

# Full wwPDB X-ray Structure Validation Report (i)

### Oct 16, 2023 – 12:37 AM EDT

PDB ID	:	8DBA
Title	:	Crystal structure of dodecameric KaiC
Authors	:	Padua, R.A.P.; Grant, T.; Pitsawong, W.; Hoemberger, M.S.; Otten, R.; Brad-
		shaw, N.; Grigorieff, N.; Kern, D.
Deposited on	:	2022-06-14
Resolution	:	3.50  Å(reported)

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

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

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	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 3.50 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 <sub>free</sub>	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain		
1	А	568	2% 79%	10%	11%
1	В	568	<u>2%</u> 77%	11%	11%
1	С	568	% <b>7</b> 7%	12%	• 11%
1	D	568	<sup>2%</sup> <b>7</b> 6%	13%	• 10%
1	Е	568	% 81%	9%	• 10%



Mol	Chain	Length	Quality of chain	
1	F	568	% <b>7</b> 6%	12% 12%
1	G	568	2% 80%	10% • 9%
1	Н	568	<sup>2%</sup> 79%	10% 10%
1	Ι	568	% 	11% 13%
1	J	568	3% 77%	12% • 10%
1	Κ	568	80%	9% 11%
1	L	568	76%	13% 11%



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 93625 atoms, of which 46166 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			Atom	.s			ZeroOcc	AltConf	Trace	
1	Δ	507	Total	С	Η	Ν	0	$\mathbf{S}$	0	0	0	
	A	507	7689	2443	3810	701	719	16	0	0	0	
1	P	505	Total	С	Η	Ν	0	S	0	0	0	
	D	505	7687	2435	3812	700	724	16	0	0	0	
1	С	508	Total	С	Η	Ν	0	S	0	0	0	
	U	500	7706	2442	3821	705	722	16	0	0	0	
1	Л	510	Total	С	Η	Ν	0	S	0	0	0	
	D	510	7775	2466	3859	711	723	16	0	0	0	
1	F	511	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0	
L L	Ľ	011	7778	2460	3862	706	734	16	0	0	0	0
1	Ъ	500	Total	С	Η	Ν	0	$\mathbf{S}$	0	0	0	
L	Ľ	500	7662	2421	3810	698	717	16	0	0	0	
1	C	518	Total	$\mathbf{C}$	Η	Ν	0	$\mathbf{S}$	0	0	0	
L I	G	010	7908	2513	3913	718	748	16		0	0	
1	н	509	Total	$\mathbf{C}$	Η	Ν	0	$\mathbf{S}$	0	0	0	
1	11	505	7797	2459	3887	704	731	16	0	0	0	
1	Т	494	Total	$\mathbf{C}$	Η	Ν	Ο	$\mathbf{S}$	0	0	0	
1	1	454	7514	2402	3695	690	711	16	0	0	0	
1	Т	510	Total	$\mathbf{C}$	Η	Ν	Ο	$\mathbf{S}$	0	0	0	
1	5	510	7714	2459	3812	699	728	16	0	0	0	
1	K	508	Total	$\mathbf{C}$	Η	Ν	Ο	$\mathbf{S}$	0	0	0	
	11	000	7706	2444	3822	702	722	16	0	U	0	
1	T.	503	Total	$\mathbf{C}$	Η	Ν	Ο	$\mathbf{S}$	0	0	0	
		000	7674	2444	3786	706	722	16		U		

• Molecule 1 is a protein called Circadian clock protein KaiC.

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-1	GLY	-	expression tag	UNP B9KWX8
А	0	ALA	-	expression tag	UNP B9KWX8
В	-1	GLY	-	expression tag	UNP B9KWX8
В	0	ALA	-	expression tag	UNP B9KWX8
С	-1	GLY	-	expression tag	UNP B9KWX8



8DBA
------

Chain	Residue	Modelled	Actual	Comment	Reference
С	0	ALA	-	expression tag	UNP B9KWX8
D	-1	GLY	-	expression tag	UNP B9KWX8
D	0	ALA	-	expression tag	UNP B9KWX8
Е	-1	GLY	-	expression tag	UNP B9KWX8
Е	0	ALA	-	expression tag	UNP B9KWX8
F	-1	GLY	-	expression tag	UNP B9KWX8
F	0	ALA	-	expression tag	UNP B9KWX8
G	-1	GLY	-	expression tag	UNP B9KWX8
G	0	ALA	-	expression tag	UNP B9KWX8
Н	-1	GLY	-	expression tag	UNP B9KWX8
Н	0	ALA	-	expression tag	UNP B9KWX8
Ι	-1	GLY	-	expression tag	UNP B9KWX8
Ι	0	ALA	-	expression tag	UNP B9KWX8
J	-1	GLY	-	expression tag	UNP B9KWX8
J	0	ALA	-	expression tag	UNP B9KWX8
K	-1	GLY	-	expression tag	UNP B9KWX8
K	0	ALA	-	expression tag	UNP B9KWX8
L	-1	GLY	-	expression tag	UNP B9KWX8
L	0	ALA	-	expression tag	UNP B9KWX8

• Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
2	А	1	Total 38	C 10	H 11	N 5	0 10	Р 2	0	0



Mol	Chain	Residues	0	A	Aton	ıs			ZeroOcc	AltConf
0	٨	1	Total	С	Η	Ν	Ο	Р	0	0
	А	1	39	10	12	5	10	2	0	0
0	р	1	Total	С	Η	Ν	Ο	Р	0	0
	D	1	39	10	12	5	10	2	0	0
0	D	1	Total	С	Н	Ν	Ο	Р	0	0
	D	1	39	10	12	5	10	2	0	0
0	C	1	Total	С	Η	Ν	Ο	Р	0	0
	C	1	38	10	11	5	10	2	0	0
0	С	1	Total	С	Η	Ν	Ο	Р	0	0
	C	1	39	10	12	5	10	2	0	0
0	р	1	Total	С	Η	Ν	Ο	Р	0	0
	D	1	38	10	11	5	10	2	0	0
0	Л	1	Total	С	Η	Ν	Ο	Р	0	0
	D	1	39	10	12	5	10	2	0	0
9	F	1	Total	С	Η	Ν	Ο	Р	0	0
	Ľ	1	38	10	11	5	10	2	0	0
9	F	1	Total	С	Η	Ν	Ο	Р	0	0
	Ľ	1	39	10	12	5	10	2	0	0
9	F	1	Total	С	Η	Ν	Ο	Р	0	0
	Г	1	38	10	11	5	10	2	0	0
9	F	1	Total	С	Η	Ν	Ο	Р	0	0
	Г	1	39	10	12	5	10	2	0	0
9	С	1	Total	С	Η	Ν	Ο	Р	0	0
	G	1	38	10	11	5	10	2	0	0
9	С	1	Total	С	Η	Ν	Ο	Р	0	0
2	G	T	39	10	12	5	10	2	0	0
2	н	1	Total	$\mathbf{C}$	Η	Ν	Ο	Р	0	0
	11	1	38	10	11	5	10	2	0	0
2	н	1	Total	$\mathbf{C}$	Η	Ν	Ο	Р	0	0
	11	T	39	10	12	5	10	2	0	0
2	T	1	Total	С	Η	Ν	Ο	Р	0	0
	1	1	38	10	11	5	10	2	0	0
2	T	1	Total	С	Η	Ν	Ο	Р	0	0
	-	-	39	10	12	5	10	2	Ŭ	
2	.I	1	Total	С	Η	Ν	Ο	Р	0	0
		-	38	10	11	5	10	2		
2	2 .I	1	Total	$\mathbf{C}$	Η	Ν	Ο	Р	0	0
		-	39	10	12	5	10	2		
2 K	1	Total	С	Н	Ν	0	Р	0	0	
	**	-	38	10	11	5	10	2		
2	K	1	Total	$\mathbf{C}$	Η	Ν	Ο	Р	0	0
			39	10	12	5	10	2		



$\alpha + 1$	C		
Continued	from	previous	page
	1	1	I = J

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf			
9	т	1	Total	С	Η	Ν	Ο	Р	0	0	
	L		38	10	11	5	10	2	0	0	
9	т	т	1	Total	С	Η	Ν	Ο	Р	0	0
		1	39	10	12	5	10	2	0	U	

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Mg 2 2	0	0
3	В	3	Total Mg 3 3	0	0
3	С	2	Total Mg 2 2	0	0
3	D	2	Total Mg 2 2	0	0
3	Е	2	Total Mg 2 2	0	0
3	F	1	Total Mg 1 1	0	0
3	G	3	Total Mg 3 3	0	0
3	Н	2	Total Mg 2 2	0	0
3	Ι	2	Total Mg 2 2	0	0
3	J	2	Total Mg 2 2	0	0
3	К	2	Total Mg 2 2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	5	Total O 5 5	0	0
4	В	4	Total O 4 4	0	0
4	С	7	Total O 7 7	0	0
4	D	6	Total O 6 6	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Е	6	Total O 6 6	0	0
4	F	6	Total O 6 6	0	0
4	G	5	Total O 5 5	0	0
4	Н	5	Total O 5 5	0	0
4	Ι	7	Total O 7 7	0	0
4	J	5	Total O 5 5	0	0
4	K	6	Total O 6 6	0	0
4	L	5	Total O 5 5	0	0



# 3 Residue-property plots (i)

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



• Molecule 1: Circadian clock protein KaiC









# 1.135 1.135 7.136 7.136 7.136 7.14

# 

### 

 $\bullet$  Molecule 1: Circadian clock protein KaiC





# Lead VIL V358 1132 GLY VIL V359 VIL V359 MAA VIL V356 F136 MAA SER MAA VIL V366 MAA SER MAA VIL VIL VIL VIL V366 F136 MAA SER MAA VIL VIL VIL VIL VIL VIL AA T197 VIL VIL AA T197 VIL VIL AA VIL VIL AA



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	105.11Å 136.09Å 146.20Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$93.13^{\circ}$ $94.43^{\circ}$ $108.09^{\circ}$	Depositor
Bosolution(A)	48.10 - 3.50	Depositor
Resolution (A)	48.10 - 3.50	EDS
% Data completeness	97.7 (48.10-3.50)	Depositor
(in resolution range)	97.7 (48.10-3.50)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.18 (at 3.48 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.236 , $0.279$	Depositor
$n, n_{free}$	0.238 , $0.281$	DCC
$R_{free}$ test set	1988 reflections $(2.11\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	90.8	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.33 , $72.5$	EDS
L-test for $twinning^2$	$ < L >=0.42, < L^2>=0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	93625	wwPDB-VP
Average B, all atoms $(Å^2)$	114.0	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.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

# 5.1 Standard geometry (i)

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

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

Mal	Chain	Bond	lengths	Bond angles	
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.26	0/3938	0.52	0/5312
1	В	0.26	0/3930	0.52	0/5296
1	С	0.26	0/3941	0.53	0/5312
1	D	0.26	0/3975	0.54	0/5361
1	Е	0.26	0/3976	0.52	0/5364
1	F	0.26	0/3910	0.52	0/5268
1	G	0.26	0/4057	0.52	0/5474
1	Н	0.26	0/3969	0.53	0/5352
1	Ι	0.25	0/3875	0.52	0/5219
1	J	0.25	0/3961	0.52	0/5344
1	Κ	0.26	0/3944	0.52	0/5320
1	L	0.26	0/3946	0.53	0/5316
All	All	0.26	0/47422	0.52	0/63938

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

# 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3879	3810	3876	40	0



	Chain	Non-H	$\mathbf{H}(\mathbf{model})$	H(addod)	Clashos	Symm_Clashos
1	D	2975	2010	2071	45	Symm-Clashes
	D C		20012	2071	40	0
1		2016	3850	3012	62	0
1		2016	2009	3929	45	2
	E	3910	3002	3900	40	2
1	F C	3002	3010	3001	32	0
	G	3995	3913	4002	47	0
	Н	3910	3887	3917	39	3
	l	3819	3095	3810	53	0
	J	3902	3812	3900	47	0
	K	3884	3822	3872	43	0
		3888	3786	3899	54	1
2	A	54	23	24	1	0
2	B	54	24	24	2	0
2	C	54	23	24	4	0
2	D	54	23	24	1	0
2	E	54	23	24	2	0
2	F	54	23	24	0	0
2	G	54	23	24	3	0
2	Н	54	23	24	1	0
2	Ι	54	23	24	1	0
2	J	54	23	24	0	0
2	K	54	23	24	3	0
2	L	54	23	24	2	0
3	А	2	0	0	0	0
3	В	3	0	0	0	0
3	С	2	0	0	0	0
3	D	2	0	0	0	0
3	Ε	2	0	0	0	0
3	F	1	0	0	0	0
3	G	3	0	0	0	0
3	Н	2	0	0	0	0
3	Ι	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
4	А	5	0	0	0	0
4	В	4	0	0	1	0
4	С	7	0	0	4	0
4	D	6	0	0	0	0
4	Е	6	0	0	1	0
4	F	6	0	0	1	0
4	G	5	0	0	0	0
4	Н	5	0	0	0	0



	5	1	1 5			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Ι	7	0	0	4	0
4	J	5	0	0	0	0
4	Κ	6	0	0	3	0
4	L	5	0	0	0	0
All	All	47459	46166	46993	507	4

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 5.

All (507) 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:D:520:LEU:HD11	1:K:509:ALA:CB	2.00	0.90
1:C:37:LYS:NZ	2:C:601:ADP:O2B	2.06	0.89
1:E:498:LEU:HD11	1:J:531:VAL:HG21	1.58	0.83
1:C:510:ARG:O	1:C:513:ILE:HG22	1.80	0.81
1:I:245:ARG:NH2	1:I:443:MET:SD	2.54	0.81
1:I:63:GLU:OE2	1:K:209:ARG:NH1	2.13	0.80
1:C:441:ARG:NH2	4:C:703:HOH:O	2.14	0.79
1:I:253:LEU:HD21	1:I:435:LEU:HD11	1.64	0.79
1:E:436:TYR:CE2	1:E:449:VAL:HG22	2.17	0.78
1:C:279:SER:N	4:C:702:HOH:O	2.13	0.76
2:C:604:ADP:O2B	4:C:701:HOH:O	2.04	0.76
1:J:264:ARG:O	1:J:393:THR:OG1	2.00	0.76
1:E:489:ILE:O	1:E:493:THR:HG23	1.86	0.75
1:K:38:THR:OG1	4:K:701:HOH:O	2.05	0.74
1:G:528:LYS:O	1:G:531:VAL:HG12	1.87	0.73
1:J:334:ARG:HG3	1:J:337:PHE:HB2	1.69	0.73
1:I:250:VAL:CG2	1:I:253:LEU:HD12	2.19	0.72
1:F:60:THR:HG21	1:F:68:ILE:HD11	1.71	0.72
2:K:601:ADP:O5'	4:K:702:HOH:O	2.07	0.72
1:I:250:VAL:HG21	1:I:253:LEU:HD12	1.70	0.71
1:L:38:THR:OG1	2:L:601:ADP:O2B	2.09	0.71
1:C:61:PHE:CE1	1:C:93:ILE:HD12	2.26	0.71
1:D:520:LEU:HD11	1:K:509:ALA:HB1	1.73	0.71
1:L:267:SER:OG	1:L:416:MET:SD	2.49	0.70
1:A:489:ILE:O	1:A:493:THR:HG23	1.91	0.70
1:C:489:ILE:O	1:C:493:THR:HG23	1.92	0.69
1:D:303:GLU:OE2	1:F:441:ARG:NH1	2.25	0.69
1:F:264:ARG:O	1:F:393:THR:OG1	2.10	0.69
1:D:520:LEU:HD21	1:K:509:ALA:HB2	1.74	0.69



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:69:VAL:HG22	1:G:79:LEU:HD23	1.73	0.69
1:D:489:ILE:O	1:D:493:THR:HG23	1.93	0.68
1:J:465:HIS:CD2	1:J:477:ARG:HG3	2.27	0.68
1:A:506:ARG:O	1:A:510:ARG:HG3	1.93	0.68
1:D:473:THR:OG1	1:D:476:ALA:HB3	1.94	0.68
1:K:54:GLU:OE1	1:K:126:ARG:NH2	2.27	0.67
1:E:435:LEU:HB3	1:E:461:LEU:HD21	1.75	0.67
1:K:437:LEU:HD23	1:K:445:HIS:HB2	1.76	0.67
1:A:278:LYS:NZ	2:A:604:ADP:O3B	2.20	0.67
1:F:509:ALA:CB	1:I:520:LEU:HD22	2.25	0.67
1:C:278:LYS:NZ	2:C:604:ADP:O3B	2.25	0.66
1:C:156:LEU:HD13	1:C:163:THR:HG21	1.78	0.66
1:E:38:THR:OG1	4:E:701:HOH:O	2.11	0.66
1:H:156:LEU:HD13	1:H:163:THR:HG21	1.78	0.66
1:E:278:LYS:NZ	2:E:604:ADP:O3B	2.27	0.66
1:G:267:SER:OG	1:G:416:MET:SD	2.53	0.66
1:G:504:GLN:O	1:G:507:ARG:HG2	1.96	0.66
1:D:385:ASP:O	1:D:389:ASN:ND2	2.23	0.65
1:F:525:ILE:HD11	1:G:501:GLN:HB2	1.77	0.65
1:I:250:VAL:CB	1:I:253:LEU:HD12	2.27	0.65
1:I:38:THR:OG1	4:I:701:HOH:O	2.14	0.65
1:I:90:ILE:O	1:I:90:ILE:HD12	1.97	0.65
1:G:436:TYR:HE1	1:G:438:LEU:HB3	1.62	0.64
1:E:139:PHE:HB2	1:E:144:ILE:HD11	1.78	0.64
1:J:521:GLN:OE1	1:J:521:GLN:N	2.31	0.64
1:D:278:LYS:NZ	2:D:604:ADP:O3B	2.30	0.64
1:G:435:LEU:HD23	1:G:436:TYR:N	2.13	0.64
1:F:284:HIS:HD2	1:F:317:LEU:HD11	1.62	0.63
1:L:471:ALA:O	1:L:473:THR:N	2.32	0.63
1:E:507:ARG:HD2	1:K:518:ALA:HB2	1.80	0.63
1:A:521:GLN:O	1:A:525:ILE:HG23	1.99	0.63
1:B:278:LYS:NZ	2:B:604:ADP:O1B	2.20	0.63
1:E:513:ILE:CG1	1:J:516:LEU:HD21	2.29	0.63
1:F:131:THR:O	1:F:131:THR:HG22	1.99	0.63
1:I:250:VAL:HB	1:I:253:LEU:HD12	1.80	0.62
1:C:431:PHE:HD1	1:E:436:TYR:HH	1.47	0.62
1:K:279:SER:OG	2:K:604:ADP:O1A	2.16	0.62
1:D:525:ILE:HD11	1:I:501:GLN:HB2	1.81	0.62
1:B:93:ILE:HD11	1:B:111:LEU:HD13	1.82	0.62
1:K:16:LEU:HD21	1:K:232:VAL:HG21	1.82	0.61
1:H:57:VAL:HG22	1:H:89:ALA:HB3	1.83	0.61



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:L:208:TYR:CD1	1:L:211:THR:HG22	2.35	0.61
1:I:306:ASP:HB2	1:K:241:VAL:HG21	1.82	0.61
1:C:513:ILE:HG13	1:L:513:ILE:HG12	1.83	0.61
1:E:194:VAL:HG22	1:E:199:SER:HB3	1.81	0.61
1:F:511:ALA:HB1	1:G:511:ALA:O	2.00	0.61
1:F:284:HIS:CD2	1:F:317:LEU:HD11	2.36	0.60
1:C:278:LYS:N	4:C:702:HOH:O	2.34	0.60
1:A:445:HIS:ND1	2:B:604:ADP:O2'	2.35	0.60
1:E:513:ILE:HG13	1:J:516:LEU:HD21	1.83	0.60
1:G:98:SER:OG	1:G:100:VAL:HG13	2.01	0.60
1:I:136:PHE:CE2	1:I:149:ILE:HD13	2.37	0.59
1:F:45:LEU:O	1:F:49:VAL:HG13	2.02	0.59
1:J:315:LEU:HD23	1:J:315:LEU:O	2.02	0.59
1:L:522:ALA:O	1:L:525:ILE:HG13	2.03	0.59
1:E:399:LEU:HD23	1:E:400:ALA:N	2.18	0.59
1:F:12:GLY:O	1:F:16:LEU:HD13	2.02	0.59
1:H:49:VAL:HG22	1:H:55:PRO:HA	1.85	0.59
1:F:451:GLU:HG2	1:F:473:THR:HB	1.84	0.58
1:D:521:GLN:O	1:D:525:ILE:HG23	2.03	0.58
1:D:525:ILE:HG21	1:I:500:GLN:NE2	2.17	0.58
1:G:465:HIS:NE2	1:G:472:LEU:HD13	2.18	0.58
1:K:287:ALA:CB	1:K:317:LEU:HD11	2.34	0.58
1:D:520:LEU:HD11	1:K:509:ALA:HB3	1.86	0.58
1:D:302:GLU:OE1	1:F:414:SER:OG	2.20	0.58
1:C:295:ARG:O	1:C:357:SER:OG	2.21	0.58
1:A:524:GLU:HG2	1:H:502:ILE:HG23	1.84	0.58
1:F:49:VAL:HG12	1:F:55:PRO:HA	1.85	0.58
1:B:364:ILE:O	1:B:368:THR:HG23	2.03	0.58
1:L:420:VAL:HG22	1:L:437:LEU:CD1	2.34	0.57
1:H:435:LEU:HD13	1:H:461:LEU:HD21	1.85	0.57
1:J:480:GLU:OE1	1:J:483:ARG:NH2	2.37	0.57
1:A:520:LEU:HD12	1:H:509:ALA:HB3	1.87	0.57
1:E:364:ILE:HD11	1:E:412:LEU:HD21	1.86	0.57
1:G:494:GLU:O	1:G:497:ARG:HG2	2.05	0.57
1:D:472:LEU:HD13	1:D:477:ARG:HD3	1.87	0.57
1:I:49:VAL:HG22	1:I:55:PRO:HA	1.85	0.57
1:F:358:VAL:HG22	1:F:393:THR:HB	1.87	0.57
1:A:474:GLY:O	1:A:476:ALA:N	2.38	0.56
1:F:381:LEU:HD21	1:F:415:LEU:HD23	1.86	0.56
1:G:118:ALA:O	1:G:122:VAL:HG22	2.04	0.56
1:B:112:PHE:HE1	1:B:155:TRP:CD2	2.23	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:95:VAL:HG23	1:G:95:VAL:O	2.05	0.56
1:C:61:PHE:HE1	1:C:93:ILE:HD12	1.68	0.56
1:H:39:LEU:HD11	2:H:601:ADP:O4'	2.05	0.56
1:J:141:ASN:HA	1:J:144:ILE:HG22	1.88	0.56
1:I:36:GLY:N	2:I:601:ADP:O2B	2.38	0.56
1:L:119:ILE:HD13	1:L:161:LEU:HD11	1.87	0.55
1:A:464:PRO:HB2	1:A:471:ALA:HB1	1.88	0.55
1:C:194:VAL:HG13	1:C:194:VAL:O	2.05	0.55
1:A:332:ALA:HB3	1:C:238:LEU:HD21	1.88	0.55
1:B:256:MET:HB3	1:B:437:LEU:HD12	1.89	0.55
1:A:525:ILE:HD11	1:L:501:GLN:CB	2.37	0.55
1:F:465:HIS:CG	1:F:465:HIS:O	2.59	0.55
4:I:702:HOH:O	1:K:209:ARG:HD3	2.06	0.55
1:B:93:ILE:CD1	1:B:111:LEU:HD22	2.37	0.55
1:K:347:ILE:O	1:K:351:VAL:HG23	2.07	0.54
1:B:111:LEU:HD23	1:B:114:ARG:NH2	2.21	0.54
1:H:361:LEU:HD12	1:H:396:PHE:CE2	2.42	0.54
1:H:39:LEU:O	1:H:43:THR:HG23	2.07	0.54
1:F:62:GLU:HB2	1:F:131:THR:HG21	1.89	0.54
1:E:436:TYR:HE2	1:E:449:VAL:HG22	1.71	0.54
1:B:209:ARG:HD2	4:F:706:HOH:O	2.07	0.54
1:D:414:SER:HB3	1:E:399:LEU:HD12	1.89	0.54
1:D:221:LEU:HG	1:D:230:LEU:HD21	1.90	0.54
1:F:58:PHE:CE2	1:F:128:VAL:HG11	2.43	0.54
1:J:48:GLY:O	1:J:54:GLU:N	2.37	0.54
1:L:521:GLN:O	1:L:525:ILE:HG23	2.08	0.54
1:G:122:VAL:HG23	1:G:124:ALA:HB2	1.90	0.54
1:C:471:ALA:O	1:C:473:THR:N	2.41	0.53
1:D:122:VAL:HG23	1:D:124:ALA:HB2	1.89	0.53
1:G:438:LEU:HD23	1:G:438:LEU:H	1.73	0.53
1:J:298:TYR:CE1	1:J:360:VAL:HG11	2.42	0.53
1:A:497:ARG:HG3	1:L:529:ALA:HB2	1.91	0.53
1:G:432:ASN:ND2	1:G:473:THR:O	2.42	0.53
1:B:498:LEU:HD11	1:G:531:VAL:HB	1.89	0.53
1:C:427:VAL:O	1:C:427:VAL:HG13	2.09	0.53
1:J:500:GLN:O	1:J:504:GLN:HG2	2.08	0.53
1:E:32:SER:O	1:E:37:LYS:NZ	2.35	0.53
1:B:465:HIS:CG	1:B:465:HIS:O	2.62	0.52
1:I:421:LEU:CB	1:I:438:LEU:HD13	2.39	0.52
1:B:433:ARG:NH1	1:B:454:MET:SD	2.82	0.52
1:J:328:LEU:HD23	1:J:329:ARG:N	2.24	0.52



	to as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:472:LEU:HD23	1:F:476:ALA:O	2.08	0.52
1:I:250:VAL:HG22	1:I:459:ILE:HG21	1.92	0.52
1:L:238:LEU:O	1:L:389:ASN:ND2	2.41	0.52
1:L:264:ARG:HG3	1:L:265:GLY:N	2.24	0.52
1:D:427:VAL:HG23	1:D:428:ASN:H	1.75	0.52
1:E:169:ARG:CZ	1:E:189:LEU:HD11	2.39	0.52
1:G:237:LEU:HD21	1:H:334:ARG:HG2	1.92	0.52
1:D:473:THR:O	1:D:476:ALA:N	2.43	0.52
1:E:497:ARG:HG3	1:K:529:ALA:HB2	1.92	0.52
1:I:136:PHE:HE2	1:I:149:ILE:HD13	1.75	0.52
1:I:250:VAL:HB	1:I:253:LEU:HB2	1.92	0.52
1:B:131:THR:HG22	1:B:131:THR:O	2.09	0.51
1:F:60:THR:CG2	1:F:68:ILE:HD11	2.38	0.51
1:H:241:VAL:HG13	1:H:241:VAL:O	2.09	0.51
1:A:525:ILE:HD11	1:L:501:GLN:HB2	1.91	0.51
1:H:436:TYR:CE2	1:H:449:VAL:HG22	2.46	0.51
1:J:328:LEU:HD22	1:J:330:PHE:CE1	2.45	0.51
1:C:16:LEU:HD13	1:C:218:TYR:CD2	2.45	0.51
1:I:109:GLU:O	1:I:112:PHE:HB2	2.10	0.51
1:A:307:GLN:HA	1:C:241:VAL:HG11	1.93	0.51
1:G:421:LEU:HD23	1:G:436:TYR:CE2	2.45	0.51
1:G:471:ALA:O	1:G:473:THR:N	2.43	0.51
1:K:16:LEU:HD22	1:K:218:TYR:CZ	2.46	0.51
1:B:58:PHE:CE2	1:B:128:VAL:HG11	2.45	0.51
1:C:93:ILE:HG22	1:C:93:ILE:O	2.10	0.51
1:G:89:ALA:HB2	1:G:122:VAL:HG11	1.92	0.51
1:I:71:ASN:OD1	1:K:209:ARG:HG3	2.11	0.51
1:E:248:SER:OG	1:E:254:ASP:OD1	2.25	0.51
1:I:122:VAL:HG12	1:I:122:VAL:O	2.11	0.51
1:J:364:ILE:O	1:J:368:THR:HG23	2.10	0.51
1:K:36:GLY:N	4:K:702:HOH:O	2.44	0.51
1:D:95:VAL:HG11	1:D:102:GLU:HG3	1.93	0.50
1:E:335:PRO:HG2	1:E:366:ALA:HB1	1.93	0.50
1:A:468:GLU:O	1:A:470:GLY:N	2.43	0.50
1:B:275:GLY:O	1:B:433:ARG:NH2	2.44	0.50
1:J:58:PHE:CE2	1:J:128:VAL:HG11	2.46	0.50
1:L:242:HIS:CB	1:L:264:ARG:HG2	2.42	0.50
1:F:473:THR:HA	1:F:477:ARG:HD3	1.93	0.50
1:K:194:VAL:HG23	1:K:194:VAL:O	2.11	0.50
1:L:420:VAL:HG22	1:L:437:LEU:HD12	1.93	0.50
1:D:273:VAL:HG22	1:D:274:ALA:H	1.77	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:J:29:VAL:HG21	1:J:40:PHE:CD2	2.46	0.50
1:L:49:VAL:HG21	1:L:87:LYS:HB3	1.94	0.50
1:J:517:GLU:O	1:J:521:GLN:OE1	2.30	0.50
1:C:144:ILE:HG23	1:C:145:LEU:N	2.27	0.50
1:C:451:GLU:O	1:C:461:LEU:HA	2.12	0.50
1:F:89:ALA:HB2	1:F:122:VAL:HG11	1.94	0.50
1:L:342:MET:O	1:L:346:VAL:HG23	2.11	0.50
1:I:80:ASP:OD1	1:I:80:ASP:N	2.45	0.50
1:B:524:GLU:OE2	1:G:506:ARG:NE	2.45	0.49
1:E:513:ILE:HG13	1:J:516:LEU:HD11	1.94	0.49
1:E:513:ILE:HG12	1:J:516:LEU:HD21	1.93	0.49
1:F:525:ILE:HD11	1:G:501:GLN:CB	2.42	0.49
1:A:307:GLN:CA	1:C:241:VAL:HG11	2.42	0.49
1:A:80:ASP:OD1	1:A:80:ASP:N	2.44	0.49
1:G:29:VAL:HG21	1:G:40:PHE:CD2	2.48	0.49
1:G:474:GLY:H	1:G:477:ARG:HB2	1.77	0.49
1:B:264:ARG:O	1:B:393:THR:OG1	2.24	0.49
1:I:421:LEU:HB2	1:I:438:LEU:HD13	1.94	0.49
1:A:501:GLN:HG3	1:L:525:ILE:HD11	1.94	0.49
1:K:497:ARG:HE	1:K:497:ARG:N	2.10	0.49
1:L:56:GLY:CA	1:L:126:ARG:O	2.60	0.49
1:A:509:ALA:HB3	1:H:520:LEU:HD12	1.93	0.49
1:E:465:HIS:NE2	1:E:472:LEU:HD22	2.28	0.49
1:F:511:ALA:HB3	1:G:515:ALA:HB2	1.95	0.49
1:H:295:ARG:HG2	1:H:354:PHE:CZ	2.47	0.49
1:F:522:ALA:O	1:F:525:ILE:HG12	2.13	0.49
1:H:295:ARG:CG	1:H:354:PHE:CZ	2.96	0.49
1:I:307:GLN:HG3	1:K:241:VAL:HG22	1.94	0.49
1:B:109:GLU:HA	1:B:112:PHE:HB2	1.94	0.48
1:C:497:ARG:NH1	1:J:529:ALA:HB1	2.27	0.48
1:G:72:VAL:HG21	1:G:79:LEU:HD22	1.95	0.48
1:F:449:VAL:HG22	1:F:450:ARG:N	2.29	0.48
1:D:473:THR:O	1:D:474:GLY:C	2.52	0.48
1:E:520:LEU:HD13	1:J:509:ALA:HB2	1.95	0.48
1:J:45:LEU:HD21	1:J:88:ILE:HD11	1.95	0.48
1:J:287:ALA:CB	1:J:317:LEU:HD11	2.42	0.48
1:I:472:LEU:HD23	1:I:476:ALA:O	2.14	0.48
1:H:489:ILE:O	1:H:493:THR:HG23	2.13	0.48
1:J:203:LEU:HD12	1:J:203:LEU:C	2.34	0.48
1:B:362:ASP:HA	1:B:397:THR:OG1	2.14	0.48
1:G:520:LEU:HD21	1:G:524:GLU:OE2	2.13	0.48



Interatomic Clash			
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:K:387:LEU:HD23	1:K:392:ILE:HD11	1.95	0.48
1:B:472:LEU:HD23	1:B:476:ALA:O	2.13	0.48
1:D:296:ALA:HB3	1:D:328:LEU:CD2	2.44	0.48
1:D:310:ARG:HD3	1:F:241:VAL:CG1	2.44	0.48
1:H:235:LEU:HD13	1:H:389:ASN:OD1	2.14	0.48
1:L:480:GLU:O	1:L:484:LEU:HD23	2.13	0.48
1:K:37:LYS:N	2:K:601:ADP:O1B	2.46	0.48
1:D:220:PHE:HA	1:D:230:LEU:HD22	1.96	0.48
1:G:465:HIS:CG	1:G:465:HIS:O	2.67	0.48
4:I:702:HOH:O	1:K:209:ARG:NH1	2.45	0.48
1:J:235:LEU:O	1:J:389:ASN:ND2	2.47	0.48
1:G:49:VAL:HG22	1:G:55:PRO:HA	1.96	0.47
1:I:209:ARG:NH2	4:I:704:HOH:O	2.47	0.47
1:L:136:PHE:CZ	1:L:149:ILE:HD11	2.50	0.47
1:D:525:ILE:C	1:D:525:ILE:HD12	2.34	0.47
1:E:513:ILE:HD11	1:J:516:LEU:HD11	1.97	0.47
1:I:298:TYR:CE2	1:I:360:VAL:HG11	2.49	0.47
1:A:385:ASP:OD1	1:B:334:ARG:NH2	2.47	0.47
1:B:498:LEU:CD1	1:G:531:VAL:HB	2.45	0.47
1:E:513:ILE:CD1	1:J:516:LEU:HD11	2.44	0.47
1:F:437:LEU:HD23	1:F:445:HIS:CG	2.49	0.47
1:I:471:ALA:O	1:I:473:THR:N	2.48	0.47
1:J:69:VAL:HA	1:J:79:LEU:HD23	1.96	0.47
1:J:420:VAL:HG22	1:J:437:LEU:HD23	1.96	0.47
1:L:60:THR:HG23	1:L:60:THR:O	2.15	0.47
1:D:194:VAL:HG23	1:D:194:VAL:O	2.14	0.47
1:E:465:HIS:CG	1:E:465:HIS:O	2.68	0.47
1:G:75:LEU:HD21	2:G:601:ADP:C6	2.50	0.47
1:I:86:GLU:O	1:I:122:VAL:HG13	2.15	0.47
1:B:414:SER:O	1:B:441:ARG:NH2	2.48	0.47
1:K:471:ALA:O	1:K:473:THR:N	2.47	0.47
1:L:185:ASP:HA	1:L:209:ARG:HH11	1.79	0.47
1:D:62:GLU:HB2	1:D:131:THR:HG21	1.97	0.46
1:F:28:LEU:HD21	1:F:180:GLU:HG2	1.97	0.46
1:J:471:ALA:O	1:J:473:THR:N	2.48	0.46
1:C:61:PHE:HD1	1:C:93:ILE:HB	1.79	0.46
1:D:269:LEU:HD12	1:D:396:PHE:O	2.15	0.46
1:A:127:VAL:HG12	1:A:162:THR:O	2.15	0.46
1:K:69:VAL:O	1:K:73:ALA:HB2	2.14	0.46
1:L:22:PRO:O	1:L:162:THR:HG23	2.16	0.46
1:B:465:HIS:NE2	1:B:472:LEU:HD22	2.31	0.46



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:222:ILE:HG21	2:C:601:ADP:H1'	1.98	0.46
1:C:246:ILE:CD1	1:C:393:THR:HG21	2.46	0.46
1:F:183:VAL:HG12	1:F:183:VAL:O	2.16	0.46
1:G:279:SER:OG	2:G:604:ADP:O2A	2.31	0.46
1:I:62:GLU:HB2	1:I:131:THR:HG21	1.97	0.46
1:D:208:TYR:CD1	1:D:211:THR:HG22	2.50	0.46
1:F:16:LEU:HD21	1:F:218:TYR:CG	2.50	0.46
2:G:604:ADP:C6	1:I:444:ALA:HB2	2.51	0.46
1:L:437:LEU:HD23	1:L:445:HIS:HB2	1.98	0.46
1:C:513:ILE:HD11	1:L:513:ILE:HG21	1.98	0.46
1:F:351:VAL:HG11	1:F:386:PHE:CE2	2.50	0.46
1:J:71:ASN:ND2	1:L:209:ARG:HB3	2.31	0.46
1:D:95:VAL:HG11	1:D:102:GLU:CG	2.45	0.46
1:D:472:LEU:HD12	1:D:473:THR:N	2.30	0.46
1:L:57:VAL:HG23	1:L:124:ALA:HB2	1.98	0.46
1:C:298:TYR:CE2	1:C:360:VAL:HG11	2.51	0.46
1:E:372:ASP:O	1:E:376:VAL:HG23	2.16	0.46
1:K:185:ASP:OD1	1:K:209:ARG:HD2	2.16	0.46
1:D:16:LEU:HD13	1:D:218:TYR:CD2	2.50	0.46
1:E:471:ALA:O	1:E:473:THR:N	2.49	0.46
1:E:472:LEU:HD23	1:E:476:ALA:O	2.15	0.46
1:B:420:VAL:HG22	1:B:437:LEU:HD23	1.98	0.45
1:F:45:LEU:HD11	1:F:56:GLY:HA3	1.98	0.45
1:J:10:ILE:O	1:J:12:GLY:N	2.49	0.45
1:D:96:ASP:OD1	1:D:96:ASP:N	2.39	0.45
1:F:460:SER:C	1:F:461:LEU:HD12	2.36	0.45
1:H:364:ILE:HG21	1:H:396:PHE:HD2	1.81	0.45
1:I:436:TYR:CE2	1:I:438:LEU:HD11	2.51	0.45
1:F:465:HIS:CE1	1:F:472:LEU:HD13	2.51	0.45
1:G:482:ALA:O	1:G:486:ARG:HG3	2.16	0.45
1:D:511:ALA:O	1:I:511:ALA:HB1	2.16	0.45
1:G:474:GLY:O	1:G:477:ARG:N	2.48	0.45
1:D:7:PRO:0	1:D:126:ARG:NH2	2.49	0.45
1:H:471:ALA:O	1:H:473:THR:N	2.49	0.45
1:I:437:LEU:HD13	1:I:445:HIS:HB2	1.99	0.45
1:E:472:LEU:N	1:E:472:LEU:HD12	2.32	0.45
1:A:414:SER:CB	1:B:399:LEU:HD11	2.46	0.45
1:C:435:LEU:HD12	1:C:435:LEU:C	2.37	0.45
1:D:381:LEU:HD22	1:E:334:ARG:HD3	1.98	0.45
1:I:58:PHE:CE2	1:I:128:VAL:HG11	2.52	0.45
1:L:56:GLY:HA2	1:L:126:ARG:O	2.16	0.45



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:394:GLY:C	1:A:395:ILE:HD12	2.37	0.45
1:C:133:GLU:OE1	1:C:177:GLN:NE2	2.50	0.45
1:D:95:VAL:HG21	1:D:138:ALA:HB1	1.99	0.45
1:G:419:TRP:CH2	1:G:438:LEU:HD11	2.52	0.45
1:L:57:VAL:HG22	1:L:89:ALA:HB3	1.99	0.45
1:D:451:GLU:HB2	1:D:472:LEU:HG	1.99	0.45
1:H:252:ASP:HB2	1:H:461:LEU:HB2	1.99	0.45
1:L:335:PRO:CG	1:L:366:ALA:HB1	2.47	0.45
1:B:420:VAL:HG22	1:B:437:LEU:CD2	2.47	0.44
1:I:306:ASP:CB	1:K:241:VAL:HG21	2.46	0.44
1:L:520:LEU:HD21	1:L:524:GLU:OE2	2.18	0.44
1:A:271:SER:OG	1:A:419:TRP:NE1	2.49	0.44
1:C:49:VAL:HG22	1:C:55:PRO:HA	1.98	0.44
1:D:508:ARG:HB2	1:I:518:ALA:HB3	1.99	0.44
1:F:3:ILE:HD11	1:F:211:THR:HB	1.98	0.44
1:F:364:ILE:HG21	1:F:396:PHE:HD2	1.81	0.44
1:L:144:ILE:O	1:L:148:GLU:HG3	2.17	0.44
1:D:232:VAL:O	1:D:235:LEU:HD22	2.17	0.44
1:H:57:VAL:HG23	1:H:124:ALA:HB2	1.99	0.44
1:D:305:ALA:O	1:D:309:VAL:HG23	2.17	0.44
1:G:421:LEU:HD23	1:G:436:TYR:CZ	2.52	0.44
1:J:307:GLN:OE1	1:J:310:ARG:NH1	2.50	0.44
1:D:12:GLY:O	1:D:16:LEU:HG	2.18	0.44
1:D:132:ILE:HG12	1:D:136:PHE:CZ	2.52	0.44
1:E:49:VAL:HG22	1:E:55:PRO:HA	1.99	0.44
1:E:93:ILE:HD12	1:E:111:LEU:HD22	1.98	0.44
1:H:230:LEU:O	1:H:232:VAL:N	2.50	0.44
1:J:362:ASP:O	1:J:363:PRO:C	2.55	0.44
1:F:509:ALA:HB3	1:I:520:LEU:HD22	1.98	0.44
1:J:208:TYR:CD1	1:J:211:THR:HG22	2.52	0.44
1:B:28:LEU:HD11	1:B:167:ALA:HB2	2.00	0.44
1:G:54:GLU:OE1	1:G:126:ARG:NE	2.51	0.44
1:B:191:ASP:OD2	1:B:202:ARG:NH2	2.44	0.44
1:C:472:LEU:HD23	1:C:476:ALA:O	2.17	0.44
1:C:513:ILE:HD11	1:L:513:ILE:CG2	2.47	0.44
1:E:335:PRO:CG	1:E:366:ALA:HB1	2.48	0.44
1:F:127:VAL:HB	1:F:163:THR:HG22	2.00	0.44
1:J:465:HIS:CG	1:J:465:HIS:O	2.71	0.44
1:E:440:ALA:O	1:E:442:GLY:N	2.50	0.44
1:E:498:LEU:HD21	1:J:531:VAL:HG21	1.99	0.44
1:L:335:PRO:HG3	1:L:366:ALA:HB1	2.00	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:154:ASP:O	1:B:158:GLU:HG3	2.18	0.43
1:B:279:SER:OG	4:B:701:HOH:O	2.19	0.43
1:C:230:LEU:HD11	1:C:345:ALA:HA	2.00	0.43
1:D:304:ALA:HB1	1:F:238:LEU:HD12	2.00	0.43
1:F:452:PHE:CZ	1:F:459:ILE:HD11	2.53	0.43
1:F:472:LEU:HD12	1:F:472:LEU:N	2.32	0.43
1:K:340:LEU:HD11	1:K:371:GLY:HA3	1.99	0.43
1:B:409:ASP:OD1	1:B:409:ASP:O	2.36	0.43
1:K:452:PHE:CZ	1:K:459:ILE:HD12	2.53	0.43
1:A:498:LEU:HD21	1:H:527:LEU:HB3	2.01	0.43
1:A:520:LEU:HD21	1:A:524:GLU:OE2	2.19	0.43
1:C:431:PHE:CD1	1:E:436:TYR:CE1	3.06	0.43
1:C:520:LEU:HD21	1:L:506:ARG:HG2	2.00	0.43
1:F:298:TYR:CE2	1:F:360:VAL:HG11	2.53	0.43
1:B:506:ARG:HA	1:G:520:LEU:HD11	1.99	0.43
1:C:145:LEU:HG	1:C:149:ILE:HD11	2.01	0.43
1:F:471:ALA:O	1:F:472:LEU:HB2	2.18	0.43
1:J:362:ASP:HB3	1:J:363:PRO:HD2	2.01	0.43
1:L:168:GLU:OE1	1:L:168:GLU:HA	2.18	0.43
1:G:194:VAL:HG23	1:G:194:VAL:O	2.18	0.43
1:H:57:VAL:HG23	1:H:124:ALA:CB	2.48	0.43
1:C:506:ARG:HG2	1:L:520:LEU:HD11	2.01	0.43
1:F:61:PHE:CE1	1:F:135:LEU:HD22	2.52	0.43
1:G:338:TYR:HB3	1:G:342:MET:HB2	2.00	0.43
1:I:257:MET:HB3	1:I:443:MET:SD	2.59	0.43
1:J:175:THR:HG21	1:J:180:GLU:OE1	2.19	0.43
1:B:22:PRO:O	1:B:162:THR:HG23	2.19	0.43
1:C:254:ASP:OD1	1:C:254:ASP:C	2.57	0.43
1:D:81:LYS:O	1:D:85:GLU:HG2	2.19	0.43
1:D:203:LEU:HD23	1:D:218:TYR:O	2.18	0.43
1:C:411:GLY:O	1:C:415:LEU:HG	2.18	0.43
1:L:74:SER:OG	2:L:601:ADP:N6	2.52	0.43
1:A:436:TYR:CZ	1:A:449:VAL:HB	2.54	0.43
1:C:362:ASP:HA	1:C:397:THR:OG1	2.18	0.43
1:C:465:HIS:O	1:C:465:HIS:CG	2.72	0.43
1:D:49:VAL:HG22	1:D:55:PRO:HA	2.00	0.43
1:A:213:HIS:CE1	1:A:215:THR:HG22	2.53	0.43
1:H:215:THR:OG1	1:L:192:HIS:NE2	2.49	0.43
1:E:75:LEU:HD21	2:E:601:ADP:C6	2.54	0.42
1:G:15:GLU:HB3	1:G:232:VAL:HG23	2.01	0.42
1:A:451:GLU:HG2	1:A:462:LEU:HB2	2.01	0.42



	jageni	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:16:LEU:HD13	1:B:218:TYR:CD2	2.54	0.42
1:E:45:LEU:HD11	1:E:128:VAL:HB	2.01	0.42
1:L:347:ILE:O	1:L:351:VAL:HG23	2.19	0.42
1:E:464:PRO:CB	1:E:471:ALA:HB1	2.49	0.42
1:K:417:ASP:HA	1:K:441:ARG:HE	1.84	0.42
1:C:58:PHE:CE2	1:C:128:VAL:HG11	2.55	0.42
1:A:127:VAL:HG11	1:A:156:LEU:HD22	2.01	0.42
1:B:372:ASP:O	1:B:376:VAL:HG23	2.19	0.42
1:B:490:GLU:O	1:B:494:GLU:OE1	2.37	0.42
1:C:513:ILE:CD1	1:L:513:ILE:HG23	2.50	0.42
1:H:297:MET:HG3	1:H:354:PHE:CD2	2.55	0.42
1:C:65:PRO:HB3	1:C:90:ILE:HD12	2.02	0.42
1:D:506:ARG:HG2	1:K:520:LEU:HD21	2.00	0.42
1:J:465:HIS:NE2	1:J:472:LEU:HD13	2.35	0.42
1:K:183:VAL:HG12	1:K:183:VAL:O	2.19	0.42
1:K:505:ARG:O	1:K:508:ARG:HG2	2.20	0.42
1:L:132:ILE:O	1:L:132:ILE:HG22	2.20	0.42
1:A:501:GLN:HB2	1:L:525:ILE:HD11	2.00	0.42
1:I:253:LEU:HG	1:I:461:LEU:CD1	2.49	0.42
1:D:381:LEU:HD22	1:E:334:ARG:HH11	1.85	0.42
1:G:103:ILE:HB	1:G:138:ALA:HB2	2.02	0.42
1:H:472:LEU:N	1:H:472:LEU:HD12	2.35	0.42
1:A:183:VAL:HG12	1:A:183:VAL:O	2.19	0.42
1:C:77:PHE:CD1	1:C:77:PHE:N	2.86	0.42
1:D:61:PHE:CD2	1:D:93:ILE:HG23	2.55	0.42
1:D:522:ALA:O	1:D:525:ILE:HG13	2.20	0.42
1:F:344:LEU:HD13	1:F:383:ILE:HG13	2.02	0.41
1:H:156:LEU:HD13	1:H:163:THR:CG2	2.48	0.41
1:H:329:ARG:HG2	1:H:354:PHE:CE1	2.55	0.41
1:H:512:GLN:O	1:H:516:LEU:HG	2.19	0.41
1:L:59:VAL:HB	1:L:129:LEU:HD23	2.01	0.41
1:A:381:LEU:HD22	1:B:334:ARG:HD2	2.02	0.41
1:F:506:ARG:HG2	1:I:520:LEU:HD21	2.02	0.41
1:G:417:ASP:OD1	1:G:417:ASP:N	2.51	0.41
1:H:231:PRO:HB2	1:H:234:ALA:HB2	2.01	0.41
1:H:329:ARG:HG3	1:H:354:PHE:CD1	2.55	0.41
1:H:364:ILE:HG21	1:H:396:PHE:CD2	2.55	0.41
1:K:360:VAL:O	1:K:361:LEU:HD12	2.19	0.41
1:L:242:HIS:HB2	1:L:264:ARG:HG2	2.02	0.41
1:L:358:VAL:HG22	1:L:393:THR:HB	2.02	0.41
1:A:28:LEU:HD11	1:A:167:ALA:HB2	2.02	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:283:ALA:HB1	1:B:319:LEU:HD11	2.00	0.41
1:D:16:LEU:HD22	1:D:218:TYR:CZ	2.55	0.41
1:K:449:VAL:HG22	1:K:450:ARG:N	2.35	0.41
1:L:362:ASP:HA	1:L:363:PRO:HA	1.95	0.41
1:A:133:GLU:O	1:A:134:SER:C	2.58	0.41
1:B:335:PRO:HG2	1:B:366:ALA:HB1	2.01	0.41
1:D:516:LEU:O	1:D:520:LEU:HG	2.21	0.41
1:J:132:ILE:HG21	1:J:165:ILE:HD11	2.01	0.41
1:K:16:LEU:HD22	1:K:218:TYR:CE2	2.54	0.41
1:B:8:THR:HG21	1:B:13:PHE:CE2	2.56	0.41
1:I:317:LEU:HD23	1:I:318:ASP:N	2.35	0.41
1:F:229:VAL:HG12	1:F:230:LEU:N	2.36	0.41
1:F:509:ALA:HB2	1:I:520:LEU:HD22	2.00	0.41
1:G:103:ILE:HG22	1:G:104:GLY:N	2.35	0.41
1:K:480:GLU:O	1:K:484:LEU:HD13	2.21	0.41
1:L:525:ILE:C	1:L:525:ILE:HD12	2.41	0.41
1:C:254:ASP:OD1	1:C:255:ALA:N	2.53	0.41
1:L:108:LEU:HD11	1:L:148:GLU:HG2	2.02	0.41
1:A:208:TYR:CD1	1:A:211:THR:HG22	2.56	0.41
1:D:273:VAL:HG13	1:D:274:ALA:N	2.36	0.41
1:D:319:LEU:HD13	1:D:330:PHE:HZ	1.85	0.41
1:D:436:TYR:CZ	1:D:449:VAL:HG22	2.56	0.41
1:H:58:PHE:CE2	1:H:128:VAL:HG11	2.56	0.41
1:A:12:GLY:O	1:A:16:LEU:HG	2.20	0.41
1:A:241:VAL:HG21	1:B:306:ASP:HB2	2.02	0.41
1:C:79:LEU:HD12	1:C:88:ILE:HG21	2.02	0.41
1:E:252:ASP:HB2	1:E:461:LEU:HB2	2.02	0.41
1:H:299:PHE:HB2	1:H:361:LEU:HD23	2.02	0.41
1:I:55:PRO:HB2	1:I:124:ALA:HA	2.02	0.41
1:J:365:SER:O	1:J:369:GLU:HG3	2.21	0.41
1:K:231:PRO:C	1:K:232:VAL:HG23	2.41	0.41
1:B:180:GLU:HA	1:B:183:VAL:HG22	2.03	0.41
1:C:289:ALA:HB2	1:C:358:VAL:HG21	2.02	0.41
1:D:65:PRO:HB3	1:D:90:ILE:HG21	2.03	0.41
1:D:95:VAL:HG21	1:D:138:ALA:CB	2.51	0.41
1:D:183:VAL:HG12	1:D:183:VAL:O	2.21	0.41
1:D:450:ARG:CB	1:D:461:LEU:HD13	2.51	0.41
1:G:29:VAL:HG21	1:G:40:PHE:CE2	2.56	0.41
1:H:362:ASP:HA	1:H:363:PRO:HA	1.98	0.41
1:H:520:LEU:C	1:H:520:LEU:HD23	2.41	0.41
1:L:3:ILE:O	1:L:5:LYS:NZ	2.54	0.41



A + a 1	A + 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:E:464:PRO:HB3	1:E:473:THR:HG22	2.03	0.40
1:J:22:PRO:O	1:J:162:THR:HG23	2.21	0.40
1:J:347:ILE:O	1:J:351:VAL:HG23	2.21	0.40
1:L:362:ASP:HA	1:L:397:THR:OG1	2.20	0.40
1:B:209:ARG:HG2	1:F:71:ASN:ND2	2.36	0.40
1:C:437:LEU:HD23	1:C:445:HIS:HB2	2.03	0.40
1:G:149:ILE:HG22	1:G:183:VAL:HG11	2.02	0.40
1:I:5:LYS:HZ2	1:I:18:LEU:HB2	1.86	0.40
1:I:122:VAL:O	1:I:122:VAL:CG1	2.69	0.40
1:J:493:THR:O	1:J:497:ARG:HG3	2.20	0.40
1:A:332:ALA:CB	1:C:238:LEU:HD21	2.52	0.40
1:D:472:LEU:HD13	1:D:477:ARG:CD	2.51	0.40
1:F:107:ASP:OD1	1:F:108:LEU:N	2.55	0.40
1:H:329:ARG:CG	1:H:354:PHE:CE1	3.03	0.40
1:I:291:ALA:HA	1:I:322:TRP:CH2	2.57	0.40
1:I:307:GLN:CG	1:K:241:VAL:HG22	2.52	0.40
1:I:464:PRO:O	1:I:466:LEU:N	2.55	0.40
1:K:508:ARG:HG3	1:K:509:ALA:N	2.36	0.40
1:A:332:ALA:HB3	1:C:238:LEU:CD2	2.52	0.40
1:B:194:VAL:HA	1:B:199:SER:HA	2.04	0.40
1:C:472:LEU:HD23	1:C:476:ALA:C	2.42	0.40
1:D:520:LEU:CD2	1:K:509:ALA:HB2	2.47	0.40
1:I:305:ALA:O	1:I:309:VAL:HG23	2.21	0.40
1:B:203:LEU:C	1:B:203:LEU:HD12	2.42	0.40
1:H:141:ASN:O	1:H:142:PRO:C	2.60	0.40
1:I:253:LEU:O	1:I:257:MET:SD	2.80	0.40
1:L:298:TYR:CE2	1:L:360:VAL:HG11	2.56	0.40

All (4) 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:485:ARG:HH12	1:L:294:GLU:OE2[1_445]	1.49	0.11
1:E:245:ARG:O	1:H:485:ARG:NH1[1_545]	2.14	0.06
1:E:245:ARG:NH2	1:H:481:GLU:OE2[1_545]	2.15	0.05
1:D:87:LYS:NZ	1:H:51:ASP:OD1[1_435]	2.19	0.01



# 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	499/568~(88%)	466 (93%)	31~(6%)	2~(0%)	34	72
1	В	495/568~(87%)	473 (96%)	21 (4%)	1 (0%)	47	81
1	С	498/568~(88%)	472 (95%)	25~(5%)	1 (0%)	47	81
1	D	502/568~(88%)	460 (92%)	36 (7%)	6 (1%)	13	50
1	Е	505/568~(89%)	481 (95%)	23~(5%)	1 (0%)	47	81
1	F	492/568~(87%)	463 (94%)	28~(6%)	1 (0%)	47	81
1	G	514/568~(90%)	476 (93%)	34 (7%)	4 (1%)	19	58
1	Н	503/568~(89%)	476 (95%)	27~(5%)	0	100	100
1	Ι	484/568~(85%)	455 (94%)	26~(5%)	3 (1%)	25	64
1	J	504/568~(89%)	472 (94%)	28~(6%)	4 (1%)	19	58
1	Κ	502/568~(88%)	479 (95%)	19 (4%)	4 (1%)	19	58
1	L	495/568~(87%)	462 (93%)	32~(6%)	1 (0%)	47	81
All	All	5993/6816 (88%)	5635 (94%)	330 (6%)	28 (0%)	29	68

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	95	VAL
1	D	474	GLY
1	J	363	PRO
1	Κ	232	VAL
1	А	469	GLY
1	В	473	THR
1	G	472	LEU
1	Ι	465	HIS
1	Ι	473	THR
1	J	11	GLN
1	J	472	LEU
1	С	472	LEU



Mol	Chain	Res	Type
1	D	141	ASN
1	Е	441	ARG
1	G	440	ALA
1	L	472	LEU
1	А	475	THR
1	G	97	PRO
1	J	231	PRO
1	Κ	196	ASN
1	Κ	472	LEU
1	F	138	ALA
1	G	196	ASN
1	K	411	GLY
1	D	97	PRO
1	D	427	VAL
1	D	273	VAL
1	Ι	363	PRO

### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	398/457~(87%)	392~(98%)	6(2%)	65 84
1	В	398/457~(87%)	393~(99%)	5 (1%)	69 86
1	С	397/457~(87%)	389~(98%)	8 (2%)	55 79
1	D	403/457~(88%)	402 (100%)	1 (0%)	93 98
1	Ε	403/457~(88%)	397~(98%)	6 (2%)	65 84
1	F	397/457~(87%)	394 (99%)	3~(1%)	81 91
1	G	415/457~(91%)	412 (99%)	3~(1%)	84 93
1	Н	404/457~(88%)	397~(98%)	7(2%)	60 82
1	Ι	394/457~(86%)	388~(98%)	6(2%)	65 84
1	J	$40\overline{1/457}\ (88\%)$	395~(98%)	6 (2%)	65 84
1	K	397/457~(87%)	393(99%)	4 (1%)	76 88



Continued	from	previous	page
contentaca	<i>J</i> <sup>1</sup> <i>O</i> 110	proceed ac	pago

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	402/457~(88%)	397~(99%)	5 (1%)	71 87	
All	All	4809/5484~(88%)	4749 (99%)	60 (1%)	71 87	

All (60) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	208	TYR
1	А	257	MET
1	А	298	TYR
1	А	334	ARG
1	А	373	ARG
1	А	507	ARG
1	В	112	PHE
1	В	159	ARG
1	В	208	TYR
1	В	448	GLN
1	В	456	ASP
1	С	6	SER
1	С	199	SER
1	С	208	TYR
1	С	257	MET
1	С	271	SER
1	С	285	PHE
1	С	431	PHE
1	С	497	ARG
1	D	208	TYR
1	Е	70	ASN
1	Е	208	TYR
1	Е	245	ARG
1	Е	285	PHE
1	Е	436	TYR
1	Е	497	ARG
1	F	202	ARG
1	F	208	TYR
1	F	465	HIS
1	G	208	TYR
1	G	417	ASP
1	G	497	ARG
1	Н	154	ASP
1	Н	192	HIS
1	Н	208	TYR
1	Н	425	ARG



7 4 1		- T	
Mol	Chain	Res	Type
1	Н	445	HIS
1	Н	497	ARG
1	Н	504	GLN
1	Ι	208	TYR
1	Ι	227	PHE
1	Ι	285	PHE
1	Ι	330	PHE
1	Ι	343	HIS
1	Ι	457	ARG
1	J	208	TYR
1	J	362	ASP
1	J	414	SER
1	J	436	TYR
1	J	452	PHE
1	J	456	ASP
1	Κ	208	TYR
1	Κ	370	SER
1	Κ	399	LEU
1	К	497	ARG
1	L	64	ARG
1	L	245	ARG
1	L	330	PHE
1	L	337	PHE
1	L	456	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	521	GLN
1	Е	239	HIS
1	Е	343	HIS
1	F	284	HIS
1	F	465	HIS
1	Ι	239	HIS
1	J	445	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)

Of 47 ligands modelled in this entry, 23 are monoatomic - leaving 24 for Mogul analysis.

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

Mal	Tuno	Chain	Dog	Link	Bo	Bond lengths		Bond angles		
	туре	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	D	604	3	24,29,29	0.92	1 (4%)	29,45,45	1.52	5 (17%)
2	ADP	F	603	3	24,29,29	0.92	1 (4%)	29,45,45	1.49	5 (17%)
2	ADP	В	604	3	24,29,29	0.93	1 (4%)	29,45,45	1.44	4 (13%)
2	ADP	L	601	-	24,29,29	0.92	1 (4%)	29,45,45	1.47	4 (13%)
2	ADP	Ι	601	-	24,29,29	0.92	1 (4%)	29,45,45	1.44	4 (13%)
2	ADP	С	601	3	24,29,29	0.91	1 (4%)	29,45,45	1.49	4 (13%)
2	ADP	Н	601	3	24,29,29	0.93	1 (4%)	29,45,45	1.53	5 (17%)
2	ADP	K	604	3	24,29,29	0.92	1 (4%)	29,45,45	1.53	5 (17%)
2	ADP	G	604	3	24,29,29	0.91	1 (4%)	29,45,45	1.50	5 (17%)
2	ADP	Н	603	3	24,29,29	0.91	1 (4%)	29,45,45	1.50	5 (17%)
2	ADP	D	601	-	24,29,29	0.93	1 (4%)	29,45,45	1.51	4 (13%)
2	ADP	А	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.51	5 (17%)
2	ADP	Е	601	-	24,29,29	0.93	1 (4%)	29,45,45	1.45	4 (13%)
2	ADP	G	601	3	24,29,29	0.92	1 (4%)	29,45,45	1.46	4 (13%)
2	ADP	K	601	-	24,29,29	0.92	1 (4%)	29,45,45	1.45	4 (13%)
2	ADP	F	601	-	24,29,29	0.92	1 (4%)	29,45,45	1.48	4 (13%)
2	ADP	L	602	3	24,29,29	0.93	1 (4%)	29,45,45	1.49	4 (13%)
2	ADP	В	601	3	24,29,29	0.95	1 (4%)	29,45,45	1.48	4 (13%)



Mal Turna C		Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Dog	Tink	Bo	ond leng	$\mathbf{ths}$	В	ond ang	les
	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2										
2	ADP	Е	604	3	24,29,29	0.91	1 (4%)	$29,\!45,\!45$	1.50	5 (17%)										
2	ADP	А	604	3	24,29,29	0.92	1 (4%)	29,45,45	1.50	5 (17%)										
2	ADP	J	604	3	24,29,29	0.92	1 (4%)	29,45,45	1.46	5 (17%)										
2	ADP	J	601	-	24,29,29	0.94	1 (4%)	$29,\!45,\!45$	1.45	5 (17%)										
2	ADP	С	604	3	24,29,29	0.92	1 (4%)	$29,\!45,\!45$	1.52	5 (17%)										
2	ADP	Ι	604	3,1	24,29,29	0.91	1 (4%)	29,45,45	1.52	5 (17%)										

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	D	604	3	-	5/12/32/32	0/3/3/3
2	ADP	F	603	3	-	5/12/32/32	0/3/3/3
2	ADP	В	604	3	-	5/12/32/32	0/3/3/3
2	ADP	L	601	-	-	0/12/32/32	0/3/3/3
2	ADP	Ι	601	-	-	6/12/32/32	0/3/3/3
2	ADP	С	601	3	-	5/12/32/32	0/3/3/3
2	ADP	Н	601	3	-	7/12/32/32	0/3/3/3
2	ADP	К	604	3	-	2/12/32/32	0/3/3/3
2	ADP	G	604	3	-	4/12/32/32	0/3/3/3
2	ADP	Н	603	3	-	4/12/32/32	0/3/3/3
2	ADP	D	601	-	-	5/12/32/32	0/3/3/3
2	ADP	А	601	-	-	6/12/32/32	0/3/3/3
2	ADP	Е	601	-	-	2/12/32/32	0/3/3/3
2	ADP	G	601	3	-	4/12/32/32	0/3/3/3
2	ADP	K	601	-	-	6/12/32/32	0/3/3/3
2	ADP	F	601	-	-	0/12/32/32	0/3/3/3
2	ADP	L	602	3	-	4/12/32/32	0/3/3/3
2	ADP	В	601	3	-	4/12/32/32	0/3/3/3
2	ADP	Е	604	3	-	1/12/32/32	0/3/3/3
2	ADP	А	604	3	-	4/12/32/32	0/3/3/3
2	ADP	J	604	3	-	3/12/32/32	0/3/3/3
2	ADP	J	601	-	-	5/12/32/32	0/3/3/3
2	ADP	C	604	3	_	5/12/32/32	0/3/3/3



Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	Ι	604	3,1	-	5/12/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	Н	601	ADP	C5-C4	2.43	1.47	1.40
2	D	601	ADP	C5-C4	2.41	1.47	1.40
2	А	601	ADP	C5-C4	2.41	1.47	1.40
2	В	601	ADP	C5-C4	2.40	1.47	1.40
2	J	604	ADP	C5-C4	2.39	1.47	1.40
2	F	603	ADP	C5-C4	2.39	1.47	1.40
2	L	602	ADP	C5-C4	2.39	1.47	1.40
2	J	601	ADP	C5-C4	2.39	1.47	1.40
2	Н	603	ADP	C5-C4	2.39	1.47	1.40
2	В	604	ADP	C5-C4	2.38	1.47	1.40
2	Κ	604	ADP	C5-C4	2.38	1.47	1.40
2	Е	601	ADP	C5-C4	2.37	1.47	1.40
2	С	604	ADP	C5-C4	2.37	1.47	1.40
2	Ε	604	ADP	C5-C4	2.36	1.47	1.40
2	F	601	ADP	C5-C4	2.36	1.47	1.40
2	А	604	ADP	C5-C4	2.36	1.47	1.40
2	G	601	ADP	C5-C4	2.36	1.47	1.40
2	Ι	601	ADP	C5-C4	2.35	1.47	1.40
2	D	604	ADP	C5-C4	2.35	1.47	1.40
2	Κ	601	ADP	C5-C4	2.35	1.47	1.40
2	С	601	ADP	C5-C4	2.35	1.47	1.40
2	L	601	ADP	C5-C4	2.35	1.47	1.40
2	G	604	ADP	C5-C4	2.34	1.47	1.40
2	Ι	604	ADP	C5-C4	2.34	1.47	1.40

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	D	601	ADP	PA-O3A-PB	-3.89	119.47	132.83
2	А	601	ADP	PA-O3A-PB	-3.78	119.86	132.83
2	Н	601	ADP	PA-O3A-PB	-3.77	119.88	132.83
2	Ι	604	ADP	N3-C2-N1	-3.73	122.85	128.68
2	А	604	ADP	N3-C2-N1	-3.70	122.90	128.68
2	Е	604	ADP	N3-C2-N1	-3.70	122.90	128.68
2	G	604	ADP	N3-C2-N1	-3.70	122.90	128.68
2	H	601	ADP	N3-C2-N1	-3.68	122.92	128.68
2	D	604	ADP	N3-C2-N1	-3.68	122.92	128.68


Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	G	601	ADP	N3-C2-N1	-3.67	122.94	128.68
2	L	601	ADP	N3-C2-N1	-3.67	122.95	128.68
2	В	604	ADP	N3-C2-N1	-3.66	122.96	128.68
2	Κ	604	ADP	N3-C2-N1	-3.66	122.96	128.68
2	F	601	ADP	N3-C2-N1	-3.66	122.96	128.68
2	С	604	ADP	N3-C2-N1	-3.65	122.97	128.68
2	Н	603	ADP	N3-C2-N1	-3.65	122.98	128.68
2	J	601	ADP	N3-C2-N1	-3.64	122.99	128.68
2	L	602	ADP	N3-C2-N1	-3.64	122.99	128.68
2	D	604	ADP	PA-O3A-PB	-3.64	120.35	132.83
2	J	604	ADP	N3-C2-N1	-3.63	123.00	128.68
2	В	601	ADP	N3-C2-N1	-3.63	123.01	128.68
2	D	601	ADP	N3-C2-N1	-3.63	123.01	128.68
2	С	601	ADP	N3-C2-N1	-3.63	123.01	128.68
2	F	603	ADP	N3-C2-N1	-3.62	123.02	128.68
2	А	601	ADP	N3-C2-N1	-3.62	123.02	128.68
2	Е	601	ADP	N3-C2-N1	-3.62	123.02	128.68
2	Ι	601	ADP	N3-C2-N1	-3.61	123.04	128.68
2	А	604	ADP	PA-O3A-PB	-3.60	120.47	132.83
2	С	604	ADP	PA-O3A-PB	-3.58	120.53	132.83
2	Κ	601	ADP	N3-C2-N1	-3.58	123.08	128.68
2	L	602	ADP	PA-O3A-PB	-3.55	120.66	132.83
2	В	601	ADP	PA-O3A-PB	-3.53	120.70	132.83
2	L	601	ADP	PA-O3A-PB	-3.52	120.73	132.83
2	F	601	ADP	PA-O3A-PB	-3.50	120.81	132.83
2	Н	603	ADP	PA-O3A-PB	-3.49	120.83	132.83
2	F	603	ADP	PA-O3A-PB	-3.49	120.86	132.83
2	Κ	604	ADP	PA-O3A-PB	-3.48	120.87	132.83
2	G	604	ADP	PA-O3A-PB	-3.42	121.10	132.83
2	J	601	ADP	PA-O3A-PB	-3.38	121.24	132.83
2	Ι	604	ADP	PA-O3A-PB	-3.37	121.25	132.83
2	В	604	ADP	PA-O3A-PB	-3.36	121.30	132.83
2	С	601	ADP	C3'-C2'-C1'	3.35	106.02	100.98
2	J	604	ADP	PA-O3A-PB	-3.32	121.45	132.83
2	Е	604	ADP	PA-O3A-PB	-3.30	121.50	132.83
2	L	601	ADP	C3'-C2'-C1'	3.27	105.90	100.98
2	Е	604	ADP	C3'-C2'-C1'	3.27	105.90	100.98
2	Ι	604	ADP	C3'-C2'-C1'	3.26	105.88	100.98
2	K	601	ADP	PA-O3A-PB	-3.24	121.69	132.83
2	F	601	ADP	C3'-C2'-C1'	3.23	105.84	100.98
2	Ι	601	ADP	PA-O3A-PB	-3.19	121.89	132.83
2	G	601	ADP	PA-O3A-PB	-3.19	121.89	132.83



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Κ	601	ADP	C3'-C2'-C1'	3.16	105.73	100.98
2	Ι	601	ADP	C3'-C2'-C1'	3.15	105.72	100.98
2	Ε	601	ADP	PA-O3A-PB	-3.14	122.05	132.83
2	D	601	ADP	C3'-C2'-C1'	3.11	105.66	100.98
2	G	604	ADP	C3'-C2'-C1'	3.11	105.66	100.98
2	Н	603	ADP	C3'-C2'-C1'	3.07	105.61	100.98
2	В	601	ADP	C3'-C2'-C1'	3.07	105.60	100.98
2	Н	601	ADP	C3'-C2'-C1'	3.07	105.59	100.98
2	С	601	ADP	PA-O3A-PB	-3.06	122.31	132.83
2	А	601	ADP	C3'-C2'-C1'	3.01	105.51	100.98
2	С	604	ADP	C3'-C2'-C1'	2.99	105.48	100.98
2	D	604	ADP	C4-C5-N7	-2.95	106.32	109.40
2	D	604	ADP	C3'-C2'-C1'	2.94	105.40	100.98
2	Ε	601	ADP	C4-C5-N7	-2.93	106.35	109.40
2	L	602	ADP	C4-C5-N7	-2.92	106.35	109.40
2	Н	601	ADP	C4-C5-N7	-2.92	106.35	109.40
2	В	601	ADP	C4-C5-N7	-2.92	106.36	109.40
2	С	604	ADP	C4-C5-N7	-2.91	106.37	109.40
2	Ε	604	ADP	C4-C5-N7	-2.90	106.38	109.40
2	J	604	ADP	C4-C5-N7	-2.89	106.39	109.40
2	J	601	ADP	C4-C5-N7	-2.89	106.39	109.40
2	J	601	ADP	C3'-C2'-C1'	2.89	105.32	100.98
2	Κ	604	ADP	C4-C5-N7	-2.87	106.40	109.40
2	F	603	ADP	C3'-C2'-C1'	2.87	105.30	100.98
2	А	604	ADP	C3'-C2'-C1'	2.86	105.29	100.98
2	F	603	ADP	C4-C5-N7	-2.86	106.42	109.40
2	D	601	ADP	C4-C5-N7	-2.86	106.42	109.40
2	А	601	ADP	C4-C5-N7	-2.85	106.42	109.40
2	Κ	604	ADP	C3'-C2'-C1'	2.85	105.27	100.98
2	G	604	ADP	C4-C5-N7	-2.84	106.44	109.40
2	В	604	ADP	C4-C5-N7	-2.83	106.45	109.40
2	Ε	601	ADP	C3'-C2'-C1'	2.83	105.24	100.98
2	Ι	604	ADP	C4-C5-N7	-2.82	106.46	109.40
2	А	604	ADP	C4-C5-N7	-2.82	106.46	109.40
2	Н	603	ADP	C4-C5-N7	-2.78	106.51	109.40
2	G	601	ADP	C4-C5-N7	-2.76	106.52	109.40
2	F	601	ADP	C4-C5-N7	-2.75	106.54	109.40
2	L	601	ADP	C4-C5-N7	-2.68	106.61	109.40
2	G	601	ADP	C3'-C2'-C1'	2.66	104.99	100.98
2	Ι	601	ADP	C4-C5-N7	-2.63	106.66	109.40
2	$\mathbf{C}$	601	ADP	C4-C5-N7	-2.54	106.75	109.40
2	Κ	601	ADP	C4-C5-N7	-2.50	106.79	109.40

Continued from previous page...



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	J	604	ADP	C3'-C2'-C1'	2.20	104.29	100.98
2	Η	601	ADP	C2-N1-C6	2.15	122.43	118.75
2	Κ	604	ADP	C2-N1-C6	2.09	122.33	118.75
2	Ι	604	ADP	C2-N1-C6	2.08	122.32	118.75
2	D	604	ADP	C2-N1-C6	2.08	122.31	118.75
2	Е	604	ADP	C2-N1-C6	2.06	122.28	118.75
2	L	602	ADP	C2-N1-C6	2.06	122.27	118.75
2	С	604	ADP	C2-N1-C6	2.06	122.27	118.75
2	А	604	ADP	C2-N1-C6	2.05	122.27	118.75
2	В	604	ADP	C2-N1-C6	2.05	122.26	118.75
2	F	603	ADP	C2-N1-C6	2.04	122.25	118.75
2	Н	603	ADP	C2-N1-C6	2.04	122.24	118.75
2	G	604	ADP	C2-N1-C6	2.03	122.23	118.75
2	J	601	ADP	C2-N1-C6	2.03	122.23	118.75
2	А	601	ADP	C2-N1-C6	2.03	122.23	118.75
2	J	604	ADP	C2-N1-C6	2.02	122.22	118.75

There are no chirality outliers.

All (	(97)	torsion	outliers	$\operatorname{are}$	listed	below:	

Mol	Chain	$\mathbf{Res}$	Type	Atoms
2	А	601	ADP	C5'-O5'-PA-O1A
2	А	601	ADP	C5'-O5'-PA-O2A
2	А	601	ADP	C5'-O5'-PA-O3A
2	А	604	ADP	C5'-O5'-PA-O1A
2	В	601	ADP	O4'-C4'-C5'-O5'
2	В	601	ADP	C3'-C4'-C5'-O5'
2	В	604	ADP	PA-O3A-PB-O3B
2	В	604	ADP	C5'-O5'-PA-O2A
2	С	601	ADP	PA-O3A-PB-O3B
2	С	601	ADP	C5'-O5'-PA-O3A
2	С	604	ADP	C5'-O5'-PA-O2A
2	С	604	ADP	C5'-O5'-PA-O3A
2	С	604	ADP	C3'-C4'-C5'-O5'
2	D	601	ADP	C5'-O5'-PA-O1A
2	D	601	ADP	C5'-O5'-PA-O3A
2	D	604	ADP	C5'-O5'-PA-O1A
2	D	604	ADP	C5'-O5'-PA-O2A
2	D	604	ADP	C3'-C4'-C5'-O5'
2	F	603	ADP	C5'-O5'-PA-O1A
2	F	603	ADP	C5'-O5'-PA-O2A
2	G	601	ADP	C5'-O5'-PA-O1A



Mol	Chain	Res	Type	Atoms
2	G	601	ADP	C5'-O5'-PA-O3A
2	G	604	ADP	C5'-O5'-PA-O1A
2	Н	601	ADP	C5'-O5'-PA-O1A
2	Н	601	ADP	C5'-O5'-PA-O3A
2	Н	603	ADP	C5'-O5'-PA-O1A
2	Ι	601	ADP	C5'-O5'-PA-O1A
2	Ι	604	ADP	C5'-O5'-PA-O1A
2	Ι	604	ADP	C5'-O5'-PA-O2A
2	J	601	ADP	O4'-C4'-C5'-O5'
2	J	601	ADP	C3'-C4'-C5'-O5'
2	J	604	ADP	C5'-O5'-PA-O1A
2	J	604	ADP	C5'-O5'-PA-O2A
2	K	601	ADP	PB-O3A-PA-O5'
2	K	601	ADP	C5'-O5'-PA-O1A
2	K	601	ADP	C5'-O5'-PA-O2A
2	K	601	ADP	C3'-C4'-C5'-O5'
2	K	604	ADP	C5'-O5'-PA-O2A
2	L	602	ADP	C5'-O5'-PA-O1A
2	Ι	604	ADP	C3'-C4'-C5'-O5'
2	F	603	ADP	C3'-C4'-C5'-O5'
2	K	601	ADP	O4'-C4'-C5'-O5'
2	Ι	601	ADP	O4'-C4'-C5'-O5'
2	С	604	ADP	O4'-C4'-C5'-O5'
2	D	604	ADP	O4'-C4'-C5'-O5'
2	Ι	601	ADP	C3'-C4'-C5'-O5'
2	Ι	604	ADP	O4'-C4'-C5'-O5'
2	В	604	ADP	PA-O3A-PB-O1B
2	А	604	ADP	C5'-O5'-PA-O3A
2	В	604	ADP	C5'-O5'-PA-O3A
2	F	603	ADP	C5'-O5'-PA-O3A
2	G	604	ADP	C5'-O5'-PA-O3A
2	Н	603	ADP	C5'-O5'-PA-O3A
2	Ι	601	ADP	C5'-O5'-PA-O3A
2	L	602	ADP	C5'-O5'-PA-O3A
2	В	601	ADP	PB-O3A-PA-O1A
2	D	601	ADP	PB-O3A-PA-O2A
2	Н	601	ADP	PB-O3A-PA-O1A
2	Ι	601	ADP	PB-O3A-PA-O2A
2	J	601	ADP	PB-O3A-PA-O1A
2	A	604	ADP	C5'-O5'-PA-O2A
2	В	604	ADP	C5'-O5'-PA-O1A
2		601	ADP	C5'-O5'-PA-O1A



Mol	Chain	Res	Type	Atoms
2	G	604	ADP	C5'-O5'-PA-O2A
2	Н	601	ADP	C5'-O5'-PA-O2A
2	Н	603	ADP	C5'-O5'-PA-O2A
2	L	602	ADP	C5'-O5'-PA-O2A
2	F	603	ADP	O4'-C4'-C5'-O5'
2	А	604	ADP	C3'-C4'-C5'-O5'
2	Н	603	ADP	C3'-C4'-C5'-O5'
2	L	602	ADP	C3'-C4'-C5'-O5'
2	G	601	ADP	PB-O3A-PA-O1A
2	G	601	ADP	PB-O3A-PA-O2A
2	G	604	ADP	C3'-C4'-C5'-O5'
2	Н	601	ADP	PB-O3A-PA-O2A
2	Н	601	ADP	C3'-C4'-C5'-O5'
2	Н	601	ADP	O4'-C4'-C5'-O5'
2	С	601	ADP	O4'-C4'-C5'-O5'
2	С	601	ADP	PA-O3A-PB-O2B
2	D	604	ADP	C5'-O5'-PA-O3A
2	Ι	604	ADP	C5'-O5'-PA-O3A
2	J	604	ADP	C5'-O5'-PA-O3A
2	K	601	ADP	C5'-O5'-PA-O3A
2	K	604	ADP	C5'-O5'-PA-O3A
2	Е	604	ADP	C3'-C4'-C5'-O5'
2	А	601	ADP	PB-O3A-PA-O1A
2	А	601	ADP	PB-O3A-PA-O2A
2	D	601	ADP	PB-O3A-PA-O1A
2	Е	601	ADP	PB-O3A-PA-O1A
2	Е	601	ADP	PB-O3A-PA-O2A
2	Ι	601	ADP	PB-O3A-PA-O1A
2	J	601	ADP	PB-O3A-PA-O2A
2	В	601	ADP	C5'-O5'-PA-O1A
2	С	604	ADP	C5'-O5'-PA-O1A
2	D	601	ADP	C5'-O5'-PA-O2A
2	J	601	ADP	C5'-O5'-PA-O1A
2	A	601	ADP	C3'-C4'-C5'-O5'

Continued from previous page...

There are no ring outliers.

14 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	604	ADP	1	0
2	В	604	ADP	2	0
2	L	601	ADP	2	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Ι	601	ADP	1	0
2	С	601	ADP	2	0
2	Н	601	ADP	1	0
2	K	604	ADP	1	0
2	G	604	ADP	2	0
2	Е	601	ADP	1	0
2	G	601	ADP	1	0
2	K	601	ADP	2	0
2	E	604	ADP	1	0
2	А	604	ADP	1	0
2	С	604	ADP	2	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	А	507/568~(89%)	0.12	13 (2%) 56 49	55, 98, 161, 204	0
1	В	505/568~(88%)	-0.03	9 (1%) 68 62	51, 99, 142, 165	0
1	С	508/568~(89%)	-0.03	7 (1%) 75 69	54, 98, 150, 186	0
1	D	510/568~(89%)	0.00	11 (2%) 62 56	57, 90, 146, 211	0
1	Ε	511/568~(89%)	-0.17	3 (0%) 89 86	51, 89, 139, 177	0
1	F	500/568~(88%)	-0.14	4 (0%) 86 81	42, 94, 138, 200	0
1	G	518/568~(91%)	-0.01	10 (1%) 66 61	53, 99, 161, 216	0
1	Н	509/568~(89%)	0.05	13 (2%) 56 49	41, 92, 149, 206	0
1	Ι	494/568~(86%)	0.02	7 (1%) 75 69	58, 101, 149, 175	0
1	J	510/568~(89%)	0.09	19 (3%) 41 37	65, 121, 171, 202	0
1	Κ	508/568~(89%)	0.25	16 (3%) 49 43	63, 115, 165, 195	0
1	L	503/568~(88%)	-0.02	10 (1%) 65 60	47, 106, 165, 180	0
All	All	6083/6816 (89%)	0.01	122 (2%) 65 60	41, 99, 157, 216	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	87	LYS	6.6
1	Н	143	ALA	5.9
1	Κ	91	GLU	4.6
1	В	468	GLU	4.5
1	L	88	ILE	4.2
1	А	98	SER	4.1
1	L	77	PHE	4.1
1	Н	142	PRO	4.1
1	D	178	GLY	4.0
1	Ι	468	GLU	3.8
1	Е	140	SER	3.8



Mol	Chain	Res	Type	RSRZ
1	D	141	ASN	3.7
1	Κ	2	GLY	3.5
1	В	471	ALA	3.5
1	F	529	ALA	3.4
1	А	115	LEU	3.3
1	Н	141	ASN	3.3
1	А	113	LEU	3.3
1	F	142	PRO	3.2
1	А	95	VAL	3.2
1	А	153	PHE	3.2
1	J	124	ALA	3.2
1	С	2	GLY	3.2
1	D	140	SER	3.2
1	В	470	GLY	3.1
1	G	96	ASP	3.1
1	F	141	ASN	3.1
1	L	139	PHE	3.0
1	J	473	THR	3.0
1	Ι	161	LEU	3.0
1	D	139	PHE	3.0
1	А	57	VAL	3.0
1	А	91	GLU	2.9
1	С	59	VAL	2.9
1	J	294	GLU	2.9
1	J	140	SER	2.9
1	D	371	GLY	2.9
1	D	448	GLN	2.8
1	G	101	ALA	2.8
1	Н	109	GLU	2.8
1	В	465	HIS	2.8
1	D	136	PHE	2.8
1	J	8	THR	2.8
1	J	119	ILE	2.7
1	J	123	GLY	2.7
1	G	99	GLU	2.7
1	L	501	GLN	2.7
1	K	356	PRO	2.7
1	J	58	PHE	2.7
1	G	179	LEU	2.6
1	Н	132	ILE	2.6
1	K	126	ARG	2.6
1	G	103	ILE	2.6



Mol	Chain	Res	Type	RSRZ
1	Н	165	ILE	2.6
1	K	158	GLU	2.6
1	В	467	GLY	2.6
1	Н	182	TYR	2.5
1	J	242	HIS	2.5
1	J	112	PHE	2.5
1	K	252	ASP	2.5
1	В	124	ALA	2.5
1	В	469	GLY	2.5
1	С	470	GLY	2.5
1	G	98	SER	2.5
1	D	177	GLN	2.4
1	J	55	PRO	2.4
1	D	99	GLU	2.4
1	Н	468	GLU	2.4
1	Η	233	SER	2.4
1	J	354	PHE	2.4
1	А	111	LEU	2.4
1	А	466	LEU	2.4
1	K	171	ASP	2.4
1	J	88	ILE	2.4
1	Н	140	SER	2.4
1	G	140	SER	2.3
1	F	530	LEU	2.3
1	Н	181	GLU	2.3
1	K	160	GLY	2.3
1	Е	468	GLU	2.3
1	J	77	PHE	2.3
1	J	89	ALA	2.3
1	Ι	240	GLN	2.3
1	L	2	GLY	2.3
1	А	93	ILE	2.3
1	J	536	ALA	2.3
1	K	161	LEU	2.3
1	K	129	LEU	2.2
1	J	91	GLU	2.2
1	А	124	ALA	2.2
1	D	260	GLY	2.2
1	Е	407	THR	2.2
1	J	225	ASP	2.2
1	L	170	GLY	2.2
1	K	127	VAL	2.2



Mol	Chain	Res	Type	RSRZ
1	А	122	VAL	2.2
1	L	75	LEU	2.2
1	J	20	GLY	2.1
1	K	232	VAL	2.1
1	С	347	ILE	2.1
1	G	102	GLU	2.1
1	K	435	LEU	2.1
1	K	473	THR	2.1
1	Н	230	LEU	2.1
1	L	91	GLU	2.1
1	В	472	LEU	2.1
1	Ι	135	LEU	2.1
1	С	145	LEU	2.1
1	Ι	115	LEU	2.1
1	Н	178	GLY	2.1
1	А	119	ILE	2.1
1	K	182	TYR	2.1
1	G	138	ALA	2.1
1	D	227	PHE	2.0
1	С	129	LEU	2.0
1	Ι	111	LEU	2.0
1	С	124	ALA	2.0
1	Ι	432	ASN	2.0
1	К	143	ALA	2.0
1	L	82	LEU	2.0
1	В	159	ARG	2.0
1	G	104	GLY	2.0

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

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

#### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	<b>B-factors</b> ( $Å^2$ )	Q<0.9
3	MG	Ι	603	1/1	0.67	0.28	79,79,79,79	0
3	MG	С	603	1/1	0.71	0.26	98,98,98,98	0
2	ADP	L	601	27/27	0.81	0.27	94,126,152,158	0
2	ADP	J	601	27/27	0.84	0.29	105,136,162,167	0
2	ADP	F	601	27/27	0.87	0.29	72,117,146,151	0
3	MG	J	603	1/1	0.88	0.29	104,104,104,104	0
2	ADP	G	604	27/27	0.89	0.27	47,77,119,137	0
2	ADP	С	601	27/27	0.89	0.27	73,95,115,117	0
2	ADP	В	601	27/27	0.90	0.27	87,114,141,141	0
2	ADP	G	601	27/27	0.90	0.30	89,114,139,143	0
3	MG	В	605	1/1	0.91	0.24	84,84,84,84	0
2	ADP	Ι	604	27/27	0.91	0.21	69,104,130,139	0
3	MG	K	603	1/1	0.91	0.23	85,85,85,85	0
2	ADP	K	604	27/27	0.92	0.23	77,106,129,131	0
2	ADP	А	604	27/27	0.92	0.29	$69,\!88,\!114,\!127$	0
3	MG	K	602	1/1	0.92	0.23	70,70,70,70	0
3	MG	Ι	602	1/1	0.92	0.13	$53,\!53,\!53,\!53$	0
2	ADP	A	601	27/27	0.93	0.24	95,112,137,158	0
2	ADP	Ι	601	27/27	0.93	0.27	100,123,156,158	0
2	ADP	K	601	27/27	0.93	0.22	108,131,158,171	0
2	ADP	D	601	27/27	0.94	0.27	72,97,132,137	0
2	ADP	Н	603	27/27	0.94	0.28	65,93,117,137	0
3	MG	С	602	1/1	0.94	0.35	63,63,63,63	0
2	ADP	E	601	27/27	0.94	0.22	60,91,112,122	0
3	MG	D	602	1/1	0.94	0.28	85,85,85,85	0
3	MG	G	603	1/1	0.94	0.25	98,98,98,98	0
3	MG	Н	604	1/1	0.94	0.16	77,77,77,77	0
2	ADP	E	604	27/27	0.94	0.26	51,78,112,113	0
2	ADP	В	604	27/27	0.94	0.23	58,75,91,106	0
2	ADP	J	604	27/27	0.94	0.29	64,84,108,124	0
2	ADP	F	603	27/27	0.94	0.25	58,94,119,126	0
2	ADP	C	604	27/27	0.94	0.26	72,87,114,123	0
3	MG	B	602	1/1	0.95	0.13	36,36,36,36	0
2	ADP	D	604	27/27	0.95	0.27	57,77,98,106	0
2	ADP	H	601	27/27	0.95	0.23	68,95,134,137	0
2	ADP		602	27/27	0.96	0.18	41,78,99,103	
3	MG	H	602	1/1	0.96	0.24	77,77,77,77	0
3	MG	A	602	1/1	0.97	0.17	76,76,76,76	
3	MG		603		0.97	0.42	66,66,66,66	
3	MG	<u> </u>	602	1/1	0.97	0.24	82,82,82,82	
3	MG	G	602	1/1	0.97	0.33	46, 46, 46, 46	0

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 <sup>2</sup> )	Q<0.9
3	MG	G	605	1/1	0.98	0.23	$58,\!58,\!58,\!58$	0
3	MG	J	602	1/1	0.98	0.34	62,62,62,62	0
3	MG	В	603	1/1	0.98	0.19	$65,\!65,\!65,\!65$	0
3	MG	Е	602	1/1	0.98	0.21	46,46,46,46	0
3	MG	А	603	1/1	0.98	0.17	98,98,98,98	0
3	MG	D	603	1/1	0.99	0.29	$68,\!68,\!68,\!68$	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.

