



	Interstomic		
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:G:82:ASP:C	1:G:104:THR:HG23	2.41	0.41
1:H:42:ILE:HG21	1:H:42:ILE:HD13	1.74	0.41
1:B:266:ARG:NH2	1:B:284:GLU:HB2	2.36	0.41
1:D:32:HIS:ND1	1:D:33:PRO:HD2	2.36	0.41
1:E:85:PHE:CD1	1:E:107:ILE:HB	2.56	0.41
1:H:183:VAL:HG22	1:H:240:THR:HB	2.01	0.41
1:A:82:ASP:C	1:A:104:THR:HG23	2.42	0.41
1:B:25:ILE:HG13	1:B:25:ILE:H	1.62	0.41
1:B:273:TYR:CD2	1:B:279:ILE:HG21	2.56	0.41
1:C:73:THR:C	1:C:74:GLU:HG2	2.41	0.41
1:C:150:THR:OG1	1:C:151:ARG:N	2.54	0.41
1:C:166:ALA:HB1	1:C:314:ALA:HB1	2.03	0.41
1:C:269:TYR:HB3	1:C:281:LEU:HD21	2.02	0.41
1:D:220:THR:N	1:D:221:PRO:HD2	2.36	0.41
1:E:282:MET:HE3	1:E:286:GLN:HB3	2.03	0.41
1:E:319:ASP:HB3	1:E:322:VAL:CG1	2.48	0.41
1:F:23:GLY:HA2	1:F:26:LEU:HD12	2.03	0.41
1:G:13:ALA:HB2	1:G:81:HIS:CD2	2.56	0.41
1:G:55:LEU:HD23	1:G:65:LEU:HB3	2.02	0.41
1:H:24:GLU:OE2	1:H:27:ARG:NE	2.52	0.41
1:H:165:LEU:HB3	1:H:301:ILE:HD11	2.03	0.41
1:C:137:LEU:HG	1:C:137:LEU:O	2.21	0.41
1:E:107:ILE:HG23	1:E:153:ILE:HG22	2.03	0.41
1:H:16:GLY:HA3	1:H:88:LEU:CD1	2.50	0.41
1:E:140:LEU:HD23	1:E:141:PRO:O	2.21	0.40
1:A:137:LEU:C	1:A:139:GLU:H	2.23	0.40
1:A:172:ALA:C	1:A:174:ASP:H	2.24	0.40
1:C:55:LEU:O	1:C:55:LEU:HG	2.20	0.40
1:D:159:TYR:HB2	1:D:160:PRO:HD3	2.03	0.40
1:D:255:THR:HA	1:D:312:PHE:O	2.21	0.40
1:E:42:ILE:O	1:E:68:ARG:NH2	2.24	0.40
1:F:213:ILE:HG22	1:F:240:THR:HG23	2.03	0.40
1:H:161:THR:HG21	1:H:323:LYS:O	2.21	0.40
1:B:168:PHE:CD1	1:B:168:PHE:C	2.94	0.40
1:A:34:ALA:HA	1:A:37:ASP:OD1	2.21	0.40
1:E:248:ARG:HB2	1:E:294:ILE:HD12	2.04	0.40
1:F:213:ILE:HB	1:G:313:VAL:HG11	2.04	0.40
1:H:330:VAL:HB	1:H:345:LEU:HD21	2.03	0.40
1:A:98:GLN:O	1:A:98:GLN:CG	2.70	0.40
1:A:162:ALA:HB2	1:A:318:ILE:HD13	2.02	0.40
1:B:213:ILE:HD12	1:C:313:VAL:HG11	2.03	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:MET:HG2	1:B:301:ILE:O	2.22	0.40
1:D:289:ARG:HG3	1:D:292:ALA:N	2.36	0.40
1:E:153:ILE:O	1:E:153:ILE:CG2	2.70	0.40
1:E:177:GLU:HB2	1:E:257:ARG:O	2.21	0.40
1:H:168:PHE:CD1	1:H:168:PHE:C	2.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	P	erc	entile	es
1	А	342/354~(97%)	296 (86%)	34 (10%)	12 (4%)		3	11	
1	В	342/354~(97%)	296~(86%)	41 (12%)	5 (2%)		10	31	
1	С	342/354~(97%)	292 (85%)	41 (12%)	9 (3%)		5	17	
1	D	342/354~(97%)	313 (92%)	28 (8%)	1 (0%)		41	70	
1	Е	342/354~(97%)	293 (86%)	38 (11%)	11 (3%)		4	13	
1	F	342/354~(97%)	295~(86%)	39 (11%)	8 (2%)		6	20	
1	G	342/354~(97%)	294 (86%)	42 (12%)	6 (2%)		8	26	
1	Н	342/354~(97%)	301 (88%)	36 (10%)	5 (2%)		10	31	
All	All	2736/2832 (97%)	2380 (87%)	299 (11%)	57 (2%)		7	22	

All (57) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	194	ALA
1	А	322	VAL
1	В	89	PRO
1	С	49	THR
1	Е	134	PRO



Mol	Chain	Res	Type
1	А	87	ALA
1	А	99	GLN
1	А	148	ARG
1	А	150	THR
1	D	50	SER
1	F	77	VAL
1	F	141	PRO
1	F	275	ALA
1	G	148	ARG
1	G	347	VAL
1	В	129	HIS
1	С	48	ALA
1	C	233	ARG
1	С	337	LEU
1	Е	58	HIS
1	Е	167	LEU
1	Е	259	ARG
1	F	271	LYS
1	G	73	THR
1	Н	30	LEU
1	Н	323	LYS
1	А	48	ALA
1	А	195	ALA
1	В	195	ALA
1	В	342	THR
1	С	126	GLY
1	С	148	ARG
1	Е	21	ALA
1	E	54	THR
1	E	76	ALA
1	E	132	SER
1	E	320	ASN
1	F	43	GLY
1	F	68	ARG
1	F	103	GLU
1	G	325	THR
1	Н	216	VAL
1	В	327	GLY
1	C	89	PRO
1	E	70	VAL
1	A	60	PRO
1	A	343	ASP



Mol	Chain	Res	Type
1	С	178	PRO
1	С	325	THR
1	Ε	71	GLU
1	G	64	PRO
1	А	192	GLY
1	G	322	VAL
1	Н	230	VAL
1	F	245	PRO
1	А	138	PRO
1	Н	322	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	209/255~(82%)	203~(97%)	6 (3%)	42	74
1	В	221/255~(87%)	205~(93%)	16 (7%)	14	37
1	С	231/255~(91%)	212~(92%)	19 (8%)	11	31
1	D	221/255~(87%)	203~(92%)	18 (8%)	11	32
1	Е	203/255~(80%)	187 (92%)	16 (8%)	12	33
1	F	169/255~(66%)	158 (94%)	11 (6%)	17	43
1	G	182/255~(71%)	166 (91%)	16 (9%)	10	28
1	Н	184/255~(72%)	175~(95%)	9(5%)	25	55
All	All	1620/2040~(79%)	1509 (93%)	111 (7%)	15	40

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

Mol	Chain	Res	Type
1	А	60	PRO
1	А	74	GLU
1	А	158	CYS
1	А	168	PHE
1	А	189	SER



Mol	Chain	Res	Type
1	А	232	ASP
1	В	10	THR
1	В	112	ASP
1	В	123	ARG
1	В	132	SER
1	В	158	CYS
1	В	188	THR
1	В	197	THR
1	В	205	ILE
1	В	207	SER
1	В	259	ARG
1	В	260	SER
1	В	266	ARG
1	В	281	LEU
1	В	300	HIS
1	В	343	ASP
1	В	348	VAL
1	С	54	THR
1	С	88	LEU
1	С	90	HIS
1	С	92	HIS
1	С	96	LEU
1	С	132	SER
1	С	135	TYR
1	С	158	CYS
1	С	168	PHE
1	С	186	SER
1	С	198	ASP
1	С	204	VAL
1	С	211	TYR
1	С	236	SER
1	C	251	LEU
1	С	255	THR
1	C	296	SER
1	С	308	ASP
1	C	342	THR
1	D	11	LYS
1	D	54	THR
1	D	82	ASP
1	D	101	SER
1	D	128	SER
1	D	135	TYR



Mol	Chain	Res	Type
1	D	168	PHE
1	D	176	ILE
1	D	180	VAL
1	D	197	THR
1	D	198	ASP
1	D	211	TYR
1	D	250	ILE
1	D	254	CYS
1	D	308	ASP
1	D	320	ASN
1	D	347	VAL
1	D	348	VAL
1	Е	14	VAL
1	Е	39	ARG
1	Е	74	GLU
1	Е	90	HIS
1	Е	145	ASP
1	Е	153	ILE
1	Е	155	VAL
1	Е	158	CYS
1	Е	165	LEU
1	Е	167	LEU
1	Е	168	PHE
1	Е	189	SER
1	Е	270	GLU
1	Е	281	LEU
1	Е	288	PRO
1	Е	350	VAL
1	F	82	ASP
1	F	127	SER
1	F	135	TYR
1	F	155	VAL
1	F	168	PHE
1	F	174	ASP
1	F	209	ARG
1	F	218	ARG
1	F	255	THR
1	F	297	ASN
1	F	300	HIS
1	G	10	THR
1	G	45	LEU
1	G	93	SER



Mol	Chain	Res	Type
1	G	101	SER
1	G	115	LEU
1	G	127	SER
1	G	145	ASP
1	G	168	PHE
1	G	181	THR
1	G	204	VAL
1	G	236	SER
1	G	263	SER
1	G	308	ASP
1	G	320	ASN
1	G	333	MET
1	G	348	VAL
1	Н	10	THR
1	Н	40	LEU
1	Н	92	HIS
1	Н	168	PHE
1	Н	225	GLN
1	Н	235	VAL
1	Н	247	SER
1	Н	296	SER
1	Н	325	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Tuno	Chain	Dog	Link	Bo	ond leng	\mathbf{ths}	В	ond ang	les
	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UKK	В	401	-	$15,\!15,\!15$	1.77	3 (20%)	$19,\!19,\!19$	2.34	8 (42%)

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
2	UKK	В	401	-	-	0/4/4/4	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	В	401	UKK	O08-C05	5.41	1.43	1.36
2	В	401	UKK	C02-N01	2.43	1.46	1.38
2	В	401	UKK	C05-N04	2.21	1.35	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	401	UKK	C03-N04-C05	5.35	121.33	116.63
2	В	401	UKK	C06-C05-N04	-3.94	118.99	124.87
2	В	401	UKK	O08-C05-C06	3.10	121.57	115.35
2	В	401	UKK	C07-C06-C05	2.95	121.53	117.72
2	В	401	UKK	C14-C09-C10	-2.56	116.24	120.18
2	В	401	UKK	C06-C07-C02	-2.42	117.56	120.67
2	В	401	UKK	C07-C02-N01	-2.26	116.71	120.91
2	В	401	UKK	C07-C02-C03	2.01	119.32	116.91

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	401	UKK	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 any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	$Q{<}0.9$
1	А	344/354~(97%)	0.28	11 (3%) 47 37	30, 79, 115, 163	0
1	В	344/354~(97%)	0.14	6 (1%) 70 63	37, 68, 104, 150	0
1	С	344/354~(97%)	0.11	6 (1%) 70 63	30, 68, 103, 158	0
1	D	344/354~(97%)	0.17	5 (1%) 73 67	41, 70, 103, 134	0
1	E	344/354~(97%)	0.47	22 (6%) 19 12	30, 93, 120, 154	0
1	F	344/354~(97%)	0.83	51 (14%) 2 1	68, 117, 149, 198	0
1	G	344/354~(97%)	0.65	36 (10%) 6 3	60, 104, 137, 170	0
1	Н	344/354~(97%)	0.23	12 (3%) 44 34	54, 78, 108, 145	0
All	All	2752/2832 (97%)	0.36	149 (5%) 25 17	30, 84, 130, 198	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	285	GLY	7.1
1	F	51	ALA	6.7
1	F	180	VAL	6.4
1	F	80	GLY	5.5
1	Ε	310	GLN	5.2
1	Е	181	THR	5.1
1	F	325	THR	4.9
1	G	180	VAL	4.8
1	F	324	GLY	4.7
1	В	89	PRO	4.7
1	Е	255	THR	4.4
1	А	87	ALA	4.4
1	G	316	ALA	4.3
1	Н	90	HIS	4.2
1	G	131	GLY	4.2
1	Е	154	ALA	4.2



7NPJ

Mol	Chain	Res Type		RSRZ	
1	G	229	ALA	4.1	
1	В	142	GLY	4.0	
1	F	200	LEU	4.0	
1	Н	97	ALA	4.0	
1	Е	309	ALA	3.9	
1	F	326	ALA	3.8	
1	Е	226	GLY	3.8	
1	F	94	ALA	3.8	
1	F	320	ASN	3.8	
1	А	72	PRO	3.6	
1	F	216	VAL	3.6	
1	В	325	THR	3.5	
1	F	135	TYR	3.5	
1	G	252	ALA	3.4	
1	G	317	ALA	3.4	
1	G	255	THR	3.3	
1	F	311	THR	3.3	
1	С	92	HIS	3.2	
1	G	226	GLY	3.2	
1	А	147	LEU	3.2	
1	Н	268	ALA	3.2	
1	F	231	THR	3.1	
1	F	85	PHE	3.1	
1	G	256	ALA	3.1	
1	F	349	GLY	3.1	
1	G	149	GLY	3.1	
1	F	286	GLN	3.1	
1	Н	311	THR	3.1	
1	G	130	ALA	3.1	
1	G	87	ALA	3.0	
1	G	66	ALA	3.0	
1	Е	311	THR	3.0	
1	F	84	VAL	3.0	
1	F	126	GLY	3.0	
1	F	263	263 SER		
1	H	76	ALA	2.9	
1	F	210 ALA		2.9	
1	F	266 ARG		2.9	
1	F	130	ALA	2.8	
1	F	156	PRO	2.8	
1	E	182	VAL	2.8	
1	F	318	ILE	2.8	



Mol	Chain	Res	Type	RSRZ	
1	Е	258	THR	2.8	
1	G	191	ALA	2.8	
1	Н	91	GLY	2.8	
1	G	325	THR	2.8	
1	G	72	PRO	2.7	
1	F	87	ALA	2.7	
1	F	173	ALA	2.7	
1	F	267	ALA	2.7	
1	F	15	ALA	2.7	
1	F	90	HIS	2.7	
1	G	51	ALA	2.7	
1	Н	94	ALA	2.7	
1	F	141	PRO	2.7	
1	Е	9	ALA	2.7	
1	G	181	THR	2.7	
1	G	63	THR	2.6	
1	А	155	VAL	2.6	
1	Е	295	GLY	2.6	
1	Е	155	VAL	2.6	
1	Н	187	GLY	2.6	
1	D	285 GLY		2.6	
1	F	167 LEU		2.6	
1	Е	275	ALA	2.6	
1	F	230 VAL		2.6	
1	Е	197	THR	2.5	
1	D	345	LEU	2.5	
1	Н	283	PRO	2.5	
1	G	45	LEU	2.5	
1	F	316	ALA	2.5	
1	F	301	ILE	2.5	
1	G	338	GLY	2.5	
1	F	154	ALA	2.5	
1	F	179	ALA	2.5	
1	А	93	SER	2.5	
1	G	127	SER	2.4	
1	F	317	ALA	2.4	
1	G	171	LEU	2.4	
1	G	159	TYR	2.4	
1	G	106	ILE	2.4	
1	А	73	THR	2.4	
1	G	192	GLY	2.4	
1	Е	135	TYR 2.4		



Mol	Chain	Res	Type	RSRZ	
1	G	334	ASN	2.4	
1	Е	168	PHE	2.4	
1	Е	90	HIS	2.3	
1	F	287 LEU		2.3	
1	А	114	ARG	2.3	
1	С	106	ILE	2.3	
1	Е	352	PRO	2.3	
1	В	13	ALA	2.3	
1	F	86	LEU	2.3	
1	В	83	ALA	2.3	
1	Н	253	THR	2.3	
1	F	305	VAL	2.3	
1	Ε	13	ALA	2.3	
1	A	148	ARG	2.3	
1	D	88	LEU	2.2	
1	G	250	ILE	2.2	
1	В	12	VAL	2.2	
1	G	249	GLY	2.2	
1	D	273	TYR	2.2	
1	G	285	GLY	2.2	
1	А	115	LEU	2.2	
1	F	240	THR	2.2	
1	Ε	296	SER	2.2	
1	Н	130	ALA	2.2	
1	G	172	ALA	2.1	
1	G	169	PRO	2.1	
1	F	125	TYR	2.1	
1	F	21	ALA	2.1	
1	F	294	ILE	2.1	
1	G	313	VAL	2.1	
1	С	96	LEU	2.1	
1	F	296	SER	2.1	
1	С	78	LEU	2.1	
1	C	141	PRO	2.1	
1	F	261	PRO	2.1	
1	F	237	VAL	2.1	
1	Н	180	VAL	2.1	
1	G	300	HIS	2.1	
1	A	243	LEU	2.1	
1	E	170	ALA	2.1	
1	G	86	LEU	2.1	
1	D	298	ALA	2.1	



Mol	Chain	Res Type		RSRZ
1	Ε	173	ALA	2.1
1	С	348	VAL	2.1
1	F	74	GLU	2.1
1	F	128	SER	2.0
1	F	132	SER	2.0
1	G	80	GLY	2.0
1	А	309	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UKK	В	401	14/14	0.73	0.35	$63,\!70,\!81,\!89$	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.

