

Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2020 - 01:08 am BST

PDB ID	:	6DHN
Title	:	Bovine glutamate dehydrogenase complexed with $Eu3+$
Authors	:	Smith, T.J.
Deposited on	:	2018-05-20
$\operatorname{Resolution}$:	3.30 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	:	2.11
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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	Λ	500	6%								
	A	382	47%	35%	•• 14%						
	Ð		3%								
1	В	582	47%	35%	•• 14%						
			8%								
1	С	582	46%	36%	•• 14%						
			3%								
1	D	582	48%	34%	•• 14%						
			10%								
1	E	582	45%	37%	•• 14%						
			4%								
1	F	582	45%	36%	• • 14%						



The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLU	А	601	-	-	Х	-
2	GLU	В	601	-	- X		-
2	GLU	С	601	-	- X		-
2	GLU	D	601	_	- X		-
2	GLU	Е	601	-	-	Х	-
2	GLU	F	602	_	-	Х	-
3	GTP	А	602	-	-	Х	-
4	NAI	А	604	_	-	-	Х
4	NAI	С	603	-	-	-	Х
4	NAI	F	601	_	-	-	Х
4	NAI	F	603	-	-	-	Х



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 24276 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	501	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	Π	501	3916	2473	687	737	19	0	0	0
1	р	501	Total	С	Ν	Ο	S	0	0	0
	D	001	3916	2473	687	737	19	0	0	0
1	C	501	Total	С	Ν	Ο	S	0	0	0
		501	3916	2473	687	737	19	0		0
1	р	501	Total	С	Ν	Ο	S	0	0	0
		501	3916	2473	687	737	19	0	0	
1	Б	501	Total	С	Ν	Ο	S	0	0	0
		106	3916	2473	687	737	19	0	0	0
1	1 F	501	Total	С	Ν	Ο	S	0	0	0
		501	3916	2473	687	737	19		U	

• Molecule 1 is a protein called Glutamate dehydrogenase 1, mitochondrial.

• Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).





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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf			
2	Δ	1	Total C N O	0	0			
2 11	±	10 5 1 4	0	0				
2	В	1	Total C N O	0	0			
		1	$10 \ 5 \ 1 \ 4$	0	0			
2	C	C	C	C	1	Total C N O	0	0
			$10 \ 5 \ 1 \ 4$	0				
2	Л	1	Total C N O	0	0			
	D	*	$10 \ 5 \ 1 \ 4$	0	0			
2	E	1	Total C N O	0	0			
		*	$10 \ 5 \ 1 \ 4$	0	0			
2	F	1	Total C N O	0				
	Ľ	r 1	10 5 1 4	0	0			

• Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf			
3	Λ	1	Total	С	Ν	Ο	Р	0	0			
	I	32	10	5	14	3	0	0				
3	В	1	Total	С	Ν	Ο	Р	0	0			
0	D	L	32	10	5	14	3		0			
3	С	C 1	Total	С	Ν	Ο	Р	0	0			
0	U		32	10	5	14	3		0			
3	3 D	П	Л	n	1	Total	С	Ν	Ο	Р	0	0
0		I	32	10	5	14	3	0	0			
3	F	D 1	Total	С	Ν	Ο	Р	0	0			
J	Ľ	Ľ	Ŀ	T	32	10	5	14	3	Ū		



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total 32	C 10	N 5	0 14	Р 3	0	0

• Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf								
4	Λ	1	Total	С	Ν	Ο	Р	0	0								
4	1 11	T	44	21	7	14	2	0	0								
4	Δ	1	Total	С	Ν	Ο	Р	19	0								
	11		44	21	7	14	2	12	0								
	В	1	Total	\mathbf{C}	Ν	Ο	Р	0	0								
	D	T	44	21	7	14	2	0	0								
4	В	1	Total	С	Ν	Ο	Р	11	0								
	D	L	44	21	7	14	2	11									
4	С	C 1	Total	\mathbf{C}	Ν	Ο	Р	16	0								
			44	21	7	14	2										
	C	C	С	С	С	С	С	С	C	1	Total	\mathbf{C}	Ν	Ο	Р	0	0
-		L	44	21	7	14	2	0	0								
4	D	1	Total	С	Ν	Ο	Р	0	0								
		±	44	21	7	14	2	0									
4	D	1	Total	С	Ν	Ο	Р	10	0								
		-	44	21	7	14	2	10									
4	E	1	Total	\mathbf{C}	Ν	Ο	Р	0	0								
	1	44	21	7	14	2	Ŭ										
4	F	1	Total	\mathbf{C}	Ν	Ο	Р	13	0								
	-	-	44	21	7	14	2	10									



001000	nucu jion	i preciouo pu	90						
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	Б	1	Total	С	Ν	Ο	Р	16	0
4	4 F	1	44	21	7	14	2	10	0
4 F	1	Total	С	Ν	Ο	Р	0	0	
	L L		44	21	7	14	2	0	U

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3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.



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• Molecule 1: Glutamate dehydrogenase 1, mitochondrial







• Molecule 1: Glutamate dehydrogenase 1, mitochondrial











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	121.11Å 98.76Å 165.64Å	Depositor
a, b, c, α , β , γ	90.00° 101.55° 90.00°	Depositor
$\mathbf{Bosolution} \left(\overset{\wedge}{\mathbf{A}} \right)$	43.89 - 3.30	Depositor
Resolution (A)	47.44 - 3.23	EDS
% Data completeness	92.3 (43.89-3.30)	Depositor
(in resolution range)	90.2 (47.44-3.23)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.69 (at 3.25 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
D D	0.260 , 0.301	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.260 , 0.302	DCC
R_{free} test set	2842 reflections $(5.10%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	36.0	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.27, 13.5	EDS
L-test for twinning ²	$ \langle L \rangle = 0.43, \langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	24276	wwPDB-VP
Average B, all atoms $(Å^2)$	37.0	wwPDB-VP

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

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



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	Bo	ond lengths	Bond angles		
MOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.46	0/3999	1.06	26/5396~(0.5%)	
1	В	0.48	3/3999~(0.1%)	1.01	21/5396~(0.4%)	
1	С	0.46	2/3999~(0.1%)	0.89	16/5396~(0.3%)	
1	D	0.57	3/3999~(0.1%)	1.45	32/5396~(0.6%)	
1	Е	0.55	6/3999~(0.2%)	1.08	31/5396~(0.6%)	
1	F	0.60	6/3999~(0.2%)	2.03	52/5396~(1.0%)	
All	All	0.52	20/23994~(0.1%)	1.31	178/32376~(0.5%)	

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	15
1	В	0	8
1	С	0	12
1	D	0	14
1	Е	0	14
1	F	2	18
All	All	2	81

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	D	73	GLU	CD-OE1	-15.37	1.08	1.25
1	Е	247	PHE	CG-CD1	-10.53	1.23	1.38
1	F	31	ASP	CG-OD1	-10.08	1.02	1.25
1	D	247	PHE	CG-CD1	-9.71	1.24	1.38
1	F	447	ASP	CG-OD1	-9.37	1.03	1.25
1	Е	38	GLU	CD-OE1	-8.80	1.16	1.25



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Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	Е	205	GLN	CD-OE1	-7.61	1.07	1.24
1	F	471	TYR	CG-CD1	-7.33	1.29	1.39
1	F	63	PHE	CE1-CZ	-6.95	1.24	1.37
1	D	297	GLN	CB-CG	-6.50	1.35	1.52
1	В	19	ARG	CG-CD	-6.33	1.36	1.51
1	В	205	GLN	CD-OE1	-6.27	1.10	1.24
1	Е	38	GLU	CB-CG	-6.24	1.40	1.52
1	С	471	TYR	CG-CD1	-5.68	1.31	1.39
1	F	355	GLU	CB-CG	-5.44	1.41	1.52
1	Ε	36	GLU	CB-CG	-5.41	1.41	1.52
1	В	388	ASN	CG-OD1	-5.23	1.12	1.24
1	С	38	GLU	CD-OE1	-5.21	1.20	1.25
1	F	471	TYR	CE2-CZ	-5.18	1.31	1.38
1	E	73	GLU	CD-OE1	-5.17	1.20	1.25

An (176) bond angle outliers are listed beid	All (78) bond	angle	outliers	are	listed	below
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	F	63	PHE	CB-CG-CD1	77.11	174.77	120.80
1	F	63	PHE	CB-CG-CD2	-59.42	79.20	120.80
1	F	447	ASP	CB-CG-OD1	-47.16	75.86	118.30
1	D	73	GLU	OE1-CD-OE2	-45.39	68.84	123.30
1	D	31	ASP	CB-CG-OD1	44.55	158.39	118.30
1	D	31	ASP	CB-CG-OD2	-31.75	89.72	118.30
1	F	447	ASP	OD1-CG-OD2	-30.56	65.24	123.30
1	В	19	ARG	NE-CZ-NH1	-29.88	105.36	120.30
1	А	261	ARG	NE-CZ-NH1	-28.41	106.10	120.30
1	D	31	ASP	OD1-CG-OD2	-27.36	71.31	123.30
1	F	447	ASP	CB-CG-OD2	25.31	141.08	118.30
1	В	19	ARG	NE-CZ-NH2	24.34	132.47	120.30
1	А	261	ARG	NE-CZ-NH2	23.92	132.26	120.30
1	F	478	ARG	NE-CZ-NH1	-23.37	108.61	120.30
1	Е	50	ARG	NE-CZ-NH2	21.60	131.10	120.30
1	Е	50	ARG	NE-CZ-NH1	-21.18	109.71	120.30
1	Е	217	ARG	NE-CZ-NH1	-21.00	109.80	120.30
1	С	490	PHE	CB-CG-CD2	-20.82	106.22	120.80
1	F	490	PHE	CB-CG-CD2	-20.80	106.24	120.80
1	F	294	PHE	CB-CG-CD2	-20.20	106.66	120.80
1	D	294	PHE	CB-CG-CD2	-20.13	106.71	120.80
1	Е	217	ARG	NE-CZ-NH2	19.79	130.19	120.30
1	F	478	ARG	NE-CZ-NH2	19.74	130.17	120.30
1	D	73	GLU	CG-CD-OE1	-19.36	79.58	118.30



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	455	TYR	CB-CG-CD2	-18.65	109.81	121.00
	F	31	ASP	CB-CG-OD2	18.44	134.89	118.30
1	A	261	ARG	CD-NE-CZ	18.08	148.92	123.60
1	В	19	ARG	CD-NE-CZ	17.69	148.36	123.60
1	A	455	TYR	CB-CG-CD2	-17.54	110.48	121.00
1	F	63	PHE	CD1-CG-CD2	-17.14	96.01	118.30
1	F	19	ARG	NE-CZ-NH1	-15.75	112.42	120.30
1	D	10	PHE	CB-CG-CD2	-15.00	110.30	120.80
1	F	68	ASP	CB-CG-OD1	14.53	131.37	118.30
1	D	295	LYS	CD-CE-NZ	14.23	144.43	111.70
1	F	19	ARG	NE-CZ-NH2	13.33	126.96	120.30
1	F	63	PHE	CG-CD1-CE1	13.08	135.19	120.80
1	F	295	LYS	CD-CE-NZ	12.92	141.41	111.70
1	D	73	GLU	CG-CD-OE2	12.66	143.62	118.30
1	С	19	ARG	NE-CZ-NH2	-11.78	114.41	120.30
1	F	478	ARG	CD-NE-CZ	11.58	139.81	123.60
1	С	19	ARG	NE-CZ-NH1	11.27	125.94	120.30
1	Е	19	ARG	NE-CZ-NH2	-11.27	114.67	120.30
1	F	68	ASP	CB-CG-OD2	-11.09	108.32	118.30
1	F	238	MET	CA-CB-CG	10.93	131.88	113.30
1	А	19	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	Ε	19	ARG	NE-CZ-NH1	10.81	125.70	120.30
1	D	401	TYR	CB-CG-CD2	-10.80	114.52	121.00
1	D	19	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	Ε	50	ARG	CD-NE-CZ	10.70	138.59	123.60
1	F	68	ASP	OD1-CG-OD2	-10.48	103.39	123.30
1	F	457	MET	CA-CB-CG	-10.39	95.63	113.30
1	D	19	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	А	19	ARG	NE-CZ-NH1	10.31	125.45	120.30
1	Е	247	PHE	CD1-CG-CD2	-10.30	104.91	118.30
1	F	50	ARG	CD-NE-CZ	10.14	137.79	123.60
1	F	50	ARG	NE-CZ-NH1	-9.75	115.42	120.30
1	D	247	PHE	CD1-CG-CD2	-9.60	105.82	118.30
1	F	401	TYR	CB-CG-CD2	-9.21	115.47	121.00
1	В	275	GLU	CG-CD-OE2	9.14	136.57	118.30
1	F	471	TYR	CD1-CG-CD2	-9.12	107.86	117.90
1	А	195	HIS	N-CA-CB	-9.00	94.39	110.60
1	А	401	TYR	CB-CG-CD2	-8.96	115.62	121.00
1	F	287	ASP	CB-CG-OD2	-8.96	110.23	118.30
1	F	287	ASP	CB-CG-OD1	8.96	126.36	118.30
1	F	310	TYR	CB-CG-CD2	-8.74	115.76	121.00
1	Ε	217	ARG	CD-NE-CZ	8.39	135.34	123.60



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	$Ideal(^{o})$
1	D	297	GLN	CA-CB-CG	-8.31	95.12	113.40
1	B	275	GLU	CG-CD-OE1	-8.30	101.71	118.30
1	A	295	LYS	CD-CE-NZ	8.28	130.74	111.70
1	Е	455	TYR	CD1-CG-CD2	-8.25	108.82	117.90
1	В	295	LYS	CD-CE-NZ	8.24	130.65	111.70
1	С	295	LYS	CD-CE-NZ	8.22	130.60	111.70
1	Е	295	LYS	CD-CE-NZ	8.19	130.53	111.70
1	С	19	ARG	CD-NE-CZ	7.88	134.64	123.60
1	F	471	TYR	CB-CG-CD2	-7.86	116.28	121.00
1	D	294	PHE	CB-CG-CD1	7.84	126.29	120.80
1	Е	247	PHE	CB-CA-C	7.78	125.97	110.40
1	F	294	PHE	CB-CG-CD1	7.77	126.24	120.80
1	А	402	GLU	OE1-CD-OE2	-7.73	114.02	123.30
1	А	455	TYR	CD1-CG-CD2	-7.70	109.42	117.90
1	Е	78	TYR	CB-CG-CD2	-7.70	116.38	121.00
1	D	262	TYR	CB-CG-CD2	-7.68	116.39	121.00
1	F	19	ARG	CD-NE-CZ	7.65	134.31	123.60
1	F	63	PHE	CG-CD2-CE2	7.63	129.19	120.80
1	Е	247	PHE	N-CA-CB	-7.59	96.94	110.60
1	F	490	PHE	CB-CG-CD1	7.54	126.08	120.80
1	Е	19	ARG	CD-NE-CZ	7.53	134.14	123.60
1	D	446	LYS	CD-CE-NZ	7.52	128.99	111.70
1	А	78	TYR	CB-CG-CD2	-7.52	116.49	121.00
1	В	275	GLU	CB-CG-CD	7.42	134.23	114.20
1	D	247	PHE	CB-CA-C	7.36	125.11	110.40
1	С	490	PHE	CD1-CG-CD2	-7.31	108.80	118.30
1	F	331	LEU	CB-CG-CD2	-7.18	98.80	111.00
1	Е	38	GLU	OE1-CD-OE2	-7.12	114.76	123.30
1	D	247	PHE	N-CA-CB	-7.07	97.87	110.60
1	F	490	PHE	CD1-CG-CD2	-7.07	109.11	118.30
1	F	31	ASP	CB-CA-C	-7.06	96.27	110.40
1	F	31	ASP	CB-CG-OD1	-7.06	111.95	118.30
1	D	10	PHE	CD1-CG-CD2	-7.05	109.13	118.30
1	В	388	ASN	N-CA-CB	-7.04	97.92	110.60
1	D	19	ARG	CD-NE-CZ	6.97	133.36	123.60
1	F	294	PHE	CD1-CG-CD2	-6.97	109.24	118.30
1	С	490	PHE	CB-CA-C	-6.93	96.53	110.40
1	D	294	PHE	CD1-CG-CD2	-6.92	109.31	118.30
1	D	183	TYR	CB-CG-CD2	-6.85	116.89	121.00
1	С	471	TYR	CD1-CG-CD2	-6.81	110.41	117.90
1	В	310	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	С	50	ARG	NE-CZ-NH2	-6.77	116.92	120.30



Continued from previous page							
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Е	247	PHE	CB-CG-CD2	-6.76	116.07	120.80
1	С	490	PHE	CB-CG-CD1	6.75	125.52	120.80
1	А	402	GLU	CA-CB-CG	6.70	128.13	113.40
1	F	183	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	В	183	TYR	CB-CG-CD2	-6.67	117.00	121.00
1	А	19	ARG	CD-NE-CZ	6.63	132.88	123.60
1	А	183	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	С	183	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	D	275	GLU	OE1-CD-OE2	-6.53	115.46	123.30
1	С	38	GLU	OE1-CD-OE2	-6.49	115.51	123.30
1	D	10	PHE	CB-CA-C	-6.47	97.47	110.40
1	В	50	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	Е	183	TYR	CB-CG-CD2	-6.37	117.18	121.00
1	Е	455	TYR	CB-CA-C	-6.36	97.68	110.40
1	А	50	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	Е	78	TYR	CB-CG-CD1	6.32	124.79	121.00
1	В	317	VAL	CG1-CB-CG2	6.25	120.91	110.90
1	А	455	TYR	CB-CA-C	-6.20	97.99	110.40
1	F	501	THR	CA-CB-OG1	6.18	121.97	109.00
1	D	50	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	F	490	PHE	CB-CA-C	-6.17	98.07	110.40
1	В	470	LYS	CD-CE-NZ	6.13	125.81	111.70
1	А	31	ASP	CB-CG-OD1	6.08	123.77	118.30
1	С	50	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	F	317	VAL	CG1-CB-CG2	6.02	120.53	110.90
1	D	470	LYS	CD-CE-NZ	-6.00	97.90	111.70
1	F	31	ASP	OD1-CG-OD2	-5.97	111.96	123.30
1	F	294	PHE	CB-CA-C	-5.94	98.53	110.40
1	D	294	PHE	CB-CA-C	-5.92	98.56	110.40
1	А	471	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	А	78	TYR	CB-CG-CD1	5.84	124.50	121.00
1	F	287	ASP	OD1-CG-OD2	-5.80	112.28	123.30
1	В	102	ASP	CB-CG-OD1	5.80	123.52	118.30
1	Е	205	GLN	CB-CG-CD	5.79	126.66	111.60
1	Е	469	MET	CG-SD-CE	5.72	109.35	100.20
1	D	50	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	В	102	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	F	102	ASP	CB-CG-OD1	5.66	123.39	118.30
1	В	50	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	F	86	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	Е	78	TYR	CA-CB-CG	5.61	124.06	113.40
1	С	291	LEU	CB-CG-CD2	5.60	120.52	111.00



Continued from previous page							
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	78	TYR	CA-CB-CG	5.57	123.98	113.40
1	F	245	LYS	CD-CE-NZ	5.56	124.48	111.70
1	F	102	ASP	OD1-CG-OD2	-5.55	112.75	123.30
1	В	317	VAL	CA-CB-CG1	5.51	119.16	110.90
1	А	471	TYR	CB-CG-CD1	5.49	124.30	121.00
1	Е	317	VAL	CG1-CB-CG2	-5.49	102.12	110.90
1	В	466	ARG	CA-CB-CG	5.44	125.37	113.40
1	F	338	ARG	CG-CD-NE	5.39	123.13	111.80
1	Е	217	ARG	CG-CD-NE	-5.37	100.53	111.80
1	Е	139	ASN	CB-CA-C	-5.31	99.77	110.40
1	Е	447	ASP	CB-CG-OD2	5.31	123.08	118.30
1	С	391	HIS	N-CA-CB	-5.29	101.08	110.60
1	Е	245	LYS	CD-CE-NZ	5.28	123.85	111.70
1	D	471	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	D	401	TYR	CD1-CG-CD2	-5.23	112.15	117.90
1	Е	469	MET	CA-CB-CG	5.23	122.18	113.30
1	F	317	VAL	CA-CB-CG1	5.19	118.69	110.90
1	В	275	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	А	50	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	А	195	HIS	CB-CA-C	5.14	120.68	110.40
1	D	247	PHE	CB-CG-CD2	-5.13	117.21	120.80
1	В	424	HIS	C-N-CA	5.06	132.93	122.30
1	А	32	LEU	CB-CG-CD1	-5.05	102.42	111.00
1	В	78	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	А	406	ASN	N-CA-CB	-5.03	101.54	110.60
1	F	433	THR	CA-CB-OG1	5.02	119.54	109.00
1	С	420	LYS	CD-CE-NZ	5.01	123.23	111.70
1	Е	469	MET	CB-CG-SD	5.00	127.40	112.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	433	THR	CB
1	F	501	THR	CB

All (81) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	183	TYR	Sidechain
1	А	195	HIS	Sidechain
1	А	209	HIS	Sidechain
1	А	221	HIS	Sidechain



6DHN

Mal	Chain	Dec	T -m	Creare
	Chain	nes	Type	Group
1	A	261	ARG	Sidechain
1	A	275	GLU	Sidechain
1	A	31	ASP	Sidechain
1	A	38	GLU	Peptide
1	A	391	HIS	Sidechain
1	А	401	TYR	Sidechain
1	А	402	GLU	Sidechain
1	А	406	ASN	Sidechain
1	А	455	TYR	Sidechain
1	А	490	PHE	Sidechain
1	А	78	TYR	Sidechain
1	В	102	ASP	Sidechain
1	В	139	ASN	Sidechain
1	В	183	TYR	Sidechain
1	В	209	HIS	Sidechain
1	В	221	HIS	Sidechain
1	В	388	ASN	Sidechain
1	В	401	TYR	Sidechain
1	В	78	TYR	Sidechain
1	С	183	TYR	Sidechain
1	С	209	HIS	Sidechain
1	С	35	ARG	Peptide
1	С	38	GLU	Sidechain
1	С	391	HIS	Sidechain
1	С	40	GLN	Peptide
1	С	401	TYR	Sidechain
1	С	455	TYR	Sidechain
1	С	471	TYR	Sidechain
1	С	484	ASN	Sidechain
1	С	490	PHE	Sidechain
1	С	78	TYR	Sidechain
1	D	10	PHE	Sidechain
1	D	183	TYR	Sidechain
1	D	209	HIS	Sidechain
1	D	247	PHE	Sidechain
1	D	262	TYR	Sidechain
1	D	275	GLU	Sidechain
1	D	294	PHE	Sidechain
1	D	297	GLN	Sidechain
1	D	38	GLU	Peptide
1	D	391	HIS	Sidechain
1	D	401	TYR	Sidechain



Mol	Chain	Res	Type	Group
1	D	406	ASN	Sidechain
1	D	490	PHE	Sidechain
1	D	73	GLU	Sidechain
1	Е	139	ASN	Sidechain
1	Е	183	TYR	Sidechain
1	Е	205	GLN	Sidechain
1	Е	209	HIS	Sidechain
1	Е	247	PHE	Sidechain
1	Е	254	ASN	Sidechain
1	Е	340	LYS	Peptide
1	Е	38	GLU	Sidechain,Peptide
1	Е	39	GLU	Peptide
1	Е	401	TYR	Sidechain
1	Е	455	TYR	Sidechain
1	Е	490	PHE	Sidechain
1	Е	78	TYR	Sidechain
1	F	102	ASP	Sidechain
1	F	183	TYR	Sidechain
1	F	19	ARG	Sidechain
1	F	195	HIS	Sidechain
1	F	209	HIS	Sidechain
1	F	226	PHE	Sidechain
1	F	287	ASP	Sidechain
1	F	294	PHE	Sidechain
1	F	310	TYR	Sidechain
1	F	38	GLU	Peptide
1	F	401	TYR	Sidechain
1	F	406	ASN	Sidechain
1	F	432	PRO	Peptide
1	F	471	TYR	Sidechain
1	F	490	PHE	Sidechain
1	F	50	ARG	Sidechain
1	F	68	ASP	Sidechain
1	F	78	TYR	Sidechain

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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	3916	0	3879	210	0
1	В	3916	0	3880	223	0
1	С	3916	0	3879	214	0
1	D	3916	0	3878	209	0
1	Е	3916	0	3879	238	0
1	F	3916	0	3880	224	0
2	А	10	0	5	7	0
2	В	10	0	5	7	0
2	С	10	0	5	4	0
2	D	10	0	5	4	0
2	Ε	10	0	5	6	0
2	F	10	0	5	5	0
3	А	32	0	12	13	0
3	В	32	0	12	2	0
3	С	32	0	12	0	0
3	D	32	0	12	1	0
3	Ε	32	0	12	1	0
3	F	32	0	12	2	0
4	А	88	0	51	11	0
4	В	88	0	51	15	0
4	С	88	0	50	10	0
4	D	88	0	50	9	0
4	Е	44	0	25	10	0
4	F	132	0	75	23	0
All	All	24276	0	23679	1210	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (1210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:604:NAI:O4B	4:C:604:NAI:C1B	1.63	1.23
1:B:458:GLU:OE2	1:B:462:ARG:NH1	1.80	1.12
1:A:463:GLN:HG2	1:A:466:ARG:HH12	1.18	1.09
1:F:38:GLU:HB2	1:F:40:GLN:H	1.19	1.07
1:C:303:GLY:H	1:C:309:ILE:HD11	1.21	1.04
1:A:38:GLU:HB2	1:A:40:GLN:H	1.29	0.97
1:E:339:VAL:O	1:E:340:LYS:HD3	1.66	0.96
1:E:315:LEU:O	1:E:340:LYS:NZ	2.00	0.94
1:C:337:PRO:O	1:C:363:ARG:NH1	2.00	0.94
1:B:30:GLU:O	1:B:33:LYS:NZ	2.02	0.93



		Interatomic Clash			
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:F:337:PRO:O	1:F:363:ARG:NH1	2.02	0.93		
1:B:337:PRO:O	1:B:363:ARG:NH1	2.02	0.92		
1:A:261:ARG:NH2	3:A:602:GTP:O2G	2.02	0.92		
1:D:396:ARG:NH1	1:F:119:ASP:O	2.03	0.92		
1:D:337:PRO:O	1:D:363:ARG:NH1	2.05	0.90		
1:D:3:ARG:NH1	1:D:4:GLU:HG3	1.87	0.90		
1:A:463:GLN:HG2	1:A:466:ARG:NH1	1.87	0.90		
1:E:337:PRO:O	1:E:363:ARG:NH1	2.04	0.90		
1:E:339:VAL:O	1:E:341:ALA:N	2.04	0.89		
1:A:337:PRO:O	1:A:363:ARG:NH1	2.06	0.89		
1:B:221:HIS:CD2	1:B:454:ALA:HA	2.09	0.88		
1:D:374:ASN:HB2	4:D:603:NAI:H5N	1.55	0.86		
2:A:601:GLU:HA	4:A:603:NAI:H4N	1.57	0.85		
1:C:183:TYR:HD1	1:C:187:ILE:HG23	1.40	0.85		
1:E:303:GLY:H	1:E:309:ILE:HD11	1.40	0.85		
1:B:29:VAL:HG21	1:B:42:ARG:HG3	1.58	0.85		
1:A:183:TYR:HD1	1:A:187:ILE:HG23	1.41	0.84		
1:A:29:VAL:HG21	1:A:42:ARG:HG3	1.60	0.83		
1:C:147:ARG:NH1	1:F:499:THR:OG1	2.12	0.83		
1:A:119:ASP:O	1:C:396:ARG:NH1	2.10	0.82		
1:B:488:LYS:HA	1:B:491:ARG:HH12	1.45	0.82		
1:C:29:VAL:HG21	1:C:42:ARG:HG3	1.61	0.82		
1:D:183:TYR:HD1	1:D:187:ILE:HG23	1.41	0.82		
1:B:499:THR:OG1	1:E:147:ARG:NH1	2.12	0.81		
1:E:487:GLU:HG2	1:E:491:ARG:HH12	1.46	0.81		
1:F:28:LEU:HB3	1:F:490:PHE:HE2	1.47	0.80		
1:B:459:ARG:HH21	1:B:463:GLN:NE2	1.79	0.80		
1:A:499:THR:OG1	1:D:147:ARG:NH1	2.14	0.80		
1:B:221:HIS:HD2	1:B:454:ALA:HA	1.44	0.80		
1:C:458:GLU:HG2	1:C:462:ARG:NH1	1.97	0.80		
1:E:462:ARG:NH1	1:E:466:ARG:HH22	1.81	0.79		
1:A:333:LYS:NZ	1:A:355:GLU:OE1	2.13	0.79		
1:E:435:GLU:OE2	1:E:435:GLU:N	2.17	0.78		
1:E:27:LYS:NZ	1:E:31:ASP:OD2	2.16	0.77		
1:E:29:VAL:HG21	1:E:42:ARG:HG3	1.64	0.77		
1:E:322:LEU:HD22	1:E:340:LYS:NZ	2.00	0.77		
1:B:488:LYS:HA	1:B:491:ARG:NH1	1.99	0.77		
1:B:387:LYS:HE2	4:B:604:NAI:H3D	1.67	0.77		
1:C:146:ARG:HH11	1:C:182:THR:HG22	1.50	0.77		
1:A:413:VAL:HG11	1:C:413:VAL:HG13	1.67	0.77		
1:A:146:ARG:HH11	1:A:182:THR:HG22	1.50	0.76		



	lowe page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:147:ARG:NH1	1:D:499:THR:OG1	2.18	0.76	
4:D:604:NAI:H4N	1:E:195:HIS:CD2	2.21	0.76	
1:A:443:ALA:HA	1:C:401:TYR:CE2	2.20	0.76	
1:B:90:LYS:NZ	2:B:601:GLU:OE2	2.19	0.76	
1:F:146:ARG:HH11	1:F:182:THR:HG22	1.50	0.76	
1:E:318:ASP:HA	1:E:340:LYS:HG3	1.67	0.76	
1:B:147:ARG:NH1	1:E:499:THR:OG1	2.18	0.76	
1:F:5:ASP:HB3	1:F:332:THR:HB	1.68	0.76	
4:F:601:NAI:H6N	4:F:601:NAI:H52N	1.68	0.76	
1:D:5:ASP:HB3	1:D:332:THR:HB	1.67	0.75	
1:E:119:ASP:O	1:F:396:ARG:NH1	2.20	0.75	
1:F:34:THR:HG21	1:F:44:ARG:HH22	1.52	0.75	
1:E:339:VAL:C	1:E:340:LYS:HD3	2.07	0.75	
1:A:262:TYR:OH	3:A:602:GTP:O1G	2.03	0.75	
1:C:141:LEU:O	1:C:145:THR:HG23	1.87	0.74	
1:C:190:TYR:OH	1:E:190:TYR:OH	2.06	0.74	
1:A:409:LEU:HD22	1:C:409:LEU:HD21	1.68	0.74	
1:D:146:ARG:HH11	1:D:182:THR:HG22	1.51	0.74	
1:C:183:TYR:CD1	1:C:187:ILE:HG23	2.22	0.73	
1:F:29:VAL:HG21	1:F:42:ARG:HG3	1.70	0.73	
1:B:146:ARG:HH11	1:B:182:THR:HG22	1.51	0.73	
1:A:303:GLY:H	1:A:309:ILE:HD11	1.54	0.73	
1:D:38:GLU:HB2	1:D:40:GLN:H	1.53	0.73	
1:E:247:PHE:CE2	1:E:270:CYS:HA	2.24	0.73	
1:A:5:ASP:HB3	1:A:332:THR:HB	1.68	0.73	
1:C:90:LYS:NZ	2:C:601:GLU:OE1	2.21	0.73	
1:D:183:TYR:CD1	1:D:187:ILE:HG23	2.24	0.73	
1:E:403:ARG:HH11	1:E:441:SER:HG	1.36	0.73	
1:D:141:LEU:O	1:D:145:THR:HG23	1.87	0.73	
1:D:3:ARG:HH12	1:D:4:GLU:HG3	1.50	0.72	
1:B:141:LEU:O	1:B:145:THR:HG23	1.88	0.72	
1:F:90:LYS:NZ	2:F:602:GLU:OE2	2.21	0.72	
1:F:387:LYS:HE2	4:F:603:NAI:H52N	1.70	0.72	
1:E:239:THR:O	1:E:245:LYS:NZ	2.22	0.72	
1:F:38:GLU:HB2	1:F:40:GLN:N	2.01	0.72	
1:F:294:PHE:CE2	1:F:304:PHE:HA	2.25	0.72	
1:C:27:LYS:NZ	1:C:31:ASP:OD2	2.22	0.72	
1:E:141:LEU:O	1:E:145:THR:HG23	1.90	0.72	
1:E:247:PHE:CD2	1:E:270:CYS:HA	2.24	0.72	
1:E:146:ARG:HH11	1:E:182:THR:HG22	1.53	0.72	
1:F:141:LEU:O	1:F:145:THR:HG23	1.90	0.72	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:401:TYR:CE2	1:F:443:ALA:HA	2.25	0.72
1:E:38:GLU:OE2	1:E:40:GLN:OE1	2.07	0.72
1:A:221:HIS:CD2	1:A:454:ALA:HA	2.24	0.72
1:D:294:PHE:CE2	1:D:304:PHE:HA	2.24	0.71
1:A:428:ILE:HG12	1:C:420:LYS:NZ	2.05	0.71
1:F:239:THR:O	1:F:245:LYS:NZ	2.22	0.71
1:A:141:LEU:O	1:A:145:THR:HG23	1.90	0.71
1:D:401:TYR:HE2	1:F:443:ALA:HA	1.54	0.71
1:E:12:MET:HG3	1:E:354:PRO:HD3	1.72	0.71
1:A:183:TYR:CD1	1:A:187:ILE:HG23	2.24	0.71
1:A:265:ARG:NH2	3:A:602:GTP:O3G	2.23	0.71
1:D:247:PHE:CE2	1:D:270:CYS:HA	2.26	0.71
1:C:415:GLU:O	1:C:419:ARG:HG2	1.91	0.70
1:B:337:PRO:HD3	1:B:359:ILE:HD13	1.72	0.70
1:F:280:ILE:HD11	1:F:291:LEU:HD11	1.73	0.70
2:A:601:GLU:HA	4:A:603:NAI:C4N	2.21	0.70
1:A:265:ARG:HH22	3:A:602:GTP:PG	2.15	0.70
1:E:5:ASP:HB3	1:E:332:THR:HB	1.74	0.70
1:A:90:LYS:NZ	2:A:601:GLU:OE1	2.23	0.70
1:B:38:GLU:HG3	1:B:40:GLN:HB3	1.74	0.69
1:A:206:GLY:HA2	4:A:604:NAI:H3D	1.74	0.69
1:B:12:MET:HG3	1:B:354:PRO:HD3	1.75	0.69
1:B:459:ARG:HH21	1:B:463:GLN:HE21	1.38	0.69
1:A:499:THR:HG1	1:D:147:ARG:HH12	1.39	0.69
1:E:463:GLN:HA	1:E:466:ARG:HH11	1.58	0.69
1:A:65:ILE:HG21	1:A:144:ILE:HG12	1.75	0.69
1:E:247:PHE:HE2	1:E:270:CYS:CB	2.06	0.69
1:D:12:MET:HG3	1:D:354:PRO:HD3	1.74	0.69
1:D:90:LYS:NZ	2:D:601:GLU:OE2	2.24	0.69
1:E:280:ILE:HD11	1:E:291:LEU:HD11	1.74	0.69
1:D:247:PHE:CD2	1:D:270:CYS:HA	2.27	0.69
1:B:27:LYS:NZ	1:B:31:ASP:OD2	2.26	0.68
1:E:317:VAL:O	1:E:340:LYS:HG3	1.93	0.68
1:E:95:TYR:HB3	1:E:133:PRO:HG3	1.75	0.68
1:E:274:GLY:O	1:E:275:GLU:HG2	1.94	0.68
1:A:126:LYS:NZ	2:A:601:GLU:OXT	2.27	0.67
1:C:126:LYS:NZ	2:C:601:GLU:O	2.27	0.67
1:D:280:ILE:HD11	1:D:291:LEU:HD11	1.76	0.67
1:E:322:LEU:HD13	1:E:340:LYS:HZ1	1.57	0.67
1:A:26:ASP:OD1	1:A:42:ARG:NH2	2.28	0.67
1:C:12:MET:HG3	1:C:354:PRO:HD3	1.75	0.67



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:12:MET:HG3	1:A:354:PRO:HD3	1.76	0.67
1:D:126:LYS:NZ	2:D:601:GLU:OXT	2.28	0.67
1:D:85:HIS:O	4:D:604:NAI:N7N	2.28	0.67
1:C:28:LEU:HB3	1:C:490:PHE:HE2	1.59	0.67
1:E:439:ARG:NH1	1:F:401:TYR:CD1	2.63	0.67
1:E:252:PHE:HB3	1:E:275:GLU:OE2	1.94	0.67
1:F:349:ASN:N	4:F:605:NAI:O2D	2.26	0.67
1:C:5:ASP:HB3	1:C:332:THR:HB	1.77	0.67
1:E:439:ARG:NH1	1:F:401:TYR:CE1	2.62	0.67
1:C:303:GLY:N	1:C:309:ILE:HD11	2.04	0.66
1:C:26:ASP:OD1	1:C:42:ARG:NH2	2.28	0.66
1:F:346:GLU:OE2	1:F:478:ARG:NH1	2.28	0.66
1:F:68:ASP:OD1	1:F:140:GLU:HG3	1.94	0.66
1:A:95:TYR:HB3	1:A:133:PRO:HG3	1.76	0.66
1:F:95:TYR:HB3	1:F:133:PRO:HG3	1.77	0.66
1:B:339:VAL:O	1:B:341:ALA:N	2.29	0.66
1:C:57:HIS:HD2	1:F:155:LYS:HG3	1.61	0.66
1:A:37:THR:HA	1:A:41:LYS:HE3	1.77	0.66
1:A:261:ARG:NH1	3:A:602:GTP:O2G	2.29	0.66
1:E:126:LYS:NZ	2:E:601:GLU:OXT	2.28	0.66
1:D:37:THR:HA	1:D:41:LYS:HE3	1.77	0.66
1:F:18:ASP:OD1	1:F:53:LYS:NZ	2.23	0.66
1:C:3:ARG:NH1	1:C:3:ARG:HB2	2.11	0.66
1:F:126:LYS:NZ	2:F:602:GLU:O	2.28	0.66
1:B:95:TYR:HB3	1:B:133:PRO:HG3	1.77	0.66
1:D:339:VAL:O	1:D:341:ALA:N	2.29	0.65
1:E:95:TYR:OH	1:E:145:THR:HG22	1.96	0.65
1:C:455:TYR:O	1:C:459:ARG:N	2.28	0.65
1:D:29:VAL:HG21	1:D:42:ARG:HG3	1.77	0.65
1:F:12:MET:HG3	1:F:354:PRO:HD3	1.76	0.65
1:A:95:TYR:OH	1:A:145:THR:HG22	1.97	0.65
1:B:77:GLY:C	1:B:78:TYR:HD2	2.00	0.65
1:D:95:TYR:HB3	1:D:133:PRO:HG3	1.79	0.65
1:B:190:TYR:OH	1:D:190:TYR:OH	2.15	0.64
1:E:37:THR:HA	1:E:41:LYS:HE3	1.79	0.64
1:E:90:LYS:NZ	2:E:601:GLU:OE1	2.27	0.64
1:E:374:ASN:HB2	4:E:603:NAI:H5N	1.79	0.64
1:F:28:LEU:HB3	1:F:490:PHE:CE2	2.31	0.64
1:B:126:LYS:NZ	2:B:601:GLU:O	2.30	0.64
1:A:339:VAL:O	1:A:341:ALA:N	2.31	0.64
1:C:458:GLU:CD	1:C:462:ARG:HH12	2.00	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:2:ASP:O	1:B:3:ARG:HD3	1.98	0.64
1:B:246:THR:HG22	1:B:269:LYS:HE3	1.78	0.64
1:B:5:ASP:HB3	1:B:332:THR:HB	1.80	0.64
1:A:396:ARG:NH1	1:B:119:ASP:O	2.30	0.64
1:D:420:LYS:CE	1:F:428:ILE:HG12	2.28	0.64
2:E:601:GLU:HA	4:E:603:NAI:H4N	1.80	0.64
1:B:211:ARG:NH1	1:B:211:ARG:O	2.29	0.63
1:B:396:ARG:NH1	1:C:119:ASP:O	2.31	0.63
1:E:26:ASP:OD1	1:E:42:ARG:NH2	2.31	0.63
1:C:499:THR:OG1	1:F:147:ARG:NH1	2.31	0.63
1:F:95:TYR:OH	1:F:145:THR:HG22	1.99	0.63
1:A:287:ASP:OD2	1:A:289:LYS:HG2	1.97	0.63
1:F:25:GLU:OE1	1:F:46:ARG:NH1	2.32	0.63
1:A:38:GLU:OE2	1:A:40:GLN:HB2	1.99	0.63
1:C:95:TYR:HB3	1:C:133:PRO:HG3	1.79	0.63
1:E:260:MET:HG2	1:E:288:PRO:HG3	1.80	0.63
1:E:46:ARG:O	1:E:50:ARG:HG3	1.97	0.63
1:D:66:ARG:HG2	1:D:67:ARG:O	1.98	0.63
1:F:339:VAL:O	1:F:341:ALA:N	2.31	0.63
1:F:77:GLY:C	1:F:78:TYR:HD2	2.02	0.63
1:B:95:TYR:OH	1:B:145:THR:HG22	1.99	0.63
1:E:302:LEU:HD22	1:E:309:ILE:HD12	1.81	0.63
1:A:221:HIS:HD2	1:A:454:ALA:HA	1.62	0.63
1:C:77:GLY:C	1:C:78:TYR:HD2	2.02	0.63
1:D:215:THR:OG1	4:D:603:NAI:H42N	1.97	0.63
1:B:26:ASP:OD1	1:B:42:ARG:NH2	2.32	0.62
1:A:261:ARG:CZ	3:A:602:GTP:O2G	2.47	0.62
1:E:77:GLY:C	1:E:78:TYR:HD2	2.02	0.62
1:D:247:PHE:HE2	1:D:270:CYS:CB	2.11	0.62
1:E:282:ASN:ND2	1:E:306:LYS:O	2.31	0.62
1:F:260:MET:HG2	1:F:288:PRO:HG3	1.82	0.62
1:C:209:HIS:CD2	1:C:446:LYS:HB2	2.33	0.62
1:A:456:THR:HA	1:A:459:ARG:HB3	1.81	0.62
1:D:26:ASP:OD1	1:D:42:ARG:NH2	2.33	0.62
1:C:37:THR:HA	1:C:41:LYS:HE3	1.80	0.62
1:D:95:TYR:OH	1:D:145:THR:HG22	2.00	0.61
1:E:317:VAL:O	1:E:340:LYS:HE3	1.99	0.61
1:A:260:MET:HG2	1:A:288:PRO:HG3	1.81	0.61
1:D:77:GLY:C	1:D:78:TYR:HD2	2.04	0.61
1:F:86:ARG:HE	4:F:601:NAI:H62A	1.47	0.61
1:B:196:ALA:HB2	1:B:388:ASN:HB3	1.81	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:458:GLU:OE1	1:C:462:ARG:NH1	2.26	0.61
1:F:26:ASP:OD1	1:F:42:ARG:NH2	2.33	0.61
1:D:470:LYS:HB3	1:D:471:TYR:CD2	2.35	0.61
1:B:260:MET:HG2	1:B:288:PRO:HG3	1.82	0.61
1:B:392:VAL:HG22	1:C:386:LEU:HD13	1.82	0.61
1:D:470:LYS:HB3	1:D:471:TYR:HD2	1.63	0.61
4:B:604:NAI:H2A	1:C:492:VAL:CG2	2.31	0.61
1:D:456:THR:HG21	1:E:396:ARG:NH2	2.15	0.61
1:F:282:ASN:ND2	1:F:306:LYS:O	2.33	0.61
1:A:315:LEU:HD13	1:A:331:LEU:HD12	1.83	0.60
1:B:280:ILE:HD11	1:B:291:LEU:HD11	1.83	0.60
1:D:387:LYS:HE2	4:F:601:NAI:H51N	1.82	0.60
1:A:396:ARG:HH21	1:B:456:THR:HG21	1.66	0.60
1:C:95:TYR:OH	1:C:145:THR:HG22	2.01	0.60
1:C:339:VAL:O	1:C:341:ALA:N	2.35	0.60
1:C:387:LYS:HE2	4:C:603:NAI:H3D	1.84	0.60
1:E:455:TYR:CE2	1:F:399:PHE:HD2	2.18	0.60
1:B:117:VAL:HG21	1:B:371:LEU:HB3	1.84	0.60
1:B:412:SER:HA	1:C:433:THR:HG23	1.84	0.60
1:E:2:ASP:O	1:E:3:ARG:HD2	2.02	0.60
1:E:340:LYS:HE2	1:E:341:ALA:HB2	1.84	0.59
1:C:117:VAL:HG21	1:C:371:LEU:HB3	1.84	0.59
1:E:403:ARG:NH1	1:E:441:SER:OG	2.29	0.59
1:F:331:LEU:HD23	1:F:360:PHE:HZ	1.66	0.59
1:C:230:ALA:HA	1:C:233:MET:HB2	1.83	0.59
1:E:415:GLU:O	1:E:419:ARG:HB2	2.02	0.59
1:F:471:TYR:N	1:F:471:TYR:HD2	1.99	0.59
1:D:315:LEU:HD13	1:D:331:LEU:HD12	1.84	0.59
1:A:209:HIS:CD2	1:A:446:LYS:HB2	2.37	0.59
1:A:428:ILE:HA	1:C:420:LYS:HE3	1.85	0.59
1:F:209:HIS:CD2	1:F:446:LYS:HB2	2.38	0.59
1:A:211:ARG:NH1	1:A:211:ARG:O	2.33	0.59
1:E:316:GLU:C	1:E:340:LYS:HD2	2.23	0.59
1:B:55:CYS:O	1:E:62:SER:HB2	2.03	0.59
1:D:211:ARG:NH1	1:D:211:ARG:O	2.30	0.59
1:D:247:PHE:HE1	1:D:263:LEU:HB2	1.67	0.59
1:E:211:ARG:O	1:E:211:ARG:NH1	2.30	0.59
1:E:315:LEU:HD13	1:E:331:LEU:HD12	1.85	0.59
1:C:57:HIS:CD2	1:F:155:LYS:HG3	2.37	0.59
1:F:211:ARG:NH1	1:F:211:ARG:O	2.29	0.59
1:F:331:LEU:HB2	1:F:352:THR:HG22	1.85	0.59



	ious puge	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:44:ARG:NH1	1:A:494:ASN:OD1	2.34	0.58
1:E:209:HIS:CD2	1:E:446:LYS:HB2	2.38	0.58
1:B:79:ARG:HH11	1:B:127:ALA:HB2	1.69	0.58
1:E:322:LEU:HD22	1:E:340:LYS:HZ3	1.68	0.58
1:D:260:MET:HG2	1:D:288:PRO:HG3	1.86	0.58
1:B:154:LYS:HB3	1:F:189:HIS:NE2	2.18	0.58
1:F:79:ARG:HH11	1:F:127:ALA:HB2	1.69	0.58
1:A:333:LYS:HE3	1:A:355:GLU:HB3	1.84	0.58
1:B:190:TYR:HH	1:D:190:TYR:HH	1.48	0.58
1:E:126:LYS:HZ1	2:E:601:GLU:N	2.01	0.58
1:E:339:VAL:HG12	1:E:339:VAL:O	2.03	0.58
1:A:79:ARG:HH11	1:A:127:ALA:HB2	1.68	0.58
1:E:230:ALA:HA	1:E:233:MET:HB2	1.84	0.58
1:F:169:MET:HA	4:F:605:NAI:O1N	2.04	0.58
1:C:211:ARG:NH1	1:C:211:ARG:O	2.30	0.58
1:A:386:LEU:HD22	1:C:392:VAL:HG22	1.86	0.58
1:A:117:VAL:HG21	1:A:371:LEU:HB3	1.86	0.58
1:B:150:MET:HG3	1:E:500:PHE:CE2	2.38	0.58
1:A:500:PHE:CZ	1:D:150:MET:HG3	2.38	0.58
1:F:126:LYS:HZ1	2:F:602:GLU:N	2.00	0.58
1:B:154:LYS:HD2	1:F:189:HIS:ND1	2.18	0.57
1:A:500:PHE:HZ	1:D:150:MET:HG3	1.69	0.57
1:D:117:VAL:HG21	1:D:371:LEU:HB3	1.86	0.57
1:E:462:ARG:NH1	1:E:466:ARG:NH2	2.51	0.57
1:E:463:GLN:HA	1:E:466:ARG:NH1	2.19	0.57
1:B:241:GLY:O	1:B:245:LYS:NZ	2.37	0.57
1:D:247:PHE:HE2	1:D:270:CYS:SG	2.28	0.57
1:D:386:LEU:HD13	1:E:392:VAL:HG22	1.86	0.57
1:C:208:ILE:HG13	1:C:445:GLU:OE2	2.04	0.57
1:A:393:SER:HB3	4:A:604:NAI:O3	2.05	0.57
1:B:500:PHE:HE2	1:E:150:MET:HG3	1.69	0.57
1:D:289:LYS:NZ	3:D:602:GTP:O6	2.37	0.57
1:D:282:ASN:ND2	1:D:306:LYS:O	2.36	0.57
1:F:253:GLY:HA3	4:F:605:NAI:PA	2.44	0.57
1:A:391:HIS:HD1	1:B:385:TRP:HH2	1.51	0.57
1:E:423:LYS:O	1:E:425:GLY:N	2.38	0.57
1:F:86:ARG:HD2	4:F:601:NAI:C3N	2.35	0.57
2:A:601:GLU:CA	4:A:603:NAI:H4N	2.32	0.57
1:A:77:GLY:C	1:A:78:TYR:HD2	2.08	0.57
1:B:331:LEU:HD23	1:B:360:PHE:CZ	2.39	0.57
1:A:401:TYR:CE1	1:B:439:ARG:NH1	2.71	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:396:ARG:NH2	1:B:456:THR:HG21	2.18	0.56
1:D:303:GLY:H	1:D:309:ILE:HD11	1.69	0.56
1:A:282:ASN:ND2	1:A:306:LYS:O	2.37	0.56
4:C:604:NAI:H2N	4:C:604:NAI:O1N	2.05	0.56
1:B:37:THR:HA	1:B:41:LYS:HE3	1.86	0.56
1:C:79:ARG:HH11	1:C:127:ALA:HB2	1.70	0.56
1:C:331:LEU:HD23	1:C:360:PHE:CZ	2.40	0.56
1:B:208:ILE:HG13	1:B:445:GLU:OE2	2.04	0.56
1:C:3:ARG:HB2	1:C:3:ARG:CZ	2.34	0.56
1:D:167:PRO:HD3	1:D:176:MET:HG3	1.87	0.56
1:D:150:MET:HE1	1:D:186:THR:HG21	1.86	0.56
1:E:171:THR:HG22	1:E:175:GLU:HG2	1.86	0.56
1:B:126:LYS:HZ1	2:B:601:GLU:N	2.03	0.56
1:C:171:THR:HG22	1:C:175:GLU:HG2	1.87	0.56
1:C:260:MET:HG2	1:C:288:PRO:HG3	1.87	0.56
1:D:331:LEU:HB2	1:D:352:THR:HG22	1.88	0.56
1:D:409:LEU:HD21	1:F:409:LEU:HD22	1.88	0.56
1:E:331:LEU:HD23	1:E:360:PHE:CZ	2.40	0.56
1:F:331:LEU:HD23	1:F:360:PHE:CZ	2.40	0.56
1:F:117:VAL:HG21	1:F:371:LEU:HB3	1.87	0.56
1:F:403:ARG:NH1	1:F:407:TYR:HE2	2.02	0.56
1:A:401:TYR:CD1	1:B:439:ARG:NH1	2.74	0.56
1:A:428:ILE:HG12	1:C:420:LYS:HZ2	1.71	0.56
1:B:150:MET:CE	1:B:186:THR:HG21	2.36	0.56
1:B:281:TRP:HB2	1:B:310:TYR:HB2	1.87	0.56
1:D:390:ASN:O	1:D:392:VAL:HG23	2.05	0.56
1:E:169:MET:HG2	4:E:603:NAI:H52N	1.88	0.56
1:F:390:ASN:O	1:F:392:VAL:HG23	2.06	0.56
1:D:230:ALA:HA	1:D:233:MET:HB2	1.87	0.56
1:E:247:PHE:HE1	1:E:263:LEU:HB2	1.70	0.56
1:B:331:LEU:HB2	1:B:352:THR:HG22	1.87	0.56
1:B:392:VAL:CG2	1:C:386:LEU:HD13	2.36	0.56
1:C:126:LYS:HZ1	2:C:601:GLU:N	2.04	0.56
1:E:499:THR:HG23	1:E:501:THR:HB	1.88	0.56
1:F:455:TYR:CE1	1:F:459:ARG:HD2	2.41	0.56
1:B:185:SER:O	1:F:154:LYS:HD3	2.07	0.55
1:E:167:PRO:HD3	1:E:176:MET:HG3	1.88	0.55
1:F:252:PHE:HB3	1:F:275:GLU:OE2	2.06	0.55
1:B:499:THR:HG23	1:B:501:THR:HB	1.88	0.55
1:F:169:MET:HG2	4:F:605:NAI:H52N	1.87	0.55
1:F:221:HIS:CD2	1:F:454:ALA:HA	2.42	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:331:LEU:HB2	1:A:352:THR:HG22	1.89	0.55
1:D:3:ARG:HH12	1:D:4:GLU:CG	2.18	0.55
1:F:34:THR:HG21	1:F:44:ARG:NH2	2.22	0.55
1:A:331:LEU:HD23	1:A:360:PHE:CZ	2.41	0.55
1:D:221:HIS:CD2	1:D:454:ALA:HA	2.42	0.55
1:C:331:LEU:HB2	1:C:352:THR:HG22	1.88	0.55
4:B:604:NAI:H2A	1:C:492:VAL:HG23	1.89	0.55
1:E:117:VAL:HG21	1:E:371:LEU:HB3	1.87	0.55
1:A:126:LYS:HZ1	2:A:601:GLU:N	2.05	0.55
1:A:220:PHE:HD2	1:A:221:HIS:HD1	1.55	0.55
1:D:79:ARG:HH11	1:D:127:ALA:HB2	1.70	0.55
1:E:459:ARG:HA	1:E:462:ARG:HD3	1.87	0.55
1:B:62:SER:HB2	1:E:55:CYS:O	2.06	0.55
1:F:37:THR:HA	1:F:41:LYS:HE3	1.89	0.55
1:B:167:PRO:HD3	1:B:176:MET:HG3	1.88	0.55
1:B:169:MET:HG2	4:B:603:NAI:H52N	1.88	0.55
2:E:601:GLU:HA	4:E:603:NAI:C4N	2.37	0.55
1:A:91:GLY:HA3	1:A:125:ALA:O	2.06	0.55
1:E:390:ASN:O	1:E:392:VAL:HG23	2.07	0.55
1:F:167:PRO:HD3	1:F:176:MET:HG3	1.88	0.55
1:A:413:VAL:HG11	1:C:413:VAL:CG1	2.35	0.55
1:E:150:MET:CE	1:E:186:THR:HG21	2.37	0.55
1:C:282:ASN:ND2	1:C:306:LYS:O	2.36	0.55
1:C:471:TYR:N	1:C:471:TYR:HD2	2.04	0.55
1:E:79:ARG:HH11	1:E:127:ALA:HB2	1.71	0.55
1:F:402:GLU:HG3	1:F:406:ASN:OD1	2.06	0.55
1:D:247:PHE:C	1:D:247:PHE:CD2	2.81	0.54
1:D:126:LYS:HZ1	2:D:601:GLU:N	2.05	0.54
1:E:331:LEU:HB2	1:E:352:THR:HG22	1.90	0.54
1:C:150:MET:CE	1:C:186:THR:HG21	2.37	0.54
1:D:150:MET:CE	1:D:186:THR:HG21	2.37	0.54
1:D:91:GLY:HA3	1:D:125:ALA:O	2.07	0.54
1:E:455:TYR:CZ	1:F:399:PHE:HD2	2.26	0.54
1:F:406:ASN:ND2	1:F:436:PHE:HZ	2.05	0.54
1:A:406:ASN:ND2	1:A:436:PHE:HZ	2.06	0.54
1:B:230:ALA:HA	1:B:233:MET:HB2	1.89	0.54
1:E:279:SER:OG	1:E:314:ILE:HB	2.06	0.54
1:A:213:SER:HA	1:A:258:HIS:ND1	2.22	0.54
1:C:91:GLY:HA3	1:C:125:ALA:O	2.07	0.54
1:C:390:ASN:O	1:C:392:VAL:HG23	2.08	0.54
1:E:53:LYS:HB2	1:E:54:PRO:HD3	1.89	0.54



<i>5</i> 1		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap(Å)
1·E·254·ASN·HB2	$4 \cdot E \cdot 603 \cdot N AI \cdot O2N$	2.07	0.54
1:F:209:HIS:HD2	1:F:446:LYS:HB2	1.72	0.54
$1 \cdot B \cdot 24 \cdot VAL \cdot HG13$	1·B·483·VAL·HG13	1.88	0.54
1:C:470:LYS:HG3	$1 \cdot C \cdot 471 \cdot TYB \cdot CD2$	2.42	0.54
1:F:281:TRP:HB2	1:F:310:TYR:HB2	1.89	0.54
1.F.345.ALA.HB1	$1 \cdot F \cdot 373 \cdot LEU \cdot HD21$	1.89	0.54
1.C·252·PHE·HB3	1:C.275:GLU:OE2	2.08	0.54
1.D.331.LEU.HD23	$1 \cdot D \cdot 360 \cdot PHE \cdot CZ$	2.00	0.54
1:F:34:THR:HG21	1:F:44:ABG:HH12	1 73	0.54
$1 \cdot B \cdot 150 \cdot MET \cdot HG3$	$1 \cdot E \cdot 500 \cdot PHE \cdot HE2$	1.73	0.54
1·B·375·ALA·O	1.B.379.THB.OG1	2 20	0.54
1·B·414·GLN·HG3	1.B.428.ILE.O	2.08	0.54
1.D.119.ASP.O	1.E.396.ABG.NH1	2 41	0.54
1:F:171:THR:HG22	1:E:175:GLU:HG2	1.89	0.54
$1 \cdot C \cdot 167 \cdot PRO \cdot HD3$	1.C.176.MET.HG3	1.00	0.54
$1 \cdot F \cdot 23 \cdot ILE \cdot HG 22$	$1 \cdot F \cdot 471 \cdot TVR \cdot HD1$	1.73	0.54
1.1.29.1112.11022 1.A.27.LYS.NZ	$1 \cdot A \cdot 31 \cdot A \text{SP} \cdot \text{OD} 2$	2.38	0.54
$1 \cdot C \cdot 501 \cdot THB \cdot OG1$	1.F.66.ABG.NH1	2.30	0.54
1.0.32.LEU.HD11	$1 \cdot D \cdot 494 \cdot A SN \cdot OD1$	2.10	0.54
$1 \cdot E \cdot 247 \cdot PHE \cdot CE2$	1:E:270:CVS:CA	2.90	0.54
$\frac{1.1.2.217.1}{1.1.7}$	$1 \cdot E \cdot 471 \cdot T \times B \cdot CD2$	2.56	0.53
$\frac{1 \cdot A \cdot 390 \cdot A \text{SN} \cdot 0}{1 \cdot A \cdot 390 \cdot A \text{SN} \cdot 0}$	1.A.392.VAL.:HG23	2.06	0.53
1:F:274:GLY:0	1.F.275.GLU.HG2	2.00	0.53
1.F.42.ABG.O	1.F.46.ABG.HG3	2.00	0.53
1.B.357.ASP.OD2	1:B:478:ABG:NE	2.36	0.53
1:B:91:GLY:HA3	1.B.125.ALA.O	2.00	0.53
$1 \cdot C \cdot 150 \cdot MET \cdot HE1$	1.C.186.THB.HG21	1 90	0.53
1.D.244.ASP.HA	$1 \cdot D \cdot 269 \cdot I \cdot VS \cdot NZ$	2.23	0.53
1.E.91.GLV.HA3	1.E.125.ALA.O	2.28	0.55
$1 \cdot B \cdot 90 \cdot LYS \cdot HD2$	1.B.120.HBH.0	2.00	0.53
1.E.24.VAL:HG13	1.E.483.VAL.HG13	1.91	0.53
1.A.167.PRO.HD3	1.A.176.MET.HG3	1.89	0.53
1: A · 230: AL A · H A	1.A.233.MET.HB2	1.00	0.53
1.C·275·GLU·HG3	$1 \cdot C \cdot 301 \cdot ILE \cdot HD13$	1.91	0.53
1.C.315.LEU.HD13	$1 \cdot C \cdot 331 \cdot LEU \cdot HD12$	1.90	0.53
1:E:79:ARG·HD2	1:E:127:ALA·HB2	1.88	0.53
1:E:221:HIS:CD2	1:E:454:ALA·HA	2 43	0.53
1:F:27:LYS·NZ	1:F:31:ASP:OD2	2.42	0.53
1:F:358·LVS·O	1:F:362:GLU·HG3	2.09	0.53
1:A:252:PHE·HB3	1:A:275:GLU:OE2	2.09	0.53
1:A:399:PHE:HD2	1:B:455:TYR:HH	1.56	0.53



	lo uo pugo	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:C:388:ASN:O	1:C:391:HIS:CD2	2.62	0.53
1:A:368:ILE:HG21	1:A:373:LEU:HD13	1.91	0.53
1:B:169:MET:HA	4:B:603:NAI:O1N	2.09	0.53
1:B:279:SER:OG	1:B:314:ILE:HB	2.08	0.53
1:C:221:HIS:CD2	1:C:454:ALA:HA	2.44	0.53
1:E:345:ALA:HB1	1:E:373:LEU:HD21	1.91	0.53
1:F:32:LEU:HD11	1:F:494:ASN:OD1	2.08	0.53
1:A:24:VAL:HG13	1:A:483:VAL:HG13	1.90	0.53
1:B:282:ASN:ND2	1:B:306:LYS:O	2.37	0.53
1:C:345:ALA:HB1	1:C:373:LEU:HD21	1.91	0.53
1:C:471:TYR:N	1:C:471:TYR:CD2	2.77	0.53
1:D:279:SER:OG	1:D:314:ILE:HB	2.09	0.53
1:D:10:PHE:HE1	1:D:53:LYS:NZ	2.07	0.53
1:F:406:ASN:HD22	1:F:436:PHE:HZ	1.57	0.53
1:D:10:PHE:CD2	1:D:105:LYS:HE2	2.44	0.52
1:F:91:GLY:HA3	1:F:125:ALA:O	2.09	0.52
1:A:499:THR:HG23	1:A:501:THR:HB	1.91	0.52
1:C:458:GLU:CG	1:C:462:ARG:NH1	2.71	0.52
1:B:35:ARG:O	1:B:37:THR:N	2.36	0.52
1:E:368:ILE:HG21	1:E:373:LEU:HD13	1.92	0.52
1:B:345:ALA:HB1	1:B:373:LEU:HD21	1.90	0.52
1:D:247:PHE:CE2	1:D:270:CYS:CA	2.91	0.52
1:A:488:LYS:HG2	1:A:491:ARG:NH2	2.23	0.52
1:B:315:LEU:HD22	1:B:331:LEU:HD11	1.92	0.52
1:C:279:SER:OG	1:C:314:ILE:HB	2.09	0.52
1:C:458:GLU:CG	1:C:462:ARG:HH12	2.22	0.52
1:C:499:THR:HG23	1:C:501:THR:HB	1.91	0.52
1:C:53:LYS:HB2	1:C:54:PRO:HD3	1.91	0.52
1:D:398:THR:O	1:D:401:TYR:N	2.42	0.52
1:F:382:TYR:CZ	1:F:386:LEU:HD11	2.45	0.52
1:B:396:ARG:NH2	1:C:456:THR:HG21	2.25	0.52
1:D:24:VAL:CG1	1:D:483:VAL:HG13	2.39	0.52
1:E:24:VAL:HG13	1:E:483:VAL:HG13	1.91	0.52
1:A:115:CYS:SG	1:A:378:VAL:HG11	2.50	0.52
1:B:215:THR:HB	4:B:603:NAI:H42N	1.91	0.52
1:B:390:ASN:O	1:B:392:VAL:HG23	2.09	0.52
1:B:33:LYS:HD3	1:B:41:LYS:NZ	2.25	0.52
1:F:239:THR:HG21	1:F:244:ASP:OD2	2.10	0.52
1:C:458:GLU:HG2	1:C:462:ARG:HH11	1.73	0.52
1:E:25:GLU:OE1	1:E:46:ARG:NH1	2.43	0.52
1:F:186:THR:OG1	1:F:187:ILE:N	2.43	0.52



	louis pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:279:SER:OG	1:A:314:ILE:HB	2.10	0.52
1:A:388:ASN:O	1:A:391:HIS:CD2	2.63	0.52
1:C:458:GLU:HG2	1:C:462:ARG:HH12	1.74	0.52
1:D:294:PHE:CD2	1:D:304:PHE:HD1	2.28	0.52
1:F:368:ILE:HG21	1:F:373:LEU:HD13	1.91	0.52
1:F:372:TYR:O	1:F:457:MET:HE3	2.10	0.52
1:B:24:VAL:CG1	1:B:483:VAL:HG13	2.40	0.52
1:C:28:LEU:HB3	1:C:490:PHE:CE2	2.42	0.52
1:A:345:ALA:HB1	1:A:373:LEU:HD21	1.91	0.51
1:E:247:PHE:CD2	1:E:247:PHE:C	2.84	0.51
1:E:280:ILE:HG22	1:E:309:ILE:HD13	1.93	0.51
1:B:159:GLY:HA2	1:B:183:TYR:HE2	1.75	0.51
1:B:150:MET:HE1	1:B:186:THR:HG21	1.91	0.51
1:C:24:VAL:HG13	1:C:483:VAL:HG13	1.93	0.51
1:C:280:ILE:HD11	1:C:291:LEU:HD11	1.92	0.51
1:C:238:MET:HE1	1:C:343:ILE:HG13	1.92	0.51
1:A:427:THR:O	1:C:420:LYS:HE3	2.11	0.51
1:D:427:THR:O	1:E:420:LYS:HE2	2.10	0.51
1:B:403:ARG:HA	1:B:440:ILE:O	2.10	0.51
1:C:78:TYR:HD1	1:C:101:VAL:HG23	1.75	0.51
1:F:236:LEU:HD22	1:F:342:LYS:HD2	1.92	0.51
1:A:186:THR:OG1	1:A:187:ILE:N	2.43	0.51
1:A:24:VAL:CG1	1:A:483:VAL:HG13	2.40	0.51
1:B:115:CYS:SG	1:B:378:VAL:HG11	2.50	0.51
1:E:172:GLY:N	1:E:175:GLU:OE2	2.42	0.51
1:F:159:GLY:HA2	1:F:183:TYR:HE2	1.76	0.51
1:F:294:PHE:CD2	1:F:304:PHE:HD1	2.28	0.51
1:A:192:ILE:HG12	1:A:391:HIS:HE1	1.75	0.51
1:A:406:ASN:HD22	1:A:436:PHE:HZ	1.56	0.51
1:D:269:LYS:N	1:D:269:LYS:HD2	2.25	0.51
1:F:279:SER:OG	1:F:314:ILE:HB	2.11	0.51
1:F:222:GLY:HA3	1:F:373:LEU:HD12	1.92	0.51
1:A:155:LYS:HG3	1:D:57:HIS:CD2	2.46	0.51
1:D:345:ALA:HB1	1:D:373:LEU:HD21	1.92	0.51
1:E:247:PHE:HE2	1:E:270:CYS:SG	2.32	0.51
1:E:5:ASP:HB2	1:E:333:LYS:HG2	1.93	0.51
1:F:115:CYS:SG	1:F:378:VAL:HG11	2.50	0.51
1:D:413:VAL:HG13	1:F:413:VAL:HG11	1.93	0.51
1:A:336:ALA:HB3	1:A:359:ILE:HD12	1.92	0.51
1:B:399:PHE:HD2	1:C:455:TYR:CE2	2.29	0.51
1:C:115:CYS:SG	1:C:378:VAL:HG11	2.51	0.51



	ious puge	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap(Å)
1:F:287:ASP:HB3	1:F:290:GLU:HG3	1.93	0.51
1:A:459:ARG:HG3	1:A:459:ABG:NH1	2.24	0.51
1:D:402:GLU:OE2	1:E:402:GLU:OE2	2 29	0.51
1:E:487:GLU:HG2	1:E:491:ARG:NH1	2.21	0.51
1:B:39:GLU:OE2	1:B:42:ARG:HD2	2.11	0.51
1:C:118:VAL:HG21	1:C:375:ALA:HB1	1.93	0.51
1:C:382:TYR:CZ	1:C:386:LEU:HD11	2.46	0.51
1:D:209:HIS:CD2	1:D:446:LYS:HB2	2.45	0.51
1:C:375:ALA:O	1:C:379:THR:OG1	2.22	0.51
1:F:269:LYS:HD2	1:F:284:ASP:O	2.11	0.51
1:A:357:ASP:OD2	1:A:478:ARG:NE	2.35	0.50
1:A:36:GLU:HB3	1:A:40:GLN:HG2	1.91	0.50
1:B:32:LEU:HD11	1:B:494:ASN:OD1	2.11	0.50
1:C:222:GLY:HA3	1:C:373:LEU:HD12	1.93	0.50
1:B:51:ILE:HG12	1:E:64:PRO:HB3	1.93	0.50
1:B:292:GLU:OE1	3:B:602:GTP:N2	2.32	0.50
1:D:336:ALA:HB3	1:D:359:ILE:HD12	1.93	0.50
1:D:403:ARG:HA	1:D:440:ILE:O	2.12	0.50
1:E:222:GLY:HA3	1:E:373:LEU:HD12	1.93	0.50
1:F:24:VAL:CG1	1:F:483:VAL:HG13	2.42	0.50
1:A:118:VAL:HG21	1:A:375:ALA:HB1	1.94	0.50
1:A:463:GLN:HA	1:A:466:ARG:NH1	2.26	0.50
1:D:436:PHE:HB2	1:E:408:HIS:HB3	1.93	0.50
1:D:495:GLU:O	1:E:205:GLN:OE1	2.28	0.50
1:E:159:GLY:HA2	1:E:183:TYR:HE2	1.75	0.50
1:E:213:SER:O	1:E:215:THR:N	2.45	0.50
1:F:213:SER:O	1:F:215:THR:N	2.45	0.50
1:C:68:ASP:OD2	1:C:137:THR:OG1	2.27	0.50
1:D:24:VAL:HG13	1:D:483:VAL:HG13	1.92	0.50
1:C:23:ILE:HG22	1:C:471:TYR:HD1	1.77	0.50
1:B:396:ARG:CZ	1:C:456:THR:HG21	2.42	0.50
1:E:118:VAL:HG21	1:E:375:ALA:HB1	1.92	0.50
1:A:90:LYS:HD2	1:A:164:VAL:O	2.11	0.50
1:B:222:GLY:HA3	1:B:373:LEU:HD12	1.93	0.50
1:D:382:TYR:CZ	1:D:386:LEU:HD11	2.47	0.50
1:F:398:THR:O	1:F:401:TYR:N	2.42	0.50
1:C:32:LEU:HD11	1:C:494:ASN:OD1	2.11	0.50
1:C:43:ASN:O	1:C:44:ARG:NH1	2.45	0.50
1:D:118:VAL:HG21	1:D:375:ALA:HB1	1.93	0.50
1:F:403:ARG:HA	1:F:440:ILE:O	2.11	0.50
1:A:315:LEU:HD22	1:A:331:LEU:HD11	1.94	0.50



	ious puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:A:604:NAI:H71N	1:B:86:ARG:HD3	1.76	0.50
1:C:368:ILE:HG21	1:C:373:LEU:HD13	1.92	0.50
1:D:247:PHE:C	1:D:247:PHE:HD2	2.14	0.50
1:B:500:PHE:CE2	1:E:150:MET:HG3	2.46	0.50
1:F:241:GLY:O	1:F:245:LYS:NZ	2.45	0.50
1:A:213:SER:O	1:A:215:THR:N	2.45	0.50
1:A:241:GLY:O	1:A:245:LYS:NZ	2.44	0.50
1:B:213:SER:O	1:B:215:THR:N	2.45	0.50
1:B:239:THR:HG21	1:B:244:ASP:OD2	2.12	0.50
1:B:368:ILE:HG21	1:B:373:LEU:HD13	1.93	0.50
1:C:65:ILE:HD13	1:C:144:ILE:HG12	1.93	0.50
1:D:213:SER:O	1:D:215:THR:N	2.45	0.50
1:E:303:GLY:N	1:E:309:ILE:HD11	2.19	0.50
1:E:315:LEU:HD22	1:E:331:LEU:HD11	1.92	0.50
1:E:318:ASP:CA	1:E:340:LYS:HG3	2.40	0.50
1:D:432:PRO:HA	1:E:412:SER:OG	2.12	0.50
1:E:496:ALA:HA	1:F:177:SER:OG	2.12	0.50
1:A:209:HIS:HD2	1:A:446:LYS:HB2	1.76	0.49
1:C:66:ARG:HG2	1:C:71:SER:O	2.12	0.49
1:E:209:HIS:HD2	1:E:446:LYS:HB2	1.75	0.49
1:E:94:ARG:HG3	1:E:169:MET:HB2	1.94	0.49
1:C:67:ARG:HD3	1:C:73:GLU:OE1	2.12	0.49
1:F:372:TYR:O	1:F:457:MET:CE	2.60	0.49
1:B:465:MET:O	1:B:469:MET:HG2	2.12	0.49
1:B:396:ARG:NE	1:C:456:THR:HG21	2.28	0.49
1:E:171:THR:HA	1:E:175:GLU:OE2	2.12	0.49
1:E:382:TYR:CZ	1:E:386:LEU:HD11	2.47	0.49
1:A:403:ARG:HA	1:A:440:ILE:O	2.12	0.49
1:C:470:LYS:HG3	1:C:471:TYR:CE2	2.47	0.49
1:D:386:LEU:HD13	1:E:392:VAL:CG2	2.43	0.49
1:D:375:ALA:O	1:D:379:THR:OG1	2.19	0.49
1:A:155:LYS:HG3	1:D:57:HIS:HD2	1.77	0.49
1:E:247:PHE:CE2	1:E:270:CYS:CB	2.92	0.49
1:E:32:LEU:HD11	1:E:494:ASN:OD1	2.12	0.49
1:F:391:HIS:HA	4:F:603:NAI:H4D	1.95	0.49
1:A:67:ARG:NH1	1:A:136:TYR:CE2	2.81	0.49
1:A:32:LEU:HD11	1:A:494:ASN:OD1	2.11	0.49
1:C:186:THR:OG1	1:C:187:ILE:N	2.44	0.49
1:C:24:VAL:CG1	1:C:483:VAL:HG13	2.43	0.49
1:D:357:ASP:OD2	1:D:478:ARG:NE	2.39	0.49
1:A:57:HIS:HA	1:D:60:SER:O	2.11	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:213:SER:O	1:C:215:THR:N	2.46	0.49
1:D:315:LEU:HD22	1:D:331:LEU:HD11	1.94	0.49
1:F:23:ILE:HG22	1:F:471:TYR:CD1	2.48	0.49
1:C:315:LEU:HD22	1:C:331:LEU:HD11	1.94	0.49
1:D:247:PHE:CD1	1:D:263:LEU:HD12	2.48	0.49
1:F:34:THR:OG1	1:F:35:ARG:N	2.46	0.49
1:A:177:SER:OG	1:B:496:ALA:HA	2.13	0.49
1:C:403:ARG:HA	1:C:440:ILE:O	2.13	0.49
1:D:443:ALA:HA	1:E:401:TYR:CE2	2.48	0.49
1:B:388:ASN:N	1:B:388:ASN:HD22	2.11	0.49
1:D:247:PHE:O	1:D:247:PHE:HD2	1.96	0.49
1:E:403:ARG:HA	1:E:440:ILE:O	2.12	0.49
1:E:24:VAL:CG1	1:E:483:VAL:HG13	2.42	0.49
1:F:230:ALA:HA	1:F:233:MET:HB2	1.95	0.49
1:F:247:PHE:CE1	1:F:263:LEU:HB2	2.48	0.49
1:F:336:ALA:HB3	1:F:359:ILE:HD12	1.94	0.49
1:F:118:VAL:HG21	1:F:375:ALA:HB1	1.94	0.49
1:B:337:PRO:HD3	1:B:359:ILE:CD1	2.41	0.48
1:B:60:SER:O	1:E:57:HIS:HA	2.13	0.48
1:D:456:THR:HG21	1:E:396:ARG:CZ	2.43	0.48
1:B:331:LEU:HD23	1:B:360:PHE:HZ	1.77	0.48
1:E:150:MET:HE1	1:E:186:THR:HG21	1.95	0.48
1:B:118:VAL:HG21	1:B:375:ALA:HB1	1.95	0.48
1:D:289:LYS:HD2	1:D:289:LYS:HA	1.59	0.48
1:E:239:THR:HG21	1:E:244:ASP:OD2	2.13	0.48
1:A:382:TYR:CZ	1:A:386:LEU:HD11	2.47	0.48
1:A:417:LEU:CD1	1:C:417:LEU:HD21	2.43	0.48
1:D:209:HIS:HD2	1:D:446:LYS:HB2	1.78	0.48
1:F:146:ARG:NH1	1:F:182:THR:HG22	2.26	0.48
1:A:462:ARG:HD2	1:A:465:MET:CE	2.43	0.48
1:C:239:THR:HG21	1:C:244:ASP:OD2	2.14	0.48
1:C:65:ILE:O	1:C:65:ILE:HG13	2.13	0.48
1:D:346:GLU:OE1	1:D:352:THR:OG1	2.24	0.48
1:D:368:ILE:HG21	1:D:373:LEU:HD13	1.96	0.48
1:D:222:GLY:HA3	1:D:373:LEU:HD12	1.94	0.48
1:D:208:ILE:HG13	1:D:445:GLU:OE2	2.13	0.48
1:D:53:LYS:O	1:D:82:HIS:NE2	2.46	0.48
4:E:603:NAI:O1N	4:E:603:NAI:H2N	2.14	0.48
1:F:400:LYS:HG2	1:F:400:LYS:O	2.13	0.48
1:A:208:ILE:HG13	1:A:445:GLU:OE2	2.14	0.48
1:D:209:HIS:HD2	1:D:446:LYS:HA	1.78	0.48


	lous pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:48:ILE:O	1:E:52:ILE:HG13	2.14	0.48
1:F:53:LYS:HB2	1:F:54:PRO:HD3	1.95	0.48
1:A:171:THR:HG22	1:A:175:GLU:HG2	1.96	0.48
1:B:213:SER:HB3	3:B:602:GTP:O2'	2.14	0.48
1:C:286:ILE:HG21	1:C:291:LEU:HD12	1.94	0.48
1:C:209:HIS:HD2	1:C:446:LYS:HB2	1.74	0.48
1:E:107:LEU:HB2	1:E:126:LYS:HG2	1.95	0.48
1:E:265:ARG:O	1:E:267:GLY:N	2.47	0.48
1:E:398:THR:O	1:E:401:TYR:N	2.45	0.48
1:E:68:ASP:OD2	1:E:137:THR:OG1	2.28	0.48
4:F:605:NAI:O1A	4:F:605:NAI:O1N	2.32	0.48
1:D:294:PHE:HD1	1:D:298:HIS:ND1	2.11	0.48
1:E:456:THR:HG21	1:F:396:ARG:NE	2.29	0.48
1:F:374:ASN:HB2	4:F:605:NAI:H5N	1.95	0.48
1:A:346:GLU:OE1	1:A:351:PRO:HD2	2.14	0.48
2:B:601:GLU:HA	4:B:603:NAI:C4N	2.43	0.48
4:A:604:NAI:N7N	1:B:86:ARG:NH1	2.61	0.48
1:D:115:CYS:SG	1:D:378:VAL:HG11	2.54	0.48
1:D:3:ARG:NH1	1:D:4:GLU:CG	2.70	0.48
1:A:222:GLY:HA3	1:A:373:LEU:HD12	1.95	0.47
1:A:82:HIS:CG	1:A:109:SER:HA	2.49	0.47
1:E:115:CYS:SG	1:E:378:VAL:HG11	2.54	0.47
1:D:420:LYS:NZ	1:F:428:ILE:HG12	2.29	0.47
1:A:432:PRO:HB3	1:A:436:PHE:CD2	2.49	0.47
4:A:604:NAI:H8A	4:A:604:NAI:H2B	1.64	0.47
1:F:294:PHE:HD1	1:F:298:HIS:ND1	2.12	0.47
1:A:148:PHE:CE2	1:A:152:LEU:HD11	2.50	0.47
1:A:247:PHE:CE1	1:A:263:LEU:HB2	2.49	0.47
1:A:398:THR:O	1:A:401:TYR:N	2.43	0.47
1:B:382:TYR:CZ	1:B:386:LEU:HD11	2.49	0.47
1:B:455:TYR:CE1	1:B:459:ARG:HG3	2.49	0.47
1:E:247:PHE:HA	1:E:321:ILE:O	2.14	0.47
1:F:346:GLU:CD	1:F:478:ARG:HH12	2.17	0.47
1:E:86:ARG:HG3	4:F:603:NAI:H62A	1.80	0.47
1:E:159:GLY:HA2	1:E:183:TYR:CE2	2.50	0.47
1:E:90:LYS:HD2	1:E:164:VAL:O	2.15	0.47
1:E:186:THR:OG1	1:E:187:ILE:N	2.45	0.47
1:F:172:GLY:N	1:F:175:GLU:OE2	2.42	0.47
1:A:239:THR:HG21	1:A:244:ASP:OD2	2.14	0.47
1:A:292:GLU:CD	3:A:602:GTP:HN1	2.17	0.47
1:B:38:GLU:HG3	1:B:40:GLN:CB	2.44	0.47



	lous puge	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap(Å)
1:D:14:GLU:HA	1:D:53:LYS:HE3	1.96	0.47
1:A:177:SER:HB2	1:A:202:PRO:HG2	1.96	0.47
1:B:246:THB:HG22	1:B:269:LYS:CE	2.45	0.47
1:B:169:MET:HA	4:B:603:NAI:O1A	2.15	0.47
1:C:166:ALA:HB1	1:C:167:PRO:HD2	1.95	0.47
1:E:38:GLU:HB3	1:E:40:GLN:H	1.78	0.47
1:A:67:ARG:HD3	1:A:73:GLU:OE1	2.15	0.47
1:B:159:GLY:HA2	1:B:183:TYR:CE2	2.49	0.47
1:B:303:GLY:H	1:B:309:ILE:HD12	1.80	0.47
1:D:239:THR:HG21	1:D:244:ASP:OD2	2.15	0.47
1:D:213:SER:HB2	1:D:262:TYR:HE2	1.80	0.47
1:D:247:PHE:HA	1:D:321:ILE:O	2.15	0.47
1:E:471:TYR:N	1:E:471:TYR:CD2	2.83	0.47
1:A:265:ARG:O	1:A:267:GLY:N	2.46	0.47
1:A:274:GLY:O	1:A:275:GLU:HG3	2.14	0.47
1:B:432:PRO:HB3	1:B:436:PHE:CD2	2.49	0.47
1:D:172:GLY:N	1:D:175:GLU:OE2	2.40	0.47
1:F:23:ILE:CG2	1:F:471:TYR:HD1	2.27	0.47
1:F:369:PRO:HB3	1:F:478:ARG:HA	1.97	0.47
1:F:470:LYS:HG3	1:F:471:TYR:CD2	2.50	0.47
1:A:429:PRO:O	1:C:416:SER:HB3	2.15	0.47
1:C:67:ARG:NH1	1:C:136:TYR:CE2	2.83	0.47
1:E:353:THR:HB	1:E:354:PRO:HD2	1.97	0.47
1:E:456:THR:HG21	1:F:396:ARG:NH2	2.30	0.47
1:D:77:GLY:C	1:D:78:TYR:CD2	2.88	0.47
4:E:603:NAI:O1N	4:E:603:NAI:H2D	2.15	0.47
1:F:159:GLY:HA2	1:F:183:TYR:CE2	2.50	0.47
1:F:465:MET:O	1:F:469:MET:HG2	2.15	0.47
1:A:57:HIS:CE1	1:A:84:GLN:HE22	2.33	0.47
1:B:183:TYR:O	1:B:183:TYR:HD1	1.98	0.47
1:C:331:LEU:HD23	1:C:360:PHE:HZ	1.80	0.47
1:D:67:ARG:NH1	1:D:136:TYR:CE2	2.83	0.47
1:B:209:HIS:CD2	1:B:446:LYS:HB2	2.50	0.46
1:C:78:TYR:HE1	1:C:101:VAL:HB	1.79	0.46
1:C:432:PRO:HB3	1:C:436:PHE:CD2	2.50	0.46
1:D:39:GLU:O	1:D:43:ASN:ND2	2.48	0.46
1:D:471:TYR:CD2	1:D:471:TYR:N	2.83	0.46
1:E:177:SER:HB2	1:E:202:PRO:HG2	1.97	0.46
1:B:111:MET:HE1	2:B:601:GLU:HG3	1.97	0.46
1:B:172:GLY:N	1:B:175:GLU:OE2	2.39	0.46
1:B:401:TYR:HE2	1:C:447:ASP:CB	2.28	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (\mathbf{A})	overlap(Å)
1·A·444·SEB·OG	$1 \cdot A \cdot 447 \cdot ASP \cdot OD1$	2.25	0.46
1:C:357:ASP:OD2	1:C:478:ABG:NE	2.34	0.46
1.C.196.ALA.HB2	1.C.388.ASN.HB2	1 97	0.16
1.C.398.THB.O	$1 \cdot C \cdot 401 \cdot T \text{YB} \cdot \text{N}$	2.46	0.46
1.0.000.1111.0	$1 \cdot D \cdot 436 \cdot PHE \cdot CD2$	2.10	0.46
1.F.209.HIS.HE1	$3 \cdot F \cdot 604 \cdot GTP \cdot H5$ "	1.80	0.46
1.A.146.ARG.NH1	1·A·182·THB·HG22	$\frac{1.00}{2.25}$	0.46
1.B.33.LVS.HD3	1.B.41.LVS.HZ3	1.80	0.16
$1 \cdot C \cdot 78 \cdot TYB \cdot CE1$	$1 \cdot C \cdot 101 \cdot VAL \cdot HB$	$\frac{1.00}{2.50}$	0.46
$1 \cdot C \cdot 265 \cdot ABG \cdot O$	1.C.267.GLY.N	2.36	0.46
1.C.44.ABG·HD3	1·C·44·ABG·HA	1.37	0.46
1.D.353.THB.HB	$1 \cdot D \cdot 354 \cdot PRO \cdot HD2$	1.98	0.46
1.F.67.ABG·NH1	$\frac{1.\text{E}\cdot301.1\text{ R}\cdot0.1\text{H}\cdot2}{1.\text{F}\cdot1.36\cdot\text{TYB}\cdot\text{CE}2}$	2.83	0.46
1.A.432.PRO.HB3	1.A.436.PHE.HD2	1.81	0.46
1.B.346.GLU.OE1	$1 \cdot B \cdot 352 \cdot THB \cdot OG1$	2.24	0.46
1.B.470.LVS.HB3	1.B.471.TVR.HD2	1 79	0.46
1:B:67:ABG:HD3	1.B.73.GLU.OE1	2.15	0.10
1.C.146.ARG.HH11	1.C.182.THB.CG2	2.10	0.46
1.0.110.110.1110	1.D.298.HIS.ND1	2.20	0.46
$1 \cdot D \cdot 369 \cdot PRO \cdot HB3$	1:D:478:ABG:HA	1.98	0.46
1.E.247.PHE.C	$1 \cdot E \cdot 247 \cdot PHE \cdot HD2$	2 19	0.46
$1 \cdot E \cdot 247 \cdot PHE \cdot CE1$	$1 \cdot E \cdot 263 \cdot L E U \cdot H D 12$	2.50	0.10
1.E.211.1 HE.011	$1 \cdot E \cdot 340 \cdot LVS \cdot CG$	2.30	0.46
1.E.010RDF	1.E.010.ET5.000	2.33	0.46
1.B.281.TRP.CG	1.B.310.TYB.HD2	2.33	0.46
1:C:336:ALA:HB3	1:C:359:ILE:HD12	1.97	0.46
1.C.255.VAL:HG23	$4 \cdot C \cdot 604 \cdot N A I \cdot O2N$	2.15	0.46
1.0.200.0111.11020	$1 \cdot D \cdot 109 \cdot SEB \cdot HA$	2.10	0.46
1:E:67:ABG:NH1	1:E:136:TYB:CE2	2.83	0.46
1:E:455:TYB:HH	1:F:399:PHE:HD2	1 64	0.46
1:B:303:GLY:H	1:B:309:ILE:CD1	2.28	0.46
1:C:172:GLY:N	1:C:175:GLU:OE2	2.42	0.46
1:C:280:ILE:HG22	1:C:309:ILE:HD13	1.97	0.46
1:D:400:LYS:O	1:D:400:LYS:HG2	2.15	0.46
1:D:433:THR:HG23	1:E:412:SER:HA	1.97	0.46
1:F:323:ILE:HG12	1:F:345:ALA:HB3	1.97	0.46
1:C:107:LEU:HB2	1:C:126:LYS:HG2	1.97	0.46
1:A:24:VAL:O	1:A:27:LYS:N	2.49	0.46
1:B:275:GLU:HG3	4:B:603:NAI:H1B	1.97	0.46
1:B:353:THR:HB	1:B:354:PRO:HD2	1.97	0.46
1:B:420:LYS:HG2	1:B:421:PHE:CE1	2.51	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap(Å)
1:C:28:LEU:HD13	1:C:490:PHE:CD2	2.50	0.46
1:E:336:ALA:HB3	1:E:359:ILE:HD12	1.98	0.46
1:E:82:HIS:CG	1:E:109:SER:HA	2.50	0.46
1:A:150:MET:CE	1:A:186:THR:HG21	2.46	0.46
1:A:375:ALA:O	1:A:379:THR:OG1	2.24	0.46
1:B:432:PRO:HB3	1:B:436:PHE:HD2	1.81	0.46
1:C:23:ILE:HG22	1:C:471:TYR:CD1	2.51	0.46
1:F:166:ALA:HB1	1:F:167:PRO:HD2	1.98	0.46
1:F:48:ILE:O	1:F:52:ILE:HG13	2.16	0.46
1:A:471:TYR:CD2	1:A:471:TYR:N	2.84	0.45
1:A:77:GLY:O	1:A:78:TYR:HD2	1.99	0.45
1:C:82:HIS:CG	1:C:109:SER:HA	2.51	0.45
1:D:420:LYS:HE2	1:F:427:THR:O	2.16	0.45
1:D:53:LYS:O	1:D:53:LYS:HD3	2.16	0.45
1:E:241:GLY:O	1:E:245:LYS:NZ	2.48	0.45
1:E:294:PHE:CE2	1:E:304:PHE:HA	2.51	0.45
1:B:67:ARG:NH1	1:B:136:TYR:CE2	2.84	0.45
1:B:336:ALA:HB3	1:B:359:ILE:HD12	1.98	0.45
1:C:17:PHE:CE2	1:C:486:ILE:HG12	2.50	0.45
1:C:302:LEU:HD22	1:C:309:ILE:HD12	1.99	0.45
1:E:323:ILE:HG12	1:E:345:ALA:HB3	1.99	0.45
1:E:369:PRO:HB3	1:E:478:ARG:HA	1.98	0.45
1:A:96:SER:O	1:A:130:LYS:HA	2.17	0.45
1:E:247:PHE:HD2	1:E:247:PHE:O	1.99	0.45
1:E:67:ARG:HD3	1:E:73:GLU:OE1	2.16	0.45
1:B:154:LYS:HD2	1:F:189:HIS:CG	2.51	0.45
1:F:208:ILE:HG13	1:F:445:GLU:OE2	2.16	0.45
1:A:192:ILE:CG1	1:A:391:HIS:HE1	2.29	0.45
1:A:205:GLN:CD	1:B:495:GLU:O	2.55	0.45
1:C:323:ILE:HG12	1:C:345:ALA:HB3	1.99	0.45
1:D:191:ASP:HB3	1:D:194:ALA:HB2	1.98	0.45
1:D:432:PRO:HB3	1:D:436:PHE:HD2	1.81	0.45
1:E:247:PHE:CD1	1:E:263:LEU:HD12	2.52	0.45
1:F:183:TYR:HD1	1:F:183:TYR:O	2.00	0.45
1:F:353:THR:HB	1:F:354:PRO:HD2	1.98	0.45
2:F:602:GLU:HA	4:F:605:NAI:H4N	1.99	0.45
1:A:382:TYR:O	1:A:386:LEU:HG	2.17	0.45
1:B:209:HIS:HD2	1:B:446:LYS:HA	1.82	0.45
1:D:166:ALA:HB1	1:D:167:PRO:HD2	1.99	0.45
1:D:281:TRP:HB2	1:D:310:TYR:HB2	1.98	0.45
1:B:57:HIS:HA	1:E:60:SER:O	2.17	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:396:ARG:NE	1:B:456:THR:HG21	2.32	0.45
1:B:48:ILE:O	1:B:52:ILE:HG13	2.17	0.45
1:C:185:SER:O	1:D:154:LYS:HD3	2.17	0.45
1:A:385:TRP:HH2	1:C:391:HIS:HD1	1.62	0.45
1:C:432:PRO:HB3	1:C:436:PHE:HD2	1.82	0.45
1:C:150:MET:CE	1:D:186:THR:HG22	2.47	0.45
1:D:323:ILE:HG12	1:D:345:ALA:HB3	1.98	0.45
1:D:403:ARG:HB2	1:D:441:SER:HA	1.99	0.45
1:D:456:THR:HG21	1:E:396:ARG:HH21	1.82	0.45
1:F:82:HIS:CG	1:F:109:SER:HA	2.52	0.45
1:F:90:LYS:HD2	1:F:164:VAL:O	2.17	0.45
1:A:491:ARG:HE	4:C:603:NAI:H2B	1.82	0.45
1:D:24:VAL:O	1:D:27:LYS:N	2.50	0.45
1:D:252:PHE:HB3	1:D:275:GLU:OE2	2.16	0.45
1:E:166:ALA:HB1	1:E:167:PRO:HD2	1.99	0.45
1:E:253:GLY:HA3	4:E:603:NAI:O5B	2.17	0.45
1:E:500:PHE:HA	1:F:146:ARG:CZ	2.47	0.45
3:E:602:GTP:O5'	3:E:602:GTP:H8	2.00	0.45
1:A:166:ALA:HB1	1:A:167:PRO:HD2	1.98	0.45
1:A:369:PRO:HB3	1:A:478:ARG:HA	1.98	0.45
1:A:48:ILE:HG21	1:A:490:PHE:HD1	1.82	0.45
1:D:281:TRP:CG	1:D:310:TYR:HD2	2.35	0.45
3:A:602:GTP:H2'	3:A:602:GTP:O1G	2.16	0.45
1:B:205:GLN:OE1	1:C:495:GLU:O	2.35	0.45
1:D:57:HIS:CE1	1:D:84:GLN:HE22	2.35	0.45
1:E:57:HIS:CE1	1:E:84:GLN:HE22	2.35	0.45
1:A:294:PHE:CE2	1:A:304:PHE:HA	2.52	0.44
1:B:209:HIS:CD2	1:B:446:LYS:HA	2.52	0.44
1:C:18:ASP:OD1	1:C:53:LYS:HD3	2.17	0.44
1:B:498:VAL:HB	1:E:72:TRP:CH2	2.53	0.44
1:F:244:ASP:N	1:F:244:ASP:OD1	2.50	0.44
1:F:69:ASP:OD1	1:F:71:SER:OG	2.25	0.44
1:A:292:GLU:OE2	3:A:602:GTP:N1	2.48	0.44
1:A:36:GLU:O	1:A:40:GLN:HB3	2.18	0.44
1:F:265:ARG:O	1:F:267:GLY:N	2.46	0.44
1:A:213:SER:HB3	3:A:602:GTP:O2'	2.17	0.44
1:C:199:THR:HA	1:C:384:GLU:OE1	2.16	0.44
1:C:294:PHE:CE2	1:C:304:PHE:HA	2.52	0.44
1:F:236:LEU:O	1:F:342:LYS:HE2	2.17	0.44
1:F:346:GLU:OE1	1:F:351:PRO:HD2	2.17	0.44
1:A:209:HIS:HE1	3:A:602:GTP:H5"	1.82	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap(Å)
1·A·281·TBP·CZ2	1·A·283·PBO·HG3	2.52	0.44
1:A:396:ARG:HE	1:B:456:THR:HG21	1.81	0.44
1:B:186:THB:OG1	1:B:187:ILE:N	2 44	0.44
1:B:215:THB:CB	4:B:603:NAI:H42N	2.46	0.44
1:B:388:ASN:H	1:B:388:ASN:HD22	1.66	0.44
1:B:388:ASN:N	1:B:388:ASN:ND2	2.66	0.44
1:B:471:TYB:N	1:B:471:TYR:CD2	2.84	0.44
1:A:204:SER:HB3	1:B:491:ARG:HG2	1.99	0.44
1:E:95:TYR:HH	1:E:145:THR:HG22	1.81	0.44
1:E:183:TYR:HD1	1:E:183:TYR:O	1.99	0.44
1:E:317:VAL:O	1:E:340:LYS:CE	2.63	0.44
1:F:126:LYS:HG3	1:F:127:ALA:H	1.82	0.44
1:F:66:ARG:NH1	1:F:143:LYS:HE2	2.32	0.44
1:F:315:LEU:HD22	1:F:331:LEU:HD11	1.98	0.44
1:A:261:ARG:HH12	3:A:602:GTP:PG	2.40	0.44
1:A:213:SER:HB2	1:A:262:TYR:HE2	1.83	0.44
1:A:39:GLU:OE1	1:A:42:ARG:HD2	2.17	0.44
1:A:455:TYR:O	1:A:459:ARG:N	2.36	0.44
1:B:244:ASP:N	1:B:244:ASP:OD1	2.51	0.44
1:B:369:PRO:HB3	1:B:478:ARG:HA	1.98	0.44
1:E:375:ALA:O	1:E:379:THR:OG1	2.24	0.44
1:F:150:MET:CE	1:F:186:THR:HG21	2.48	0.44
1:E:456:THR:HG21	1:F:396:ARG:HE	1.81	0.44
1:F:94:ARG:HG3	1:F:169:MET:HB2	2.00	0.44
1:B:82:HIS:CG	1:B:109:SER:HA	2.52	0.44
2:B:601:GLU:HA	4:B:603:NAI:C3N	2.48	0.44
1:D:210:GLY:O	1:D:214:ALA:HB2	2.17	0.44
1:D:339:VAL:O	1:D:340:LYS:C	2.55	0.44
1:D:401:TYR:CE2	1:F:443:ALA:CA	2.99	0.44
1:D:17:PHE:CE2	1:D:486:ILE:HG12	2.52	0.44
4:A:604:NAI:H71N	1:B:86:ARG:HH11	1.65	0.44
1:B:171:THR:HG22	1:B:175:GLU:HG2	2.00	0.44
1:B:208:ILE:HA	1:B:445:GLU:OE2	2.18	0.44
1:B:247:PHE:CE1	1:B:263:LEU:HB2	2.53	0.44
1:B:400:LYS:HG2	1:B:400:LYS:O	2.17	0.44
1:B:410:LEU:HG	1:B:430:ILE:HG22	2.00	0.44
1:B:86:ARG:HD3	1:B:86:ARG:HH11	1.64	0.44
1:E:172:GLY:O	1:E:176:MET:HG2	2.18	0.44
1:E:429:PRO:HG2	1:F:419:ARG:NH2	2.33	0.44
2:E:601:GLU:HA	4:E:603:NAI:C3N	2.48	0.44
1:F:209:HIS:CD2	1:F:446:LYS:HA	2.52	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap(Å)
1:F:215:THR:HG21	4:F:605:NAL:N7N	2.32	0.44
1:A:358:LYS:NZ	1:A:361:LEU:HD13	2.33	0.44
1·A·402·GLU·O	$1 \cdot A \cdot 406 \cdot A SN \cdot OD1$	2.36	0.44
1:A:86:ABG:NH2	4·C·603·NAI·N3A	2.66	0.11
1:B:146:ARG:NH1	1:B:182:THB:HG22	$\frac{2.00}{2.27}$	0.44
1.B.326.ALA.HB1	4·B·603·NAI·C6A	2.48	0.44
1.C·208·ILE·HA	1.C·445·GLU·OE2	2.18	0.44
1.C.353.THB.HB	$1 \cdot C \cdot 354 \cdot PRO \cdot HD2$	1 99	0.11
1:C:215:THR:OG1	4:C:604:NAI:H42N	2.18	0.44
1.D.195.HIS.CD2	$4 \cdot F \cdot 601 \cdot N AI \cdot 07N$	2.10	0.44
1.E.252.PHE.CB	$1 \cdot E \cdot 275 \cdot GLU \cdot OE2$	2.65	0.44
1.E.202.THE.0B	$\frac{1 \cdot E \cdot 2 \cdot 6 \cdot G \pm 0 \cdot O \pm 2}{1 \cdot F \cdot 384 \cdot G \pm 0 \cdot O \pm 1}$	2.00	0.44
1.C·281·TRP·CG	$1 \cdot C \cdot 310 \cdot TYB \cdot HD2$	2.36	0.44
1:D:172:GLY:0	1:D:176:MET:HG2	2.38	0.44
$1 \cdot D \cdot 48 \cdot ILE \cdot HG21$	$1 \cdot D \cdot 490 \cdot PHE \cdot HD1$	1.83	0.44
1.A.498.VAL.HB	$1 \cdot D \cdot 72 \cdot TBP \cdot CZ2$	2.53	0.11
1.F.339.VAL:O	1.E.339.VAL.HG12	2.33	0.44
1.R.247.PHE.C	$1 \cdot B \cdot 247 \cdot PHE \cdot CD2$	2.11	0.43
1.B.323.ILE.HG12	1.B.345.ALA.HB3	1 99	0.43
1.B.209.HIS.HD2	1.B.446.LVS.HB2	1.80	0.43
1.C.90.LYS.HD2	1.C.164.VAL:O	2.18	0.43
1:D:48:ILE:O	1:D:52:ILE:HG13	2.13	0.43
1:E:346:GLU:OE1	1:E:351:PRO:HD2	2.18	0.43
1:F:209:HIS:HD2	1:F:446:LYS:HA	1.82	0.43
1:E:456:THR:HG21	1:F:396:ARG:HH21	1.83	0.43
1:A:244:ASP:OD1	1:A:244:ASP:N	2.51	0.43
1:A:432:PRO:HA	1:C:412:SER:OG	2.18	0.43
2:B:601:GLU:HA	4:B:603:NAI:H4N	1.99	0.43
1:D:372:TYR:OH	1:D:461:ALA:HB2	2.18	0.43
1:E:17:PHE:CE2	1:E:486:ILE:HG12	2.53	0.43
1:B:58:VAL:O	1:E:59:LEU:HA	2.18	0.43
1:A:369:PRO:HD3	1:A:477:LEU:HB2	2.00	0.43
1:C:369:PRO:HB3	1:C:478:ARG:HA	1.99	0.43
1:E:423:LYS:C	1:E:425:GLY:H	2.22	0.43
1:F:269:LYS:HD2	1:F:284:ASP:C	2.38	0.43
1:B:126:LYS:HG3	1:B:127:ALA:H	1.83	0.43
1:B:148:PHE:CE2	1:B:152:LEU:HD11	2.53	0.43
1:B:57:HIS:CE1	1:B:84:GLN:HE22	2.36	0.43
1:B:61:LEU:HD21	1:E:57:HIS:CD2	2.53	0.43
1:C:281:TRP:CZ2	1:C:283:PRO:HG3	2.54	0.43
1:E:432:PRO:HB3	1:E:436:PHE:CD2	2.54	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:F:403:ARG:HB2	1:F:441:SER:HA	2.00	0.43
1:A:208:ILE:HA	1:A:445:GLU:OE2	2.19	0.43
1:B:91:GLY:O	1:B:165:PRO:HA	2.19	0.43
1:C:274:GLY:O	1:C:275:GLU:HG2	2.18	0.43
1:C:372:TYR:OH	1:C:461:ALA:HB2	2.18	0.43
4:D:604:NAI:H3D	1:E:387:LYS:HE2	2.01	0.43
1:D:90:LYS:HD2	1:D:164:VAL:O	2.19	0.43
1:D:96:SER:O	1:D:130:LYS:HA	2.18	0.43
1:E:148:PHE:CE2	1:E:152:LEU:HD11	2.54	0.43
1:F:146:ARG:HH11	1:F:182:THR:CG2	2.27	0.43
1:B:294:PHE:CE2	1:B:304:PHE:HA	2.53	0.43
1:B:320:ASP:HA	1:B:342:LYS:CD	2.48	0.43
1:B:470:LYS:HG2	1:B:471:TYR:CE2	2.54	0.43
1:A:409:LEU:CD2	1:C:409:LEU:HD21	2.44	0.43
1:D:169:MET:HA	4:D:603:NAI:O1A	2.18	0.43
1:E:220:PHE:HD1	1:E:263:LEU:HD23	1.83	0.43
1:E:316:GLU:O	1:E:340:LYS:HD2	2.19	0.43
1:B:392:VAL:HG22	1:C:386:LEU:CD1	2.47	0.43
1:C:27:LYS:HD2	1:C:471:TYR:OH	2.19	0.43
1:D:412:SER:HA	1:F:433:THR:HG23	2.00	0.43
1:E:244:ASP:OD1	1:E:244:ASP:N	2.49	0.43
1:E:357:ASP:OD2	1:E:478:ARG:NE	2.39	0.43
1:F:196:ALA:HB2	1:F:388:ASN:HB2	2.01	0.43
1:F:28:LEU:HD13	1:F:490:PHE:CD2	2.54	0.43
1:F:67:ARG:HD3	1:F:73:GLU:OE1	2.18	0.43
1:A:17:PHE:CE2	1:A:486:ILE:HG12	2.54	0.43
1:A:206:GLY:CA	4:A:604:NAI:H3D	2.47	0.43
1:B:96:SER:O	1:B:130:LYS:HA	2.19	0.43
1:B:265:ARG:O	1:B:267:GLY:N	2.47	0.43
1:B:48:ILE:HG21	1:B:490:PHE:HD1	1.83	0.43
1:C:410:LEU:HG	1:C:430:ILE:HG22	2.00	0.43
1:C:48:ILE:O	1:C:52:ILE:HG13	2.19	0.43
1:A:491:ARG:HG2	4:C:603:NAI:O2B	2.18	0.43
1:D:10:PHE:CE1	1:D:53:LYS:NZ	2.84	0.43
1:F:402:GLU:O	1:F:406:ASN:OD1	2.36	0.43
1:A:172:GLY:N	1:A:175:GLU:OE2	2.40	0.43
1:A:465:MET:O	1:A:469:MET:HG2	2.19	0.43
1:B:78:TYR:N	1:B:78:TYR:HD2	2.16	0.43
1:C:382:TYR:O	1:C:386:LEU:HG	2.19	0.43
1:D:94:ARG:O	1:D:128:GLY:HA2	2.19	0.43
1:C:154:LYS:HB3	1:D:189:HIS:NE2	2.34	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:210:GLY:O	1:E:214:ALA:HB2	2.19	0.43
1:D:433:THR:N	1:E:412:SER:OG	2.48	0.43
1:A:77:GLY:C	1:A:78:TYR:CD2	2.90	0.43
1:B:315:LEU:HD13	1:B:331:LEU:HD12	2.01	0.43
1:B:398:THR:O	1:B:401:TYR:N	2.46	0.43
1:C:213:SER:HB2	1:C:262:TYR:HE2	1.84	0.43
1:D:160:PRO:HD3	1:D:183:TYR:CE2	2.54	0.43
1:D:29:VAL:HG13	1:D:41:LYS:HB2	2.00	0.43
1:E:133:PRO:HG2	1:E:170:SER:HB3	2.00	0.43
1:E:150:MET:HE2	1:E:186:THR:HG21	2.00	0.43
1:E:355:GLU:OE1	1:E:358:LYS:HD2	2.19	0.43
1:F:213:SER:HB2	1:F:262:TYR:HE2	1.84	0.43
1:F:294:PHE:CD1	1:F:298:HIS:ND1	2.86	0.43
1:F:57:HIS:CE1	1:F:84:GLN:HE22	2.36	0.43
1:A:353:THR:HB	1:A:354:PRO:HD2	2.00	0.42
1:B:166:ALA:HB1	1:B:167:PRO:HD2	2.01	0.42
1:B:57:HIS:CD2	1:E:61:LEU:HD21	2.54	0.42
1:C:96:SER:O	1:C:130:LYS:HA	2.19	0.42
1:D:247:PHE:CE1	1:D:263:LEU:HD12	2.54	0.42
1:D:281:TRP:CZ2	1:D:283:PRO:HG3	2.54	0.42
4:D:604:NAI:H4N	1:E:195:HIS:NE2	2.33	0.42
1:E:199:THR:HA	1:E:384:GLU:OE1	2.19	0.42
1:E:211:ARG:HA	1:E:380:VAL:HG11	2.01	0.42
1:F:281:TRP:CG	1:F:310:TYR:CD2	3.07	0.42
1:F:213:SER:HB3	3:F:604:GTP:O2'	2.20	0.42
1:A:68:ASP:OD2	1:A:137:THR:OG1	2.26	0.42
1:C:247:PHE:CE1	1:C:263:LEU:HB2	2.54	0.42
1:C:281:TRP:HB2	1:C:310:TYR:HB2	2.00	0.42
1:D:410:LEU:HG	1:D:430:ILE:HG22	1.99	0.42
1:D:209:HIS:CD2	1:D:446:LYS:HA	2.54	0.42
1:D:465:MET:O	1:D:469:MET:HG2	2.18	0.42
1:E:65:ILE:HD13	1:E:144:ILE:CG1	2.50	0.42
1:F:247:PHE:C	1:F:247:PHE:CD2	2.92	0.42
1:E:119:ASP:C	1:F:396:ARG:HH12	2.21	0.42
1:A:212:ILE:HG22	1:A:258:HIS:HE1	1.85	0.42
1:B:363:ARG:HB3	1:B:363:ARG:HE	1.69	0.42
1:C:154:LYS:HD2	1:D:189:HIS:ND1	2.35	0.42
1:C:369:PRO:HD3	1:C:477:LEU:HB2	2.01	0.42
1:D:215:THR:CB	4:D:603:NAI:H42N	2.48	0.42
1:E:208:ILE:HA	1:E:445:GLU:OE2	2.19	0.42
1:F:34:THR:CG2	1:F:44:ARG:HH22	2.25	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap(Å)
$1 \cdot B \cdot 401 \cdot TYB \cdot CE2$	1.C.447.ASP.HB3	2.54	0.42
1:D:247:PHE:CE2	1:D:270:CYS:CB	2.97	0.42
1:E:281:TRP:CG	1:E:310:TYR:HD2	2.37	0.42
1:F:96:SER:O	1:F:130:LYS:HA	2.20	0.42
1:A:126:LYS:HG3	1:A:127:ALA:H	1.84	0.42
1:C:8:ASN:ND2	1:C:102:ASP:OD2	2.45	0.42
1:C:111:MET:HE1	2:C:601:GLU:HG3	2.01	0.42
1:D:10:PHE:CE2	1:D:105:LYS:HE2	2.54	0.42
1:E:94:ARG:O	1:E:128:GLY:HA2	2.19	0.42
1:E:247:PHE:HE2	1:E:270:CYS:HB2	1.82	0.42
1:E:433:THR:HG23	1:F:412:SER:HA	2.01	0.42
1:E:48:ILE:HG21	1:E:490:PHE:HD1	1.83	0.42
1:F:209:HIS:HD2	1:F:446:LYS:CA	2.33	0.42
1:F:247:PHE:HE1	1:F:263:LEU:HB2	1.84	0.42
1:F:294:PHE:HE2	1:F:304:PHE:HA	1.81	0.42
1:F:372:TYR:OH	1:F:461:ALA:HB2	2.19	0.42
1:F:17:PHE:CE2	1:F:486:ILE:HG12	2.54	0.42
1:A:281:TRP:CG	1:A:310:TYR:HD2	2.37	0.42
1:B:213:SER:HB2	1:B:262:TYR:HE2	1.83	0.42
1:C:94:ARG:O	1:C:128:GLY:HA2	2.20	0.42
1:C:159:GLY:HA2	1:C:183:TYR:CE2	2.55	0.42
1:C:241:GLY:O	1:C:245:LYS:NZ	2.45	0.42
1:E:208:ILE:HG13	1:E:445:GLU:OE2	2.20	0.42
1:A:150:MET:HE1	1:A:186:THR:HG21	2.00	0.42
1:B:295:LYS:O	1:B:295:LYS:HG3	2.19	0.42
1:C:247:PHE:CD2	1:C:247:PHE:C	2.93	0.42
1:D:159:GLY:HA2	1:D:183:TYR:CE2	2.55	0.42
1:D:265:ARG:O	1:D:267:GLY:N	2.46	0.42
1:E:24:VAL:O	1:E:27:LYS:N	2.52	0.42
1:E:331:LEU:HD23	1:E:360:PHE:HZ	1.82	0.42
1:E:495:GLU:O	1:F:205:GLN:CD	2.58	0.42
1:C:60:SER:O	1:F:57:HIS:HA	2.20	0.42
1:A:133:PRO:HG2	1:A:170:SER:HB3	2.01	0.42
1:A:403:ARG:HD2	1:A:441:SER:OG	2.19	0.42
1:A:462:ARG:O	1:A:465:MET:N	2.53	0.42
1:B:10:PHE:CD2	1:B:105:LYS:HE2	2.54	0.42
1:B:403:ARG:O	1:B:406:ASN:N	2.53	0.42
1:C:210:GLY:O	1:C:214:ALA:HB2	2.20	0.42
1:D:209:HIS:HD2	1:D:446:LYS:CA	2.31	0.42
1:F:238:MET:HE1	1:F:342:LYS:HB3	2.02	0.42
1:F:2:ASP:OD1	1:F:3:ARG:N	2.42	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap(Å)
1·A·160·PRO·HD3	$1 \cdot A \cdot 183 \cdot TYB \cdot CE2$	2.55	0.42
1:A:337:PRO:HG3	1:A:359:ILE:HD13	$\frac{2.00}{2.00}$	0.12
1.B.210.GLY.O	$1 \cdot B \cdot 214 \cdot ALA \cdot HB2$	2.20	0.42
$1 \cdot A \cdot 396 \cdot ABG \cdot CZ$	$1 \cdot B \cdot 456 \cdot THB \cdot HG21$	2.50	0.12
1:C:247:PHE:HB3	1:C:321:ILE:HB	$\frac{2.00}{2.02}$	0.12
1.A.409.LEU.HD13	$1 \cdot C \cdot 409 \cdot LEU \cdot HD11$	2.02	0.42
$1 \cdot D \cdot 274 \cdot GLY \cdot O$	1.D.275.GLU.HG3	$\frac{2.01}{2.20}$	0.42
$\frac{1.D.271.0L1.0}{1.D.382.TYB.0}$	1.D.386.LEU.HG	2.20	0.12
1:D:444:SER:OG	1:D:447:ASP:OD1	2.23	0.12
1:E:400:LYS:HG2	1:E:400:LYS:O	2 20	0.42
$1 \cdot F \cdot 281 \cdot TBP \cdot CZ2$	1·F·283·PBO·HG3	2.54	0.42
1.F.77.GLY.C	$1 \cdot F \cdot 78 \cdot TYB \cdot CD2$	2.88	0.42
1·A·281·TBP·HB2	$1 \cdot A \cdot 310 \cdot TYB \cdot HB2$	2.02	0.42
1:B:281:TBP:CZ2	1:B:283:PBO:HG3	2.55	0.42
1.B.78.TYB.N	1·B·78·TYB·CD2	2.88	0.42
1.C.89.CVS.HB3	1.C.125.ALA.HB2	2.02	0.42
1.C.172.GLY.O	1.C.176.MET.HG2	2.02	0.12
1.D.208.ILE.HA	$1 \cdot D \cdot 445 \cdot GLU \cdot OE2$	2.10	0.12
$\frac{1.D.200.1122.1111}{1.D.493.TYB.0}$	1.D.498.VAL:HG22	2.20	0.12
$1 \cdot F \cdot 210 \cdot GLY \cdot O$	$1 \cdot F \cdot 214 \cdot ALA \cdot HB2$	2.20	0.12
1.F.363.ABG.HE	1.F.363.ABG.HB3	1.72	0.12
1.F.432.PRO.HB3	$1 \cdot F \cdot 436 \cdot PHE \cdot CD2$	2 55	0.12
$1 \cdot F \cdot 86 \cdot ABG \cdot HD2$	$4 \cdot F \cdot 601 \cdot N AI \cdot C2N$	2.50	0.12
1:F:91:GLY:0	1:F:165:PRO:HA	$\frac{2.30}{2.20}$	0.12
1:A:199:THB:HA	1:A:384:GLU:OE1	2.19	0.41
1:B:172:GLY:O	1:B:176:MET:HG2	2 20	0.41
1:B:336:ALA:N	1:B:337:PRO:HD2	2.35	0.41
1:C:148:PHE:CE2	1:C:152:LEU:HD11	2.55	0.41
1:C:338:ARG:O	1:C:340:LYS:HG2	2.20	0.41
1:D:32:LEU:HD12	1:D:32:LEU:HA	1.80	0.41
1:D:346:GLU:OE1	1:D:351:PRO:HD2	2.20	0.41
1:E:27:LYS:O	1:E:30:GLU:HB3	2.20	0.41
1:F:211:ARG:HA	1:F:380:VAL:HG11	2.01	0.41
1:F:86:ARG:HG3	4:F:601:NAI:H62A	1.84	0.41
1:A:20:GLY:O	1:A:24:VAL:HG22	2.20	0.41
1:B:493:TYR:O	1:B:498:VAL:HG22	2.19	0.41
1:D:209:HIS:HD2	1:D:446:LYS:CB	2.32	0.41
1:E:91:GLY:O	1:E:165:PRO:HA	2.19	0.41
1:E:281:TRP:CZ2	1:E:283:PRO:HG3	2.54	0.41
1:E:339:VAL:O	1:E:340:LYS:CD	2.52	0.41
1:E:317:VAL:C	1:E:340:LYS:HG3	2.40	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:340:LYS:HG2	1:E:341:ALA:HB2	2.02	0.41
1:E:372:TYR:OH	1:E:461:ALA:HB2	2.19	0.41
1:E:403:ARG:NH1	1:E:440:ILE:HG23	2.34	0.41
1:C:143:LYS:HE3	1:F:501:THR:HA	2.02	0.41
1:F:78:TYR:N	1:F:78:TYR:CD2	2.88	0.41
1:A:48:ILE:O	1:A:52:ILE:HG13	2.20	0.41
1:B:310:TYR:CE2	1:B:317:VAL:HG22	2.54	0.41
1:B:211:ARG:HA	1:B:380:VAL:HG11	2.02	0.41
1:B:422:GLY:C	1:B:424:HIS:H	2.23	0.41
1:B:374:ASN:HB2	4:B:603:NAI:H5N	2.02	0.41
1:C:244:ASP:OD1	1:C:244:ASP:N	2.54	0.41
1:C:265:ARG:C	1:C:267:GLY:H	2.24	0.41
1:C:400:LYS:O	1:C:400:LYS:HG2	2.20	0.41
1:D:148:PHE:CE2	1:D:152:LEU:HD11	2.55	0.41
1:A:189:HIS:ND1	1:E:154:LYS:HD2	2.35	0.41
1:E:459:ARG:NH1	1:E:459:ARG:HG3	2.35	0.41
1:F:209:HIS:HD2	1:F:446:LYS:CB	2.34	0.41
1:F:65:ILE:HG22	1:F:66:ARG:O	2.19	0.41
1:A:146:ARG:HH11	1:A:182:THR:CG2	2.26	0.41
1:A:210:GLY:O	1:A:214:ALA:HB2	2.20	0.41
1:A:94:ARG:HG3	1:A:169:MET:HB2	2.03	0.41
1:C:177:SER:HB2	1:C:202:PRO:HG2	2.02	0.41
1:C:211:ARG:HA	1:C:380:VAL:HG11	2.03	0.41
1:C:91:GLY:O	1:C:165:PRO:HA	2.20	0.41
1:D:111:MET:HE1	2:D:601:GLU:HG3	2.01	0.41
1:D:387:LYS:HE2	4:F:601:NAI:C5D	2.50	0.41
1:D:77:GLY:O	1:D:78:TYR:HD2	2.03	0.41
1:E:382:TYR:O	1:E:386:LEU:HG	2.20	0.41
1:E:5:ASP:HB2	1:E:333:LYS:HE3	2.02	0.41
1:F:41:LYS:O	1:F:45:VAL:HG23	2.20	0.41
1:A:94:ARG:O	1:A:128:GLY:HA2	2.20	0.41
1:B:150:MET:HE2	1:B:186:THR:HG21	2.02	0.41
1:B:211:ARG:NH2	4:B:603:NAI:O7N	2.36	0.41
1:C:65:ILE:HG21	1:C:144:ILE:HG12	2.03	0.41
1:C:69:ASP:OD1	1:C:71:SER:OG	2.25	0.41
1:D:146:ARG:HH11	1:D:182:THR:CG2	2.25	0.41
1:D:37:THR:HG23	1:D:41:LYS:HE3	2.03	0.41
1:F:375:ALA:O	1:F:379:THR:OG1	2.24	0.41
1:A:211:ARG:O	1:A:214:ALA:HB3	2.20	0.41
1:A:220:PHE:HD1	1:A:263:LEU:HD23	1.86	0.41
1:B:20:GLY:O	1:B:24:VAL:HG22	2.20	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:24:VAL:O	1:B:27:LYS:N	2.54	0.41
1:F:337:PRO:HG3	1:F:359:ILE:HD13	2.01	0.41
1:F:433:THR:HG23	1:F:433:THR:H	1.61	0.41
1:F:86:ARG:NE	4:F:601:NAI:H62A	2.17	0.41
1:A:29:VAL:HG13	1:A:41:LYS:HB2	2.02	0.41
1:B:94:ARG:O	1:B:128:GLY:HA2	2.21	0.41
1:D:20:GLY:O	1:D:24:VAL:HG22	2.21	0.41
1:E:410:LEU:HG	1:E:430:ILE:HG22	2.03	0.41
1:F:24:VAL:O	1:F:27:LYS:N	2.53	0.41
1:A:265:ARG:NH2	3:A:602:GTP:PG	2.89	0.41
1:B:17:PHE:CE2	1:B:486:ILE:HG12	2.55	0.41
1:B:491:ARG:HB2	1:B:491:ARG:CZ	2.50	0.41
1:C:211:ARG:O	1:C:214:ALA:HB3	2.21	0.41
1:C:20:GLY:O	1:C:24:VAL:HG22	2.21	0.41
1:A:448:ILE:HD12	1:C:397:LEU:O	2.21	0.41
1:C:169:MET:CG	4:C:604:NAI:H3D	2.51	0.41
1:F:406:ASN:ND2	1:F:436:PHE:CZ	2.88	0.41
4:F:601:NAI:C6N	4:F:601:NAI:H52N	2.44	0.41
1:F:121:PRO:HA	4:F:601:NAI:N6A	2.36	0.41
1:A:410:LEU:HG	1:A:430:ILE:HG22	2.02	0.41
1:A:91:GLY:O	1:A:165:PRO:HA	2.20	0.41
1:B:211:ARG:O	1:B:214:ALA:HB3	2.21	0.41
1:C:374:ASN:HB2	4:C:604:NAI:C5N	2.51	0.41
1:D:265:ARG:C	1:D:267:GLY:H	2.24	0.41
1:D:25:GLU:O	1:D:29:VAL:HG23	2.21	0.41
1:E:96:SER:O	1:E:130:LYS:HA	2.20	0.41
1:E:493:TYR:O	1:E:498:VAL:HG22	2.21	0.41
1:A:247:PHE:C	1:A:247:PHE:CD2	2.94	0.41
1:B:154:LYS:HB3	1:F:189:HIS:CE1	2.56	0.41
1:B:133:PRO:HG2	1:B:170:SER:HB3	2.03	0.41
1:B:320:ASP:HA	1:B:342:LYS:HD2	2.03	0.41
1:B:61:LEU:HD23	1:B:61:LEU:HA	1.91	0.41
1:B:77:GLY:C	1:B:78:TYR:CD2	2.88	0.41
1:F:374:ASN:HB2	4:F:605:NAI:C5N	2.51	0.41
1:B:38:GLU:HB2	1:B:39:GLU:H	1.74	0.41
$1:D:164:VAL:H\overline{A}$	1:D:197:CYS:O	2.21	0.41
1:D:239:THR:O	1:D:245:LYS:NZ	2.39	0.41
1:D:27:LYS:O	1:D:30:GLU:HB3	2.21	0.41
1:D:339:VAL:O	1:D:339:VAL:HG12	2.19	0.41
1:F:211:ARG:O	1:F:214:ALA:HB3	2.21	0.41
1:B:146:ARG:HH11	1:B:182:THR:CG2	2.30	0.40



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:B:403:ARG:NH1	1:B:441:SER:OG	2.54	0.40
1:C:189:HIS:CE1	1:D:154:LYS:HB3	2.56	0.40
1:A:406:ASN:ND2	1:C:409:LEU:HD12	2.37	0.40
1:C:29:VAL:HG13	1:C:41:LYS:HB2	2.03	0.40
1:C:43:ASN:HB3	1:C:44:ARG:CZ	2.51	0.40
1:D:253:GLY:HA3	4:D:603:NAI:PA	2.60	0.40
1:D:91:GLY:O	1:D:165:PRO:HA	2.21	0.40
1:E:20:GLY:O	1:E:24:VAL:HG22	2.21	0.40
1:A:246:THR:HB	1:A:271:VAL:CG2	2.51	0.40
1:A:211:ARG:HA	1:A:380:VAL:HG11	2.03	0.40
1:A:372:TYR:OH	1:A:461:ALA:HB2	2.21	0.40
1:C:45:VAL:HG22	1:C:490:PHE:CZ	2.56	0.40
1:D:131:ILE:HB	1:D:136:TYR:CE1	2.56	0.40
1:C:154:LYS:HB3	1:D:189:HIS:CE1	2.56	0.40
1:D:220:PHE:HD1	1:D:263:LEU:HD23	1.86	0.40
1:D:224:GLU:HA	1:D:227:ILE:HG22	2.03	0.40
1:D:331:LEU:HD23	1:D:360:PHE:HZ	1.85	0.40
1:E:211:ARG:O	1:E:214:ALA:HB3	2.21	0.40
1:E:27:LYS:HD2	1:E:471:TYR:OH	2.21	0.40
1:E:281:TRP:HB2	1:E:310:TYR:HB2	2.02	0.40
1:E:61:LEU:N	1:E:77:GLY:O	2.54	0.40
1:E:78:TYR:HD2	1:E:78:TYR:N	2.20	0.40
1:F:369:PRO:HD3	1:F:477:LEU:HB2	2.03	0.40
1:F:357:ASP:OD2	1:F:478:ARG:HD2	2.21	0.40
1:F:69:ASP:O	1:F:71:SER:N	2.54	0.40
2:A:601:GLU:CB	4:A:603:NAI:H4N	2.52	0.40
1:B:17:PHE:CD1	1:B:53:LYS:HG2	2.57	0.40
1:B:220:PHE:HD1	1:B:263:LEU:HD23	1.86	0.40
1:B:25:GLU:OE1	1:B:46:ARG:NE	2.54	0.40
1:C:133:PRO:HG2	1:C:170:SER:HB3	2.03	0.40
1:C:339:VAL:O	1:C:339:VAL:HG12	2.21	0.40
1:C:65:ILE:HD13	1:C:144:ILE:CG1	2.52	0.40
1:E:247:PHE:CE1	1:E:263:LEU:HB2	2.53	0.40
1:F:94:ARG:O	1:F:128:GLY:HA2	2.21	0.40
1:F:432:PRO:HB3	1:F:436:PHE:HD2	1.86	0.40
1:A:400:LYS:O	1:A:400:LYS:HG2	2.20	0.40
1:B:89:CYS:HB3	1:B:125:ALA:HB2	2.03	0.40
1:C:470:LYS:CG	1:C:471:TYR:CE2	3.04	0.40
1:D:27:LYS:HD2	1:D:471:TYR:OH	2.21	0.40
1:E:131:ILE:HB	1:E:136:TYR:CE1	2.56	0.40
1:F:86:ARG:HB3	1:F:121:PRO:O	2.22	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:GLY:O	1:F:176:MET:HG2	2.20	0.40
1:F:414:GLN:HG3	1:F:428:ILE:O	2.22	0.40
1:F:111:MET:HE1	2:F:602:GLU:HG3	2.03	0.40
1:A:134:LYS:HD3	1:A:134:LYS:HA	1.64	0.40
1:A:225:ASN:OD1	1:A:458:GLU:HG2	2.20	0.40
1:B:27:LYS:HD2	1:B:471:TYR:OH	2.22	0.40
1:C:160:PRO:HD3	1:C:183:TYR:CE2	2.56	0.40
1:C:192:ILE:HG12	1:C:391:HIS:HE1	1.85	0.40
1:C:69:ASP:O	1:C:71:SER:N	2.54	0.40
1:E:215:THR:HB	4:E:603:NAI:H42N	2.02	0.40
1:F:131:ILE:HB	1:F:136:TYR:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	499/582~(86%)	448 (90%)	42 (8%)	9~(2%)	8	35
1	В	499/582~(86%)	444 (89%)	41 (8%)	14 (3%)	5	25
1	С	499/582~(86%)	448 (90%)	43 (9%)	8 (2%)	9	36
1	D	499/582~(86%)	447 (90%)	40 (8%)	12 (2%)	6	28
1	Е	499/582~(86%)	444 (89%)	43 (9%)	12 (2%)	6	28
1	F	499/582~(86%)	446 (89%)	38 (8%)	15 (3%)	4	24
All	All	2994/3492~(86%)	2677(89%)	247 (8%)	70 (2%)	6	29

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	HIS



Mol	Chain	Res	Type
1	А	214	ALA
1	А	340	LYS
1	В	33	LYS
1	В	214	ALA
1	С	214	ALA
1	D	214	ALA
1	D	340	LYS
1	Е	214	ALA
1	Е	340	LYS
1	F	214	ALA
1	F	340	LYS
1	F	433	THR
1	А	498	VAL
1	В	67	ARG
1	В	340	LYS
1	В	403	ARG
1	В	424	HIS
1	В	498	VAL
1	С	340	LYS
1	С	498	VAL
1	D	276	SER
1	D	436	PHE
1	D	498	VAL
1	Е	317	VAL
1	Ε	498	VAL
1	F	33	LYS
1	F	498	VAL
1	В	391	HIS
1	С	266	PHE
1	D	266	PHE
1	D	500	PHE
1	E	266	PHE
1	E	391	HIS
1	E	424	HIS
1	F	66	ARG
1	F	309	ILE
1	F	403	ARG
1	A	70	GLY
1	A	276	SER
1	А	400	LYS
1	A	403	ARG
1	В	70	GLY



Mol	Chain	Res	Type
1	В	310	TYR
1	В	423	LYS
1	С	70	GLY
1	С	276	SER
1	С	400	LYS
1	D	70	GLY
1	D	400	LYS
1	Е	70	GLY
1	Е	276	SER
1	Е	400	LYS
1	Е	403	ARG
1	F	70	GLY
1	F	266	PHE
1	F	391	HIS
1	F	400	LYS
1	F	435	GLU
1	В	36	GLU
1	В	400	LYS
1	D	363	ARG
1	F	276	SER
1	В	266	PHE
1	Е	363	ARG
1	F	496	ALA
1	D	317	VAL
1	A	317	VAL
1	С	317	VAL
1	D	309	ILE

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	Percei	ntiles
1	А	417/471~(88%)	409~(98%)	8 (2%)	57	77
1	В	417/471~(88%)	410 (98%)	7 (2%)	60	78
1	С	417/471~(88%)	409 (98%)	8 (2%)	57	77



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	417/471~(88%)	407~(98%)	10~(2%)	49 73
1	Ε	417/471~(88%)	407~(98%)	10~(2%)	49 73
1	F	417/471~(88%)	408~(98%)	9~(2%)	52 74
All	All	2502/2826~(88%)	2450~(98%)	52 (2%)	53 75

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All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	9	PHE
1	А	35	ARG
1	А	78	TYR
1	А	195	HIS
1	А	221	HIS
1	А	357	ASP
1	А	450	HIS
1	А	455	TYR
1	В	9	PHE
1	В	31	ASP
1	В	78	TYR
1	В	183	TYR
1	В	310	TYR
1	В	338	ARG
1	В	357	ASP
1	С	3	ARG
1	С	9	PHE
1	С	31	ASP
1	С	44	ARG
1	С	78	TYR
1	С	102	ASP
1	С	357	ASP
1	С	490	PHE
1	D	9	PHE
1	D	10	PHE
1	D	78	TYR
1	D	238	MET
1	D	247	PHE
1	D	294	PHE
1	D	357	ASP
1	D	424	HIS
1	D	462	ARG
1	D	491	ARG



Mol	Chain	Res	Type
1	Е	9	PHE
1	Е	31	ASP
1	Е	79	ARG
1	Е	183	TYR
1	Е	247	PHE
1	Е	340	LYS
1	Е	357	ASP
1	Е	401	TYR
1	Е	455	TYR
1	Е	469	MET
1	F	9	PHE
1	F	19	ARG
1	F	98	ASP
1	F	183	TYR
1	F	294	PHE
1	F	310	TYR
1	F	357	ASP
1	F	423	LYS
1	F	490	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	205	GLN
1	В	209	HIS
1	D	209	HIS
1	D	391	HIS
1	Е	195	HIS
1	F	195	HIS
1	F	209	HIS
1	F	391	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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



5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

24 ligands are modelled in this entry.

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

Mal	Tune	Chain	Dec	Tink	B	ond leng	gths	E	Bond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	NAI	Е	603	-	42,48,48	4.76	19 (45%)	47,73,73	1.90	8 (17%)
3	GTP	F	604	-	$26,\!34,\!34$	1.02	1 (3%)	33,54,54	2.08	10 (30%)
4	NAI	F	605	-	42,48,48	4.75	19 (45%)	47,73,73	2.06	11 (23%)
4	NAI	С	603	-	42,48,48	4.77	19 (45%)	47,73,73	1.95	5(10%)
4	NAI	В	604	-	42,48,48	4.70	18 (42%)	47,73,73	1.81	<mark>6 (12%)</mark>
4	NAI	F	601	-	42,48,48	4.71	19 (45%)	47,73,73	2.15	10 (21%)
4	NAI	А	603	-	42,48,48	4.72	19 (45%)	47,73,73	2.10	<mark>8 (17%)</mark>
3	GTP	С	602	1	$26,\!34,\!34$	0.96	1 (3%)	33,54,54	1.74	<mark>6 (18%)</mark>
3	GTP	В	602	-	$26,\!34,\!34$	0.93	1 (3%)	33,54,54	1.82	7 (21%)
3	GTP	А	602	-	$26,\!34,\!34$	1.11	1 (3%)	33,54,54	2.13	<mark>9 (27%)</mark>
4	NAI	С	604	-	42,48,48	4.81	20 (47%)	47,73,73	1.87	<mark>9 (19%)</mark>
4	NAI	А	604	1	42,48,48	4.71	19 (45%)	47,73,73	2.20	8 (17%)
3	GTP	Е	602	1	26,34,34	0.97	1 (3%)	33,54,54	1.69	7 (21%)
3	GTP	D	602	1	$26,\!34,\!34$	0.98	1 (3%)	33,54,54	1.82	<mark>6 (18%)</mark>
4	NAI	В	603	-	42,48,48	4.68	20 (47%)	47,73,73	2.13	10 (21%)
4	NAI	D	603	-	42,48,48	4.74	19 (45%)	47,73,73	1.82	5(10%)
4	NAI	D	604	1	42,48,48	4.71	19 (45%)	47,73,73	2.01	<mark>9 (19%)</mark>
4	NAI	F	603	-	42,48,48	4.73	20 (47%)	47,73,73	1.85	7 (14%)

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.



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAI	Е	603	-	-	11/25/72/72	0/5/5/5
3	GTP	F	604	-	-	1/18/38/38	0/3/3/3
4	NAI	F	605	-	-	13/25/72/72	0/5/5/5
4	NAI	С	603	-	-	12/25/72/72	0/5/5/5
4	NAI	В	604	-	-	11/25/72/72	0/5/5/5
4	NAI	F	601	-	-	8/25/72/72	0/5/5/5
4	NAI	А	603	-	-	7/25/72/72	0/5/5/5
3	GTP	С	602	1	-	5/18/38/38	0/3/3/3
3	GTP	В	602	-	-	3/18/38/38	0/3/3/3
3	GTP	А	602	-	-	4/18/38/38	0/3/3/3
4	NAI	С	604	-	-	15/25/72/72	0/5/5/5
4	NAI	А	604	1	-	13/25/72/72	0/5/5/5
3	GTP	Е	602	1	-	2/18/38/38	0/3/3/3
3	GTP	D	602	1	-	3/18/38/38	0/3/3/3
4	NAI	В	603	-	-	9/25/72/72	0/5/5/5
4	NAI	D	603	-	-	13/25/72/72	0/5/5/5
4	NAI	D	604	1	-	11/25/72/72	0/5/5/5
4	NAI	F	603	-	-	10/25/72/72	0/5/5/5

All (236) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
4	С	604	NAI	O4B-C1B	16.15	1.63	1.41
4	F	605	NAI	O4B-C1B	15.83	1.63	1.41
4	А	603	NAI	O4B-C1B	15.72	1.63	1.41
4	А	604	NAI	O4B-C1B	15.63	1.62	1.41
4	В	604	NAI	O4B-C1B	15.59	1.62	1.41
4	В	603	NAI	O4B-C1B	15.50	1.62	1.41
4	Е	603	NAI	O4B-C1B	15.42	1.62	1.41
4	D	603	NAI	O4B-C1B	15.39	1.62	1.41
4	С	603	NAI	O4B-C1B	15.37	1.62	1.41
4	D	604	NAI	O4B-C1B	15.33	1.62	1.41
4	F	603	NAI	O4B-C1B	15.29	1.62	1.41
4	F	601	NAI	O4B-C1B	15.16	1.62	1.41
4	С	604	NAI	C2B-C1B	-15.05	1.30	1.53
4	С	603	NAI	C2B-C1B	-14.85	1.31	1.53
4	В	604	NAI	C2B-C1B	-14.82	1.31	1.53
4	D	603	NAI	C2B-C1B	-14.81	1.31	1.53
4	Е	603	NAI	C2B-C1B	-14.75	1.31	1.53



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Mol	Chain	Res	Type	Atoms		Observed(A)	$\operatorname{Ideal}(\operatorname{\AA})$
4	А	603	NAI	C2B-C1B	-14.50	1.31	1.53
4	F	601	NAI	C2B-C1B	-14.48	1.31	1.53
4	D	604	NAI	C2B-C1B	-14.48	1.31	1.53
4	F	605	NAI	C2B-C1B	-14.47	1.31	1.53
4	F	603	NAI	C2B-C1B	-14.47	1.31	1.53
4	А	604	NAI	C2B-C1B	-14.08	1.32	1.53
4	В	603	NAI	C2B-C1B	-13.89	1.32	1.53
4	С	603	NAI	C6N-C5N	11.34	1.53	1.33
4	А	604	NAI	C6N-C5N	11.15	1.53	1.33
4	F	603	NAI	C6N-C5N	11.07	1.53	1.33
4	Е	603	NAI	C6N-C5N	11.06	1.53	1.33
4	D	603	NAI	C6N-C5N	10.96	1.52	1.33
4	D	604	NAI	C6N-C5N	10.94	1.52	1.33
4	F	601	NAI	C6N-C5N	10.89	1.52	1.33
4	С	604	NAI	C6N-C5N	10.83	1.52	1.33
4	F	605	NAI	C6N-C5N	10.79	1.52	1.33
4	В	603	NAI	C6N-C5N	10.63	1.52	1.33
4	А	603	NAI	C6N-C5N	10.62	1.52	1.33
4	В	604	NAI	C6N-C5N	10.27	1.51	1.33
4	С	603	NAI	O4D-C1D	9.05	1.63	1.42
4	F	603	NAI	O4D-C1D	9.03	1.63	1.42
4	F	605	NAI	O4D-C1D	8.82	1.62	1.42
4	А	603	NAI	O4D-C1D	8.73	1.62	1.42
4	С	604	NAI	O4D-C1D	8.68	1.62	1.42
4	А	604	NAI	O4D-C1D	8.67	1.62	1.42
4	D	603	NAI	O4D-C1D	8.66	1.62	1.42
4	Е	603	NAI	O4D-C1D	8.60	1.62	1.42
4	F	601	NAI	O4D-C1D	8.54	1.62	1.42
4	D	604	NAI	O4D-C1D	8.51	1.62	1.42
4	В	603	NAI	O4D-C1D	8.44	1.62	1.42
4	В	604	NAI	O4D-C1D	8.29	1.61	1.42
4	В	603	NAI	C2D-C1D	-7.34	1.30	1.53
4	Е	603	NAI	C2D-C1D	-7.18	1.30	1.53
4	F	603	NAI	C2D-C1D	-7.15	1.30	1.53
4	F	605	NAI	C2D-C1D	-7.15	1.30	1.53
4	С	603	NAI	C2D-C1D	-7.15	1.30	1.53
4	А	603	NAI	C2N-C3N	7.08	1.54	1.34
4	F	601	NAI	C2D-C1D	-7.05	1.30	1.53
4	С	604	NAI	C2D-C1D	-7.03	1.31	1.53
4	В	603	NAI	C2N-C3N	7.03	1.54	1.34
4	В	604	NAI	C2D-C1D	-7.01	1.31	1.53
4	D	603	NAI	C2D-C1D	-7.00	1.31	1.53

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Mol	Chain	\mathbf{Res}	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
4	А	604	NAI	C2D-C1D	-6.96	1.31	1.53
4	А	603	NAI	C2D-C1D	-6.81	1.31	1.53
4	D	604	NAI	C2D-C1D	-6.81	1.31	1.53
4	С	604	NAI	C2N-C3N	6.77	1.53	1.34
4	Е	603	NAI	C2N-C3N	6.73	1.53	1.34
4	D	604	NAI	C2N-C3N	6.69	1.53	1.34
4	F	605	NAI	C2N-C3N	6.63	1.53	1.34
4	D	603	NAI	C2N-C3N	6.58	1.53	1.34
4	В	604	NAI	C2N-C3N	6.55	1.53	1.34
4	В	604	NAI	O4D-C4D	-6.44	1.30	1.45
4	F	605	NAI	O4D-C4D	-6.38	1.30	1.45
4	С	603	NAI	C2N-C3N	6.33	1.52	1.34
4	А	604	NAI	C2N-C3N	6.30	1.52	1.34
4	F	603	NAI	C2N-C3N	6.29	1.52	1.34
4	D	603	NAI	O4B-C4B	-6.29	1.30	1.45
4	Е	603	NAI	O4B-C4B	-6.24	1.31	1.45
4	F	601	NAI	C2N-C3N	6.22	1.52	1.34
4	А	603	NAI	O4D-C4D	-6.21	1.31	1.45
4	F	601	NAI	O4D-C4D	-6.21	1.31	1.45
4	D	604	NAI	O4D-C4D	-6.19	1.31	1.45
4	А	604	NAI	O4B-C4B	-6.15	1.31	1.45
4	A	604	NAI	O4D-C4D	-6.13	1.31	1.45
4	F	603	NAI	O4D-C4D	-6.13	1.31	1.45
4	В	603	NAI	O4D-C4D	-6.07	1.31	1.45
4	D	604	NAI	O4B-C4B	-6.06	1.31	1.45
4	F	603	NAI	O4B-C4B	-6.05	1.31	1.45
4	С	604	NAI	O4D-C4D	-6.02	1.31	1.45
4	Е	603	NAI	O4D-C4D	-6.02	1.31	1.45
4	F	601	NAI	O4B-C4B	-6.00	1.31	1.45
4	С	603	NAI	O4B-C4B	-5.99	1.31	1.45
4	D	603	NAI	O4D-C4D	-5.98	1.31	1.45
4	В	604	NAI	O4B-C4B	-5.98	1.31	1.45
4	А	603	NAI	O4B-C4B	-5.97	1.31	1.45
4	В	603	NAI	O4B-C4B	-5.96	1.31	1.45
4	С	603	NAI	O4D-C4D	-5.94	1.31	1.45
4	С	604	NAI	O4B-C4B	-5.87	1.31	1.45
4	F	605	NAI	O4B-C4B	-5.76	1.32	1.45
4	В	603	NAI	C7N-N7N	4.79	1.46	1.33
4	F	603	NAI	C7N-N7N	4.70	1.45	1.33
4	A	603	NAI	C7N-N7N	4.68	1.45	1.33
4	Е	603	NAI	C7N-N7N	4.68	1.45	1.33
4	С	603	NAI	C7N-N7N	4.67	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
4	D	603	NAI	C7N-N7N	4.67	1.45	1.33
4	D	604	NAI	C7N-N7N	4.66	1.45	1.33
4	В	604	NAI	C7N-N7N	4.60	1.45	1.33
4	F	601	NAI	C7N-N7N	4.59	1.45	1.33
4	A	604	NAI	C7N-N7N	4.57	1.45	1.33
4	С	604	NAI	C7N-N7N	4.55	1.45	1.33
4	F	605	NAI	C7N-N7N	4.52	1.45	1.33
3	A	602	GTP	C6-N1	3.44	1.39	1.33
4	F	601	NAI	O3D-C3D	-3.41	1.34	1.43
3	F	604	GTP	C6-N1	3.39	1.38	1.33
4	Ε	603	NAI	C6N-N1N	3.28	1.45	1.37
4	F	605	NAI	O3D-C3D	-3.28	1.35	1.43
4	В	603	NAI	O2B-C2B	3.25	1.50	1.43
4	А	604	NAI	C6A-N6A	3.25	1.45	1.34
4	А	603	NAI	C6A-N6A	3.24	1.45	1.34
4	F	603	NAI	O2B-C2B	3.23	1.50	1.43
4	С	604	NAI	C6A-N6A	3.23	1.45	1.34
4	Е	603	NAI	C6A-N6A	3.22	1.45	1.34
4	В	604	NAI	O2D-C2D	3.20	1.50	1.43
4	В	604	NAI	C6A-N6A	3.20	1.45	1.34
4	F	603	NAI	C6A-N6A	3.20	1.45	1.34
4	В	603	NAI	C6A-N6A	3.19	1.45	1.34
4	D	603	NAI	C6A-N6A	3.19	1.45	1.34
4	С	604	NAI	O2B-C2B	3.18	1.50	1.43
4	С	603	NAI	C6N-N1N	3.18	1.45	1.37
4	F	605	NAI	C6A-N6A	3.17	1.45	1.34
4	D	603	NAI	O2B-C2B	3.16	1.50	1.43
4	Е	603	NAI	O2B-C2B	3.16	1.50	1.43
4	D	604	NAI	O2B-C2B	3.16	1.50	1.43
4	Е	603	NAI	O3D-C3D	-3.15	1.35	1.43
4	D	604	NAI	C6A-N6A	3.15	1.45	1.34
4	С	603	NAI	C6A-N6A	3.15	1.45	1.34
4	A	604	NAI	O2B-C2B	3.15	1.50	1.43
4	F	601	NAI	O2B-C2B	3.14	1.50	1.43
4	D	604	NAI	C6N-N1N	3.11	1.45	1.37
3	С	602	GTP	C6-N1	3.10	1.38	1.33
4	F	603	NAI	C6N-N1N	3.08	1.45	1.37
4	В	604	NAI	O2B-C2B	3.08	1.50	1.43
4	F	601	NAI	O2D-C2D	3.06	1.50	1.43
3	Е	602	GTP	C6-N1	3.04	1.38	1.33
4	D	603	NAI	O2D-C2D	3.04	1.50	1.43
4	F	601	NAI	C6A-N6A	3.03	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
4	С	604	NAI	C6N-N1N	3.03	1.44	1.37
4	D	603	NAI	C6N-N1N	3.03	1.44	1.37
4	A	604	NAI	O2D-C2D	3.03	1.50	1.43
4	D	604	NAI	O3D-C3D	-3.02	1.35	1.43
4	F	603	NAI	O3D-C3D	-2.99	1.35	1.43
4	F	605	NAI	O2B-C2B	2.97	1.50	1.43
4	С	603	NAI	O2B-C2B	2.96	1.50	1.43
3	D	602	GTP	C6-N1	2.96	1.38	1.33
4	F	603	NAI	O3B-C3B	-2.94	1.36	1.43
4	F	605	NAI	C6N-N1N	2.94	1.44	1.37
4	В	603	NAI	O2D-C2D	2.94	1.49	1.43
4	С	604	NAI	O2D-C2D	2.93	1.49	1.43
4	А	603	NAI	C6N-N1N	2.93	1.44	1.37
4	С	603	NAI	O2D-C2D	2.93	1.49	1.43
4	D	604	NAI	C7N-C3N	2.93	1.55	1.48
4	F	601	NAI	C6N-N1N	2.92	1.44	1.37
4	A	603	NAI	O3D-C3D	-2.92	1.36	1.43
4	С	604	NAI	O3B-C3B	-2.91	1.36	1.43
4	С	603	NAI	O3D-C3D	-2.91	1.36	1.43
4	С	603	NAI	O3B-C3B	-2.90	1.36	1.43
4	A	603	NAI	O2D-C2D	2.89	1.49	1.43
3	В	602	GTP	C6-N1	2.89	1.38	1.33
4	Е	603	NAI	O2D-C2D	2.89	1.49	1.43
4	D	603	NAI	O3D-C3D	-2.87	1.36	1.43
4	D	603	NAI	O3B-C3B	-2.86	1.36	1.43
4	В	603	NAI	C6N-N1N	2.85	1.44	1.37
4	Е	603	NAI	O3B-C3B	-2.84	1.36	1.43
4	F	601	NAI	O7N-C7N	-2.82	1.17	1.24
4	В	604	NAI	O3B-C3B	-2.81	1.36	1.43
4	В	604	NAI	O3D-C3D	-2.81	1.36	1.43
4	F	605	NAI	O3B-C3B	-2.80	1.36	1.43
4	В	603	NAI	C5A-C4A	-2.79	1.33	1.40
4	A	603	NAI	O2B-C2B	2.78	1.49	1.43
4	A	604	NAI	O3B-C3B	-2.75	1.36	1.43
4	F	601	NAI	O3B-C3B	-2.75	1.36	1.43
4	F	603	NAI	C5A-C4A	-2.75	1 33	1 40
$\frac{1}{4}$	F	605	NAI	O2D-C2D	2.75	1.49	1.43
4	D	603	NAI	C5A-C4A	-2.73	1.33	1.40
4	D	604	NAI	O2D-C2D	2.72	1.49	1.43
4	C	603	NAI	C5A-C4A	-2 70	1 33	1 40
	A	603	NAI	C5A-C4A	-2.68	1 33	1.10
4	D	604	NAI	O3B-C3B	-2.68	1.36	1.43

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6DHN

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Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
4	С	604	NAI	C5A-C4A	-2.67	1.33	1.40
4	E	603	NAI	C5A-C4A	-2.67	1.33	1.40
4	С	604	NAI	O3D-C3D	-2.65	1.36	1.43
4	В	604	NAI	C6N-N1N	2.64	1.43	1.37
4	В	603	NAI	O3D-C3D	-2.63	1.36	1.43
4	А	604	NAI	C6N-N1N	2.62	1.43	1.37
4	F	601	NAI	C5A-C4A	-2.60	1.34	1.40
4	А	603	NAI	O3B-C3B	-2.57	1.36	1.43
4	F	603	NAI	O7N-C7N	-2.55	1.18	1.24
4	F	601	NAI	C2A-N3A	2.55	1.36	1.32
4	А	604	NAI	C2A-N3A	2.55	1.36	1.32
4	В	603	NAI	O3B-C3B	-2.54	1.37	1.43
4	А	603	NAI	C7N-C3N	2.52	1.54	1.48
4	F	605	NAI	C2A-N3A	2.50	1.36	1.32
4	F	605	NAI	C5A-C4A	-2.50	1.34	1.40
4	А	604	NAI	O3D-C3D	-2.48	1.37	1.43
4	F	603	NAI	O2D-C2D	2.46	1.48	1.43
4	В	604	NAI	C5A-C4A	-2.45	1.34	1.40
4	А	604	NAI	O7N-C7N	-2.45	1.18	1.24
4	В	604	NAI	O7N-C7N	-2.44	1.18	1.24
4	F	605	NAI	O7N-C7N	-2.44	1.18	1.24
4	D	604	NAI	C2A-N3A	2.43	1.36	1.32
4	В	603	NAI	C7N-C3N	2.42	1.53	1.48
4	D	604	NAI	C5A-C4A	-2.40	1.34	1.40
4	А	604	NAI	C5A-C4A	-2.39	1.34	1.40
4	С	604	NAI	O7N-C7N	-2.32	1.19	1.24
4	С	603	NAI	O7N-C7N	-2.31	1.19	1.24
4	A	604	NAI	C7N-C3N	2.29	1.53	1.48
4	В	603	NAI	C2A-N3A	2.28	1.35	1.32
4	Е	603	NAI	O7N-C7N	-2.25	1.19	1.24
4	F	605	NAI	PA-O5B	2.25	1.68	1.59
4	С	604	NAI	C2A-N3A	2.23	1.35	1.32
4	С	603	NAI	C7N-C3N	2.23	1.53	1.48
4	Е	603	NAI	C2A-N3A	2.22	1.35	1.32
4	С	604	NAI	C7N-C3N	2.20	1.53	1.48
4	Е	603	NAI	C7N-C3N	2.20	1.53	1.48
4	A	603	NAI	O7N-C7N	-2.19	1.19	1.24
4	В	603	NAI	O7N-C7N	-2.19	1.19	1.24
4	D	603	NAI	O7N-C7N	-2.18	1.19	1.24
4	В	604	NAI	C2A-N3A	2.16	1.35	1.32
4	D	603	NAI	C2A-N3A	2.14	1.35	1.32
4	F	601	NAI	C4N-C3N	2.14	1.54	1.49

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Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
4	С	604	NAI	PA-O5B	2.12	1.67	1.59
4	F	603	NAI	C7N-C3N	2.11	1.53	1.48
4	С	603	NAI	C2A-N3A	2.10	1.35	1.32
4	D	604	NAI	C4N-C3N	2.08	1.54	1.49
4	F	603	NAI	C2A-N3A	2.06	1.35	1.32
4	В	603	NAI	PA-O5B	2.05	1.67	1.59
4	D	603	NAI	C7N-C3N	2.01	1.53	1.48
4	А	603	NAI	C2A-N3A	2.01	1.35	1.32
4	F	603	NAI	C5B-C4B	2.01	1.57	1.51

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	F	601	NAI	C3N-C2N-N1N	-9.42	109.65	123.10
4	В	604	NAI	C5A-C6A-N6A	7.43	131.64	120.35
4	С	603	NAI	C5A-C6A-N6A	7.36	131.54	120.35
4	В	603	NAI	C5A-C6A-N6A	7.28	131.41	120.35
4	Е	603	NAI	C5A-C6A-N6A	7.22	131.32	120.35
4	А	603	NAI	C5A-C6A-N6A	7.18	131.26	120.35
4	А	604	NAI	C3N-C2N-N1N	-7.06	113.02	123.10
4	А	604	NAI	C5A-C6A-N6A	7.04	131.06	120.35
4	D	603	NAI	C5A-C6A-N6A	6.96	130.93	120.35
4	С	604	NAI	C5A-C6A-N6A	6.93	130.88	120.35
4	D	604	NAI	C5A-C6A-N6A	6.66	130.47	120.35
4	F	605	NAI	C5A-C6A-N6A	6.59	130.36	120.35
4	А	603	NAI	N3A-C2A-N1A	-6.09	119.16	128.68
4	F	603	NAI	C5A-C6A-N6A	6.06	129.56	120.35
4	В	603	NAI	N3A-C2A-N1A	-5.91	119.44	128.68
3	А	602	GTP	N3-C2-N1	-5.85	119.42	127.22
4	С	603	NAI	N3A-C2A-N1A	-5.80	119.61	128.68
4	С	604	NAI	N3A-C2A-N1A	-5.71	119.75	128.68
4	Е	603	NAI	N3A-C2A-N1A	-5.65	119.84	128.68
4	D	603	NAI	N3A-C2A-N1A	-5.64	119.86	128.68
3	F	604	GTP	N3-C2-N1	-5.63	119.72	127.22
3	А	602	GTP	O2G-PG-O3B	5.44	122.89	104.64
4	D	604	NAI	C4D-O4D-C1D	-5.22	97.96	109.47
4	D	604	NAI	N3A-C2A-N1A	-5.22	120.53	128.68
4	F	605	NAI	N3A-C2A-N1A	-5.20	120.56	128.68
4	В	603	NAI	N6A-C6A-N1A	-5.18	107.82	118.57
4	F	603	NAI	N3A-C2A-N1A	-5.14	120.64	128.68
3	F	604	GTP	PB-O3B-PG	-5.14	115.19	132.83
4	С	603	NAI	N6A-C6A-N1A	-5.12	107.95	118.57



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	602	GTP	N3-C2-N1	-5.11	120.40	127.22
4	F	601	NAI	N3A-C2A-N1A	-5.10	120.70	128.68
4	A	604	NAI	N3A-C2A-N1A	-5.10	120.71	128.68
3	С	602	GTP	N3-C2-N1	-5.07	120.46	127.22
4	A	603	NAI	N6A-C6A-N1A	-4.99	108.21	118.57
3	В	602	GTP	N3-C2-N1	-4.92	120.66	127.22
3	D	602	GTP	N3-C2-N1	-4.91	120.67	127.22
4	В	604	NAI	N6A-C6A-N1A	-4.88	108.45	118.57
4	Е	603	NAI	N6A-C6A-N1A	-4.80	108.61	118.57
3	В	602	GTP	C2-N3-C4	4.69	120.71	115.36
4	А	604	NAI	N6A-C6A-N1A	-4.66	108.91	118.57
3	Е	602	GTP	C2-N3-C4	4.65	120.67	115.36
4	В	604	NAI	N3A-C2A-N1A	-4.61	121.48	128.68
4	С	604	NAI	N6A-C6A-N1A	-4.58	109.07	118.57
4	D	603	NAI	N6A-C6A-N1A	-4.58	109.07	118.57
3	С	602	GTP	C2-N3-C4	4.55	120.56	115.36
4	F	601	NAI	C5A-C6A-N6A	4.49	127.18	120.35
3	D	602	GTP	C2-N3-C4	4.45	120.44	115.36
4	D	604	NAI	C3B-C2B-C1B	4.44	107.67	100.98
4	D	604	NAI	N6A-C6A-N1A	-4.42	109.40	118.57
4	F	605	NAI	N6A-C6A-N1A	-4.39	109.47	118.57
3	D	602	GTP	PB-O3B-PG	-4.39	117.77	132.83
4	А	604	NAI	C2D-C1D-N1N	-4.35	102.40	113.30
4	А	604	NAI	C3B-C2B-C1B	4.33	107.50	100.98
3	F	604	GTP	C2-N3-C4	4.33	120.30	115.36
4	С	603	NAI	C3N-C2N-N1N	-4.32	116.93	123.10
3	A	602	GTP	C2-N3-C4	4.32	120.29	115.36
4	A	603	NAI	C3B-C2B-C1B	4.23	107.34	100.98
4	В	603	NAI	C3B-C2B-C1B	4.15	107.22	100.98
4	F	605	NAI	O4D-C1D-N1N	4.15	116.16	108.06
4	В	604	NAI	C4D-O4D-C1D	-4.09	100.45	109.47
4	D	603	NAI	PN-O3-PA	-4.02	119.04	132.83
4	F	603	NAI	N6A-C6A-N1A	-4.00	110.27	118.57
4	F	603	NAI	C3N-C2N-N1N	-3.93	117.48	123.10
4	F	605	NAI	C3B-C2B-C1B	3.89	106.83	100.98
3	B	602	GTP	C3'-C2'-C1'	3.88	106.82	100.98
4	A	603	NAI	C1D-N1N-C2N	3.75	127.35	121.11
4	A	603	NAI	C3N-C7N-N7N	3.60	124.07	117.67
4	F	601	NAI	C3B-C2B-C1B	3.54	106.31	100.98
4	C	603	NAI	C3B-C2B-C1B	3.53	106.29	100.98
4	F	603	NAI	O4D-C1D-N1N	3.48	114.86	108.06
4	B	603	NAI	04D-C1D-N1N	3.44	114.78	108.06



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	604	NAI	C3D-C2D-C1D	3.44	107.96	101.43
4	F	605	NAI	PN-O3-PA	-3.42	121.10	132.83
4	F	603	NAI	C3B-C2B-C1B	3.38	106.07	100.98
4	С	604	NAI	C3B-C2B-C1B	-3.37	95.90	100.98
4	В	603	NAI	C3N-C7N-N7N	3.36	123.64	117.67
3	F	604	GTP	C5-C6-N1	-3.32	118.88	123.43
3	А	602	GTP	PB-O3B-PG	-3.30	121.50	132.83
4	В	604	NAI	C3N-C2N-N1N	-3.14	118.61	123.10
3	F	604	GTP	C3'-C2'-C1'	3.07	105.60	100.98
4	F	601	NAI	C2D-C1D-N1N	-3.04	105.69	113.30
3	А	602	GTP	C5-C6-N1	-3.02	119.30	123.43
3	F	604	GTP	N2-C2-N1	2.99	121.90	117.25
3	С	602	GTP	C5-C6-N1	-2.94	119.41	123.43
3	D	602	GTP	PA-O3A-PB	-2.91	122.85	132.83
4	Е	603	NAI	O4D-C1D-C2D	-2.90	100.33	106.64
3	А	602	GTP	C6-N1-C2	2.89	120.52	115.93
3	D	602	GTP	C5-C6-N1	-2.87	119.51	123.43
3	F	604	GTP	C6-N1-C2	2.87	120.48	115.93
4	F	601	NAI	N6A-C6A-N1A	-2.84	112.68	118.57
3	Е	602	GTP	C5-C6-N1	-2.81	119.59	123.43
4	В	603	NAI	C1D-N1N-C2N	2.79	125.75	121.11
3	В	602	GTP	C5-C6-N1	-2.78	119.62	123.43
3	С	602	GTP	PA-O3A-PB	-2.76	123.34	132.83
4	С	604	NAI	O4B-C1B-C2B	-2.70	102.99	106.93
4	F	603	NAI	C2D-C1D-N1N	-2.67	106.61	113.30
4	F	605	NAI	C2D-C1D-N1N	-2.67	106.62	113.30
3	Е	602	GTP	PA-O3A-PB	-2.64	123.76	132.83
4	F	601	NAI	C3D-C2D-C1D	2.63	106.42	101.43
4	А	603	NAI	C1D-N1N-C6N	-2.56	115.32	120.83
3	A	602	GTP	C1'-N9-C4	-2.55	122.16	126.64
4	D	603	NAI	O5D-C5D-C4D	2.50	117.61	108.99
3	A	602	GTP	N2-C2-N1	2.50	121.14	117.25
4	F	605	NAI	C1D-N1N-C2N	2.49	125.26	121.11
4	F	601	NAI	O7N-C7N-C3N	-2.47	116.25	120.90
3	В	602	GTP	O3G-PG-O3B	2.44	112.82	104.64
4	F	601	NAI	C2D-C3D-C4D	2.44	107.39	102.64
4	E	603	NAI	O4D-C1D-N1N	2.43	112.80	108.06
4	F	605	NAI	C3N-C2N-N1N	-2.42	119.64	123.10
3	C	602	GTP	C6-N1-C2	2.41	119.77	115.93
3	В	602	GTP	PB-O3B-PG	-2.40	124.60	132.83
4	D	604	NAI	O4D-C1D-N1N	2.38	112.71	108.06
3	Ε	602	GTP	C6-N1-C2	2.37	119.69	115.93



Mol	Chain	\mathbf{Res}	\mathbf{Type}	Atoms		$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	Е	603	NAI	C3D-C2D-C1D	-2.36	96.95	101.43
4	В	603	NAI	C3N-C2N-N1N	-2.36	119.73	123.10
3	С	602	GTP	C3'-C2'-C1'	2.33	104.48	100.98
4	F	605	NAI	C4D-O4D-C1D	-2.30	104.39	109.47
4	А	603	NAI	C3N-C2N-N1N	-2.30	119.82	123.10
4	F	601	NAI	C3N-C7N-N7N	2.28	121.71	117.67
4	А	604	NAI	C3N-C7N-N7N	2.22	121.61	117.67
3	D	602	GTP	C6-N1-C2	2.22	119.45	115.93
4	В	603	NAI	C1D-N1N-C6N	-2.22	116.05	120.83
4	F	605	NAI	O4D-C4D-C3D	-2.20	100.76	105.11
4	С	604	NAI	O5B-C5B-C4B	2.18	116.50	108.99
3	Е	602	GTP	PB-O3B-PG	-2.17	125.37	132.83
4	D	604	NAI	C3N-C2N-N1N	-2.17	120.00	123.10
3	В	602	GTP	C6-N1-C2	2.16	119.36	115.93
4	Е	603	NAI	PN-O3-PA	-2.15	125.46	132.83
3	Е	602	GTP	C3'-C2'-C1'	2.10	104.14	100.98
4	D	604	NAI	O4D-C4D-C3D	-2.10	100.96	105.11
4	Е	603	NAI	C5D-C4D-C3D	-2.10	107.33	115.18
3	F	604	GTP	C4-C5-N7	-2.10	107.22	109.40
4	D	604	NAI	C2B-C3B-C4B	2.08	106.68	102.64
4	С	604	NAI	C3N-C7N-N7N	2.05	121.31	117.67
4	В	604	NAI	O5D-C5D-C4D	2.05	116.05	108.99
3	F	604	GTP	PA-O3A-PB	-2.05	125.80	132.83
3	F	604	GTP	C1'-N9-C4	-2.04	123.06	126.64
4	С	604	NAI	O4B-C4B-C3B	-2.03	101.10	105.11
4	С	604	NAI	O4D-C1D-N1N	2.02	112.00	108.06
4	В	603	NAI	PN-O3-PA	-2.01	125.94	132.83
3	A	602	GTP	C6-C5-C4	-2.00	118.89	120.80

There are no chirality outliers.

All (151) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Е	603	NAI	PA-O3-PN-O5D
4	Е	603	NAI	O4D-C4D-C5D-O5D
4	Е	603	NAI	C3D-C4D-C5D-O5D
3	В	602	GTP	C5'-O5'-PA-O1A
3	А	602	GTP	PB-O3A-PA-O5'
4	С	604	NAI	C5B-O5B-PA-O1A
4	С	604	NAI	C5B-O5B-PA-O2A
4	С	604	NAI	C5B-O5B-PA-O3
4	С	604	NAI	C3B-C4B-C5B-O5B



Mol	Chain	Res		Atoms
4	С	604	NAI	C5D-O5D-PN-O1N
4	С	604	NAI	C5D-O5D-PN-O2N
4	С	604	NAI	C2N-C3N-C7N-N7N
4	A	604	NAI	C5B-O5B-PA-O1A
4	A	604	NAI	C5B-O5B-PA-O3
4	A	604	NAI	C5D-O5D-PN-O1N
4	A	604	NAI	O4D-C1D-N1N-C2N
4	A	604	NAI	C2N-C3N-C7N-N7N
4	F	605	NAI	O4B-C4B-C5B-O5B
4	F	605	NAI	C3B-C4B-C5B-O5B
4	F	605	NAI	C5D-O5D-PN-O1N
4	F	605	NAI	C5D-O5D-PN-O2N
4	F	605	NAI	O4D-C4D-C5D-O5D
4	F	605	NAI	O4D-C1D-N1N-C6N
4	F	605	NAI	C2N-C3N-C7N-N7N
3	С	602	GTP	O4'-C4'-C5'-O5'
3	С	602	GTP	C3'-C4'-C5'-O5'
4	D	603	NAI	O4B-C4B-C5B-O5B
4	D	603	NAI	C3B-C4B-C5B-O5B
4	D	603	NAI	C5D-O5D-PN-O1N
4	D	603	NAI	C5D-O5D-PN-O2N
4	D	603	NAI	O4D-C4D-C5D-O5D
4	D	603	NAI	C3D-C4D-C5D-O5D
4	С	603	NAI	O4D-C4D-C5D-O5D
4	С	603	NAI	O4D-C1D-N1N-C2N
4	С	603	NAI	C2N-C3N-C7N-N7N
4	В	604	NAI	C5B-O5B-PA-O3
4	В	604	NAI	C5D-O5D-PN-O3
4	В	604	NAI	C5D-O5D-PN-O1N
4	В	604	NAI	C5D-O5D-PN-O2N
4	В	604	NAI	C4D-C5D-O5D-PN
4	В	604	NAI	O4D-C1D-N1N-C2N
4	D	604	NAI	C4B-C5B-O5B-PA
4	D	604	NAI	O4B-C4B-C5B-O5B
4	D	604	NAI	C3B-C4B-C5B-O5B
4	D	604	NAI	C5D-O5D-PN-O3
4	В	603	NAI	C3B-C4B-C5B-O5B
4	В	603	NAI	C5D-O5D-PN-O1N
4	В	603	NAI	C5D-O5D-PN-O2N
4	В	603	NAI	O4D-C4D-C5D-O5D
4	В	603	NAI	C3D-C4D-C5D-O5D
4	F	601	NAI	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	F	601	NAI	C5B-O5B-PA-O2A
4	F	601	NAI	C5D-O5D-PN-O1N
4	F	601	NAI	C5D-O5D-PN-O2N
4	A	603	NAI	C3B-C4B-C5B-O5B
4	F	603	NAI	C5B-O5B-PA-O1A
4	F	603	NAI	C5B-O5B-PA-O2A
4	F	603	NAI	C5B-O5B-PA-O3
4	F	603	NAI	C5D-O5D-PN-O1N
4	F	603	NAI	O4D-C4D-C5D-O5D
4	F	603	NAI	C3D-C4D-C5D-O5D
4	F	603	NAI	O4D-C1D-N1N-C2N
4	Е	603	NAI	O4B-C4B-C5B-O5B
3	А	602	GTP	O4'-C4'-C5'-O5'
4	С	604	NAI	O4B-C4B-C5B-O5B
4	F	605	NAI	C3D-C4D-C5D-O5D
4	В	604	NAI	O4B-C4B-C5B-O5B
4	А	603	NAI	O4B-C4B-C5B-O5B
4	D	604	NAI	O4D-C1D-N1N-C6N
4	Е	603	NAI	C3B-C4B-C5B-O5B
3	А	602	GTP	C3'-C4'-C5'-O5'
4	А	604	NAI	O4B-C4B-C5B-O5B
4	А	604	NAI	C3B-C4B-C5B-O5B
4	С	603	NAI	C3D-C4D-C5D-O5D
4	В	604	NAI	C3B-C4B-C5B-O5B
3	D	602	GTP	O4'-C4'-C5'-O5'
3	D	602	GTP	C3'-C4'-C5'-O5'
4	D	604	NAI	C3D-C4D-C5D-O5D
4	В	603	NAI	O4B-C4B-C5B-O5B
4	D	604	NAI	O4D-C4D-C5D-O5D
4	С	603	NAI	C2D-C1D-N1N-C6N
3	С	602	GTP	PG-O3B-PB-O3A
4	A	603	NAI	C2D-C1D-N1N-C6N
4	Е	603	NAI	PN-O3-PA-O5B
4	С	604	NAI	PN-O3-PA-O5B
4	С	604	NAI	PA-O3-PN-O5D
4	D	604	NAI	PN-O3-PA-O5B
3	D	602	GTP	PB-O3A-PA-O5'
4	F	603	NAI	C4D-C5D-O5D-PN
4	А	603	NAI	O4D-C1D-N1N-C6N
3	В	602	GTP	C5'-O5'-PA-O3A
4	А	604	NAI	C5D-O5D-PN-O3
4	D	603	NAI	C5B-O5B-PA-O3



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Mol	Chain	Res	Type	Atoms
4	D	603	NAI	C5D-O5D-PN-O3
4	D	604	NAI	C5B-O5B-PA-O3
4	В	603	NAI	C5D-O5D-PN-O3
4	F	603	NAI	C5D-O5D-PN-O3
4	С	603	NAI	PA-O3-PN-O2N
4	В	603	NAI	O4D-C1D-N1N-C6N
4	F	601	NAI	O4D-C1D-N1N-C2N
4	С	603	NAI	C2D-C1D-N1N-C2N
4	Е	603	NAI	C4D-C5D-O5D-PN
3	В	602	GTP	C5'-O5'-PA-O2A
4	А	604	NAI	C5B-O5B-PA-O2A
4	А	604	NAI	C5D-O5D-PN-O2N
4	F	605	NAI	C5B-O5B-PA-O2A
4	В	604	NAI	C5B-O5B-PA-O1A
4	В	604	NAI	C5B-O5B-PA-O2A
4	D	604	NAI	C5D-O5D-PN-O1N
4	F	603	NAI	C5D-O5D-PN-O2N
4	А	603	NAI	C2D-C1D-N1N-C2N
4	А	604	NAI	C2N-C3N-C7N-O7N
4	С	603	NAI	C2N-C3N-C7N-O7N
4	А	603	NAI	O4D-C1D-N1N-C2N
4	А	603	NAI	O4D-C4D-C5D-O5D
4	С	604	NAI	O4D-C1D-N1N-C6N
4	D	603	NAI	O4D-C1D-N1N-C6N
3	А	602	GTP	PA-O3A-PB-O3B
4	F	605	NAI	PA-O3-PN-O2N
4	D	603	NAI	PA-O3-PN-O2N
4	D	603	NAI	C2D-C1D-N1N-C6N
4	F	601	NAI	C4B-C5B-O5B-PA
4	С	604	NAI	C2D-C1D-N1N-C6N
4	Е	603	NAI	O4D-C1D-N1N-C6N
4	А	604	NAI	C2D-C1D-N1N-C6N
4	Е	603	NAI	C2D-C1D-N1N-C6N
3	F	604	GTP	PA-O3A-PB-O1B
3	Е	602	GTP	PA-O3A-PB-O1B
4	А	604	NAI	C2D-C1D-N1N-C2N
4	В	603	NAI	C4B-C5B-O5B-PA
4	С	603	NAI	O4B-C4B-C5B-O5B
3	Е	602	GTP	PA-O3A-PB-O3B
4	Е	603	NAI	C5B-O5B-PA-O3
4	С	604	NAI	C5D-O5D-PN-O3
4	F	605	NAI	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
4	F	605	NAI	C5D-O5D-PN-O3
4	С	603	NAI	C5D-O5D-PN-O3
4	F	601	NAI	C5B-O5B-PA-O3
4	F	601	NAI	C5D-O5D-PN-O3
4	С	604	NAI	PN-O3-PA-O1A
4	С	604	NAI	PN-O3-PA-O2A
4	F	605	NAI	PA-O3-PN-O1N
3	С	602	GTP	PG-O3B-PB-O1B
3	С	602	GTP	PB-O3A-PA-O2A
4	D	603	NAI	PA-O3-PN-O1N
4	В	604	NAI	PN-O3-PA-O2A
4	Е	603	NAI	C5B-O5B-PA-O2A
4	D	603	NAI	C5B-O5B-PA-O2A
4	C	603	NAI	C5B-O5B-PA-O1A
4	С	603	NAI	C5D-O5D-PN-O2N
4	D	604	NAI	C5B-O5B-PA-O2A

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There are no ring outliers.

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Е	603	NAI	10	0
3	F	604	GTP	2	0
4	F	605	NAI	9	0
4	С	603	NAI	4	0
4	В	604	NAI	3	0
4	F	601	NAI	11	0
4	А	603	NAI	4	0
3	В	602	GTP	2	0
3	А	602	GTP	13	0
4	С	604	NAI	6	0
4	А	604	NAI	7	0
3	Е	602	GTP	1	0
3	D	602	GTP	1	0
4	В	603	NAI	12	0
4	D	603	NAI	5	0
4	D	604	NAI	4	0
4	F	603	NAI	3	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	$Q{<}0.9$
1	А	501/582~(86%)	0.43	35 (6%) 16 16	8, 34, 69, 101	0
1	В	501/582~(86%)	0.25	19 (3%) 40 37	7, 29, 65, 94	0
1	С	501/582~(86%)	0.53	44 (8%) 10 10	12, 37, 72, 99	0
1	D	501/582~(86%)	0.38	17 (3%) 45 43	8, 30, 62, 89	0
1	Ε	501/582~(86%)	0.66	60 (11%) 4 3	7, 41, 78, 95	0
1	F	501/582~(86%)	0.38	25 (4%) 28 27	9,35,66,95	0
All	All	3006/3492~(86%)	0.44	200 (6%) 17 17	7, 34, 73, 101	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	37	THR	10.3
1	F	501	THR	8.2
1	В	501	THR	7.4
1	С	499	THR	7.4
1	D	499	THR	6.9
1	В	499	THR	6.9
1	А	501	THR	6.2
1	С	424	HIS	6.2
1	В	498	VAL	5.7
1	А	37	THR	5.6
1	F	499	THR	5.0
1	Е	334	SER	4.9
1	Е	284	ASP	4.9
1	D	498	VAL	4.9
1	С	319	CYS	4.8
1	D	500	PHE	4.7
1	F	223	ILE	4.6
1	С	305	PRO	4.6
1	С	298	HIS	4.6



Mol	Chain	Res	Type	RSRZ
1	Е	285	GLY	4.6
1	С	31	ASP	4.6
1	D	424	HIS	4.5
1	Е	237	GLY	4.5
1	Е	227	ILE	4.5
1	А	413	VAL	4.5
1	Е	313	SER	4.3
1	Е	365	ILE	4.1
1	F	2	ASP	4.1
1	Е	355	GLU	4.1
1	В	497	GLY	4.0
1	Е	319	CYS	3.9
1	С	342	LYS	3.9
1	Е	250	GLN	3.9
1	D	425	GLY	3.9
1	А	23	ILE	3.8
1	С	68	ASP	3.8
1	Е	270	CYS	3.8
1	С	286	ILE	3.7
1	Е	1	ALA	3.6
1	А	499	THR	3.6
1	Е	341	ALA	3.6
1	F	500	PHE	3.5
1	С	498	VAL	3.5
1	Е	476	ASP	3.5
1	D	501	THR	3.5
1	Е	501	THR	3.5
1	Е	321	ILE	3.4
1	F	4	GLU	3.4
1	C	501	THR	3.4
1	Е	464	ILE	3.4
1	F	430	ILE	3.4
1	C	244	ASP	3.4
1	Е	226	PHE	3.4
1	В	428	ILE	3.3
1	Е	344	ILE	3.3
1	Е	249	VAL	3.3
1	E	305	PRO	3.3
1	F	440	ILE	3.3
1	A	498	VAL	3.3
1	E	318	ASP	3.3
1	E	475	LEU	3.3



Mol	Chain	Res	Type	RSRZ
1	Е	4	GLU	3.2
1	В	426	GLY	3.2
1	С	300	THR	3.2
1	А	429	PRO	3.2
1	F	412	SER	3.1
1	А	490	PHE	3.1
1	С	329	LYS	3.1
1	В	242	PHE	3.1
1	F	293	ASP	3.1
1	Е	232	TYR	3.1
1	Е	2	ASP	3.1
1	F	428	ILE	3.1
1	С	469	MET	3.1
1	С	423	LYS	3.0
1	С	72	TRP	3.0
1	Е	345	ALA	3.0
1	А	26	ASP	3.0
1	Е	223	ILE	3.0
1	F	3	ARG	3.0
1	Е	32	LEU	3.0
1	Е	252	PHE	3.0
1	D	286	ILE	2.9
1	Е	359	ILE	2.9
1	Е	33	LYS	2.9
1	С	365	ILE	2.9
1	F	250	GLN	2.9
1	F	298	HIS	2.9
1	Е	339	VAL	2.9
1	Е	500	PHE	2.9
1	F	498	VAL	2.8
1	F	426	GLY	2.8
1	Е	315	LEU	2.8
1	F	72	TRP	2.8
1	С	283	PRO	2.8
1	А	410	LEU	2.8
1	Е	310	TYR	2.8
1	А	484	ASN	2.8
1	С	318	ASP	2.8
1	А	22	SER	2.8
1	Е	360	PHE	2.8
1	А	431	VAL	2.7
1	С	500	PHE	2.7



Mol	Chain	Res	Type	RSRZ
1	F	427	THR	2.7
1	Е	283	PRO	2.7
1	D	413	VAL	2.7
1	D	285	GLY	2.7
1	D	417	LEU	2.7
1	А	43	ASN	2.6
1	D	37	THR	2.6
1	Е	236	LEU	2.6
1	В	416	SER	2.6
1	Е	41	LYS	2.6
1	Е	224	GLU	2.6
1	В	419	ARG	2.6
1	Е	497	GLY	2.6
1	F	473	LEU	2.6
1	С	270	CYS	2.6
1	С	1	ALA	2.6
1	С	133	PRO	2.6
1	В	417	LEU	2.5
1	Е	31	ASP	2.5
1	Е	311	GLU	2.5
1	А	412	SER	2.5
1	А	424	HIS	2.5
1	В	237	GLY	2.5
1	Е	304	PHE	2.5
1	Е	337	PRO	2.5
1	В	500	PHE	2.5
1	Е	335	ASN	2.5
1	F	429	PRO	2.5
1	А	279	SER	2.5
1	Е	267	GLY	2.5
1	D	1	ALA	2.5
1	А	268	ALA	2.4
1	С	409	LEU	2.4
1	С	320	ASP	2.4
1	А	33	LYS	2.4
1	А	425	GLY	2.4
1	А	1	ALA	2.4
1	А	366	MET	2.4
1	А	472	ASN	2.4
1	F	21	ALA	2.4
1	С	302	LEU	2.4
1	D	70	GLY	2.3



Mol	Chain	Res	Type	RSRZ
1	В	3	ARG	2.3
1	В	101	VAL	2.3
1	Е	251	GLY	2.3
1	С	4	GLU	2.3
1	А	228	ASN	2.3
1	А	426	GLY	2.3
1	В	414	GLN	2.3
1	Е	499	THR	2.3
1	Е	317	VAL	2.3
1	С	285	GLY	2.3
1	В	418	GLU	2.3
1	С	30	GLU	2.3
1	С	251	GLY	2.3
1	Е	34	THR	2.3
1	Е	3	ARG	2.3
1	Е	19	ARG	2.3
1	А	434	ALA	2.3
1	Е	247	PHE	2.3
1	С	278	GLY	2.3
1	F	64	PRO	2.3
1	D	137	THR	2.2
1	А	304	PHE	2.2
1	С	297	GLN	2.2
1	С	314	ILE	2.2
1	А	417	LEU	2.2
1	А	500	PHE	2.2
1	А	278	GLY	2.2
1	С	330	GLN	2.2
1	С	427	THR	2.2
1	А	497	GLY	2.2
1	А	223	ILE	2.2
1	А	246	THR	2.1
1	А	320	ASP	2.1
1	Е	293	ASP	2.1
1	D	139	ASN	2.1
1	D	66	ARG	2.1
1	В	223	ILE	2.1
1	В	427	THR	2.1
1	F	304	PHE	2.1
1	С	242	PHE	2.1
1	С	303	GLY	2.1
1	Е	322	LEU	2.1



		-		Daba
Mol	Chain	\mathbf{Res}	Type	RSRZ
1	F	35	ARG	2.1
1	F	407	TYR	2.1
1	С	344	ILE	2.0
1	А	242	PHE	2.0
1	Е	300	THR	2.0
1	С	441	SER	2.0
1	Е	235	ILE	2.0
1	D	276	SER	2.0
1	Е	281	TRP	2.0
1	С	339	VAL	2.0
1	В	364	ASN	2.0
1	С	360	PHE	2.0
1	С	413	VAL	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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	NAI	F	603	44/44	0.64	0.49	$16,\!43,\!66,\!71$	17
4	NAI	С	603	44/44	0.67	0.42	$7,\!46,\!62,\!83$	18
4	NAI	D	604	44/44	0.69	0.39	10,32,61,93	11
3	GTP	Е	602	32/32	0.69	0.32	$56,\!83,\!98,\!104$	0
4	NAI	А	604	44/44	0.72	0.41	$12,\!33,\!59,\!76$	13
4	NAI	F	601	44/44	0.73	0.40	11,31,69,97	14
3	GTP	А	602	32/32	0.74	0.27	$30,\!51,\!81,\!91$	0
3	GTP	С	602	32/32	0.76	0.24	41,73,95,108	0
3	GTP	D	602	32/32	0.77	0.28	34,65,87,94	0
4	NAI	В	604	44/44	0.78	0.34	$19,\!37,\!52,\!71$	14



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	GLU	Е	601	10/10	0.85	0.31	21,22,26,36	0
3	GTP	F	604	32/32	0.85	0.25	$34,\!50,\!77,\!85$	0
2	GLU	A	601	10/10	0.88	0.27	$16,\!20,\!25,\!30$	0
4	NAI	В	603	44/44	0.88	0.23	$9,\!17,\!36,\!44$	0
3	GTP	В	602	32/32	0.89	0.20	$23,\!37,\!48,\!50$	0
4	NAI	A	603	44/44	0.90	0.22	$10,\!23,\!37,\!44$	0
4	NAI	D	603	44/44	0.90	0.21	$15,\!24,\!45,\!55$	0
2	GLU	В	601	10/10	0.90	0.22	$9,\!15,\!19,\!21$	0
4	NAI	F	605	44/44	0.90	0.22	$12,\!27,\!44,\!47$	0
4	NAI	С	604	44/44	0.91	0.20	$18,\!31,\!53,\!66$	0
2	GLU	F	602	10/10	0.92	0.21	$11,\!14,\!18,\!24$	0
2	GLU	Ċ	601	10/10	0.92	0.19	15,19,25,25	0
4	NAI	E	603	44/44	0.92	0.18	25,41,72,75	0
2	GLU	D	601	10/10	0.95	0.19	$10,\!15,\!21,\!27$	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.

