

Full wwPDB X-ray Structure Validation Report (i)

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

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

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

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

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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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

Mol	Chain	Length	Quality	of chain		
1	D	377	55%	33%	6%	6%
1	F	377	% 55%	34%	6%	6%
1	G	377	54%	35%	5%	6%
1	Н	377	% 52%	37%	5%	6%
2	А	402	51%	30% 7	% • 11	.%



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Mol	Chain	Length	Quality	of chain	
2	В	402	50%	30%	8% • 11%
2	С	402	51%	29%	7% • 11%
2	Е	402	49%	32%	7% • 11%

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
3	ACT	В	1001	-	-	Х	-
3	ACT	D	401	-	-	Х	-
3	ACT	F	401	-	-	-	Х
3	ACT	G	401	-	-	Х	-
3	ACT	Н	401	-	-	Х	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22892 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	а	356	Total C N O S		0	0				
	D	550	2785	1766	468	533	18	121	0	0
1	ц	256	Total	С	Ν	0	S	192	0	0
	11	550	2785	1766	468	533	18	120	0	
1	C	256	Total	С	Ν	0	S	120	0	0
	G	390	2785	1766	468	533	18	132	0	0
1	1 F	256	Total	С	Ν	0	S	65	0	0
	Г	300	2785	1766	468	533	18	05	0	0

• Molecule 1 is a protein called Actin, alpha skeletal muscle.

• Molecule 2 is a protein called Formin-like protein 3.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	Λ	357	Total	С	Ν	0	\mathbf{S}	265	265 0	
	A	- 357	2895	1848	502	533	12	205	0	0
0	F	257	Total	С	Ν	0	S	979	0	0
	Ľ	- 357	2895	1848	502	533	12	212	0	U
0	C	257	Total	С	Ν	0	S	252	0	0
	U		2895	1848	502	533	12	232	0	0
0	Р	257	Total	С	Ν	0	S	260	0	0
	D	- 337	2895	1848	502	533	12	200		U

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	553	GLY	-	expression tag	UNP Q6ZPF4
А	554	SER	-	expression tag	UNP Q6ZPF4
E	553	GLY	-	expression tag	UNP Q6ZPF4
Е	554	SER	-	expression tag	UNP Q6ZPF4
С	553	GLY	-	expression tag	UNP Q6ZPF4
С	554	SER	-	expression tag	UNP Q6ZPF4
В	553	GLY	-	expression tag	UNP Q6ZPF4
В	554	SER	-	expression tag	UNP Q6ZPF4



- 4EAH
- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	Ε	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:



$C_{10}H_{16}N_5O_{13}P_3).$



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	
4	Л	1	Total	С	Ν	Ο	Р	0	0	
4	D	1	31	10	5	13	3	0	0	
4	ц	1	Total	С	Ν	Ο	Р	0	0	
4	П	1	31	10	5	13	3	0	0	
4	С	1	Total	С	Ν	Ο	Р	0	0	
4	G	1	31	10	5	13	3	0	0	
4	Б	D 1		С	Ν	Ο	Р	0	0	
4	F,		31	10	5	13	3	U	U	



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Actin, alpha skeletal muscle



GLN GLY ALA ALA LEU LEU LEU LEU



• Molecule 1: Actin, alpha skeletal muscle









8375 8375 1877 1877 1876 1877 1877 1877 1877 1877 1877 1877 1877 1877 1877 1887 1886 1883 1886 1883 1886 1884 1886 1883 1886 1883 1886 1884 1886 1884 1886 1884 1886 1884 1886 1884 1886 1884 1886 1884 1886 1884 1886 1886 1886 1895 1995 1995 1996 1996 1996 1996 1996 1996 1996 1996 1996 1996 1996 1996 1996 110 110 111 111

• Molecule 2: Formin-like protein 3





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	125.98Å 126.05 Å 129.62 Å	Deperitor
a, b, c, α , β , γ	90.00° 93.17° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	19.82 - 3.40	Depositor
Resolution (A)	19.82 - 3.40	EDS
% Data completeness	99.8 (19.82-3.40)	Depositor
(in resolution range)	99.8(19.82-3.40)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	$2.92 (at 3.44 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
P. P.	0.230 , 0.277	Depositor
n, n_{free}	0.225 , 0.274	DCC
R_{free} test set	2894 reflections (5.22%)	wwPDB-VP
Wilson B-factor $(Å^2)$	98.3	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29, 62.6	EDS
L-test for $twinning^2$	$< L >=0.43, < L^2>=0.26$	Xtriage
Estimated twinning fraction	0.037 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22892	wwPDB-VP
Average B, all atoms $(Å^2)$	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.14% 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: ATP, ACT

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

Mol Chain		Bond	lengths	Bond angles	
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	D	0.51	0/2845	0.70	0/3858
1	F	0.48	0/2845	0.69	0/3858
1	G	0.48	0/2845	0.70	0/3858
1	Н	0.48	0/2845	0.70	0/3858
2	А	0.48	0/2942	0.70	1/3956~(0.0%)
2	В	0.49	0/2942	0.69	1/3956~(0.0%)
2	С	0.49	0/2942	0.70	1/3956~(0.0%)
2	Е	0.49	0/2942	0.70	1/3956~(0.0%)
All	All	0.49	0/23148	0.70	4/31256~(0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Е	740	LEU	CA-CB-CG	5.37	127.64	115.30
2	С	740	LEU	CA-CB-CG	5.25	127.37	115.30
2	А	740	LEU	CA-CB-CG	5.15	127.14	115.30
2	В	740	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2785	0	2758	100	1
1	F	2785	0	2758	97	1
1	G	2785	0	2758	105	0
1	Н	2785	0	2758	111	0
2	А	2895	0	2971	101	0
2	В	2895	0	2971	104	0
2	С	2895	0	2971	99	0
2	Ε	2895	0	2971	105	0
3	А	12	0	9	1	0
3	В	4	0	3	2	0
3	С	8	0	6	2	0
3	D	4	0	3	2	0
3	Ε	4	0	3	1	0
3	F	8	0	6	1	0
3	G	4	0	3	2	0
3	Н	4	0	3	2	0
4	D	31	0	12	5	0
4	F	31	0	12	1	0
4	G	31	0	12	2	0
4	Н	31	0	12	2	0
All	All	22892	0	23000	776	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (776) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:147:ARG:HH12	1:H:330:ILE:HG12	1.29	0.94
1:H:261:LEU:HB3	1:H:274:ILE:HD11	1.54	0.90
1:D:261:LEU:HB3	1:D:274:ILE:HD11	1.55	0.89
1:D:147:ARG:HH12	1:D:330:ILE:HG12	1.36	0.88
1:G:261:LEU:HB3	1:G:274:ILE:HD11	1.55	0.88
1:G:137:GLN:NE2	4:G:402:ATP:O3G	2.08	0.87
1:G:147:ARG:HH12	1:G:330:ILE:HG12	1.39	0.86
1:F:147:ARG:HH12	1:F:330:ILE:HG12	1.41	0.85
1:F:261:LEU:HB3	1:F:274:ILE:HD11	1.58	0.85
1:H:137:GLN:NE2	4:H:402:ATP:O3G	2.11	0.83
2:B:746:GLN:HE22	1:H:323:SER:HB3	1.44	0.82
2:A:778:ASN:ND2	3:A:1003:ACT:O	2.14	0.81
2:A:758:LYS:HB2	2:A:898:VAL:HG13	1.62	0.81
2:E:789:LYS:O	2:E:792:SER:OG	1.97	0.81



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:789:LYS:O	2:C:792:SER:OG	2.00	0.79
2:B:807:THR:HG23	2:B:810:HIS:H	1.48	0.79
2:E:758:LYS:HB2	2:E:898:VAL:HG13	1.65	0.78
1:F:111:ASN:ND2	1:F:115:ASN:OD1	2.17	0.77
1:D:173:HIS:O	1:D:173:HIS:ND1	2.17	0.77
1:H:128:ASN:OD1	1:H:359:LYS:NZ	2.13	0.77
2:A:637:THR:HG22	2:A:639:LEU:H	1.50	0.77
2:A:789:LYS:O	2:A:792:SER:OG	2.03	0.76
2:B:789:LYS:O	2:B:792:SER:OG	2.01	0.76
2:C:758:LYS:HB2	2:C:898:VAL:HG13	1.68	0.75
1:F:173:HIS:O	1:F:173:HIS:ND1	2.19	0.75
1:H:173:HIS:O	1:H:173:HIS:ND1	2.20	0.74
2:E:765:GLN:HG2	2:E:823:LEU:HD11	1.69	0.74
1:G:173:HIS:ND1	1:G:173:HIS:O	2.19	0.74
2:B:758:LYS:HB2	2:B:898:VAL:HG13	1.70	0.74
1:G:164:PRO:HG2	1:G:174:ALA:HB1	1.69	0.73
1:D:164:PRO:HG2	1:D:174:ALA:HB1	1.69	0.73
2:C:637:THR:HG22	2:C:639:LEU:H	1.52	0.73
1:F:106:THR:HB	1:F:137:GLN:HG2	1.71	0.73
2:E:637:THR:HG22	2:E:639:LEU:H	1.54	0.73
2:E:807:THR:HG23	2:E:810:HIS:H	1.52	0.73
2:B:765:GLN:HG2	2:B:823:LEU:HD11	1.71	0.72
2:C:807:THR:HG23	2:C:810:HIS:H	1.53	0.72
1:D:106:THR:HB	1:D:137:GLN:HG2	1.71	0.72
2:A:765:GLN:HG2	2:A:823:LEU:HD11	1.71	0.72
1:G:106:THR:HB	1:G:137:GLN:HG2	1.71	0.72
2:B:637:THR:HG22	2:B:639:LEU:H	1.55	0.71
2:B:757:VAL:HA	2:B:830:LEU:HD23	1.72	0.71
2:E:598:LEU:HD12	2:E:599:GLU:H	1.55	0.71
1:F:20:GLY:HA2	1:F:94:LEU:HD21	1.70	0.71
2:C:598:LEU:HD12	2:C:599:GLU:H	1.55	0.71
1:H:164:PRO:HG2	1:H:174:ALA:HB1	1.72	0.71
2:A:807:THR:HG23	2:A:810:HIS:H	1.54	0.71
2:C:746:GLN:HE22	1:F:323:SER:HB3	1.55	0.71
1:H:106:THR:HB	1:H:137:GLN:HG2	1.71	0.71
1:G:20:GLY:HA2	1:G:94:LEU:HD21	1.73	0.71
2:B:598:LEU:HD12	2:B:599:GLU:H	1.57	0.70
1:H:20:GLY:HA2	1:H:94:LEU:HD21	1.73	0.70
2:C:757:VAL:HA	2:C:830:LEU:HD23	1.73	0.70
1:F:16:LEU:HD12	1:F:32:PRO:HA	1.73	0.70
1:H:111:ASN:ND2	1:H:115:ASN:OD1	2.21	0.70



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:D:323:SER:HB3	2:A:746:GLN:HE22	1.56	0.70
2:B:565:ILE:HD13	2:B:566:LYS:H	1.55	0.70
2:C:643:ARG:NH2	2:C:690:GLU:OE2	2.24	0.69
1:G:25:ASP:OD2	1:G:28:ARG:NH2	2.24	0.69
1:G:25:ASP:N	3:G:401:ACT:OXT	2.24	0.69
1:G:16:LEU:HD12	1:G:32:PRO:HA	1.74	0.69
1:H:16:LEU:HD12	1:H:32:PRO:HA	1.74	0.69
1:G:260:THR:HG23	1:G:266:PHE:HB2	1.73	0.69
1:D:20:GLY:HA2	1:D:94:LEU:HD21	1.73	0.69
2:A:598:LEU:HD12	2:A:599:GLU:H	1.55	0.69
2:E:746:GLN:HE22	1:G:323:SER:HB3	1.57	0.69
2:B:643:ARG:NH2	2:B:690:GLU:OE2	2.26	0.69
2:E:858:ILE:HG22	2:E:874:LEU:HD12	1.75	0.69
2:A:645:LYS:NZ	2:A:646:ASN:OD1	2.25	0.69
2:A:757:VAL:HA	2:A:830:LEU:HD23	1.74	0.69
1:F:260:THR:HG23	1:F:266:PHE:HB2	1.75	0.68
2:E:757:VAL:HA	2:E:830:LEU:HD23	1.73	0.68
1:F:164:PRO:HG2	1:F:174:ALA:HB1	1.75	0.68
1:D:278:THR:O	1:D:282:ILE:HD12	1.93	0.68
2:E:643:ARG:NH2	2:E:690:GLU:OE2	2.27	0.68
2:A:669:ASP:HB3	2:A:673:LEU:HB2	1.76	0.67
1:D:128:ASN:OD1	1:D:359:LYS:NZ	2.18	0.67
2:A:643:ARG:NH2	2:A:690:GLU:OE2	2.28	0.67
1:G:111:ASN:ND2	1:G:115:ASN:OD1	2.25	0.67
2:C:765:GLN:HG2	2:C:823:LEU:HD11	1.77	0.67
2:B:605:ARG:HG2	2:B:609:LEU:HD12	1.77	0.67
2:B:840:SER:N	1:H:323:SER:OG	2.20	0.67
1:H:25:ASP:OD2	1:H:28:ARG:NH2	2.27	0.67
1:D:136:ILE:HD12	1:D:136:ILE:H	1.60	0.67
1:H:217:CYS:HA	1:H:254:ARG:HG3	1.75	0.67
1:G:128:ASN:OD1	1:G:359:LYS:NZ	2.17	0.67
1:H:107:GLU:O	1:H:137:GLN:HG3	1.95	0.66
1:G:157:ASP:HB2	4:G:402:ATP:H5'1	1.77	0.66
2:A:605:ARG:HG2	2:A:609:LEU:HD12	1.77	0.66
1:G:217:CYS:HA	1:G:254:ARG:HG3	1.77	0.66
2:A:858:ILE:HG22	2:A:874:LEU:HD12	1.77	0.66
2:E:823:LEU:O	2:E:826:PHE:HB3	1.97	0.65
1:G:136:ILE:H	1:G:136:ILE:HD12	1.61	0.65
2:B:823:LEU:O	2:B:826:PHE:HB3	1.96	0.65
1:D:260:THR:HG23	1:D:266:PHE:HB2	1.79	0.64
1:D:16:LEU:HD12	1:D:32:PRO:HA	1.78	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:111:ASN:ND2	1:D:115:ASN:OD1	2.24	0.64
2:C:823:LEU:O	2:C:826:PHE:HB3	1.96	0.64
1:F:136:ILE:HD12	1:F:136:ILE:H	1.63	0.64
1:F:25:ASP:OD2	1:F:28:ARG:NH2	2.30	0.64
1:F:217:CYS:HA	1:F:254:ARG:HG3	1.78	0.64
1:H:136:ILE:HD12	1:H:136:ILE:H	1.62	0.64
2:E:605:ARG:HG2	2:E:609:LEU:HD12	1.79	0.64
2:C:858:ILE:HG22	2:C:874:LEU:HD12	1.79	0.64
1:D:25:ASP:OD2	1:D:28:ARG:NH2	2.31	0.64
2:C:669:ASP:HB3	2:C:673:LEU:HB2	1.79	0.64
2:C:866:ASP:N	2:C:867:ASN:OD1	2.31	0.64
2:A:823:LEU:O	2:A:826:PHE:HB3	1.98	0.64
1:H:260:THR:HG23	1:H:266:PHE:HB2	1.80	0.64
1:D:157:ASP:HB2	4:D:402:ATP:H5'1	1.79	0.63
1:H:96:VAL:HB	1:H:101:HIS:CE1	2.33	0.63
1:D:217:CYS:HA	1:D:254:ARG:HG3	1.79	0.63
2:C:762:LYS:HB3	2:C:826:PHE:HB2	1.78	0.63
2:A:654:ALA:HB2	2:A:677:PHE:CE1	2.34	0.63
1:D:25:ASP:N	3:D:401:ACT:OXT	2.32	0.63
2:A:762:LYS:HB3	2:A:826:PHE:HB2	1.80	0.63
2:E:654:ALA:HB2	2:E:677:PHE:CE1	2.33	0.63
2:E:669:ASP:HB3	2:E:673:LEU:HB2	1.81	0.63
1:D:107:GLU:O	1:D:137:GLN:HG3	1.99	0.63
2:A:866:ASP:N	2:A:867:ASN:OD1	2.31	0.63
2:B:866:ASP:N	2:B:867:ASN:OD1	2.32	0.63
2:B:858:ILE:HG22	2:B:874:LEU:HD12	1.80	0.62
2:B:638:LEU:N	2:B:711:ASP:OD2	2.18	0.62
2:C:654:ALA:HB2	2:C:677:PHE:CE1	2.34	0.62
2:B:762:LYS:HB3	2:B:826:PHE:HB2	1.81	0.62
2:C:789:LYS:HG3	2:B:579:LEU:HD21	1.80	0.62
1:H:18:LYS:HA	1:H:30:VAL:HG22	1.82	0.62
2:C:913:VAL:O	2:C:916:PRO:HD2	2.00	0.61
2:A:576:TRP:HB2	2:E:792:SER:HB3	1.82	0.61
2:A:782:ARG:NH1	2:E:573:VAL:HG23	2.15	0.61
2:B:654:ALA:HB2	2:B:677:PHE:CE1	2.35	0.61
1:F:138:ALA:O	1:F:152:VAL:HG21	1.99	0.61
2:E:771:LEU:O	2:E:775:ASN:HB2	2.01	0.61
1:D:367:PRO:HD3	2:A:573:VAL:HG11	1.83	0.61
2:A:672:THR:O	2:A:672:THR:OG1	2.15	0.61
2:C:779:SER:HB3	2:B:565:ILE:H	1.64	0.61
1:F:186:THR:O	1:F:190:MET:HG2	2.00	0.61



	lo de pagen	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:743:LEU:HD22	2:C:844:VAL:HG13	1.81	0.61
1:G:18:LYS:HA	1:G:30:VAL:HG22	1.82	0.61
1:D:138:ALA:O	1:D:152:VAL:HG21	2.01	0.61
2:E:869:VAL:HA	2:E:872:ASN:HB3	1.83	0.61
2:A:913:VAL:O	2:A:916:PRO:HD2	2.01	0.60
2:B:645:LYS:NZ	2:B:646:ASN:OD1	2.34	0.60
2:B:669:ASP:HB3	2:B:673:LEU:HB2	1.83	0.60
2:E:866:ASP:N	2:E:867:ASN:OD1	2.35	0.60
2:A:573:VAL:HG23	2:E:782:ARG:NH1	2.16	0.60
2:E:743:LEU:HD22	2:E:844:VAL:HG13	1.83	0.60
1:D:137:GLN:NE2	4:D:402:ATP:O3G	2.35	0.60
1:G:272:ALA:HB1	1:G:276:GLU:HB2	1.82	0.60
1:G:96:VAL:HB	1:G:101:HIS:CE1	2.37	0.60
1:G:278:THR:O	1:G:282:ILE:HD12	2.02	0.60
2:E:762:LYS:HB3	2:E:826:PHE:HB2	1.83	0.60
2:C:579:LEU:HD21	2:B:789:LYS:HG3	1.84	0.60
1:G:280:ASN:HA	1:G:283:MET:HB2	1.84	0.60
2:C:605:ARG:HG2	2:C:609:LEU:HD12	1.83	0.59
2:C:638:LEU:N	2:C:711:ASP:OD2	2.21	0.59
1:G:107:GLU:O	1:G:137:GLN:HG3	2.01	0.59
2:A:578:ALA:HB1	2:E:785:VAL:HG21	1.83	0.59
2:A:743:LEU:HD22	2:A:844:VAL:HG13	1.83	0.59
1:H:27:PRO:HD3	1:H:340:TRP:CE3	2.38	0.59
1:F:18:LYS:HA	1:F:30:VAL:HG22	1.85	0.59
2:A:722:ARG:HA	2:A:722:ARG:NH1	2.18	0.59
2:A:875:SER:OG	2:A:876:THR:N	2.36	0.59
2:B:869:VAL:HA	2:B:872:ASN:HB3	1.84	0.58
2:C:869:VAL:HA	2:C:872:ASN:HB3	1.84	0.58
1:G:186:THR:O	1:G:190:MET:HG2	2.03	0.58
2:A:771:LEU:O	2:A:775:ASN:HB2	2.04	0.58
1:H:186:THR:O	1:H:190:MET:HG2	2.03	0.58
1:G:27:PRO:HD3	1:G:340:TRP:CE3	2.39	0.58
2:B:576:TRP:HD1	2:B:576:TRP:O	1.86	0.58
2:B:743:LEU:HD22	2:B:844:VAL:HG13	1.85	0.58
1:D:186:THR:O	1:D:190:MET:HG2	2.03	0.58
2:C:771:LEU:O	2:C:775:ASN:HB2	2.03	0.58
2:C:778:ASN:ND2	3:B:1001:ACT:O	2.37	0.57
2:B:913:VAL:O	2:B:916:PRO:HD2	2.03	0.57
1:H:222:ASP:HB3	1:H:225:ASN:HB2	1.86	0.57
1:D:222:ASP:HB3	1:D:225:ASN:HB2	1.87	0.57
2:A:869:VAL:HA	2:A:872:ASN:HB3	1.85	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:F:96:VAL:HB	1:F:101:HIS:CE1	2.40	0.57
1:D:18:LYS:HA	1:D:30:VAL:HG22	1.86	0.57
1:F:222:ASP:HB3	1:F:225:ASN:HB2	1.87	0.57
1:D:96:VAL:HB	1:D:101:HIS:CE1	2.39	0.57
2:E:576:TRP:O	2:E:576:TRP:HD1	1.86	0.57
2:B:664:ALA:HA	2:B:667:THR:HG22	1.86	0.57
1:D:9:VAL:HG22	1:D:104:LEU:HB3	1.86	0.57
2:B:570:ARG:O	2:B:570:ARG:HG3	2.04	0.57
1:G:138:ALA:O	1:G:152:VAL:HG21	2.05	0.57
1:F:9:VAL:HG12	1:F:340:TRP:NE1	2.19	0.57
2:C:570:ARG:HG3	2:C:570:ARG:O	2.04	0.57
2:C:576:TRP:HD1	2:C:576:TRP:O	1.87	0.57
1:G:222:ASP:HB3	1:G:225:ASN:HB2	1.86	0.57
1:F:333:PRO:HG2	1:F:334:GLU:HG3	1.87	0.57
1:G:9:VAL:HG22	1:G:104:LEU:HB3	1.87	0.57
2:C:565:ILE:HD13	2:C:566:LYS:H	1.69	0.56
2:C:568:LYS:HB3	2:C:569:PHE:HD1	1.70	0.56
2:A:576:TRP:HD1	2:A:576:TRP:O	1.88	0.56
1:G:151:ILE:HD12	1:G:164:PRO:HG3	1.88	0.56
2:A:578:ALA:HB1	2:E:785:VAL:HG11	1.87	0.56
2:C:672:THR:O	2:C:672:THR:OG1	2.11	0.56
1:F:107:GLU:O	1:F:137:GLN:HG3	2.05	0.56
2:C:807:THR:OG1	2:C:808:LEU:N	2.38	0.56
2:B:740:LEU:HB2	2:B:884:LEU:HD13	1.87	0.56
2:A:568:LYS:HB3	2:A:569:PHE:HD1	1.70	0.56
2:E:638:LEU:N	2:E:711:ASP:OD2	2.23	0.56
2:C:875:SER:OG	2:C:876:THR:N	2.37	0.56
2:E:649:ILE:HD13	1:G:143:TYR:CE1	2.41	0.56
1:H:218:TYR:CZ	1:H:255:PHE:HB3	2.42	0.55
2:A:570:ARG:HG3	2:A:570:ARG:O	2.07	0.55
1:D:280:ASN:HA	1:D:283:MET:HB2	1.88	0.55
1:D:272:ALA:HB1	1:D:276:GLU:HB2	1.86	0.55
2:E:573:VAL:HG11	1:G:367:PRO:HD3	1.89	0.55
2:E:570:ARG:O	2:E:570:ARG:HG3	2.07	0.55
2:B:565:ILE:CD1	2:B:566:LYS:H	2.19	0.55
2:B:771:LEU:O	2:B:775:ASN:HB2	2.06	0.55
1:H:147:ARG:NH1	1:H:330:ILE:HG12	2.12	0.55
1:H:272:ALA:HB1	1:H:276:GLU:HB2	1.87	0.55
1:F:71:ILE:HG23	1:F:76:ILE:HG12	1.88	0.55
2:C:664:ALA:HA	2:C:667:THR:HG22	1.88	0.55
1:H:138:ALA:O	1:H:152:VAL:HG21	2.05	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:278:THR:O	1:F:282:ILE:HD12	2.06	0.55
1:F:280:ASN:HA	1:F:283:MET:HB2	1.88	0.55
2:E:568:LYS:HB3	2:E:569:PHE:HD1	1.71	0.55
1:D:14:SER:OG	4:D:402:ATP:O2B	2.25	0.55
2:A:866:ASP:HB3	2:A:867:ASN:HA	1.89	0.55
1:D:71:ILE:HG23	1:D:76:ILE:HG12	1.89	0.54
2:E:913:VAL:O	2:E:916:PRO:HD2	2.07	0.54
2:C:905:SER:O	2:C:909:THR:HG23	2.08	0.54
1:H:71:ILE:HG23	1:H:76:ILE:HG12	1.88	0.54
2:E:645:LYS:NZ	2:E:646:ASN:OD1	2.41	0.54
1:F:14:SER:OG	4:F:403:ATP:O2B	2.23	0.54
1:D:151:ILE:HD12	1:D:164:PRO:HG3	1.89	0.54
1:H:278:THR:O	1:H:282:ILE:HD12	2.08	0.54
1:F:35:VAL:HG21	1:F:81:ASP:HB3	1.88	0.54
1:F:287:ILE:HG23	1:F:290:ARG:NH1	2.22	0.54
1:H:280:ASN:HA	1:H:283:MET:HB2	1.89	0.54
2:A:638:LEU:N	2:A:711:ASP:OD2	2.24	0.54
1:G:274:ILE:HG21	1:G:313:MET:HE1	1.89	0.54
2:A:792:SER:HB3	2:E:576:TRP:HB2	1.91	0.53
1:H:9:VAL:HG12	1:H:340:TRP:NE1	2.23	0.53
1:D:143:TYR:CE1	2:A:649:ILE:HD13	2.43	0.53
1:H:27:PRO:HD3	1:H:340:TRP:CD2	2.43	0.53
1:H:151:ILE:HD12	1:H:164:PRO:HG3	1.91	0.53
1:G:71:ILE:HG23	1:G:76:ILE:HG12	1.89	0.53
2:E:672:THR:O	2:E:672:THR:OG1	2.18	0.53
2:B:568:LYS:HB3	2:B:569:PHE:HD1	1.74	0.53
1:G:260:THR:HG21	1:G:267:ILE:HG23	1.90	0.53
1:G:287:ILE:HA	1:G:290:ARG:HD3	1.91	0.53
2:A:905:SER:O	2:A:909:THR:HG23	2.08	0.53
2:C:813:ALA:HB3	2:C:932:ASN:ND2	2.24	0.53
1:D:287:ILE:HA	1:D:290:ARG:HD3	1.90	0.53
2:A:827:TRP:CD1	2:A:828:GLN:HG3	2.43	0.53
1:G:178:LEU:HG	1:G:180:LEU:H	1.74	0.53
1:F:151:ILE:HD12	1:F:164:PRO:HG3	1.91	0.53
1:D:218:TYR:CZ	1:D:255:PHE:HB3	2.43	0.53
1:H:17:VAL:O	1:H:30:VAL:HA	2.09	0.53
2:C:785:VAL:HG21	2:B:578:ALA:HB1	1.91	0.53
2:C:827:TRP:CZ3	2:C:926:LYS:HG2	2.43	0.53
2:B:905:SER:O	2:B:909:THR:HG23	2.08	0.53
1:G:196:ARG:HH21	1:G:251:GLY:H	1.57	0.53
1:F:287:ILE:HA	1:F:290:ARG:HD3	1.91	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:840:SER:N	1:G:323:SER:OG	2.33	0.52
2:C:866:ASP:HB3	2:C:867:ASN:HA	1.90	0.52
2:E:664:ALA:HA	2:E:667:THR:HG22	1.91	0.52
2:C:573:VAL:HG11	1:F:367:PRO:HD3	1.91	0.52
2:B:713:PHE:O	2:B:717:PHE:HB2	2.08	0.52
2:B:813:ALA:HB3	2:B:932:ASN:ND2	2.25	0.52
1:G:264:PRO:HG2	1:G:271:SER:O	2.09	0.52
1:D:287:ILE:HG23	1:D:290:ARG:NH1	2.25	0.52
1:F:272:ALA:HB1	1:F:276:GLU:HB2	1.90	0.52
1:D:116:ARG:HG3	1:D:134:VAL:HG11	1.90	0.52
2:E:859:ARG:HB3	2:E:874:LEU:HD11	1.92	0.52
2:B:722:ARG:NH1	2:B:725:GLN:OE1	2.36	0.52
1:G:264:PRO:HG3	1:G:273:GLY:HA2	1.90	0.52
2:E:866:ASP:HB3	2:E:867:ASN:HA	1.91	0.52
2:B:807:THR:OG1	2:B:808:LEU:N	2.43	0.52
2:B:866:ASP:HB3	2:B:867:ASN:HA	1.91	0.52
1:G:218:TYR:CZ	1:G:255:PHE:HB3	2.45	0.52
1:G:333:PRO:HG2	1:G:334:GLU:HG3	1.92	0.52
2:B:692:LYS:HA	2:B:695:ARG:HG2	1.91	0.52
1:F:260:THR:HG21	1:F:267:ILE:HG23	1.91	0.52
2:E:827:TRP:CD1	2:E:828:GLN:HG3	2.45	0.51
2:C:565:ILE:H	2:B:779:SER:HB3	1.75	0.51
1:G:116:ARG:HG3	1:G:134:VAL:HG11	1.92	0.51
1:G:287:ILE:HG23	1:G:290:ARG:NH1	2.25	0.51
1:F:292:ASP:N	1:F:292:ASP:OD1	2.43	0.51
2:C:827:TRP:CD1	2:C:828:GLN:HG3	2.45	0.51
2:C:859:ARG:HB3	2:C:874:LEU:HD11	1.92	0.51
1:F:27:PRO:HD3	1:F:340:TRP:CE3	2.46	0.51
1:F:218:TYR:CZ	1:F:255:PHE:HB3	2.45	0.51
1:D:264:PRO:HG2	1:D:271:SER:O	2.11	0.51
1:H:9:VAL:HG22	1:H:104:LEU:HB3	1.92	0.51
2:E:905:SER:O	2:E:909:THR:HG23	2.10	0.51
1:H:287:ILE:HG23	1:H:290:ARG:NH1	2.25	0.51
2:A:664:ALA:HA	2:A:667:THR:HG22	1.91	0.51
2:E:737:GLN:O	2:E:741:GLN:HG2	2.11	0.51
2:E:899:VAL:HG22	2:E:914:PHE:CD1	2.45	0.51
2:C:740:LEU:HB2	2:C:884:LEU:HD13	1.92	0.51
2:B:722:ARG:NH1	2:B:722:ARG:HA	2.25	0.51
2:C:761:GLN:H	2:C:761:GLN:CD	2.14	0.51
2:B:827:TRP:CD1	2:B:828:GLN:HG3	2.45	0.51
1:H:73:HIS:HB3	1:H:177:ARG:HH22	1.75	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:9:VAL:HG12	1:F:340:TRP:CD1	2.46	0.51
2:B:746:GLN:NE2	1:H:323:SER:HB3	2.19	0.51
1:F:264:PRO:HG2	1:F:271:SER:O	2.11	0.51
1:D:9:VAL:HG12	1:D:340:TRP:NE1	2.26	0.50
2:A:750:ILE:O	2:A:754:SER:HB3	2.11	0.50
2:B:859:ARG:HB3	2:B:874:LEU:HD11	1.93	0.50
2:B:875:SER:OG	2:B:876:THR:N	2.43	0.50
1:D:125:GLU:OE1	3:E:1001:ACT:H2	2.10	0.50
1:H:313:MET:O	1:H:317:ILE:HG12	2.11	0.50
1:D:17:VAL:O	1:D:30:VAL:HA	2.12	0.50
2:C:722:ARG:HA	2:C:722:ARG:NH1	2.26	0.50
1:D:274:ILE:HG21	1:D:313:MET:HE1	1.93	0.50
1:H:9:VAL:HG12	1:H:340:TRP:CD1	2.46	0.50
1:H:157:ASP:OD2	1:H:183:ARG:NH1	2.44	0.50
2:A:775:ASN:ND2	2:A:785:VAL:O	2.36	0.50
2:A:859:ARG:HB3	2:A:874:LEU:HD11	1.94	0.50
2:E:813:ALA:HB3	2:E:932:ASN:ND2	2.27	0.50
2:B:825:ASN:O	2:B:827:TRP:N	2.44	0.50
1:G:9:VAL:HG12	1:G:340:TRP:NE1	2.27	0.50
1:D:315:LYS:HG3	1:D:316:GLU:N	2.25	0.50
2:E:827:TRP:CD1	2:E:828:GLN:N	2.80	0.50
1:H:287:ILE:HA	1:H:290:ARG:HD3	1.92	0.50
1:G:8:LEU:HD11	1:G:94:LEU:CD1	2.42	0.50
2:E:716:LEU:O	2:E:719:LYS:HB2	2.12	0.50
2:B:573:VAL:HG12	1:H:125:GLU:OE2	2.12	0.50
1:D:264:PRO:HG3	1:D:273:GLY:HA2	1.94	0.49
2:A:825:ASN:O	2:A:827:TRP:N	2.43	0.49
2:E:750:ILE:O	2:E:754:SER:HB3	2.12	0.49
1:H:315:LYS:HG3	1:H:316:GLU:N	2.27	0.49
1:H:35:VAL:HG21	1:H:81:ASP:HB3	1.94	0.49
1:G:35:VAL:HG21	1:G:81:ASP:HB3	1.92	0.49
1:F:291:LYS:HZ2	1:F:325:MET:HA	1.76	0.49
1:H:89:THR:O	1:H:94:LEU:HB2	2.13	0.49
1:H:125:GLU:OE2	1:H:362:TYR:OH	2.31	0.49
1:H:178:LEU:HG	1:H:180:LEU:H	1.77	0.49
1:G:315:LYS:HG3	1:G:316:GLU:N	2.27	0.49
1:D:27:PRO:HD3	1:D:340:TRP:CE3	2.47	0.49
2:A:761:GLN:H	2:A:761:GLN:CD	2.15	0.49
2:E:875:SER:OG	2:E:876:THR:N	2.46	0.49
2:B:738:ASP:O	2:B:741:GLN:HB2	2.12	0.49
1:H:333:PRO:HG2	1:H:334:GLU:HG3	1.95	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:722:ARG:NH1	2:C:725:GLN:OE1	2.38	0.49
1:H:264:PRO:HG2	1:H:271:SER:O	2.11	0.49
1:H:350:SER:O	1:H:353:GLN:HG2	2.13	0.49
2:B:716:LEU:O	2:B:719:LYS:HB2	2.13	0.49
1:G:17:VAL:O	1:G:30:VAL:HA	2.12	0.49
1:G:196:ARG:HG3	1:G:253:GLU:HG3	1.94	0.49
2:B:807:THR:HG22	2:B:810:HIS:ND1	2.28	0.49
1:G:27:PRO:HD3	1:G:340:TRP:CD2	2.47	0.49
1:F:313:MET:O	1:F:317:ILE:HG12	2.13	0.49
1:D:238:LYS:HB2	1:D:254:ARG:NH1	2.28	0.49
2:A:716:LEU:O	2:A:719:LYS:HB2	2.13	0.49
2:C:576:TRP:HB2	2:B:792:SER:HB3	1.93	0.49
3:C:1001:ACT:OXT	2:B:778:ASN:ND2	2.45	0.49
1:G:25:ASP:HB3	3:G:401:ACT:O	2.12	0.49
2:A:692:LYS:HA	2:A:695:ARG:HG2	1.93	0.49
2:E:790:LEU:HG	2:E:917:VAL:HG11	1.94	0.49
2:C:833:VAL:HG23	2:C:915:PHE:HB3	1.95	0.49
2:C:913:VAL:HG23	2:C:914:PHE:N	2.28	0.49
2:B:833:VAL:HG23	2:B:915:PHE:HB3	1.95	0.49
1:H:264:PRO:HG3	1:H:273:GLY:HA2	1.93	0.49
1:G:10:CYS:O	1:G:105:LEU:HA	2.13	0.49
1:G:147:ARG:NH1	1:G:330:ILE:HG12	2.17	0.49
1:G:173:HIS:O	1:G:173:HIS:CG	2.65	0.49
1:G:276:GLU:O	1:G:279:TYR:N	2.45	0.49
2:A:813:ALA:HB3	2:A:932:ASN:ND2	2.27	0.49
2:E:808:LEU:O	2:E:812:ILE:HG13	2.13	0.48
2:B:647:LEU:HD22	2:B:651:LEU:HG	1.95	0.48
1:F:17:VAL:HG23	1:F:33:SER:HB3	1.95	0.48
2:C:840:SER:N	1:F:323:SER:OG	2.34	0.48
2:A:722:ARG:HA	2:A:722:ARG:CZ	2.42	0.48
2:C:578:ALA:HB1	2:B:785:VAL:HG21	1.94	0.48
2:C:775:ASN:ND2	2:C:785:VAL:O	2.35	0.48
2:C:825:ASN:O	2:C:827:TRP:N	2.40	0.48
1:H:25:ASP:N	3:H:401:ACT:OXT	2.46	0.48
1:F:173:HIS:O	1:F:173:HIS:CG	2.64	0.48
1:D:73:HIS:HB3	1:D:177:ARG:HH22	1.79	0.48
2:E:795:LEU:HD23	2:E:795:LEU:H	1.78	0.48
1:G:89:THR:O	1:G:94:LEU:HB2	2.13	0.48
1:F:330:ILE:HG22	1:F:332:PRO:HD3	1.95	0.48
1:D:178:LEU:HG	1:D:180:LEU:H	1.78	0.48
2:A:808:LEU:O	2:A:812:ILE:HG13	2.14	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:A:722:ARG:NH1	2:A:725:GLN:OE1	2.39	0.48
2:C:649:ILE:HD13	1:F:143:TYR:CE1	2.49	0.48
1:G:102:PRO:HB3	1:G:131:ALA:HB3	1.95	0.48
1:G:157:ASP:OD2	1:G:183:ARG:NH1	2.47	0.48
1:F:276:GLU:O	1:F:279:TYR:N	2.47	0.48
1:D:196:ARG:HG3	1:D:253:GLU:HG3	1.95	0.48
2:C:877:ASN:O	2:C:880:LYS:N	2.45	0.48
1:F:8:LEU:HD11	1:F:94:LEU:CD1	2.43	0.48
1:F:262:PHE:HD1	1:F:275:HIS:ND1	2.12	0.48
2:B:575:ASN:HA	3:B:1001:ACT:H2	1.94	0.48
2:C:713:PHE:O	2:C:717:PHE:HB2	2.14	0.48
2:C:716:LEU:O	2:C:719:LYS:HB2	2.14	0.48
2:C:746:GLN:NE2	1:F:323:SER:HB3	2.27	0.48
2:A:574:PHE:CE2	2:A:576:TRP:HB3	2.49	0.48
2:A:740:LEU:HB2	2:A:884:LEU:HD13	1.95	0.48
2:A:807:THR:OG1	2:A:808:LEU:N	2.45	0.48
1:H:10:CYS:O	1:H:105:LEU:HA	2.14	0.48
1:H:292:ASP:OD1	1:H:292:ASP:N	2.47	0.48
1:F:73:HIS:HB3	1:F:177:ARG:HH22	1.78	0.48
1:F:76:ILE:HD13	1:F:82:MET:HG2	1.96	0.48
1:F:118:LYS:O	1:F:122:ILE:HG13	2.13	0.48
1:D:288:ASP:N	1:D:288:ASP:OD1	2.47	0.47
2:E:779:SER:O	2:E:780:SER:OG	2.26	0.47
1:H:173:HIS:O	1:H:173:HIS:CG	2.65	0.47
1:G:292:ASP:OD1	1:G:292:ASP:N	2.47	0.47
1:D:313:MET:O	1:D:317:ILE:HG12	2.14	0.47
2:A:647:LEU:HD22	2:A:651:LEU:HG	1.96	0.47
2:A:827:TRP:NE1	2:A:828:GLN:HG3	2.29	0.47
2:B:795:LEU:HD23	2:B:795:LEU:H	1.79	0.47
2:A:795:LEU:H	2:A:795:LEU:HD23	1.80	0.47
2:E:647:LEU:HD22	2:E:651:LEU:HG	1.96	0.47
2:E:713:PHE:O	2:E:717:PHE:HB2	2.14	0.47
2:C:899:VAL:HG22	2:C:914:PHE:CD1	2.49	0.47
1:D:323:SER:HB3	2:A:746:GLN:NE2	2.27	0.47
2:C:808:LEU:O	2:C:812:ILE:HG13	2.15	0.47
2:B:913:VAL:HG23	2:B:914:PHE:N	2.30	0.47
1:H:242:LEU:HD22	1:H:246:GLN:HG3	1.96	0.47
1:H:262:PHE:HD1	1:H:275:HIS:ND1	2.12	0.47
2:A:894:ALA:O	2:A:897:ALA:HB3	2.15	0.47
2:B:573:VAL:HG11	1:H:367:PRO:HD3	1.97	0.47
1:H:8:LEU:HD11	1:H:94:LEU:CD1	2.45	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:35:VAL:HG21	1:D:81:ASP:HB3	1.96	0.47
2:E:738:ASP:O	2:E:741:GLN:HB2	2.14	0.47
1:G:125:GLU:OE2	1:G:362:TYR:OH	2.33	0.47
1:D:173:HIS:O	1:D:173:HIS:CG	2.62	0.47
1:D:292:ASP:N	1:D:292:ASP:OD1	2.47	0.47
2:C:565:ILE:CD1	2:C:566:LYS:H	2.27	0.47
3:C:1002:ACT:OXT	1:H:121:GLN:NE2	2.47	0.47
2:B:750:ILE:O	2:B:754:SER:HB3	2.15	0.47
1:D:295:ALA:O	1:D:328:LYS:HB3	2.15	0.47
1:G:17:VAL:HG23	1:G:33:SER:HB3	1.97	0.47
1:G:73:HIS:HB3	1:G:177:ARG:HH22	1.78	0.47
1:H:238:LYS:HB2	1:H:254:ARG:NH1	2.29	0.47
1:H:260:THR:HG21	1:H:267:ILE:HG23	1.97	0.47
1:G:361:GLU:H	1:G:361:GLU:HG2	1.49	0.47
1:F:9:VAL:HG22	1:F:104:LEU:HB3	1.97	0.47
2:E:807:THR:OG1	2:E:808:LEU:N	2.48	0.47
2:C:750:ILE:O	2:C:754:SER:HB3	2.14	0.47
2:B:899:VAL:HG22	2:B:914:PHE:CD1	2.49	0.47
1:G:9:VAL:HG12	1:G:340:TRP:CD1	2.50	0.47
1:F:219:VAL:HG22	1:F:258:PRO:HB2	1.96	0.47
2:A:816:VAL:HG11	2:A:925:TYR:OH	2.15	0.46
2:A:827:TRP:CD1	2:A:828:GLN:N	2.83	0.46
2:E:656:ARG:HB3	2:E:661:ILE:HG13	1.97	0.46
2:E:796:LEU:HD23	2:E:796:LEU:HA	1.61	0.46
2:C:827:TRP:CD1	2:C:828:GLN:N	2.83	0.46
1:F:17:VAL:O	1:F:30:VAL:HA	2.15	0.46
1:F:125:GLU:OE2	1:F:362:TYR:OH	2.33	0.46
2:A:578:ALA:CB	2:E:785:VAL:HG11	2.45	0.46
2:B:808:LEU:O	2:B:812:ILE:HG13	2.15	0.46
1:G:242:LEU:HD22	1:G:246:GLN:HG3	1.97	0.46
2:B:609:LEU:C	2:B:610:PHE:HD1	2.19	0.46
1:H:73:HIS:HB3	1:H:177:ARG:NH2	2.30	0.46
1:H:276:GLU:O	1:H:279:TYR:N	2.49	0.46
1:F:140:LEU:O	1:F:342:GLY:HA3	2.16	0.46
1:D:89:THR:O	1:D:94:LEU:HB2	2.15	0.46
2:E:827:TRP:NE1	2:E:828:GLN:HG3	2.31	0.46
1:G:112:PRO:HD2	1:G:115:ASN:HB2	1.98	0.46
1:G:140:LEU:O	1:G:342:GLY:HA3	2.16	0.46
1:G:316:GLU:O	1:G:320:LEU:HD13	2.16	0.46
1:F:264:PRO:HG3	1:F:273:GLY:HA2	1.98	0.46
1:D:147:ARG:NH1	1:D:330:ILE:HG12	2.18	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:775:ASN:ND2	2:E:785:VAL:O	2.36	0.46
2:C:795:LEU:H	2:C:795:LEU:HD23	1.81	0.46
1:H:306:TYR:CE1	4:H:402:ATP:H2	2.32	0.46
1:D:262:PHE:HD1	1:D:275:HIS:ND1	2.14	0.46
2:A:713:PHE:O	2:A:717:PHE:HB2	2.14	0.46
2:B:827:TRP:NE1	2:B:828:GLN:HG3	2.31	0.46
2:B:877:ASN:O	2:B:880:LYS:N	2.48	0.46
2:E:825:ASN:O	2:E:827:TRP:N	2.42	0.46
1:D:76:ILE:HD13	1:D:82:MET:HG2	1.97	0.46
1:D:330:ILE:HG22	1:D:332:PRO:HD3	1.97	0.46
1:H:275:HIS:CD2	1:H:276:GLU:HG3	2.51	0.46
1:G:160:THR:HB	1:G:178:LEU:HB3	1.98	0.46
1:G:262:PHE:HD1	1:G:275:HIS:ND1	2.14	0.46
2:C:646:ASN:HB3	1:F:148:THR:HG21	1.97	0.46
1:H:158:GLY:HA3	1:H:183:ARG:NH2	2.31	0.46
1:H:261:LEU:HB3	1:H:274:ILE:CD1	2.37	0.46
1:F:242:LEU:HD22	1:F:246:GLN:HG3	1.96	0.46
1:D:9:VAL:HG12	1:D:340:TRP:CD1	2.51	0.45
1:D:291:LYS:HZ2	1:D:325:MET:HA	1.81	0.45
2:B:775:ASN:ND2	2:B:785:VAL:O	2.36	0.45
1:F:10:CYS:O	1:F:105:LEU:HA	2.16	0.45
1:F:257:CYS:HB3	1:F:258:PRO:HD3	1.98	0.45
1:D:140:LEU:O	1:D:342:GLY:HA3	2.16	0.45
1:H:219:VAL:HG22	1:H:258:PRO:HB2	1.98	0.45
1:F:111:ASN:HA	1:F:112:PRO:HD3	1.67	0.45
1:D:306:TYR:CE1	4:D:402:ATP:H2	2.34	0.45
2:A:802:THR:HG23	2:E:609:LEU:O	2.16	0.45
2:B:827:TRP:CD1	2:B:828:GLN:N	2.85	0.45
1:H:330:ILE:HG22	1:H:332:PRO:HD3	1.97	0.45
1:G:330:ILE:HG22	1:G:332:PRO:HD3	1.98	0.45
1:D:125:GLU:OE2	1:D:362:TYR:OH	2.34	0.45
1:D:341:ILE:HG22	1:D:345:ILE:HD12	1.97	0.45
2:E:740:LEU:HB2	2:E:884:LEU:HD13	1.98	0.45
2:E:833:VAL:HG23	2:E:915:PHE:HB3	1.99	0.45
2:C:656:ARG:HB3	2:C:661:ILE:HG13	1.99	0.45
1:G:76:ILE:HD13	1:G:82:MET:HG2	1.99	0.45
2:A:609:LEU:C	2:A:610:PHE:HD1	2.20	0.45
1:H:102:PRO:HB3	1:H:131:ALA:HB3	1.98	0.45
1:H:295:ALA:O	1:H:328:LYS:HB3	2.16	0.45
1:D:8:LEU:HD11	1:D:94:LEU:CD1	2.46	0.45
1:D:291:LYS:NZ	1:D:326:LYS:H	2.14	0.45



	lo de page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:A:737:GLN:O	2:A:741:GLN:HG2	2.17	0.45
2:E:603:LEU:O	2:E:606:PHE:HB3	2.16	0.45
2:B:825:ASN:HB2	2:B:828:GLN:OE1	2.17	0.45
1:H:17:VAL:HG23	1:H:33:SER:HB3	1.98	0.45
2:E:814:LEU:HG	2:E:932:ASN:ND2	2.32	0.45
2:E:877:ASN:O	2:E:880:LYS:N	2.50	0.45
2:B:761:GLN:H	2:B:761:GLN:CD	2.17	0.45
1:H:116:ARG:HG3	1:H:134:VAL:HG11	1.99	0.45
1:G:18:LYS:HG3	1:G:30:VAL:HG22	1.98	0.45
1:G:158:GLY:HA3	1:G:183:ARG:NH2	2.32	0.45
1:D:316:GLU:O	1:D:320:LEU:HD13	2.17	0.45
2:B:656:ARG:HB3	2:B:661:ILE:HG13	1.98	0.45
2:B:722:ARG:HA	2:B:722:ARG:CZ	2.46	0.45
1:H:99:GLU:O	1:H:130:PRO:HD3	2.17	0.45
1:F:25:ASP:N	3:F:402:ACT:OXT	2.50	0.45
1:D:10:CYS:O	1:D:105:LEU:HA	2.17	0.45
2:A:584:ILE:HD11	2:E:787:GLY:HA3	1.98	0.45
2:B:673:LEU:HA	2:B:674:PRO:HD3	1.75	0.45
1:H:316:GLU:O	1:H:320:LEU:HD13	2.17	0.45
1:H:341:ILE:HG22	1:H:345:ILE:HD12	1.99	0.45
1:D:333:PRO:HG2	1:D:334:GLU:HG3	1.98	0.45
1:D:350:SER:O	1:D:353:GLN:HG2	2.17	0.45
2:E:599:GLU:O	2:E:601:LEU:HD12	2.17	0.45
2:E:746:GLN:NE2	1:G:323:SER:HB3	2.29	0.45
1:H:288:ASP:OD1	1:H:288:ASP:N	2.50	0.45
1:G:304:THR:O	1:G:335:ARG:NH2	2.44	0.45
2:E:682:MET:O	2:E:685:LEU:HD12	2.17	0.44
2:C:738:ASP:O	2:C:741:GLN:HB2	2.16	0.44
2:C:827:TRP:NE1	2:C:828:GLN:HG3	2.32	0.44
1:H:118:LYS:O	1:H:122:ILE:HG13	2.17	0.44
1:F:112:PRO:HD2	1:F:115:ASN:HB2	1.99	0.44
1:F:217:CYS:HB2	1:F:254:ARG:O	2.17	0.44
2:A:603:LEU:O	2:A:606:PHE:HB3	2.17	0.44
2:C:581:PRO:HA	2:C:584:ILE:HB	1.99	0.44
1:G:105:LEU:HD13	1:G:134:VAL:HG22	1.99	0.44
1:F:147:ARG:NH1	1:F:330:ILE:HG12	2.21	0.44
1:D:362:TYR:O	1:D:366:GLY:N	2.40	0.44
2:C:669:ASP:HB2	2:C:730:MET:SD	2.57	0.44
2:C:707:LEU:HD23	2:C:707:LEU:HA	1.82	0.44
1:G:172:PRO:O	1:G:175:ILE:HG13	2.17	0.44
1:F:288:ASP:OD1	1:F:288:ASP:N	2.50	0.44



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	$ ext{overlap}(\text{\AA})$
2:E:913:VAL:HG23	2:E:914:PHE:N	2.33	0.44
2:B:707:LEU:HD23	2:B:707:LEU:HA	1.84	0.44
2:B:737:GLN:O	2:B:741:GLN:HG2	2.17	0.44
1:H:120:THR:HG21	1:H:370:VAL:HB	2.00	0.44
1:H:172:PRO:O	1:H:175:ILE:HG13	2.16	0.44
1:G:219:VAL:HG22	1:G:258:PRO:HB2	1.99	0.44
1:G:275:HIS:CD2	1:G:276:GLU:HG3	2.53	0.44
2:B:789:LYS:HB3	2:B:791:GLN:OE1	2.18	0.44
1:H:105:LEU:HD13	1:H:134:VAL:HG22	2.00	0.44
1:G:109:PRO:O	1:G:110:LEU:HB2	2.17	0.44
1:F:52:SER:OG	1:F:84:LYS:HD2	2.18	0.44
1:D:25:ASP:HB3	3:D:401:ACT:O	2.17	0.44
1:D:365:ALA:HB3	1:D:369:ILE:HB	2.00	0.44
2:A:874:LEU:HD23	2:A:878:GLU:HG3	2.00	0.44
2:E:669:ASP:HB2	2:E:730:MET:SD	2.58	0.44
2:C:647:LEU:HD22	2:C:651:LEU:HG	1.99	0.44
2:B:646:ASN:HB3	1:H:148:THR:HG21	1.99	0.44
1:H:124:PHE:HD1	1:H:359:LYS:HG3	1.83	0.44
2:A:599:GLU:O	2:A:601:LEU:HD12	2.17	0.44
1:H:76:ILE:HD13	1:H:82:MET:HG2	2.00	0.44
2:A:807:THR:HG22	2:A:810:HIS:ND1	2.33	0.44
2:C:677:PHE:CZ	2:C:681:LEU:HD13	2.53	0.44
2:B:649:ILE:HD13	1:H:143:TYR:CE1	2.53	0.44
1:D:276:GLU:O	1:D:279:TYR:N	2.51	0.44
2:A:790:LEU:HG	2:A:917:VAL:HG11	2.00	0.44
2:E:574:PHE:CE2	2:E:576:TRP:HB3	2.52	0.44
2:E:581:PRO:HA	2:E:584:ILE:HB	2.00	0.44
2:C:669:ASP:HB3	2:C:673:LEU:CB	2.47	0.44
2:C:722:ARG:HA	2:C:722:ARG:CZ	2.47	0.44
1:F:89:THR:O	1:F:94:LEU:HB2	2.17	0.44
2:B:581:PRO:HA	2:B:584:ILE:HB	2.01	0.43
1:F:73:HIS:HB3	1:F:177:ARG:NH2	2.32	0.43
1:F:99:GLU:O	1:F:130:PRO:HD3	2.18	0.43
1:D:105:LEU:O	1:D:134:VAL:HA	2.18	0.43
2:A:669:ASP:HB3	2:A:673:LEU:CB	2.45	0.43
2:C:609:LEU:C	2:C:610:PHE:HD1	2.21	0.43
2:C:682:MET:O	2:C:685:LEU:HD12	2.18	0.43
1:F:178:LEU:HG	1:F:180:LEU:H	1.82	0.43
1:F:352:PHE:HA	1:F:355:MET:HE2	2.00	0.43
2:A:695:ARG:HG3	2:A:696:GLN:H	1.83	0.43
1:F:6:THR:O	1:F:101:HIS:HB3	2.16	0.43



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:275:HIS:CD2	1:F:276:GLU:HG3	2.53	0.43
1:D:261:LEU:HB3	1:D:274:ILE:CD1	2.37	0.43
2:B:682:MET:O	2:B:685:LEU:HD12	2.18	0.43
2:E:874:LEU:HD23	2:E:878:GLU:HG3	2.01	0.43
2:C:874:LEU:HD23	2:C:878:GLU:HG3	2.01	0.43
2:C:905:SER:O	2:C:909:THR:N	2.50	0.43
2:B:796:LEU:HA	2:B:796:LEU:HD23	1.68	0.43
1:G:73:HIS:HB3	1:G:177:ARG:NH2	2.33	0.43
1:F:242:LEU:HB2	1:F:246:GLN:O	2.18	0.43
2:E:576:TRP:O	2:E:576:TRP:CD1	2.69	0.43
2:E:773:LEU:HD12	2:E:773:LEU:HA	1.82	0.43
1:G:341:ILE:HG22	1:G:345:ILE:HD12	2.00	0.43
1:D:73:HIS:HB3	1:D:177:ARG:NH2	2.33	0.43
2:E:606:PHE:HE1	2:E:610:PHE:CD2	2.37	0.43
2:C:599:GLU:O	2:C:601:LEU:HD12	2.18	0.43
2:B:576:TRP:O	2:B:576:TRP:CD1	2.68	0.43
2:A:840:SER:O	2:A:844:VAL:HG23	2.18	0.43
2:C:842:GLU:O	2:C:846:LEU:HG	2.18	0.43
1:H:300:SER:HB2	1:H:338:SER:HB2	2.01	0.43
1:D:94:LEU:HA	1:D:94:LEU:HD22	1.76	0.43
1:D:148:THR:HG21	2:A:646:ASN:HB3	2.00	0.43
2:E:678:VAL:O	2:E:682:MET:HG3	2.19	0.43
1:H:111:ASN:HD21	1:H:115:ASN:CG	2.15	0.43
1:H:274:ILE:HG21	1:H:313:MET:HE1	2.00	0.43
1:F:109:PRO:HG2	1:F:161:HIS:CG	2.54	0.43
1:D:264:PRO:CG	1:D:273:GLY:HA2	2.49	0.43
2:A:656:ARG:HB3	2:A:661:ILE:HG13	2.00	0.43
2:B:894:ALA:O	2:B:897:ALA:HB3	2.19	0.43
1:H:362:TYR:O	1:H:366:GLY:N	2.42	0.43
1:F:27:PRO:HD3	1:F:340:TRP:CD2	2.54	0.43
2:A:842:GLU:O	2:A:846:LEU:HG	2.19	0.42
2:E:645:LYS:HB3	2:E:645:LYS:HE3	1.74	0.42
2:B:690:GLU:O	2:B:694:LEU:HD23	2.18	0.42
1:H:112:PRO:HD2	1:H:115:ASN:HB2	2.01	0.42
2:A:637:THR:HG22	2:A:639:LEU:N	2.28	0.42
2:E:690:GLU:O	2:E:694:LEU:HD23	2.19	0.42
2:C:704:LEU:HA	2:C:704:LEU:HD13	1.77	0.42
2:C:779:SER:C	2:C:781:LYS:H	2.23	0.42
2:C:782:ARG:NH1	2:B:573:VAL:HG23	2.34	0.42
2:C:816:VAL:HG11	2:C:925:TYR:OH	2.18	0.42
2:B:677:PHE:CZ	2:B:681:LEU:HD13	2.54	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:188:TYR:HH	1:H:266:PHE:HD2	1.65	0.42
1:H:210:ARG:O	1:H:213:LYS:HB3	2.20	0.42
1:F:291:LYS:NZ	1:F:326:LYS:H	2.17	0.42
1:F:316:GLU:O	1:F:320:LEU:HD13	2.19	0.42
2:A:707:LEU:HD22	2:A:711:ASP:HB2	2.01	0.42
2:B:645:LYS:HB3	2:B:645:LYS:HE3	1.71	0.42
1:F:295:ALA:O	1:F:328:LYS:HB3	2.19	0.42
1:D:136:ILE:H	1:D:136:ILE:CD1	2.25	0.42
1:D:176:MET:HG3	1:D:281:SER:HB2	2.01	0.42
1:H:361:GLU:H	1:H:361:GLU:HG2	1.53	0.42
1:G:313:MET:O	1:G:317:ILE:HG12	2.19	0.42
1:G:350:SER:O	1:G:353:GLN:HG2	2.20	0.42
1:F:321:ALA:HB3	1:F:327:ILE:HD11	2.01	0.42
1:D:92:ASN:O	1:D:95:ARG:HD2	2.20	0.42
1:H:109:PRO:O	1:H:110:LEU:HB2	2.20	0.42
1:F:31:PHE:HZ	1:F:89:THR:HG1	1.66	0.42
1:D:120:THR:HG21	1:D:370:VAL:HB	2.01	0.42
2:A:678:VAL:O	2:A:682:MET:HG3	2.20	0.42
2:C:574:PHE:CE2	2:C:576:TRP:HB3	2.55	0.42
1:F:361:GLU:H	1:F:361:GLU:HG2	1.54	0.42
2:A:576:TRP:O	2:A:576:TRP:CD1	2.71	0.42
2:E:747:LEU:HA	2:E:747:LEU:HD23	1.79	0.42
1:H:372:ARG:H	1:H:372:ARG:HG2	1.68	0.42
1:G:196:ARG:HH21	1:G:251:GLY:N	2.17	0.42
1:F:274:ILE:HG21	1:F:313:MET:HE1	2.00	0.42
1:D:219:VAL:HG22	1:D:258:PRO:HB2	2.00	0.42
1:D:275:HIS:CD2	1:D:276:GLU:HG3	2.54	0.42
2:E:646:ASN:HB3	2:E:684:PHE:HZ	1.83	0.42
2:E:673:LEU:HA	2:E:674:PRO:HD3	1.78	0.42
2:C:576:TRP:O	2:C:576:TRP:CD1	2.70	0.42
2:C:894:ALA:O	2:C:897:ALA:HB3	2.20	0.42
2:B:816:VAL:HG11	2:B:925:TYR:OH	2.20	0.42
1:G:264:PRO:CG	1:G:273:GLY:HA2	2.49	0.42
1:F:365:ALA:HB3	1:F:369:ILE:HB	2.02	0.42
2:E:609:LEU:C	2:E:610:PHE:HD1	2.23	0.42
1:H:109:PRO:HG2	1:H:161:HIS:CG	2.54	0.42
1:G:146:GLY:C	1:G:147:ARG:HG2	2.40	0.42
2:A:645:LYS:HE3	2:A:645:LYS:HB3	1.72	0.42
2:A:863:SER:HB2	2:C:582:ASN:ND2	2.34	0.42
2:A:899:VAL:HG22	2:A:914:PHE:CD1	2.55	0.42
2:C:796:LEU:HD23	2:C:796:LEU:HA	1.57	0.42



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:H:111:ASN:HA	1:H:112:PRO:HD3	1.69	0.42
2:A:581:PRO:HA	2:A:584:ILE:HB	2.02	0.41
2:E:576:TRP:CD1	2:E:576:TRP:C	2.94	0.41
1:G:365:ALA:HB3	1:G:369:ILE:HB	2.01	0.41
1:F:120:THR:HG21	1:F:370:VAL:HB	2.02	0.41
1:F:206:ARG:HA	1:F:209:VAL:HG23	2.02	0.41
1:F:315:LYS:HG3	1:F:316:GLU:N	2.35	0.41
1:D:99:GLU:O	1:D:130:PRO:HD3	2.20	0.41
1:D:314:GLN:O	1:D:318:THR:OG1	2.38	0.41
2:E:646:ASN:HB3	1:G:148:THR:HG21	2.02	0.41
2:B:565:ILE:HG23	2:B:566:LYS:N	2.33	0.41
1:H:217:CYS:HB2	1:H:254:ARG:O	2.19	0.41
1:G:288:ASP:N	1:G:288:ASP:OD1	2.52	0.41
1:G:311:ASP:O	1:G:314:GLN:HB3	2.20	0.41
2:A:588:VAL:O	2:A:591:GLU:HB2	2.20	0.41
2:E:789:LYS:HB3	2:E:791:GLN:OE1	2.20	0.41
2:C:790:LEU:HD12	2:C:790:LEU:HA	1.90	0.41
1:H:94:LEU:HD22	1:H:94:LEU:HA	1.85	0.41
1:H:151:ILE:HD11	1:H:162:ASN:HB3	2.01	0.41
1:F:158:GLY:HA3	1:F:183:ARG:NH2	2.34	0.41
2:E:588:VAL:O	2:E:591:GLU:HB2	2.20	0.41
2:E:677:PHE:CZ	2:E:681:LEU:HD13	2.56	0.41
2:E:812:ILE:HG13	2:E:812:ILE:H	1.67	0.41
2:E:910:PRO:HD2	2:E:913:VAL:HG22	2.03	0.41
2:C:576:TRP:CD1	2:C:576:TRP:C	2.93	0.41
2:C:678:VAL:O	2:C:682:MET:HG3	2.20	0.41
2:C:779:SER:HA	2:C:783:GLY:O	2.21	0.41
2:B:603:LEU:O	2:B:606:PHE:HB3	2.20	0.41
2:B:672:THR:O	2:B:672:THR:OG1	2.17	0.41
1:G:92:ASN:O	1:G:95:ARG:HD2	2.21	0.41
1:G:120:THR:HG21	1:G:370:VAL:HB	2.00	0.41
1:F:173:HIS:CD2	1:F:173:HIS:H	2.35	0.41
1:D:302:GLY:O	4:D:402:ATP:C4	2.74	0.41
2:A:584:ILE:O	2:A:587:THR:HG23	2.20	0.41
2:A:587:THR:HB	2:E:901:TYR:O	2.21	0.41
2:C:565:ILE:HG23	2:C:566:LYS:N	2.36	0.41
2:C:790:LEU:HG	2:C:917:VAL:HG11	2.03	0.41
2:B:774:GLY:O	2:B:778:ASN:HB2	2.19	0.41
1:H:347:ALA:HA	1:H:352:PHE:CE2	2.56	0.41
1:D:17:VAL:HG23	1:D:33:SER:HB3	2.02	0.41
2:A:747:LEU:HD23	2:A:747:LEU:HA	1.73	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:704:LEU:HD13	2:E:704:LEU:HA	1.85	0.41
2:E:842:GLU:O	2:E:846:LEU:HG	2.20	0.41
2:B:850:GLU:O	2:B:853:ARG:HG3	2.21	0.41
1:G:321:ALA:HB3	1:G:327:ILE:HD11	2.03	0.41
1:D:173:HIS:CD2	1:D:173:HIS:H	2.35	0.41
2:A:606:PHE:HE1	2:A:610:PHE:CD2	2.38	0.41
2:A:913:VAL:HG23	2:A:914:PHE:N	2.35	0.41
2:E:757:VAL:HA	2:E:830:LEU:CD2	2.48	0.41
2:B:651:LEU:O	2:B:654:ALA:HB3	2.20	0.41
1:G:109:PRO:HG2	1:G:161:HIS:CG	2.55	0.41
1:G:261:LEU:HB3	1:G:274:ILE:CD1	2.38	0.41
1:G:314:GLN:O	1:G:318:THR:OG1	2.36	0.41
1:F:287:ILE:HG23	1:F:290:ARG:HH12	1.85	0.41
1:D:18:LYS:HG3	1:D:30:VAL:HG22	2.03	0.41
2:B:687:THR:O	2:B:691:VAL:HG23	2.21	0.41
2:B:807:THR:HG22	2:B:810:HIS:CG	2.56	0.41
1:H:321:ALA:HB3	1:H:327:ILE:HD11	2.02	0.41
1:G:118:LYS:O	1:G:122:ILE:HG13	2.20	0.41
2:E:652:ARG:NE	1:G:345:ILE:HG12	2.36	0.41
2:E:672:THR:O	2:E:674:PRO:HD3	2.21	0.41
2:E:756:SER:HB2	2:E:830:LEU:HA	2.03	0.41
2:E:816:VAL:HG11	2:E:925:TYR:OH	2.21	0.41
2:C:672:THR:O	2:C:674:PRO:HD3	2.21	0.41
2:B:842:GLU:O	2:B:846:LEU:HG	2.21	0.41
2:B:856:GLU:HA	2:B:859:ARG:HG2	2.03	0.41
1:H:21:PHE:HB2	3:H:401:ACT:H3	2.03	0.41
1:G:242:LEU:HB2	1:G:246:GLN:O	2.20	0.41
1:F:18:LYS:HG3	1:F:30:VAL:HG22	2.01	0.41
2:A:877:ASN:O	2:A:880:LYS:N	2.54	0.41
2:E:645:LYS:HG2	2:E:649:ILE:HD11	2.03	0.41
1:H:264:PRO:CG	1:H:273:GLY:HA2	2.51	0.41
1:D:151:ILE:HD11	1:D:162:ASN:HB3	2.03	0.40
2:C:673:LEU:HA	2:C:674:PRO:HD3	1.79	0.40
1:H:162:ASN:O	1:H:164:PRO:HD3	2.20	0.40
1:H:208:ILE:O	1:H:212:ILE:HD12	2.20	0.40
1:G:173:HIS:CD2	1:G:173:HIS:H	2.35	0.40
1:G:196:ARG:NH1	1:G:196:ARG:HB3	2.35	0.40
1:G:257:CYS:HB3	1:G:258:PRO:HD3	2.03	0.40
1:F:105:LEU:HD13	1:F:134:VAL:HG22	2.03	0.40
1:D:102:PRO:HB3	1:D:131:ALA:HB3	2.03	0.40
2:A:796:LEU:HD23	2:A:796:LEU:HA	1.65	0.40



	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:A:814:LEU:HG	2:A:932:ASN:ND2	2.35	0.40
2:A:856:GLU:HA	2:A:859:ARG:HG2	2.03	0.40
2:C:610:PHE:CE2	2:B:808:LEU:HA	2.56	0.40
2:B:678:VAL:O	2:B:682:MET:HG3	2.22	0.40
1:H:365:ALA:HB3	1:H:369:ILE:HB	2.03	0.40
1:D:160:THR:HB	1:D:178:LEU:HB3	2.03	0.40
2:A:770:ILE:HG22	2:A:788:PHE:CE2	2.57	0.40
2:B:584:ILE:HD13	2:B:584:ILE:HA	1.95	0.40
2:B:779:SER:C	2:B:781:LYS:H	2.24	0.40
1:F:124:PHE:HD1	1:F:359:LYS:HG3	1.86	0.40
1:F:287:ILE:H	1:F:287:ILE:HG12	1.65	0.40
1:D:123:MET:HG3	1:D:132:MET:HE3	2.02	0.40
1:D:361:GLU:H	1:D:361:GLU:HG2	1.51	0.40
2:A:609:LEU:O	2:E:802:THR:HG23	2.20	0.40
2:A:669:ASP:HB2	2:A:730:MET:SD	2.61	0.40
2:E:803:ASP:OD2	2:E:805:LYS:HB2	2.22	0.40
1:H:209:VAL:HA	1:H:212:ILE:HD13	2.03	0.40
1:H:257:CYS:HB3	1:H:258:PRO:HD3	2.04	0.40
1:F:210:ARG:O	1:F:213:LYS:HB3	2.21	0.40
1:D:106:THR:HA	1:D:135:ALA:O	2.21	0.40
2:A:913:VAL:C	2:A:916:PRO:HD2	2.42	0.40
2:E:774:GLY:O	2:E:778:ASN:HB2	2.22	0.40
2:B:773:LEU:HD21	2:B:811:PHE:CE2	2.56	0.40
1:H:304:THR:O	1:H:335:ARG:NH2	2.47	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:SER:OG	1:F:62:ARG:O[1_554]	2.11	0.09

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	D	352/377~(93%)	326 (93%)	25~(7%)	1 (0%)	41	72
1	F	352/377~(93%)	324 (92%)	27 (8%)	1 (0%)	41	72
1	G	352/377~(93%)	324 (92%)	27 (8%)	1 (0%)	41	72
1	Н	352/377~(93%)	325 (92%)	26 (7%)	1 (0%)	41	72
2	А	353/402~(88%)	310 (88%)	37 (10%)	6(2%)	9	34
2	В	353/402~(88%)	313 (89%)	34 (10%)	6(2%)	9	34
2	С	353/402~(88%)	313 (89%)	34 (10%)	6(2%)	9	34
2	Е	353/402~(88%)	310 (88%)	38 (11%)	5 (1%)	11	37
All	All	2820/3116 (90%)	2545 (90%)	248 (9%)	27 (1%)	15	46

analysed, and the total number of residues.

All (27) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
2	А	869	VAL
2	Е	869	VAL
2	С	869	VAL
2	В	869	VAL
2	А	598	LEU
2	А	674	PRO
2	Е	598	LEU
2	Е	674	PRO
2	С	598	LEU
2	С	674	PRO
2	В	598	LEU
2	В	674	PRO
2	С	826	PHE
2	А	826	PHE
2	А	863	SER
2	Е	826	PHE
2	Е	863	SER
2	С	863	SER
2	В	695	ARG
2	В	826	PHE
2	В	863	SER
2	А	752	ALA
2	С	695	ARG
1	D	274	ILE
1	F	274	ILE



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

Mol	Chain	Res	Type
1	G	274	ILE
1	Н	274	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	D	302/320~(94%)	262~(87%)	40 (13%)	4	15
1	F	302/320~(94%)	260 (86%)	42 (14%)	3	13
1	G	302/320~(94%)	263~(87%)	39~(13%)	4	16
1	Н	302/320~(94%)	265~(88%)	37 (12%)	4	17
2	А	316/351~(90%)	256 (81%)	60 (19%)	1	4
2	В	316/351~(90%)	255 (81%)	61 (19%)	1	4
2	С	316/351~(90%)	254 (80%)	62 (20%)	1	4
2	Е	316/351~(90%)	256 (81%)	60 (19%)	1	4
All	All	2472/2684~(92%)	2071 (84%)	401 (16%)	2	9

All (401) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	6	THR
1	D	18	LYS
1	D	28	ARG
1	D	57	GLU
1	D	66	THR
1	D	69	TYR
1	D	71	ILE
1	D	78	ASN
1	D	94	LEU
1	D	95	ARG
1	D	99	GLU
1	D	101	HIS
1	D	105	LEU



Mol	Chain	Res	Type
1	D	119	MET
1	D	120	THR
1	D	136	ILE
1	D	151	ILE
1	D	159	VAL
1	D	176	MET
1	D	179	ASP
1	D	200	PHE
1	D	202	THR
1	D	217	CYS
1	D	277	THR
1	D	280	ASN
1	D	288	ASP
1	D	289	ILE
1	D	290	ARG
1	D	292	ASP
1	D	315	LYS
1	D	318	THR
1	D	326	LYS
1	D	334	GLU
1	D	338	SER
1	D	339	VAL
1	D	349	LEU
1	D	360	GLN
1	D	368	SER
1	D	370	VAL
1	D	372	ARG
2	А	565	ILE
2	А	576	TRP
2	А	577	THR
2	А	585	ASN
2	А	587	THR
2	A	591	GLU
2	A	592	LEU
2	A	594	ASP
2	A	598	LEU
2	A	601	LEU
2	A	603	LEU
2	A	609	LEU
2	А	613	LYS
2	A	636	VAL
2	А	640	GLU



Mol	Chain	Res	Type
2	А	643	ARG
2	А	647	LEU
2	А	669	ASP
2	А	675	VAL
2	А	685	LEU
2	А	700	GLU
2	А	701	ARG
2	А	705	GLU
2	А	711	ASP
2	А	721	GLU
2	А	722	ARG
2	А	724	THR
2	А	725	GLN
2	А	738	ASP
2	А	740	LEU
2	А	742	MET
2	А	750	ILE
2	А	751	ILE
2	А	754	SER
2	А	764	LYS
2	А	765	GLN
2	А	775	ASN
2	А	781	LYS
2	А	792	SER
2	А	795	LEU
2	А	798	ASP
2	А	802	THR
2	А	808	LEU
2	А	810	HIS
2	A	815	THR
2	А	816	VAL
2	A	822	GLU
2	A	825	ASN
2	A	826	PHE
2	A	830	LEU
2	A	841	LEU
2	A	853	ARG
2	A	865	HIS
2	А	869	VAL
2	А	876	THR
2	A	882	ASP
2	А	886	ARG



Mol	Chain	Res	Type
2	А	898	VAL
2	А	909	THR
2	А	925	TYR
2	Е	565	ILE
2	Е	576	TRP
2	Е	577	THR
2	Е	585	ASN
2	Е	587	THR
2	Е	591	GLU
2	Е	592	LEU
2	Е	594	ASP
2	Е	598	LEU
2	Ε	601	LEU
2	Е	603	LEU
2	Е	609	LEU
2	Е	613	LYS
2	Е	636	VAL
2	Е	640	GLU
2	Е	643	ARG
2	Е	647	LEU
2	Е	669	ASP
2	Е	675	VAL
2	Е	685	LEU
2	Е	693	LEU
2	Е	700	GLU
2	Е	701	ARG
2	Е	705	GLU
2	Е	711	ASP
2	E	721	GLU
2	E	722	ARG
2	Е	724	THR
2	E	725	GLN
2	Е	738	ASP
2	E	740	LEU
2	Е	742	MET
2	Е	750	ILE
2	E	751	ILE
2	Е	764	LYS
2	E	765	GLN
2	Е	775	ASN
2	E	781	LYS
2	Е	792	SER



Mol	Chain	Res	Type
2	Е	795	LEU
2	Е	798	ASP
2	Е	802	THR
2	Е	808	LEU
2	Е	810	HIS
2	Е	815	THR
2	Е	816	VAL
2	Е	822	GLU
2	Е	825	ASN
2	Е	826	PHE
2	Е	830	LEU
2	Е	841	LEU
2	E	853	ARG
2	Е	865	HIS
2	Е	869	VAL
2	Е	876	THR
2	Е	882	ASP
2	Е	886	ARG
2	Е	898	VAL
2	Е	909	THR
2	Е	925	TYR
2	С	565	ILE
2	С	576	TRP
2	С	577	THR
2	С	585	ASN
2	С	587	THR
2	С	591	GLU
2	С	592	LEU
2	С	594	ASP
2	С	598	LEU
2	С	601	LEU
2	С	603	LEU
2	C	609	LEU
2	С	613	LYS
2	С	636	VAL
2	С	640	GLU
2	С	643	ARG
2	С	647	LEU
2	С	669	ASP
2	С	675	VAL
2	С	685	LEU
2	С	693	LEU



Mol	Chain	Res	Type
2	С	700	GLU
2	С	701	ARG
2	С	704	LEU
2	С	705	GLU
2	С	711	ASP
2	С	721	GLU
2	С	722	ARG
2	С	724	THR
2	С	725	GLN
2	С	738	ASP
2	С	740	LEU
2	С	742	MET
2	С	750	ILE
2	С	751	ILE
2	С	754	SER
2	С	764	LYS
2	С	765	GLN
2	С	775	ASN
2	С	781	LYS
2	С	792	SER
2	С	795	LEU
2	С	798	ASP
2	С	802	THR
2	С	808	LEU
2	С	810	HIS
2	С	815	THR
2	С	816	VAL
2	С	822	GLU
2	С	825	ASN
2	С	826	PHE
2	С	830	LEU
2	С	841	LEU
2	С	853	ARG
2	С	865	HIS
2	С	869	VAL
2	С	876	THR
2	С	882	ASP
2	С	886	ARG
2	С	898	VAL
2	С	909	THR
2	С	925	TYR
2	В	565	ILE



Mol	Chain	Res	Type
2	В	576	TRP
2	В	577	THR
2	В	585	ASN
2	В	587	THR
2	В	591	GLU
2	В	592	LEU
2	В	594	ASP
2	В	598	LEU
2	В	601	LEU
2	В	603	LEU
2	В	609	LEU
2	В	613	LYS
2	В	636	VAL
2	В	640	GLU
2	В	643	ARG
2	В	647	LEU
2	В	669	ASP
2	В	675	VAL
2	В	685	LEU
2	В	693	LEU
2	В	700	GLU
2	В	701	ARG
2	В	705	GLU
2	В	711	ASP
2	В	721	GLU
2	В	722	ARG
2	В	724	THR
2	В	725	GLN
2	В	738	ASP
2	В	740	LEU
2	В	742	MET
2	В	750	ILE
2	В	751	ILE
2	В	754	SER
2	В	764	LYS
2	В	765	GLN
2	В	775	ASN
2	В	781	LYS
2	В	792	SER
2	В	795	LEU
2	В	798	ASP
2	В	802	THR



Mol	Chain	Res	Type
2	В	808	LEU
2	В	810	HIS
2	В	815	THR
2	В	816	VAL
2	В	822	GLU
2	В	825	ASN
2	В	826	PHE
2	В	830	LEU
2	В	841	LEU
2	В	853	ARG
2	В	865	HIS
2	В	869	VAL
2	В	876	THR
2	В	882	ASP
2	В	886	ARG
2	В	898	VAL
2	В	909	THR
2	В	925	TYR
1	Н	6	THR
1	Н	18	LYS
1	Н	57	GLU
1	Н	69	TYR
1	Н	71	ILE
1	Н	78	ASN
1	Н	94	LEU
1	Н	95	ARG
1	Н	99	GLU
1	Н	101	HIS
1	Н	105	LEU
1	Н	119	MET
1	Н	120	THR
1	H	136	ILE
1	Н	151	ILE
1	H	159	VAL
1	Н	176	MET
1	Н	179	ASP
1	H	200	PHE
1	Н	202	THR
1	H	217	CYS
1	Н	277	THR
1	H	280	ASN
1	Н	288	ASP



Mol	Chain	Res	Type
1	Н	290	ARG
1	Н	292	ASP
1	Н	315	LYS
1	Н	318	THR
1	Н	326	LYS
1	Н	334	GLU
1	Н	338	SER
1	Н	339	VAL
1	Н	349	LEU
1	Н	360	GLN
1	Н	368	SER
1	Н	370	VAL
1	Н	372	ARG
1	G	6	THR
1	G	18	LYS
1	G	57	GLU
1	G	69	TYR
1	G	71	ILE
1	G	78	ASN
1	G	94	LEU
1	G	95	ARG
1	G	99	GLU
1	G	101	HIS
1	G	105	LEU
1	G	119	MET
1	G	120	THR
1	G	136	ILE
1	G	147	ARG
1	G	151	ILE
1	G	159	VAL
1	G	176	MET
1	G	179	ASP
1	G	200	PHE
1	G	202	THR
1	G	217	CYS
1	G	229	THR
1	G	277	THR
1	G	280	ASN
1	G	288	ASP
1	G	290	ARG
1	G	292	ASP
1	G	315	LYS



Mol	Chain	Res	Type
1	G	318	THR
1	G	326	LYS
1	G	334	GLU
1	G	338	SER
1	G	339	VAL
1	G	349	LEU
1	G	360	GLN
1	G	368	SER
1	G	370	VAL
1	G	372	ARG
1	F	6	THR
1	F	18	LYS
1	F	28	ARG
1	F	57	GLU
1	F	66	THR
1	F	69	TYR
1	F	71	ILE
1	F	78	ASN
1	F	94	LEU
1	F	95	ARG
1	F	99	GLU
1	F	101	HIS
1	F	105	LEU
1	F	119	MET
1	F	120	THR
1	F	136	ILE
1	F	147	ARG
1	F	151	ILE
1	F	159	VAL
1	F	176	MET
1	F	179	ASP
1	F	200	PHE
1	F	202	THR
1	F	217	CYS
1	F	229	THR
1	F	277	THR
1	F	280	ASN
1	F	288	ASP
1	F	290	ARG
1	F	292	ASP
1	F	315	LYS
1	F	318	THR



Mol	Chain	Res	Type
1	F	326	LYS
1	F	334	GLU
1	F	338	SER
1	F	339	VAL
1	F	349	LEU
1	F	351	THR
1	F	360	GLN
1	F	368	SER
1	F	370	VAL
1	F	372	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	101	HIS
1	D	137	GLN
2	А	746	GLN
2	Е	746	GLN
2	С	746	GLN
2	В	746	GLN
1	Н	101	HIS
1	G	101	HIS
1	F	101	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 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	Tuno	Chain	Dog	Link	Bo	ond leng	ths	В	ond ang	les
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	D	401	-	$3,\!3,\!3$	0.60	0	$3,\!3,\!3$	1.70	1 (33%)
3	ACT	Н	401	-	3,3,3	0.76	0	3,3,3	1.51	0
3	ACT	F	402	-	3,3,3	0.69	0	3, 3, 3	1.35	0
3	ACT	А	1001	-	3,3,3	0.76	0	$3,\!3,\!3$	0.86	0
3	ACT	F	401	-	3,3,3	0.71	0	$3,\!3,\!3$	1.41	0
3	ACT	Е	1001	-	$3,\!3,\!3$	0.80	0	$3,\!3,\!3$	1.57	1 (33%)
4	ATP	D	402	-	26,33,33	0.89	0	31,52,52	1.42	6 (19%)
3	ACT	С	1002	-	3,3,3	0.83	0	3,3,3	1.35	0
4	ATP	Н	402	-	26,33,33	1.10	3 (11%)	$31,\!52,\!52$	1.27	5 (16%)
3	ACT	G	401	-	3,3,3	0.79	0	3,3,3	1.34	0
4	ATP	F	403	-	26,33,33	0.88	1 (3%)	31,52,52	1.26	3 (9%)
3	ACT	С	1001	-	3,3,3	0.77	0	3,3,3	1.26	0
3	ACT	В	1001	-	3,3,3	0.74	0	3,3,3	1.38	0
4	ATP	G	402	-	26,33,33	0.99	1 (3%)	31,52,52	1.37	6 (19%)
3	ACT	А	1003	-	3,3,3	0.84	0	3,3,3	1.54	1 (33%)
3	ACT	А	1002	-	3,3,3	0.83	0	$3,\!3,\!3$	1.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	Н	402	-	-	4/18/38/38	0/3/3/3
4	ATP	G	402	-	-	0/18/38/38	0/3/3/3
4	ATP	F	403	-	-	0/18/38/38	0/3/3/3
4	ATP	D	402	-	-	7/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Н	402	ATP	C5-C4	2.91	1.48	1.40
4	G	402	ATP	C5-C4	2.69	1.48	1.40



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)				
4	Н	402	ATP	C2-N3	2.30	1.35	1.32				
4	F	403	ATP	C5-C4	2.14	1.46	1.40				
4	Н	402	ATP	O4'-C1'	2.09	1.44	1.41				

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	D	402	ATP	C4-C5-N7	-3.51	105.74	109.40
4	G	402	ATP	C4-C5-N7	-3.34	105.92	109.40
4	D	402	ATP	N3-C2-N1	-3.28	123.54	128.68
4	D	402	ATP	C1'-N9-C4	-3.13	121.14	126.64
4	F	403	ATP	N3-C2-N1	-2.81	124.29	128.68
4	G	402	ATP	N3-C2-N1	-2.68	124.49	128.68
4	Н	402	ATP	O3'-C3'-C2'	-2.51	103.69	111.82
4	Н	402	ATP	C2'-C3'-C4'	2.39	107.29	102.64
3	D	401	ACT	OXT-C-CH3	2.37	124.98	115.18
4	Н	402	ATP	C4-C5-N7	-2.32	106.98	109.40
4	F	403	ATP	N6-C6-N1	2.25	123.24	118.57
4	G	402	ATP	PB-O3B-PG	-2.24	125.15	132.83
4	Н	402	ATP	N3-C2-N1	-2.21	125.22	128.68
4	Н	402	ATP	C3'-C2'-C1'	2.19	104.27	100.98
4	D	402	ATP	C5-C6-N6	2.17	123.65	120.35
4	G	402	ATP	C5-C6-N6	2.17	123.65	120.35
4	D	402	ATP	C2-N1-C6	2.11	122.36	118.75
4	F	403	ATP	C4-C5-N7	-2.06	107.25	109.40
3	А	1003	ACT	OXT-C-O	-2.05	114.49	122.05
4	G	402	ATP	PA-O3A-PB	-2.03	125.88	132.83
4	G	402	ATP	C2-N1-C6	2.02	122.21	118.75
3	Е	1001	ACT	OXT-C-O	-2.02	114.60	122.05
4	D	402	ATP	C2'-C3'-C4'	2.01	106.54	102.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Н	402	ATP	C5'-O5'-PA-O1A
4	Н	402	ATP	C5'-O5'-PA-O2A
4	D	402	ATP	PG-O3B-PB-O3A
4	Н	402	ATP	C5'-O5'-PA-O3A
4	D	402	ATP	PA-O3A-PB-O1B
4	D	402	ATP	PB-O3A-PA-O2A
4	D	402	ATP	C3'-C4'-C5'-O5'



Mol	Chain	Res	Type	Atoms
4	D	402	ATP	O4'-C4'-C5'-O5'
4	Н	402	ATP	PG-O3B-PB-O3A
4	D	402	ATP	PB-O3A-PA-O1A
4	D	402	ATP	C5'-O5'-PA-O1A

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There are no ring outliers.

13 monomers are involved in 23 short contacts:

Mol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
3	D	401	ACT	2	0
3	Н	401	ACT	2	0
3	F	402	ACT	1	0
3	Ε	1001	ACT	1	0
4	D	402	ATP	5	0
3	С	1002	ACT	1	0
4	Н	402	ATP	2	0
3	G	401	ACT	2	0
4	F	403	ATP	1	0
3	С	1001	ACT	1	0
3	В	1001	ACT	2	0
4	G	402	ATP	2	0
3	А	1003	ACT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





















5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	D	356/377~(94%)	0.00	1 (0%) 94 93	58, 95, 163, 191	33~(9%)
1	F	356/377~(94%)	0.03	3 (0%) 86 85	59, 95, 164, 190	15 (4%)
1	G	356/377~(94%)	-0.14	1 (0%) 94 93	61, 97, 165, 192	33~(9%)
1	Н	356/377~(94%)	-0.03	5 (1%) 75 74	64, 97, 164, 194	28 (7%)
2	А	357/402~(88%)	-0.19	1 (0%) 94 93	64, 101, 144, 163	61 (17%)
2	В	357/402~(88%)	-0.24	0 100 100	64, 102, 144, 165	59 (16%)
2	С	357/402~(88%)	-0.16	0 100 100	65, 102, 144, 160	56 (15%)
2	Е	357/402~(88%)	-0.26	1 (0%) 94 93	65, 102, 143, 161	62 (17%)
All	All	2852/3116~(91%)	-0.12	12 (0%) 92 92	58, 99, 156, 194	347 (12%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Н	52	SER	3.6
1	F	239	SER	3.0
2	А	780	SER	2.8
1	Н	199	SER	2.8
1	Н	245	GLY	2.6
2	Е	703	PRO	2.3
1	G	53	TYR	2.3
1	D	53	TYR	2.2
1	Н	39	ARG	2.2
1	F	240	TYR	2.1
1	Н	32	PRO	2.1
1	F	241	GLU	2.1



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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ACT	F	401	4/4	0.79	0.45	88,111,123,124	0
3	ACT	С	1002	4/4	0.89	0.21	69,89,92,102	0
3	ACT	F	402	4/4	0.90	0.27	78,80,106,107	0
3	ACT	Е	1001	4/4	0.92	0.54	73,103,103,103	0
3	ACT	А	1002	4/4	0.92	0.21	80,96,99,103	0
3	ACT	С	1001	4/4	0.93	0.20	75,88,90,100	0
3	ACT	В	1001	4/4	0.93	0.17	75,94,95,97	0
3	ACT	А	1001	4/4	0.94	0.22	72,74,83,89	0
3	ACT	Н	401	4/4	0.94	0.34	70,89,100,122	0
3	ACT	А	1003	4/4	0.95	0.18	81,83,97,104	0
4	ATP	Н	402	31/31	0.95	0.17	85,109,122,133	0
4	ATP	G	402	31/31	0.96	0.19	73,104,119,122	0
3	ACT	D	401	4/4	0.97	0.26	62,66,91,110	0
3	ACT	G	401	4/4	0.97	0.26	84,88,105,122	0
4	ATP	F	403	31/31	0.97	0.18	70,91,110,116	0
4	ATP	D	402	31/31	0.98	0.21	53,86,104,106	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.

