

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

#### Oct 12, 2023 – 04:56 AM EDT

PDB ID	:	8H2A
Title	:	Crystal structure of alcohol dehydrogenase from Formosa agariphila
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Deposited on	:	2022-10-05
Resolution	:	2.50 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
$\mathrm{EDS}$	:	2.35.1
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)	:	2.35.1

# 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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	$5231 \ (2.50-2.50)$
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	Λ	370	660/	210/	
	Л	510	.%	31%	••
1	В	370	68%	29%	•••
1	C	270	2%		
1	C	370	<u> </u>	27%	•••
1	D	370	67%	29%	••••
1	Б	070	%		
	E	370	64%	33%	•••



Mol	Chain	Length	Quality of chain				
1	F	370	61%	34%	•••		
1	G	370	% 66%	31%			
1	Н	370	3% 63%	31%	•••		



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22361 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	266	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	A	300	2731	1718	459	532	22	0	0	0
1	В	366	Total	С	Ν	0	S	0	0	0
	D	500	2739	1725	459	533	22	0	0	0
1	С	363	Total	С	Ν	Ο	S	0	0	0
	U	505	2709	1704	456	528	21	0	0	0
1	Л	364	Total	С	Ν	0	S	0	0	0
	D	504	2717	1710	457	529	21	0	0	0
1	F	364	Total	С	Ν	Ο	S	0	0	0
L	Ľ	504	2717	1710	457	529	21	0	0	0
1	F	360	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0
	Ľ	502	2705	1702	455	527	21	0	0	0
1	C	365	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0
	G	505	2723	1713	458	531	21	0	0	0
1	н	356	Total	C	N	0	S	0	0	0
	11	550	2664	1678	447	519	20	0	0	U

• Molecule 1 is a protein called Alcohol dehydrogenase.

• Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf									
0	Λ	1	Total	С	Ν	Ο	Р	0	0									
	A	1	44	21	7	14	2	0	0									
9	В	1	Total	С	Ν	Ο	Р	0	0									
	D	1	44	21	7	14	2	0	0									
9	С	1	Total	С	Ν	Ο	Р	0	0									
	U	1	44	21	7	14	2	0	U									
9	Л	1	Total	С	Ν	Ο	Р	0	0									
	D		1	44	21	7	14	2	0	0								
2	F	1	Total	С	Ν	Ο	Р	0	0									
2	Ľ	T	44	21	7	14	2	0	0									
2	F	1	Total	С	Ν	Ο	Р	0	0									
2	Г	Ľ	Ľ	L,	Ľ	Ľ	T,	Г	I, I,		T	44	21	7	14	2	0	0
2	C	1	Total	С	Ν	Ο	Р	0	0									
	G	I	44	21	7	14	2	0	0									
2	н	1	Total	С	Ν	Ο	Р	0	0									
	11	1	44	21	7	14	2	0	0									

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Zn 2 2	0	0
3	В	2	Total Zn 2 2	0	0
3	С	2	Total Zn 2 2	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	2	Total Zn 2 2	0	0
3	Е	2	Total Zn 2 2	0	0
3	F	2	Total Zn 2 2	0	0
3	G	2	Total Zn 2 2	0	0
3	Н	2	Total Zn 2 2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	37	Total         O           37         37	0	0
4	В	41	Total O 41 41	0	0
4	С	37	$\begin{array}{cc} \text{Total} & \text{O} \\ 37 & 37 \end{array}$	0	0
4	D	36	$\begin{array}{cc} \text{Total} & \text{O} \\ 36 & 36 \end{array}$	0	0
4	Ε	39	Total O 39 39	0	0
4	F	34	$\begin{array}{cc} \text{Total} & \text{O} \\ 34 & 34 \end{array}$	0	0
4	G	28	Total O 28 28	0	0
4	Н	36	Total O 36 36	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: Alcohol dehydrogenase





• Molecule 1: Alcohol dehydrogenase







## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	98.49Å $157.20$ Å $98.57$ Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $103.50^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	48.19 - 2.50	Depositor
Resolution (A)	48.19 - 2.50	EDS
% Data completeness	97.3 (48.19-2.50)	Depositor
(in resolution range)	97.2 (48.19-2.50)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.84 (at 2.51 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
D D	0.225 , $0.278$	Depositor
$\Lambda, \Lambda_{free}$	0.225 , $0.278$	DCC
$R_{free}$ test set	1981 reflections $(2.02\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	46.9	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32, 28.9	EDS
L-test for $twinning^2$	$< L >=0.42, < L^2>=0.25$	Xtriage
Estimated twinning fraction	0.398 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22361	wwPDB-VP
Average B, all atoms $(Å^2)$	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.90% 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: ZN, NAD

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

Mal	Chain	Bo	ond lengths	Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.53	1/2776~(0.0%)	0.78	8/3764~(0.2%)	
1	В	0.55	1/2785~(0.0%)	0.82	8/3777~(0.2%)	
1	С	0.48	0/2754	0.79	9/3735~(0.2%)	
1	D	0.54	4/2762~(0.1%)	0.84	9/3746~(0.2%)	
1	Ε	0.50	0/2762	0.77	5/3746~(0.1%)	
1	F	0.54	3/2750~(0.1%)	0.96	12/3730~(0.3%)	
1	G	0.48	0/2768	0.77	5/3754~(0.1%)	
1	Н	0.53	4/2708~(0.1%)	0.77	5/3673~(0.1%)	
All	All	0.52	13/22065~(0.1%)	0.81	61/29925~(0.2%)	

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	1
1	В	0	2
1	С	0	2
1	D	0	3
1	Е	0	3
1	F	0	4
1	G	0	3
All	All	0	18

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	А	34	LYS	CE-NZ	6.62	1.65	1.49
1	D	65	GLU	CD-OE2	6.48	1.32	1.25
1	Н	148	LYS	CE-NZ	6.04	1.64	1.49



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	F	27	LYS	CD-CE	5.93	1.66	1.51
1	F	250	GLU	CD-OE2	5.70	1.31	1.25
1	Н	306	TRP	CB-CG	5.65	1.60	1.50
1	D	156	GLU	CD-OE1	-5.55	1.19	1.25
1	Н	148	LYS	CD-CE	5.48	1.65	1.51
1	F	250	GLU	CD-OE1	5.32	1.31	1.25
1	В	1	MET	CA-C	5.29	1.66	1.52
1	D	123	GLU	CB-CG	-5.28	1.42	1.52
1	D	123	GLU	CD-OE2	5.09	1.31	1.25
1	Н	11	LYS	CE-NZ	5.09	1.61	1.49

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	F	129	ASP	CB-CG-OD2	-20.80	99.58	118.30
1	F	129	ASP	CB-CG-OD1	17.40	133.96	118.30
1	D	356	ASP	CB-CG-OD2	-13.64	106.02	118.30
1	D	207	ARG	NE-CZ-NH2	12.45	126.52	120.30
1	В	247	LYS	CD-CE-NZ	-10.81	86.84	111.70
1	D	207	ARG	NE-CZ-NH1	-10.10	115.25	120.30
1	G	134	ARG	NE-CZ-NH2	-8.87	115.87	120.30
1	С	358	MET	CB-CG-SD	-8.43	87.11	112.40
1	F	92	PHE	CB-CG-CD2	-8.34	114.97	120.80
1	Е	319	ARG	NE-CZ-NH1	-8.01	116.30	120.30
1	Е	13	ASP	CB-CG-OD2	-7.95	111.14	118.30
1	В	1	MET	CG-SD-CE	-7.71	87.87	100.20
1	F	123	GLU	CA-CB-CG	7.69	130.32	113.40
1	С	289	GLN	N-CA-C	-7.66	90.33	111.00
1	F	92	PHE	CB-CG-CD1	7.17	125.82	120.80
1	D	207	ARG	CA-CB-CG	7.00	128.81	113.40
1	F	237	LEU	CB-CG-CD2	-6.88	99.30	111.00
1	Н	9	ILE	CG1-CB-CG2	-6.85	96.32	111.40
1	В	1	MET	CB-CA-C	6.83	124.06	110.40
1	Е	223	ARG	CG-CD-NE	6.80	126.09	111.80
1	С	289	GLN	CB-CA-C	-6.76	96.87	110.40
1	В	338	LEU	CA-CB-CG	6.74	130.81	115.30
1	А	134	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	D	123	GLU	OE1-CD-OE2	6.54	131.14	123.30
1	G	134	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	Е	74	LEU	CA-CB-CG	6.47	130.19	115.30
1	А	134	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	Н	148	LYS	CA-CB-CG	-6.47	99.17	113.40



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	G	239	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	А	307	ASP	CB-CG-OD1	6.39	124.05	118.30
1	F	123	GLU	N-CA-CB	-6.39	99.10	110.60
1	D	344	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	С	312	ASN	CB-CA-C	6.23	122.86	110.40
1	D	356	ASP	CB-CG-OD1	6.15	123.84	118.30
1	Н	352	GLN	CA-CB-CG	6.15	126.93	113.40
1	А	134	ARG	CD-NE-CZ	6.11	132.16	123.60
1	А	34	LYS	CA-CB-CG	-6.01	100.18	113.40
1	С	79	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	D	207	ARG	CD-NE-CZ	5.93	131.91	123.60
1	Е	79	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	D	226	MET	CA-CB-CG	5.76	123.10	113.30
1	В	146	LEU	CB-CG-CD2	5.68	120.66	111.00
1	С	289	GLN	CA-CB-CG	-5.62	101.03	113.40
1	Н	306	TRP	CB-CA-C	5.61	121.62	110.40
1	В	336	LEU	CB-CG-CD1	-5.60	101.47	111.00
1	В	16	PHE	CB-CG-CD2	-5.58	116.89	120.80
1	F	63	PHE	CB-CG-CD1	5.50	124.65	120.80
1	G	79	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	С	13	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	F	79	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	А	306	TRP	CB-CA-C	5.21	120.82	110.40
1	В	344	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	С	348	LEU	CB-CG-CD2	5.19	119.82	111.00
1	Н	217	ILE	CG1-CB-CG2	5.15	122.72	111.40
1	А	307	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	G	338	LEU	CA-CB-CG	5.10	127.04	115.30
1	F	306	TRP	C-N-CA	5.09	134.43	121.70
1	F	345	THR	C-N-CA	-5.08	108.99	121.70
1	F	63	PHE	CB-CG-CD2	-5.07	117.25	120.80
1	A	223	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	С	217	ILE	CG1-CB-CG2	5.01	122.43	111.40

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	305	GLU	Peptide
1	В	1	MET	Mainchain
1	В	79	TYR	Sidechain
1	С	289	GLN	Sidechain



Mol	Chain	Res	Type	Group
1	С	79	TYR	Sidechain
1	D	207	ARG	Mainchain
1	D	355	PHE	Peptide
1	D	356	ASP	Sidechain
1	Е	13	ASP	Sidechain
1	Е	319	ARG	Sidechain
1	Е	79	TYR	Sidechain
1	F	129	ASP	Sidechain
1	F	250	GLU	Mainchain
1	F	79	TYR	Sidechain
1	F	92	PHE	Sidechain
1	G	239	ASP	Sidechain
1	G	305	GLU	Peptide
1	G	79	TYR	Sidechain

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#### 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2731	0	2726	107	2
1	В	2739	0	2732	101	1
1	С	2709	0	2698	96	1
1	D	2717	0	2709	92	1
1	Е	2717	0	2709	112	1
1	F	2705	0	2695	141	1
1	G	2723	0	2714	101	0
1	Н	2664	0	2651	116	0
2	А	44	0	26	5	0
2	В	44	0	26	2	0
2	С	44	0	26	3	0
2	D	44	0	26	4	0
2	Е	44	0	26	6	0
2	F	44	0	26	2	0
2	G	44	0	26	3	0
2	Н	44	0	26	4	0
3	А	2	0	0	0	0
3	В	2	0	0	0	0
3	С	2	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2	0	0	0	0
3	Е	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	Н	2	0	0	0	0
4	А	37	0	0	11	0
4	В	41	0	0	13	0
4	С	37	0	0	11	0
4	D	36	0	0	9	0
4	Е	39	0	0	10	1
4	F	34	0	0	13	0
4	G	28	0	0	6	0
4	Н	36	0	0	11	0
All	All	22361	0	21842	814	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 19.

All (814) 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 $(\text{\AA})$	overlap (Å)
1:E:27:LYS:HG3	1:E:28:ALA:H	1.16	1.08
1:C:289:GLN:OE1	1:C:312:ASN:ND2	1.85	1.07
1:F:312:ASN:ND2	4:F:501:HOH:O	1.94	1.00
1:E:173:THR:HG22	1:E:315:TYR:HA	1.53	0.91
1:H:185:GLN:NE2	4:H:501:HOH:O	2.04	0.91
1:A:365:LYS:O	4:A:501:HOH:O	1.91	0.89
1:D:369:ILE:O	4:D:501:HOH:O	1.90	0.89
1:E:163:SER:HB3	1:E:338:LEU:HG	1.55	0.88
1:E:340:GLU:OE1	4:E:501:HOH:O	1.91	0.88
1:C:128:ASN:O	4:C:501:HOH:O	1.92	0.87
1:H:173:THR:HG22	1:H:315:TYR:HA	1.57	0.87
1:D:302:ARG:O	4:D:502:HOH:O	1.91	0.86
1:B:270:ILE:O	4:B:501:HOH:O	1.93	0.85
1:D:173:THR:HG22	1:D:315:TYR:HA	1.58	0.85
1:E:299:ILE:HD12	1:G:299:ILE:HD12	1.60	0.83
1:C:86:THR:HG22	1:C:151:ALA:HB2	1.58	0.83
1:E:21:VAL:HG11	1:E:125:THR:HG23	1.60	0.83
1:C:343:THR:OG1	1:C:363:ASN:OD1	1.96	0.83
1:F:305:GLU:O	1:F:306:TRP:HB2	1.78	0.83
1:F:343:THR:HG21	1:F:363:ASN:HA	1.60	0.83



	lous page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:223:ARG:HA	1:A:226:MET:HE3	1.60	0.83	
1:F:346:TYR:HE2	1:F:354:ALA:CA	1.92	0.83	
1:A:163:SER:HB3	1:A:338:LEU:HG	1.61	0.82	
1:E:27:LYS:HG3	1:E:28:ALA:N	1.95	0.82	
1:B:16:PHE:HB3	1:B:48:LEU:HD11	1.62	0.81	
1:H:352:GLN:O	1:H:356:ASP:N	2.11	0.81	
1:E:277:PRO:HB2	1:E:287:ALA:HB1	1.63	0.81	
1:A:305:GLU:HB3	1:A:306:TRP:CE3	2.16	0.80	
1:E:173:THR:HG21	2:E:401:NAD:H4N	1.63	0.79	
1:H:9:ILE:HD12	1:H:19:GLU:HB2	1.63	0.79	
1:G:289:GLN:HG2	1:G:310:TYR:OH	1.82	0.79	
1:D:123:GLU:OE1	1:D:126:THR:HG21	1.83	0.79	
1:E:270:ILE:O	4:E:502:HOH:O	2.02	0.78	
1:A:306:TRP:CD1	1:B:109:THR:HG22	2.19	0.78	
1:C:173:THR:HG22	1:C:315:TYR:HA	1.65	0.78	
1:C:305:GLU:N	4:C:503:HOH:O	2.16	0.78	
1:G:87:PRO:HB3	1:G:99:GLN:HB3	1.64	0.78	
1:C:305:GLU:O	1:C:306:TRP:HB2	1.81	0.78	
1:F:346:TYR:CE2	1:F:354:ALA:HB2	2.19	0.78	
1:A:173:THR:HG21	2:A:401:NAD:H4N	1.66	0.78	
1:F:204:GLN:NE2	4:F:502:HOH:O	2.07	0.77	
1:B:267:CYS:SG	4:B:540:HOH:O	2.43	0.77	
1:C:301:MET:O	4:C:503:HOH:O	2.02	0.77	
1:C:317:LYS:O	4:C:502:HOH:O	2.02	0.77	
1:E:13:ASP:OD2	1:E:15:THR:CB	2.33	0.76	
1:E:305:GLU:O	1:E:306:TRP:HB2	1.86	0.76	
1:F:346:TYR:CE2	1:F:354:ALA:CA	2.68	0.76	
1:A:266:GLU:HB3	1:A:289:GLN:HA	1.68	0.76	
1:D:127:TRP:HB2	1:D:132:ILE:HD13	1.68	0.76	
1:D:305:GLU:O	1:D:306:TRP:HB2	1.85	0.75	
1:A:52:LYS:O	4:A:503:HOH:O	2.05	0.75	
1:B:32:LEU:HD21	1:B:144:TYR:HB3	1.68	0.75	
1:D:286:THR:HG22	1:D:309:ILE:HD12	1.69	0.75	
1:B:305:GLU:O	1:B:306:TRP:HB2	1.85	0.74	
1:F:11:LYS:HE2	1:F:127:TRP:CH2	2.22	0.74	
1:F:19:GLU:HG2	1:F:127:TRP:CD1	2.22	0.74	
1:C:277:PRO:HB2	1:C:287:ALA:HB1	1.69	0.74	
1:C:18:ILE:HG22	1:C:348:LEU:HD22	1.69	0.74	
1:A:305:GLU:O	1:A:306:TRP:HB2	1.85	0.74	
1:B:118:GLY:N	4:B:502:HOH:O	2.16	0.74	
1:F:99:GLN:OE1	4:F:503:HOH:O	2.06	0.74	



	is as page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:346:TYR:CD2	1:F:354:ALA:HB2	2.22	0.73
1:E:245:LEU:HD12	4:E:504:HOH:O	1.88	0.73
1:H:305:GLU:O	1:H:306:TRP:HB2	1.85	0.73
1:G:220:ASN:OD1	1:G:222:GLU:N	2.22	0.73
1:D:116:THR:N	4:D:505:HOH:O	2.20	0.73
1:D:253:LYS:NZ	4:D:504:HOH:O	2.20	0.73
1:B:246:LEU:O	1:B:249:SER:OG	2.04	0.72
1:F:345:THR:HG23	1:F:367:VAL:HG13	1.71	0.72
1:F:99:GLN:O	4:F:504:HOH:O	2.07	0.72
1:F:271:PRO:HA	1:F:293:ILE:HD12	1.69	0.72
1:B:327:LEU:HD22	1:B:336:LEU:HD11	1.70	0.72
1:F:346:TYR:HE2	1:F:354:ALA:N	1.87	0.72
1:A:24:GLU:HB2	1:A:124:GLY:HA2	1.71	0.72
1:F:319:ARG:NH1	1:G:95:GLN:O	2.23	0.72
1:B:24:GLU:HB2	1:B:124:GLY:HA2	1.73	0.71
1:E:349:GLU:OE2	4:E:503:HOH:O	2.09	0.71
1:C:218:ASP:OD1	2:C:401:NAD:O2B	2.08	0.71
1:F:134:ARG:HD3	1:F:139:GLY:HA3	1.72	0.71
1:E:13:ASP:OD2	1:E:15:THR:HB	1.91	0.70
1:G:305:GLU:O	1:G:306:TRP:HB2	1.90	0.70
1:C:298:THR:HG22	1:D:298:THR:HG22	1.73	0.70
1:F:56:MET:HB2	1:F:141:LEU:HD12	1.72	0.70
1:C:289:GLN:NE2	1:C:293:ILE:HD12	2.06	0.70
1:D:119:HIS:HD2	1:D:137:ASN:HA	1.57	0.70
1:H:333:LYS:NZ	4:H:510:HOH:O	2.25	0.70
1:F:226:MET:SD	1:F:364:ALA:HB2	2.32	0.70
1:A:59:GLU:HA	1:A:168:SER:HB2	1.73	0.70
1:F:337:MET:N	4:F:502:HOH:O	1.96	0.70
1:F:344:ARG:HG3	1:F:346:TYR:CE1	2.26	0.70
1:G:119:HIS:HD2	1:G:137:ASN:HA	1.56	0.70
1:G:173:THR:HG22	1:G:315:TYR:HA	1.74	0.70
1:H:251:ASP:OD2	4:H:502:HOH:O	2.09	0.70
1:G:304:PHE:O	4:G:502:HOH:O	2.10	0.69
1:E:13:ASP:OD2	1:E:15:THR:N	2.25	0.69
1:H:24:GLU:HB2	1:H:124:GLY:HA2	1.74	0.69
1:C:286:THR:HG22	1:C:309:ILE:HD12	1.74	0.69
1:A:340:GLU:OE1	4:A:504:HOH:O	2.09	0.69
1:G:217:ILE:HG12	1:G:236:ILE:HB	1.74	0.69
1:E:207:ARG:NH1	1:E:230:PHE:O	2.26	0.69
1:B:173:THR:HG21	2:B:401:NAD:H4N	1.75	0.68
1:E:155:ILE:HG22	1:E:157:THR:OG1	1.93	0.68



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:E:269:ALA:O	4:E:505:HOH:O	2.12	0.68
1:A:343:THR:HG21	1:A:364:ALA:H	1.55	0.68
1:C:13:ASP:N	1:C:13:ASP:OD1	2.22	0.68
1:F:307:ASP:OD1	1:H:313:PRO:HA	1.94	0.68
1:F:346:TYR:CE2	1:F:354:ALA:HA	2.29	0.68
1:A:343:THR:N	4:A:501:HOH:O	2.25	0.68
1:C:29:ASP:OD2	1:C:148:LYS:HE3	1.93	0.68
1:F:346:TYR:HE2	1:F:354:ALA:HA	1.59	0.68
1:E:300:ASP:HB3	1:E:303:LEU:HD23	1.76	0.67
1:B:241:ASN:O	1:B:243:ILE:HD12	1.95	0.67
1:H:173:THR:HG21	2:H:401:NAD:H4N	1.76	0.67
1:C:173:THR:HG21	2:C:401:NAD:H4N	1.76	0.67
1:D:317:LYS:O	4:D:503:HOH:O	2.11	0.67
1:C:314:LEU:HD13	1:D:306:TRP:CZ2	2.30	0.67
1:E:218:ASP:OD1	2:E:401:NAD:O2B	2.12	0.67
1:E:242:ASP:O	4:E:504:HOH:O	2.12	0.66
1:G:67:VAL:HB	1:G:71:VAL:HG21	1.78	0.66
1:D:10:ALA:HB3	1:D:54:ILE:HG22	1.77	0.66
1:A:246:LEU:O	1:A:249:SER:OG	2.14	0.65
1:B:53:PRO:O	1:B:132:ILE:HD11	1.95	0.65
1:G:184:LEU:O	4:G:504:HOH:O	2.13	0.65
1:H:295:GLU:OE1	4:H:503:HOH:O	2.12	0.65
1:A:306:TRP:HD1	1:B:109:THR:HG22	1.58	0.65
1:D:173:THR:HG21	2:D:401:NAD:H4N	1.76	0.65
1:D:266:GLU:HB3	1:D:289:GLN:HA	1.77	0.65
1:F:92:PHE:HD1	1:F:92:PHE:O	1.79	0.65
1:C:27:LYS:HG2	1:C:28:ALA:H	1.62	0.64
1:F:92:PHE:CE1	1:F:96:GLU:HG3	2.31	0.64
1:G:349:GLU:O	4:G:503:HOH:O	2.13	0.64
1:B:59:GLU:HA	1:B:168:SER:HB2	1.79	0.64
1:D:345:THR:HB	1:D:369:ILE:HD13	1.79	0.64
1:G:219:ILE:HG21	1:G:240:LYS:HG3	1.80	0.64
1:G:327:LEU:HD22	1:G:336:LEU:HD11	1.78	0.64
1:F:87:PRO:HD2	1:F:150:SER:HB2	1.80	0.64
1:E:148:LYS:NZ	4:E:506:HOH:O	2.14	0.64
1:F:306:TRP:CZ2	1:H:314:LEU:HD13	2.33	0.64
1:B:346:TYR:HB2	1:B:368:ILE:HD13	1.78	0.63
1:C:223:ARG:NH1	1:C:358:MET:O	2.31	0.63
1:F:340:GLU:OE1	4:F:505:HOH:O	2.16	0.63
1:D:250:GLU:OE1	1:D:254:LYS:HE2	1.98	0.63
1:E:40:LEU:HB3	1:E:358:MET:CE	2.28	0.63



	io ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:34:LYS:HD3	1:A:144:TYR:CE1	2.33	0.63
1:A:134:ARG:HD3	1:A:139:GLY:HA3	1.80	0.63
1:C:223:ARG:HE	1:C:361:GLY:HA2	1.63	0.63
1:G:47:SER:OG	1:G:54:ILE:HD11	2.00	0.62
1:A:173:THR:HG22	1:A:315:TYR:HA	1.79	0.62
1:F:344:ARG:NH2	4:F:509:HOH:O	2.33	0.62
1:F:346:TYR:CE2	1:F:354:ALA:CB	2.81	0.62
1:A:223:ARG:NH1	4:A:502:HOH:O	1.98	0.62
1:B:289:GLN:HG2	1:B:310:TYR:OH	1.99	0.62
1:C:108:VAL:HG12	1:D:306:TRP:HE1	1.65	0.62
1:F:41:CYS:HB2	1:F:59:GLU:OE2	1.99	0.62
1:A:108:VAL:CG1	1:B:306:TRP:HE1	2.13	0.62
1:D:52:LYS:HD3	1:D:133:GLU:OE1	2.00	0.62
1:A:34:LYS:HD2	1:A:143:GLU:O	2.00	0.62
1:B:277:PRO:HB2	1:B:287:ALA:HB1	1.82	0.61
1:A:108:VAL:HG11	1:B:306:TRP:HE1	1.65	0.61
1:B:173:THR:HG22	1:B:315:TYR:HA	1.83	0.61
1:E:121:HIS:ND1	1:E:123:GLU:HG2	2.14	0.61
1:H:36:LYS:O	1:H:369:ILE:HD12	1.99	0.61
1:A:314:LEU:HD13	1:B:306:TRP:CZ2	2.36	0.61
1:D:346:TYR:HD2	1:D:354:ALA:HB2	1.64	0.61
1:A:100:HIS:CE1	1:A:317:LYS:HG3	2.35	0.61
1:G:343:THR:HG21	1:G:364:ALA:H	1.66	0.61
1:H:119:HIS:O	4:H:505:HOH:O	2.16	0.61
1:C:304:PHE:N	4:C:503:HOH:O	2.34	0.60
1:C:108:VAL:CG1	1:D:306:TRP:HE1	2.15	0.60
1:F:19:GLU:HG3	1:F:20:THR:N	2.16	0.60
1:F:162:PRO:HB3	1:F:367:VAL:HG11	1.83	0.60
1:H:134:ARG:HD3	1:H:139:GLY:HA3	1.83	0.60
1:E:24:GLU:HB2	1:E:124:GLY:HA2	1.83	0.60
1:H:32:LEU:HD22	1:H:66:GLN:OE1	2.02	0.60
1:E:207:ARG:NH2	1:E:335:ASP:O	2.35	0.60
1:G:239:ASP:HB3	1:G:241:ASN:OD1	2.02	0.60
1:D:352:GLN:HG3	1:D:356:ASP:OD2	2.02	0.60
1:E:108:VAL:CG1	1:G:306:TRP:HE1	2.16	0.59
1:H:14:GLY:HA2	1:H:48:LEU:HB3	1.82	0.59
1:A:166:ILE:HD11	1:A:338:LEU:HB2	1.84	0.59
1:F:63:PHE:CD2	1:F:77:GLY:HA2	2.37	0.59
1:F:319:ARG:HH12	1:G:96:GLU:HA	1.67	0.59
1:C:223:ARG:NE	1:C:361:GLY:HA2	2.17	0.59
1:F:266:GLU:HB3	1:F:289:GLN:HA	1.85	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:H:289:GLN:NE2	1:H:292:GLY:H	2.00	0.59
1:E:27:LYS:CG	1:E:28:ALA:H	2.04	0.59
1:H:163:SER:HB3	1:H:338:LEU:HG	1.84	0.59
1:D:367:VAL:HG13	1:D:369:ILE:HD11	1.84	0.59
1:E:289:GLN:O	1:E:289:GLN:HG3	2.03	0.59
1:H:50:TRP:HH2	1:H:136:PHE:HE1	1.51	0.59
1:C:306:TRP:HD1	1:D:109:THR:HG22	1.66	0.59
1:F:11:LYS:HE2	1:F:127:TRP:HH2	1.65	0.59
1:F:195:THR:HG21	1:F:216:ALA:HB1	1.85	0.59
1:G:277:PRO:HB2	1:G:287:ALA:HB1	1.83	0.59
1:F:289:GLN:O	1:F:289:GLN:HG3	2.01	0.59
1:D:204:GLN:HG2	1:D:336:LEU:HD12	1.83	0.59
1:E:21:VAL:CG1	1:E:125:THR:HG23	2.32	0.59
1:H:134:ARG:NH1	1:H:146:LEU:H	2.01	0.59
1:D:169:CYS:O	1:D:173:THR:HG23	2.02	0.59
1:F:198:VAL:HG13	1:F:267:CYS:HB3	1.84	0.59
1:A:306:TRP:NE1	1:B:314:LEU:HD22	2.18	0.59
1:F:41:CYS:HB3	1:F:58:HIS:CE1	2.37	0.58
1:F:289:GLN:NE2	4:F:501:HOH:O	2.36	0.58
1:A:98:ASN:HB3	1:A:101:ILE:HG22	1.85	0.58
1:C:312:ASN:OD1	1:C:312:ASN:O	2.22	0.58
1:A:1:MET:N	4:A:513:HOH:O	2.37	0.58
1:A:87:PRO:HB3	1:A:99:GLN:HB3	1.84	0.58
1:E:313:PRO:HA	1:G:307:ASP:OD1	2.04	0.58
1:F:19:GLU:HG3	1:F:20:THR:H	1.67	0.58
1:G:55:VAL:O	1:G:135:SER:HB2	2.04	0.58
1:A:305:GLU:CB	1:A:306:TRP:CE3	2.86	0.58
1:B:105:ASN:OD1	1:B:117:PRO:HB2	2.04	0.58
1:D:63:PHE:CE1	1:D:161:MET:HE3	2.39	0.58
1:H:10:ALA:O	1:H:53:PRO:HA	2.03	0.58
1:G:11:LYS:NZ	4:G:507:HOH:O	2.32	0.58
1:B:217:ILE:HD12	1:B:248:ALA:HB1	1.86	0.57
1:G:259:ARG:NH1	4:G:501:HOH:O	1.98	0.57
1:C:79:TYR:CE2	1:C:155:ILE:HD11	2.39	0.57
1:C:243:ILE:HD12	1:C:243:ILE:H	1.67	0.57
1:H:254:LYS:NZ	4:H:513:HOH:O	2.37	0.57
1:A:306:TRP:HE1	1:B:108:VAL:HG12	1.69	0.57
1:F:80:VAL:HA	1:F:153:VAL:O	2.05	0.57
1:H:344:ARG:HD2	1:H:346:TYR:OH	2.03	0.57
1:D:134:ARG:HB3	1:D:139:GLY:HA3	1.87	0.57
1:E:103:GLU:OE1	1:G:259:ARG:NH2	2.37	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:217:ILE:HG12	1:E:236:ILE:HB	1.87	0.57
1:F:109:THR:HG22	1:H:306:TRP:HD1	1.68	0.57
1:G:116:THR:N	4:G:508:HOH:O	2.38	0.57
1:H:286:THR:HG22	1:H:309:ILE:HD12	1.86	0.57
1:A:59:GLU:OE2	1:A:169:CYS:HB3	2.05	0.57
1:G:59:GLU:HA	1:G:168:SER:HB2	1.86	0.57
1:G:67:VAL:HB	1:G:71:VAL:CG2	2.35	0.57
1:A:16:PHE:CE1	1:A:351:LEU:HD23	2.40	0.57
1:E:41:CYS:HB3	1:E:58:HIS:CE1	2.40	0.57
1:E:267:CYS:O	4:E:507:HOH:O	2.17	0.57
1:F:34:LYS:O	1:F:62:GLY:HA3	2.05	0.57
1:C:134:ARG:NH1	4:C:512:HOH:O	2.38	0.56
1:H:10:ALA:HB2	1:H:56:MET:SD	2.45	0.56
1:A:100:HIS:NE2	1:B:307:ASP:OD2	2.37	0.56
1:B:223:ARG:NH2	1:B:358:MET:O	2.35	0.56
1:G:278:LEU:O	1:G:281:ILE:HG22	2.05	0.56
1:E:204:GLN:HG2	1:E:207:ARG:HH12	1.71	0.56
1:F:51:GLY:O	1:F:52:LYS:HE2	2.05	0.56
1:G:14:GLY:HA2	1:G:48:LEU:HB3	1.88	0.56
1:G:163:SER:HB3	1:G:338:LEU:HG	1.87	0.56
1:F:339:ASP:N	4:F:505:HOH:O	2.36	0.56
1:D:218:ASP:OD1	1:D:219:ILE:N	2.38	0.56
1:H:30:GLU:CG	1:H:148:LYS:HD3	2.36	0.56
1:C:8:ALA:HB2	1:C:348:LEU:HD21	1.88	0.56
1:B:194:GLY:O	1:B:199:GLY:HA3	2.06	0.56
1:E:9:ILE:HD12	1:E:19:GLU:HB2	1.88	0.56
1:F:217:ILE:HD13	1:F:248:ALA:HB1	1.87	0.56
1:F:307:ASP:OD2	1:H:100:HIS:NE2	2.37	0.56
1:G:36:LYS:HG3	1:G:63:PHE:CE2	2.41	0.56
1:C:243:ILE:O	1:C:246:LEU:HG	2.05	0.56
1:D:64:VAL:HG21	1:D:74:LEU:HD13	1.86	0.56
1:B:155:ILE:HG21	1:B:328:VAL:HG21	1.87	0.55
1:B:169:CYS:O	1:B:173:THR:HG23	2.05	0.55
1:C:127:TRP:HB2	1:C:132:ILE:HD13	1.88	0.55
1:C:306:TRP:HE1	1:D:108:VAL:HG12	1.71	0.55
1:F:345:THR:HG22	1:F:369:ILE:HB	1.87	0.55
1:F:346:TYR:CE2	1:F:354:ALA:N	2.71	0.55
1:F:348:LEU:HD23	1:F:368:ILE:HG21	1.89	0.55
1:C:306:TRP:CE2	1:D:314:LEU:HD12	2.42	0.55
1:C:41:CYS:HB3	1:C:58:HIS:CE1	2.42	0.55
1:D:306:TRP:N	1:D:306:TRP:HE3	2.05	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:32:LEU:HD11	1:G:144:TYR:HB3	1.88	0.55
1:H:277:PRO:HB2	1:H:287:ALA:HB1	1.89	0.55
1:F:27:LYS:H	1:F:30:GLU:CG	2.19	0.55
1:H:54:ILE:HD12	1:H:135:SER:HB3	1.88	0.55
1:H:56:MET:HB2	1:H:141:LEU:HD12	1.89	0.55
1:H:281:ILE:HD12	1:H:287:ALA:HB2	1.88	0.55
1:B:163:SER:HB3	1:B:338:LEU:HG	1.87	0.54
1:E:343:THR:HB	1:E:363:ASN:OD1	2.07	0.54
1:H:302:ARG:HA	1:H:305:GLU:HG3	1.87	0.54
1:G:44:ASP:O	1:G:47:SER:HB3	2.06	0.54
1:H:6:LYS:HD2	1:H:20:THR:HG23	1.88	0.54
1:A:54:ILE:HD12	1:A:135:SER:HB3	1.88	0.54
1:D:167:ILE:HA	1:D:171:VAL:HB	1.89	0.54
1:A:11:LYS:N	4:A:511:HOH:O	2.31	0.54
1:E:223:ARG:HD3	1:E:361:GLY:HA2	1.90	0.54
1:F:312:ASN:ND2	1:H:305:GLU:HG2	2.23	0.54
1:A:217:ILE:HG12	1:A:236:ILE:HB	1.90	0.54
1:C:207:ARG:NH2	1:C:230:PHE:O	2.39	0.54
1:D:13:ASP:OD1	1:D:15:THR:HG22	2.07	0.54
1:A:173:THR:HG21	2:A:401:NAD:C4N	2.37	0.54
1:C:200:LEU:HA	1:C:203:ILE:HD12	1.88	0.54
1:A:134:ARG:NH1	1:A:145:THR:HA	2.22	0.54
1:E:221:GLN:HG3	1:E:237:LEU:HD13	1.89	0.54
1:G:219:ILE:HD13	1:G:238:ALA:HB3	1.90	0.54
1:E:306:TRP:HD1	1:G:109:THR:HG22	1.73	0.54
1:C:218:ASP:HB3	1:C:224:LEU:HG	1.90	0.54
1:E:108:VAL:HG12	1:G:306:TRP:HE1	1.73	0.54
1:G:245:LEU:HB3	1:G:248:ALA:HB3	1.90	0.54
1:E:126:THR:HA	1:E:131:PRO:HA	1.90	0.53
1:G:193:LEU:O	1:G:267:CYS:N	2.39	0.53
1:H:87:PRO:HD2	1:H:150:SER:HB2	1.90	0.53
1:D:314:LEU:HD23	1:D:315:TYR:HB2	1.90	0.53
1:B:9:ILE:HD12	1:B:19:GLU:HB2	1.90	0.53
1:H:351:LEU:HG	1:H:355:PHE:CE2	2.44	0.53
1:D:352:GLN:O	1:D:356:ASP:OD2	2.25	0.53
1:E:59:GLU:HA	1:E:168:SER:HB2	1.91	0.53
1:F:44:ASP:HB2	1:F:58:HIS:CE1	2.44	0.53
1:E:98:ASN:HA	1:E:100:HIS:CE1	2.43	0.53
1:E:266:GLU:HB3	1:E:289:GLN:HA	1.89	0.53
1:E:319:ARG:HH12	1:H:96:GLU:CD	2.13	0.53
1:F:122:LEU:HD11	1:F:133:GLU:HA	1.90	0.53



	, and pagetti	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:198:VAL:HG12	2:F:401:NAD:O2N	2.08	0.53
1:D:355:PHE:O	1:D:358:MET:N	2.40	0.53
1:F:109:THR:HG22	1:H:306:TRP:CD1	2.44	0.53
1:F:306:TRP:HE3	1:F:306:TRP:N	2.07	0.53
1:F:349:GLU:OE1	1:F:349:GLU:N	2.25	0.53
1:E:67:VAL:HG22	1:E:71:VAL:HB	1.90	0.53
1:F:56:MET:CB	1:F:141:LEU:HD12	2.38	0.53
1:H:230:PHE:CZ	1:H:341:MET:HG2	2.44	0.53
1:B:16:PHE:HE2	1:B:351:LEU:HB3	1.74	0.52
1:E:348:LEU:HD22	1:E:370:PHE:HE1	1.74	0.52
1:F:86:THR:HG22	1:F:151:ALA:HB2	1.91	0.52
1:E:281:ILE:HG13	1:E:308:LYS:HE2	1.91	0.52
1:E:256:THR:HG21	1:E:260:GLY:H	1.74	0.52
1:E:311:ILE:HD12	1:G:309:ILE:HG12	1.92	0.52
1:A:167:ILE:HA	1:A:171:VAL:HB	1.91	0.52
1:C:266:GLU:HB2	1:C:277:PRO:HG3	1.90	0.52
1:B:87:PRO:HB3	1:B:99:GLN:HB3	1.92	0.52
1:C:145:THR:HA	4:C:512:HOH:O	2.09	0.52
1:C:327:LEU:HD22	1:C:336:LEU:HD11	1.91	0.52
1:D:26:PRO:HD2	1:D:66:GLN:HE21	1.74	0.52
1:A:319:ARG:NH1	4:A:512:HOH:O	2.33	0.52
1:B:10:ALA:O	1:B:53:PRO:HA	2.09	0.52
1:E:306:TRP:CE3	1:E:306:TRP:N	2.78	0.52
1:G:275:ALA:HB2	1:G:299:ILE:HG23	1.92	0.52
1:A:307:ASP:OD1	1:B:313:PRO:HA	2.09	0.52
1:C:246:LEU:O	1:C:249:SER:HB3	2.09	0.52
1:A:6:LYS:HG2	1:A:143:GLU:HG3	1.91	0.52
1:H:352:GLN:HA	1:H:355:PHE:HB2	1.91	0.52
1:F:32:LEU:HD12	1:F:145:THR:O	2.11	0.51
1:F:64:VAL:HG21	1:F:74:LEU:HD13	1.91	0.51
1:F:92:PHE:CD1	1:F:92:PHE:C	2.83	0.51
1:G:119:HIS:O	1:G:148:LYS:HE2	2.11	0.51
1:H:163:SER:OG	1:H:339:ASP:OD1	2.16	0.51
1:H:266:GLU:HB3	1:H:289:GLN:HA	1.91	0.51
1:A:235:THR:OG1	4:A:505:HOH:O	2.17	0.51
1:E:194:GLY:O	1:E:199:GLY:HA3	2.09	0.51
1:H:353:GLN:O	1:H:357:ASP:OD1	2.28	0.51
1:C:119:HIS:HD2	1:C:137:ASN:HA	1.75	0.51
1:E:121:HIS:HB2	1:E:123:GLU:OE2	2.10	0.51
1:E:312:ASN:OD1	1:E:312:ASN:O	2.29	0.51
1:E:349:GLU:O	4:E:508:HOH:O	2.19	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:265:PHE:CD1	1:D:288:VAL:HB	2.45	0.51
1:G:182:ALA:HB2	1:G:288:VAL:HG21	1.93	0.51
1:A:234:HIS:CD2	1:A:255:LEU:HD22	2.46	0.51
1:B:52:LYS:HD2	1:B:54:ILE:HD11	1.92	0.51
1:F:345:THR:CG2	1:F:369:ILE:HB	2.41	0.51
1:H:30:GLU:HG2	1:H:148:LYS:HD3	1.92	0.51
1:F:41:CYS:HB3	1:F:58:HIS:HE1	1.76	0.51
1:F:347:PRO:HD2	1:F:350:ASN:HB2	1.92	0.51
1:H:12:GLY:HA2	1:H:50:TRP:O	2.11	0.51
1:B:37:ALA:HB1	1:B:367:VAL:HG11	1.93	0.51
1:A:195:THR:HG21	1:A:216:ALA:HB1	1.93	0.51
1:A:305:GLU:HG2	1:B:312:ASN:ND2	2.25	0.51
1:C:259:ARG:NH2	4:C:504:HOH:O	2.04	0.51
1:H:289:GLN:O	1:H:312:ASN:ND2	2.44	0.51
1:B:54:ILE:CG2	1:B:135:SER:HB3	2.41	0.50
1:F:100:HIS:CD2	1:F:317:LYS:HA	2.47	0.50
1:G:80:VAL:HA	1:G:153:VAL:O	2.11	0.50
1:D:72:THR:N	4:D:512:HOH:O	2.44	0.50
1:B:137:ASN:O	4:B:506:HOH:O	2.20	0.50
1:D:306:TRP:N	1:D:306:TRP:CE3	2.80	0.50
1:A:16:PHE:HB3	1:A:48:LEU:CD2	2.41	0.50
1:A:299:ILE:HD12	1:B:299:ILE:HD12	1.92	0.50
1:D:100:HIS:CE1	1:D:317:LYS:HA	2.47	0.50
1:H:218:ASP:OD1	2:H:401:NAD:H1B	2.12	0.50
1:A:18:ILE:HD12	1:A:348:LEU:HG	1.93	0.50
1:A:338:LEU:HD23	1:A:339:ASP:H	1.77	0.50
1:B:106:SER:OG	4:B:504:HOH:O	2.19	0.50
1:C:24:GLU:HB2	1:C:124:GLY:HA2	1.94	0.50
1:F:344:ARG:CG	1:F:346:TYR:CE1	2.95	0.50
1:H:270:ILE:HB	1:H:273:LEU:HD12	1.94	0.50
1:B:242:ASP:OD1	1:B:247:LYS:HG3	2.12	0.50
1:C:25:SER:HB2	1:C:26:PRO:HD2	1.93	0.50
1:E:42:HIS:HB2	2:E:401:NAD:O3	2.11	0.50
1:A:194:GLY:O	1:A:199:GLY:HA3	2.12	0.50
1:A:306:TRP:HZ2	1:B:108:VAL:HG11	1.77	0.50
1:B:333:LYS:HE2	1:D:207:ARG:HH11	1.77	0.50
1:F:19:GLU:HG2	1:F:127:TRP:NE1	2.26	0.50
1:E:20:THR:O	4:E:509:HOH:O	2.19	0.49
1:H:59:GLU:HA	1:H:168:SER:HB2	1.94	0.49
1:B:36:LYS:O	1:B:369:ILE:HD12	2.11	0.49
1:B:269:ALA:O	4:B:505:HOH:O	2.20	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:284:ALA:HA	1:D:307:ASP:O	2.12	0.49
1:G:220:ASN:OD1	1:G:220:ASN:C	2.50	0.49
1:H:289:GLN:NE2	1:H:312:ASN:HD22	2.09	0.49
1:B:266:GLU:HB3	1:B:289:GLN:HA	1.93	0.49
1:F:299:ILE:HD12	1:H:299:ILE:HD12	1.94	0.49
1:G:100:HIS:CG	1:G:317:LYS:HA	2.47	0.49
1:C:36:LYS:HG2	1:C:36:LYS:O	2.13	0.49
1:E:26:PRO:HA	1:E:146:LEU:HD11	1.93	0.49
1:A:306:TRP:CZ2	1:B:108:VAL:HG11	2.47	0.49
1:C:19:GLU:HG3	1:C:127:TRP:NE1	2.28	0.49
1:D:173:THR:HG21	2:D:401:NAD:C4N	2.43	0.49
1:A:22:GLN:O	1:A:125:THR:HA	2.12	0.49
1:E:40:LEU:HB3	1:E:358:MET:HE3	1.95	0.49
1:F:294:GLU:HA	1:H:302:ARG:HG2	1.95	0.49
1:A:213:LYS:HG2	1:A:215:ILE:HD11	1.95	0.49
1:B:56:MET:HB2	1:B:141:LEU:HD12	1.95	0.49
1:F:134:ARG:HH12	1:F:146:LEU:H	1.61	0.49
1:H:12:GLY:O	4:H:506:HOH:O	2.20	0.49
1:H:219:ILE:HD13	1:H:240:LYS:HG3	1.95	0.49
1:G:92:PHE:O	1:G:96:GLU:HG2	2.13	0.49
1:A:169:CYS:O	1:A:173:THR:HG23	2.13	0.49
1:F:134:ARG:NH1	1:F:146:LEU:H	2.11	0.49
1:F:314:LEU:HD13	1:H:306:TRP:CZ2	2.48	0.49
1:B:281:ILE:HG22	1:B:282:ARG:O	2.12	0.49
1:C:169:CYS:O	1:C:173:THR:HG23	2.13	0.49
1:F:27:LYS:H	1:F:30:GLU:HG2	1.78	0.49
1:F:198:VAL:HG21	1:F:290:VAL:HG11	1.95	0.49
1:G:346:TYR:HB2	1:G:368:ILE:CD1	2.43	0.49
1:G:34:LYS:HD3	1:G:143:GLU:O	2.13	0.48
1:H:306:TRP:HE3	1:H:306:TRP:N	2.10	0.48
1:E:289:GLN:CG	1:E:312:ASN:HB2	2.43	0.48
1:F:24:GLU:HB2	1:F:124:GLY:HA2	1.95	0.48
1:F:313:PRO:HA	1:H:307:ASP:OD1	2.12	0.48
1:G:173:THR:HG21	2:G:401:NAD:H4N	1.94	0.48
1:H:30:GLU:CG	1:H:148:LYS:CD	2.91	0.48
1:B:54:ILE:HG21	1:B:135:SER:HB3	1.95	0.48
1:E:289:GLN:HG3	1:E:312:ASN:HB2	1.94	0.48
1:H:50:TRP:HH2	1:H:136:PHE:CE1	2.31	0.48
1:C:217:ILE:HD12	1:C:248:ALA:HB1	1.96	0.48
1:D:347:PRO:HD2	1:D:350:ASN:HB2	1.94	0.48
1:F:100:HIS:CE1	1:F:317:LYS:HA	2.48	0.48



	A	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:166:ILE:HG21	1:F:365:LYS:HG2	1.94	0.48
1:E:52:LYS:HD2	1:E:54:ILE:HD11	1.94	0.48
1:F:59:GLU:O	1:F:140:THR:OG1	2.26	0.48
1:E:40:LEU:HD23	1:E:358:MET:SD	2.54	0.48
1:F:180:ASN:O	1:F:317:LYS:HD3	2.14	0.48
1:F:207:ARG:NH1	1:F:335:ASP:O	2.47	0.48
1:G:291:SER:O	2:G:401:NAD:H1D	2.13	0.48
1:A:344:ARG:HD2	1:A:363:ASN:OD1	2.13	0.48
1:C:306:TRP:HE3	1:C:306:TRP:N	2.11	0.48
1:H:242:ASP:OD2	1:H:247:LYS:HB2	2.12	0.48
1:A:47:SER:HB3	1:A:54:ILE:HD11	1.96	0.48
1:A:360:THR:HB	1:A:362:LYS:NZ	2.29	0.48
1:B:344:ARG:HG3	1:B:344:ARG:HH11	1.78	0.48
1:G:169:CYS:O	1:G:173:THR:HG23	2.14	0.48
1:H:25:SER:OG	1:H:26:PRO:HD2	2.13	0.48
1:H:173:THR:HG21	2:H:401:NAD:C4N	2.42	0.48
1:A:59:GLU:HA	1:A:168:SER:CB	2.44	0.48
1:D:194:GLY:O	1:D:199:GLY:HA3	2.14	0.48
1:G:50:TRP:CD1	1:G:50:TRP:N	2.80	0.48
1:H:24:GLU:OE1	1:H:121:HIS:HE1	1.97	0.48
1:H:50:TRP:CH2	1:H:136:PHE:HE1	2.32	0.48
1:F:358:MET:HE3	1:F:358:MET:HB3	1.78	0.48
1:A:294:GLU:HA	1:B:302:ARG:HG3	1.97	0.47
1:H:40:LEU:HD23	1:H:41:CYS:N	2.29	0.47
1:B:44:ASP:O	1:B:47:SER:HB3	2.14	0.47
1:D:24:GLU:N	1:D:124:GLY:O	2.40	0.47
1:E:314:LEU:HD13	1:G:306:TRP:CZ2	2.49	0.47
1:G:100:HIS:CD2	1:G:317:LYS:HA	2.49	0.47
1:H:101:ILE:O	4:H:508:HOH:O	2.20	0.47
1:H:159:MET:HE2	1:H:159:MET:HB2	1.63	0.47
1:A:306:TRP:HE1	1:B:108:VAL:CG1	2.27	0.47
1:B:53:PRO:C	1:B:132:ILE:HD11	2.35	0.47
1:F:246:LEU:O	1:F:249:SER:HB3	2.15	0.47
1:G:30:GLU:HA	1:G:148:LYS:HA	1.95	0.47
1:G:81:ILE:HG12	1:G:164:ALA:HB1	1.97	0.47
1:E:47:SER:HA	1:E:50:TRP:CE2	2.49	0.47
1:H:134:ARG:HH12	1:H:146:LEU:H	1.62	0.47
1:C:195:THR:HG21	1:C:216:ALA:HB1	1.97	0.47
1:C:222:GLU:O	1:C:226:MET:HG3	2.15	0.47
1:C:266:GLU:HB2	1:C:277:PRO:CG	2.45	0.47
1:D:331:TYR:CD2	1:D:338:LEU:HD12	2.50	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:401:NAD:H6N	4:D:516:HOH:O	2.14	0.47
1:E:167:ILE:HA	1:E:171:VAL:HB	1.96	0.47
1:E:311:ILE:HG13	1:G:308:LYS:O	2.14	0.47
1:F:326:LYS:NZ	4:F:506:HOH:O	2.22	0.47
1:H:125:THR:OG1	1:H:134:ARG:NH2	2.48	0.47
1:A:312:ASN:ND2	1:B:305:GLU:HG2	2.28	0.47
1:C:306:TRP:N	1:C:306:TRP:CE3	2.83	0.47
1:F:98:ASN:HA	1:F:100:HIS:CE1	2.50	0.47
1:F:305:GLU:HB3	1:F:306:TRP:CE3	2.49	0.47
1:F:344:ARG:HG3	1:F:346:TYR:CD1	2.49	0.47
1:G:195:THR:HG21	1:G:216:ALA:HB1	1.97	0.47
1:H:157:THR:HG22	1:H:332:GLU:OE2	2.15	0.47
1:F:30:GLU:HB2	1:F:147:VAL:O	2.15	0.47
1:G:31:VAL:HG21	1:G:74:LEU:HD11	1.97	0.47
1:H:169:CYS:SG	4:H:535:HOH:O	2.61	0.47
1:A:360:THR:HB	1:A:362:LYS:HZ2	1.80	0.47
1:G:271:PRO:HB3	1:G:293:ILE:HG23	1.96	0.47
1:H:271:PRO:HA	1:H:293:ILE:HD13	1.97	0.47
1:B:126:THR:HG22	1:B:131:PRO:HA	1.97	0.47
1:H:46:ASP:OD2	4:H:507:HOH:O	2.20	0.47
1:A:195:THR:HB	1:A:200:LEU:HD23	1.96	0.46
1:A:242:ASP:OD2	1:A:245:LEU:HA	2.15	0.46
1:C:191:VAL:HG22	1:C:215:ILE:HB	1.98	0.46
1:E:198:VAL:HG12	2:E:401:NAD:O2N	2.15	0.46
1:A:117:PRO:O	1:A:148:LYS:HD2	2.14	0.46
1:F:127:TRP:O	1:F:129:ASP:N	2.48	0.46
1:F:306:TRP:N	1:F:306:TRP:CE3	2.82	0.46
2:G:401:NAD:H6N	2:G:401:NAD:H2D	1.72	0.46
1:B:100:HIS:CD2	1:B:317:LYS:HA	2.50	0.46
1:B:209:SER:OG	4:B:507:HOH:O	2.21	0.46
1:F:84:TRP:CE2	1:F:315:TYR:CE2	3.03	0.46
1:G:34:LYS:NZ	1:G:36:LYS:NZ	2.63	0.46
1:G:39:GLY:O	1:G:59:GLU:HB2	2.15	0.46
1:H:27:LYS:HE2	1:H:121:HIS:CG	2.50	0.46
1:A:133:GLU:OE1	4:A:506:HOH:O	2.20	0.46
1:C:81:ILE:HG12	1:C:164:ALA:HB1	1.96	0.46
1:C:306:TRP:CD1	1:D:109:THR:HG22	2.47	0.46
1:F:58:HIS:HA	1:F:138:ILE:HD11	1.96	0.46
1:F:92:PHE:O	1:F:92:PHE:CD1	2.65	0.46
1:H:306:TRP:N	1:H:306:TRP:CE3	2.83	0.46
1:A:284:ALA:HA	1:A:307:ASP:O	2.15	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:223:ARG:O	1:C:227:ALA:N	2.45	0.46
1:D:32:LEU:HB3	1:D:66:GLN:HB2	1.98	0.46
1:E:219:ILE:HG12	2:E:401:NAD:C5A	2.46	0.46
1:F:159:MET:HE2	1:F:164:ALA:HB2	1.97	0.46
1:G:208:ILE:HG12	1:G:335:ASP:HB3	1.97	0.46
1:H:50:TRP:CD1	1:H:50:TRP:N	2.81	0.46
1:A:13:ASP:OD1	1:A:13:ASP:N	2.49	0.46
1:B:40:LEU:HD11	1:B:351:LEU:HD12	1.96	0.46
1:E:82:LEU:HA	1:E:151:ALA:O	2.14	0.46
1:E:103:GLU:OE2	1:G:259:ARG:HD3	2.16	0.46
1:C:26:PRO:HA	1:C:146:LEU:HD11	1.97	0.46
1:D:34:LYS:HB2	1:D:144:TYR:CE1	2.50	0.46
1:D:98:ASN:HB3	1:D:101:ILE:CG1	2.45	0.46
1:H:11:LYS:HB2	1:H:13:ASP:OD1	2.15	0.46
1:H:219:ILE:CD1	1:H:240:LYS:HG3	2.46	0.46
1:B:67:VAL:HG22	1:B:71:VAL:HB	1.97	0.46
1:B:84:TRP:CH2	1:B:315:TYR:HB2	2.51	0.46
1:D:302:ARG:HA	1:D:305:GLU:HG3	1.98	0.46
1:E:198:VAL:CG1	1:E:267:CYS:HB2	2.46	0.46
1:F:63:PHE:HD2	1:F:77:GLY:HA2	1.79	0.46
1:G:245:LEU:HD12	1:G:248:ALA:HB2	1.97	0.46
1:D:26:PRO:CD	1:D:66:GLN:HE21	2.29	0.46
1:D:163:SER:HB3	1:D:338:LEU:CB	2.46	0.46
1:D:200:LEU:HA	1:D:203:ILE:HD12	1.98	0.46
1:E:346:TYR:HB2	1:E:368:ILE:HD13	1.96	0.46
1:F:207:ARG:NH2	1:F:230:PHE:O	2.49	0.46
1:F:261:ALA:O	1:F:282:ARG:HG2	2.16	0.46
1:G:116:THR:O	1:G:119:HIS:HB3	2.16	0.46
1:A:10:ALA:O	1:A:53:PRO:HA	2.16	0.46
1:C:40:LEU:HD23	1:C:41:CYS:N	2.31	0.46
1:D:175:TYR:CZ	1:D:179:VAL:HG21	2.50	0.46
1:E:172:MET:SD	1:E:324:PHE:HE1	2.39	0.46
1:F:92:PHE:CD1	1:F:96:GLU:HG3	2.51	0.46
1:H:30:GLU:HG2	1:H:148:LYS:CD	2.45	0.46
1:H:166:ILE:HD13	1:H:342:ILE:HD11	1.97	0.46
1:E:306:TRP:N	1:E:306:TRP:HE3	2.13	0.45
1:F:344:ARG:CG	1:F:346:TYR:HE1	2.30	0.45
1:C:46:ASP:HA	1:C:49:ASN:OD1	2.17	0.45
1:C:289:GLN:HB3	1:C:312:ASN:HB2	1.99	0.45
1:F:169:CYS:O	1:F:173:THR:HG23	2.17	0.45
1:H:350:ASN:HB3	1:H:353:GLN:HG2	1.97	0.45



	to do pagom	Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance (Å)		
1:B:217:ILE:HA	1:B:236:ILE:O	2.16	0.45	
1:E:81:ILE:HG13	1:E:155:ILE:HG13	1.98	0.45	
1:G:36:LYS:HG3	1:G:63:PHE:HE2	1.79	0.45	
1:G:197:GLY:O	1:G:201:ASN:ND2	2.50	0.45	
1:A:305:GLU:HB3	1:A:306:TRP:CD2	2.51	0.45	
1:C:91:CYS:O	1:C:95:GLN:HG3	2.16	0.45	
1:F:277:PRO:HB2	1:F:287:ALA:HB1	1.97	0.45	
1:H:193:LEU:HD23	1:H:217:ILE:HG23	1.99	0.45	
1:A:101:ILE:CD1	1:B:306:TRP:HD1	2.29	0.45	
1:C:34:LYS:HD3	4:C:519:HOH:O	2.16	0.45	
1:D:134:ARG:NH1	1:D:145:THR:HG22	2.31	0.45	
1:G:276:ALA:N	1:G:277:PRO:HD2	2.31	0.45	
1:C:26:PRO:HD2	1:C:66:GLN:OE1	2.17	0.45	
1:C:277:PRO:CB	1:C:287:ALA:HB1	2.44	0.45	
1:C:292:GLY:HA2	1:C:312:ASN:HD21	1.81	0.45	
1:F:27:LYS:NZ	4:F:513:HOH:O	2.48	0.45	
1:G:79:TYR:CE1	1:G:161:MET:SD	3.10	0.45	
1:A:223:ARG:CA	1:A:226:MET:HE3	2.38	0.45	
1:B:40:LEU:HD11	1:B:351:LEU:CD1	2.47	0.45	
1:C:265:PHE:HA	1:C:288:VAL:O	2.17	0.45	
1:D:21:VAL:HG21	1:D:125:THR:HG23	1.99	0.45	
1:D:352:GLN:O	1:D:356:ASP:HB2	2.17	0.45	
1:E:84:TRP:CB	1:E:136:PHE:HB3	2.47	0.45	
1:F:344:ARG:NE	1:F:345:THR:H	2.15	0.45	
1:G:98:ASN:HB3	1:G:101:ILE:HG12	1.99	0.45	
1:G:197:GLY:HA2	1:G:365:LYS:HD3	1.97	0.45	
1:G:306:TRP:N	1:G:306:TRP:HE3	2.14	0.45	
1:E:174:GLY:O	1:E:178:VAL:HG23	2.17	0.45	
1:H:73:ASN:HB2	1:H:74:LEU:HD22	1.98	0.45	
1:H:203:ILE:HG23	1:H:214:ILE:HG21	1.98	0.45	
1:B:32:LEU:CD2	1:B:144:TYR:HB3	2.43	0.45	
1:B:264:ALA:N	1:B:281:ILE:HD11	2.32	0.45	
1:C:142:SER:HB3	1:C:145:THR:HG22	1.99	0.45	
1:D:13:ASP:OD1	1:D:15:THR:N	2.48	0.45	
1:H:24:GLU:N	1:H:124:GLY:O	2.38	0.45	
1:H:34:LYS:HD2	1:H:143:GLU:O	2.17	0.45	
1:B:173:THR:HG22	1:B:315:TYR:HD1	1.82	0.45	
1:E:87:PRO:HB3	1:E:99:GLN:HB3	1.98	0.45	
1:G:346:TYR:HB2	1:G:368:ILE:HD13	1.97	0.45	
1:A:55:VAL:HG11	1:A:134:ARG:HE	1.82	0.44	
1:C:40:LEU:HD22	1:C:358:MET:SD	2.57	0.44	



	to do pagom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:305:GLU:HG2	1:D:312:ASN:ND2	2.32	0.44	
1:D:105:ASN:OD1	1:D:117:PRO:HB2	2.16	0.44	
1:F:163:SER:HB2	1:F:338:LEU:HG	1.99	0.44	
1:G:230:PHE:CZ	1:G:341:MET:HG2	2.52	0.44	
1:A:191:VAL:HG22	1:A:215:ILE:HB	1.99	0.44	
1:C:322:VAL:HG12	1:C:326:LYS:HE3	1.98	0.44	
1:D:59:GLU:HA	1:D:168:SER:OG	2.17	0.44	
1:D:82:LEU:HA	1:D:151:ALA:O	2.18	0.44	
1:D:277:PRO:HB2	1:D:287:ALA:HB1	1.99	0.44	
1:E:292:GLY:HA2	1:E:312:ASN:HD21	1.81	0.44	
1:F:108:VAL:HG12	1:H:306:TRP:HE1	1.82	0.44	
1:A:41:CYS:HB3	1:A:58:HIS:CE1	2.52	0.44	
1:B:228:LEU:HD21	1:B:235:THR:HG23	1.99	0.44	
1:C:167:ILE:HA	1:C:171:VAL:HB	1.98	0.44	
1:C:195:THR:HG22	1:C:203:ILE:HD11	2.00	0.44	
1:D:216:ALA:HB3	1:D:235:THR:HG22	2.00	0.44	
1:E:222:GLU:O	1:E:226:MET:HG3	2.17	0.44	
1:F:31:VAL:HG21	1:F:74:LEU:HD21	1.99	0.44	
1:G:119:HIS:CD2	1:G:137:ASN:HA	2.45	0.44	
1:G:238:ALA:HB1	1:G:245:LEU:HD11	1.99	0.44	
1:A:192:VAL:HG21	1:A:203:ILE:HG13	1.98	0.44	
1:F:271:PRO:HB3	1:F:293:ILE:HG23	1.99	0.44	
1:A:81:ILE:HD11	1:A:155:ILE:HD13	2.00	0.44	
1:A:266:GLU:HG2	1:A:289:GLN:HG3	1.99	0.44	
1:A:306:TRP:HE3	1:A:306:TRP:N	2.15	0.44	
1:C:19:GLU:CG	1:C:127:TRP:NE1	2.81	0.44	
1:E:13:ASP:OD2	1:E:15:THR:CA	2.65	0.44	
1:E:195:THR:HG21	1:E:216:ALA:HB1	1.99	0.44	
1:F:204:GLN:CD	4:F:502:HOH:O	2.48	0.44	
1:H:16:PHE:CZ	1:H:351:LEU:HB3	2.53	0.44	
1:H:219:ILE:HD12	4:H:511:HOH:O	2.18	0.44	
1:H:350:ASN:HB3	1:H:353:GLN:CG	2.48	0.44	
1:A:176:GLY:O	1:A:180:ASN:N	2.47	0.44	
1:B:281:ILE:HD13	1:B:281:ILE:HA	1.75	0.44	
1:C:59:GLU:HA	1:C:168:SER:HB2	2.00	0.44	
1:C:219:ILE:HD11	1:C:240:LYS:N	2.32	0.44	
1:E:16:PHE:HZ	1:E:352:GLN:HB2	1.81	0.44	
1:G:265:PHE:HA	1:G:288:VAL:O	2.18	0.44	
1:B:306:TRP:N	1:B:306:TRP:HE3	2.15	0.44	
1:C:263:TYR:HA	1:C:281:ILE:HD11	2.00	0.44	
1:D:163:SER:HB3	1:D:338:LEU:HB2	1.99	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:E:300:ASP:HB3	1:E:303:LEU:CD2	2.46	0.44	
1:G:107:PRO:HB2	1:G:136:PHE:HD1	1.81	0.44	
1:H:59:GLU:HG2	1:H:169:CYS:HB2	2.00	0.44	
1:B:277:PRO:O	1:B:281:ILE:HG12	2.18	0.44	
1:H:193:LEU:HD23	1:H:217:ILE:CG2	2.48	0.44	
1:H:216:ALA:O	1:H:235:THR:HA	2.18	0.44	
1:D:27:LYS:O	1:D:68:GLY:HA3	2.17	0.43	
1:D:173:THR:HG22	1:D:315:TYR:HD1	1.83	0.43	
1:E:246:LEU:O	1:E:249:SER:OG	2.22	0.43	
1:F:344:ARG:CB	1:F:346:TYR:HE1	2.30	0.43	
1:H:351:LEU:HG	1:H:355:PHE:CD2	2.53	0.43	
1:D:13:ASP:OD1	1:D:14:GLY:N	2.51	0.43	
1:E:305:GLU:HB3	1:E:306:TRP:CD2	2.53	0.43	
1:A:36:LYS:HG2	1:A:62:GLY:HA2	2.00	0.43	
1:B:217:ILE:CD1	1:B:248:ALA:HB1	2.47	0.43	
1:B:327:LEU:HD23	1:B:327:LEU:HA	1.87	0.43	
1:C:100:HIS:CD2	1:C:317:LYS:HA	2.54	0.43	
1:D:82:LEU:HD13	1:D:140:THR:HG22	1.99	0.43	
1:E:217:ILE:HA	1:E:236:ILE:O	2.18	0.43	
1:G:271:PRO:HA	1:G:293:ILE:HG12	2.00	0.43	
1:D:81:ILE:HD11	1:D:155:ILE:HD13	2.00	0.43	
1:E:336:LEU:HD12	1:E:336:LEU:HA	1.83	0.43	
1:H:30:GLU:HG3	1:H:148:LYS:CD	2.47	0.43	
1:H:179:VAL:O	1:H:183:LYS:HA	2.18	0.43	
1:F:358:MET:HA	1:F:363:ASN:HB2	2.00	0.43	
1:A:346:TYR:HB2	1:A:368:ILE:HD13	2.00	0.43	
1:B:121:HIS:O	4:B:508:HOH:O	2.21	0.43	
1:B:270:ILE:HB	1:B:273:LEU:HD12	1.99	0.43	
2:D:401:NAD:H6N	2:D:401:NAD:H2D	1.80	0.43	
1:F:34:LYS:NZ	1:F:35:VAL:O	2.51	0.43	
1:F:175:TYR:CZ	1:F:179:VAL:HG21	2.54	0.43	
1:F:344:ARG:HB3	1:F:346:TYR:HE1	1.82	0.43	
1:G:87:PRO:CB	1:G:99:GLN:HB3	2.43	0.43	
1:A:223:ARG:O	1:A:226:MET:HB2	2.19	0.43	
1:C:224:LEU:HD23	1:C:224:LEU:HA	1.89	0.43	
1:E:52:LYS:HG3	1:E:54:ILE:HG13	2.01	0.43	
1:G:122:LEU:O	1:G:131:PRO:HB3	2.19	0.43	
1:H:6:LYS:N	1:H:143:GLU:OE2	2.42	0.43	
1:B:29:ASP:OD1	1:B:29:ASP:N	2.45	0.43	
1:D:54:ILE:HD11	1:D:135:SER:HA	2.00	0.43	
1:D:79:TYR:CZ	1:D:155:ILE:HD11	2.53	0.43	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:F:55:VAL:HG11	1:F:134:ARG:HE	1.84	0.43	
1:H:276:ALA:N	1:H:277:PRO:HD2	2.33	0.43	
1:D:122:LEU:HD23	1:D:122:LEU:HA	1.88	0.43	
1:E:83:ASN:ND2	1:E:150:SER:O	2.46	0.43	
1:E:239:ASP:HB3	1:E:241:ASN:OD1	2.19	0.43	
1:H:41:CYS:HB2	1:H:59:GLU:OE2	2.18	0.43	
1:B:98:ASN:HB3	1:B:101:ILE:HG12	2.00	0.43	
1:B:346:TYR:O	1:B:369:ILE:HG22	2.19	0.43	
1:A:96:GLU:OE1	4:A:507:HOH:O	2.21	0.42	
1:B:178:VAL:HG22	1:B:265:PHE:CZ	2.53	0.42	
1:C:125:THR:OG1	4:C:506:HOH:O	2.22	0.42	
1:D:293:ILE:HG22	1:D:295:GLU:H	1.83	0.42	
1:E:72:THR:HG23	1:E:73:ASN:OD1	2.19	0.42	
1:E:281:ILE:HD13	1:E:287:ALA:HB2	2.00	0.42	
1:B:132:ILE:HD12	1:B:132:ILE:HA	1.83	0.42	
1:D:289:GLN:HG3	1:D:310:TYR:OH	2.18	0.42	
1:F:38:ALA:HA	1:F:60:GLY:HA2	2.01	0.42	
1:B:331:TYR:CD1	1:B:338:LEU:HD22	2.54	0.42	
1:C:276:ALA:O	1:C:280:MET:HG2	2.19	0.42	
1:G:23:VAL:HA	1:G:124:GLY:O	2.20	0.42	
1:G:34:LYS:CD	1:G:143:GLU:O	2.68	0.42	
1:F:35:VAL:HG11	1:F:140:THR:O	2.19	0.42	
1:F:166:ILE:CG2	1:F:365:LYS:HG2	2.50	0.42	
1:B:201:ASN:ND2	4:B:509:HOH:O	2.47	0.42	
1:B:222:GLU:O	1:B:225:ASP:HB2	2.19	0.42	
1:B:265:PHE:HA	1:B:288:VAL:O	2.20	0.42	
1:C:26:PRO:HG3	1:C:66:GLN:HG2	2.01	0.42	
1:C:138:ILE:HA	1:C:147:VAL:HG12	2.00	0.42	
1:G:36:LYS:HB2	1:G:161:MET:HG2	2.02	0.42	
1:G:228:LEU:HD23	1:G:232:ALA:O	2.19	0.42	
1:H:159:MET:HG3	1:H:331:TYR:CE2	2.54	0.42	
1:A:198:VAL:HG11	1:A:290:VAL:HG11	2.01	0.42	
1:E:80:VAL:HA	1:E:153:VAL:O	2.20	0.42	
1:E:100:HIS:NE2	1:G:307:ASP:OD2	2.52	0.42	
1:A:146:LEU:HD12	1:A:146:LEU:HA	1.74	0.42	
1:A:306:TRP:CZ2	1:B:314:LEU:HD13	2.55	0.42	
1:C:193:LEU:HD23	1:C:217:ILE:CG2	2.50	0.42	
1:D:108:VAL:HG11	1:D:314:LEU:HD11	2.01	0.42	
1:F:142:SER:OG	1:F:144:TYR:O	2.22	0.42	
1:F:219:ILE:HG23	1:F:238:ALA:O	2.20	0.42	
1:F:342:ILE:CG2	1:F:367:VAL:HG12	2.48	0.42	



	ti a	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:F:41:CYS:SG	1:F:42:HIS:N	2.93	0.42	
1:A:101:ILE:HD11	1:B:283:ASN:ND2	2.35	0.42	
1:D:146:LEU:HB3	4:D:509:HOH:O	2.19	0.42	
1:D:303:LEU:HA	4:D:502:HOH:O	2.20	0.42	
1:F:9:ILE:HA	1:F:54:ILE:O	2.20	0.42	
1:F:134:ARG:HD2	1:F:138:ILE:O	2.20	0.42	
1:F:167:ILE:HA	1:F:171:VAL:HB	2.00	0.42	
1:H:243:ILE:O	1:H:246:LEU:HD13	2.20	0.42	
1:H:353:GLN:O	1:H:357:ASP:HB2	2.19	0.42	
1:A:191:VAL:HG21	1:A:252:VAL:HG11	2.02	0.41	
1:A:225:ASP:HA	1:A:228:LEU:HD12	2.01	0.41	
1:A:250:GLU:O	1:A:254:LYS:HG3	2.20	0.41	
1:C:219:ILE:HD11	1:C:240:LYS:CA	2.50	0.41	
1:D:195:THR:HG21	1:D:216:ALA:HB1	2.02	0.41	
1:E:99:GLN:CD	1:E:319:ARG:HB2	2.40	0.41	
1:E:193:LEU:HD22	1:E:245:LEU:HD23	2.02	0.41	
1:F:42:HIS:O	1:F:45:HIS:HB3	2.20	0.41	
1:F:195:THR:HG22	1:F:203:ILE:HD11	2.02	0.41	
1:F:282:ARG:HH22	1:F:284:ALA:HB3	1.85	0.41	
1:H:10:ALA:HB1	1:H:48:LEU:HD23	2.01	0.41	
1:A:42:HIS:HB2	2:A:401:NAD:O3	2.20	0.41	
1:A:291:SER:O	2:A:401:NAD:H1D	2.19	0.41	
1:A:345:THR:HA	1:A:367:VAL:O	2.20	0.41	
1:B:16:PHE:HD1	4:B:503:HOH:O	2.02	0.41	
1:C:59:GLU:OE2	1:C:169:CYS:HB3	2.20	0.41	
1:E:312:ASN:OD1	1:E:312:ASN:C	2.59	0.41	
1:G:8:ALA:O	1:G:9:ILE:HD13	2.20	0.41	
1:H:30:GLU:HG3	1:H:148:LYS:HD2	2.02	0.41	
1:F:338:LEU:N	4:F:505:HOH:O	2.37	0.41	
1:B:59:GLU:HA	1:B:168:SER:CB	2.50	0.41	
1:C:193:LEU:HD21	1:C:280:MET:HG3	2.03	0.41	
1:F:293:ILE:O	1:H:301:MET:HB2	2.20	0.41	
1:G:193:LEU:HB2	1:G:266:GLU:HA	2.02	0.41	
1:A:67:VAL:HG22	1:A:71:VAL:HB	2.02	0.41	
1:A:106:SER:HB3	1:A:109:THR:HB	2.02	0.41	
1:B:202:VAL:HG21	4:B:540:HOH:O	2.20	0.41	
1:B:263:TYR:C	1:B:281:ILE:HD11	2.41	0.41	
1:B:312:ASN:ND2	4:B:520:HOH:O	2.53	0.41	
1:C:193:LEU:HD23	1:C:217:ILE:HG21	2.02	0.41	
1:E:219:ILE:HG12	2:E:401:NAD:C6A	2.50	0.41	
1:G:118:GLY:HA2 1:G:148:LYS:HD2		2.01	0.41	



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:134:ARG:HB3	1:G:138:ILE:C	2.41	0.41
1:B:134:ARG:HB3	1:B:139:GLY:N	2.35	0.41
1:G:191:VAL:HG22	1:G:215:ILE:HB	2.03	0.41
1:A:315:TYR:O	1:A:318:CYS:HB2	2.21	0.41
1:D:302:ARG:O	1:D:305:GLU:HB2	2.20	0.41
1:E:306:TRP:HE1	1:G:108:VAL:CG1	2.34	0.41
1:E:346:TYR:HB2	1:E:368:ILE:CD1	2.51	0.41
1:G:194:GLY:O	1:G:199:GLY:HA3	2.21	0.41
1:G:266:GLU:HB3	1:G:289:GLN:HA	2.03	0.41
2:H:401:NAD:H6N	2:H:401:NAD:H2D	1.88	0.41
1:A:5:SER:O	1:A:20:THR:HA	2.20	0.41
1:A:87:PRO:HD2	1:A:150:SER:HB2	2.02	0.41
1:A:305:GLU:CA	1:A:306:TRP:CE3	3.03	0.41
1:B:100:HIS:CE1	1:B:317:LYS:HA	2.56	0.41
1:B:192:VAL:HG21	1:B:203:ILE:HG13	2.02	0.41
2:B:401:NAD:H8A	2:B:401:NAD:H2B	1.81	0.41
1:C:65:GLU:O	1:C:65:GLU:HG2	2.21	0.41
2:C:401:NAD:H6N	2:C:401:NAD:H2D	1.86	0.41
1:D:55:VAL:HG23	1:D:132:ILE:HD12	2.03	0.41
1:D:125:THR:OG1	1:D:134:ARG:NH2	2.53	0.41
1:D:353:GLN:O	1:D:356:ASP:HB2	2.21	0.41
1:E:40:LEU:HD21	1:E:355:PHE:CD1	2.56	0.41
1:F:100:HIS:NE2	1:F:317:LYS:HA	2.36	0.41
1:F:219:ILE:HD11	2:F:401:NAD:N6A	2.36	0.41
1:G:30:GLU:HB2	1:G:147:VAL:O	2.21	0.41
1:G:98:ASN:HA	1:G:100:HIS:CE1	2.56	0.41
1:H:9:ILE:HD13	1:H:9:ILE:HG21	1.62	0.41
1:H:116:THR:HA	1:H:117:PRO:HD3	1.94	0.41
1:A:169:CYS:SG	2:A:401:NAD:H5N	2.61	0.41
1:C:121:HIS:HA	4:C:529:HOH:O	2.19	0.41
1:C:348:LEU:O	1:C:351:LEU:HB2	2.21	0.41
1:D:327:LEU:HD23	1:D:327:LEU:HA	1.89	0.41
1:E:223:ARG:HD3	1:E:361:GLY:CA	2.51	0.41
1:B:7:CYS:O	1:B:18:ILE:HA	2.21	0.40
1:E:331:TYR:CD1	1:E:338:LEU:CD2	3.04	0.40
1:F:344:ARG:HG3	1:F:346:TYR:HE1	1.80	0.40
1:G:289:GLN:HG2	1:G:310:TYR:CZ	2.56	0.40
1:H:28:ALA:HA	1:H:69:SER:H	1.86	0.40
1:D:22:GLN:O	1:D:125:THR:HA	2.21	0.40
1:E:198:VAL:HG11	1:E:267:CYS:HB2	2.03	0.40
1:H:185:GLN:HG3	1:H:263:TYR:OH	2.21	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:223:ARG:HD3	1:A:226:MET:HE3	2.02	0.40
1:A:230:PHE:CE1	1:A:341:MET:HG2	2.57	0.40
1:D:346:TYR:CD2	1:D:354:ALA:HB2	2.52	0.40
1:E:108:VAL:HG11	1:G:306:TRP:HE1	1.83	0.40
1:F:44:ASP:HB2	1:F:58:HIS:HE1	1.83	0.40
1:H:342:ILE:HD12	1:H:367:VAL:HG21	2.04	0.40
1:B:341:MET:SD	4:B:509:HOH:O	2.63	0.40
1:E:326:LYS:O	1:E:330:LEU:HG	2.22	0.40
1:F:342:ILE:HG21	1:F:367:VAL:HG12	2.02	0.40
1:H:36:LYS:HD2	1:H:36:LYS:HA	1.55	0.40
1:C:284:ALA:HA	1:C:307:ASP:O	2.21	0.40
1:E:184:LEU:HA	1:E:263:TYR:CZ	2.55	0.40
1:F:293:ILE:HB	1:H:301:MET:CB	2.50	0.40
1:H:12:GLY:HA3	1:H:51:GLY:HA2	2.03	0.40
1:H:80:VAL:HA	1:H:153:VAL:O	2.22	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:A:344:ARG:NH2	1:E:357:ASP:OD2[1_554]	1.97	0.23
1:C:349:GLU:OE2	1:D:344:ARG:NH2[2_546]	2.05	0.15
1:B:158:ASN:ND2	$1:F:129:ASP:O[1_455]$	2.08	0.12
1:A:339:ASP:O	4:E:503:HOH: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 analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	362/370~(98%)	345 (95%)	15 (4%)	2(1%)	25	43
1	В	362/370~(98%)	335 (92%)	26 (7%)	1 (0%)	41	61



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	С	359/370~(97%)	341~(95%)	16 (4%)	2(1%)	25 43
1	D	360/370~(97%)	336~(93%)	20~(6%)	4 (1%)	14 26
1	Ε	360/370~(97%)	341~(95%)	16 (4%)	3(1%)	19 35
1	F	358/370~(97%)	338~(94%)	17~(5%)	3~(1%)	19 35
1	G	361/370~(98%)	344~(95%)	15 (4%)	2(1%)	25 43
1	Н	350/370~(95%)	335~(96%)	12 (3%)	3 (1%)	17 31
All	All	2872/2960~(97%)	2715 (94%)	137 (5%)	20 (1%)	22 39

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All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	306	TRP
1	В	306	TRP
1	С	306	TRP
1	D	306	TRP
1	D	356	ASP
1	Е	13	ASP
1	Е	306	TRP
1	F	306	TRP
1	G	306	TRP
1	Н	306	TRP
1	D	355	PHE
1	F	128	ASN
1	А	267	CYS
1	Н	267	CYS
1	С	259	ARG
1	F	129	ASP
1	D	267	CYS
1	Е	139	GLY
1	G	292	GLY
1	Н	292	GLY

#### 5.3.2 Protein sidechains (i)

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

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


Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	296/298~(99%)	291~(98%)	5(2%)	60	82
1	В	297/298~(100%)	295~(99%)	2(1%)	84	94
1	С	293/298~(98%)	290~(99%)	3 (1%)	76	90
1	D	294/298~(99%)	291~(99%)	3~(1%)	76	90
1	Ε	294/298~(99%)	291~(99%)	3~(1%)	76	90
1	F	293/298~(98%)	288~(98%)	5(2%)	60	82
1	G	295/298~(99%)	291~(99%)	4 (1%)	67	86
1	Н	289/298~(97%)	287 (99%)	2(1%)	84	94
All	All	2351/2384 (99%)	2324 (99%)	27 (1%)	73	89

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	79	TYR
1	А	259	ARG
1	А	306	TRP
1	А	338	LEU
1	А	344	ARG
1	В	306	TRP
1	В	338	LEU
1	С	267	CYS
1	С	306	TRP
1	С	312	ASN
1	D	65	GLU
1	D	79	TYR
1	D	306	TRP
1	Е	306	TRP
1	Е	312	ASN
1	Е	338	LEU
1	F	92	PHE
1	F	247	LYS
1	F	306	TRP
1	F	315	TYR
1	F	346	TYR
1	G	239	ASP
1	G	302	ARG
1	G	306	TRP
1	G	338	LEU
1	Н	306	TRP
1	Н	315	TYR



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	185	GLN
1	А	220	ASN
1	А	312	ASN
1	В	98	ASN
1	С	289	GLN
1	С	312	ASN
1	D	66	GLN
1	D	312	ASN
1	Е	66	GLN
1	Е	312	ASN
1	Е	350	ASN
1	F	185	GLN
1	F	312	ASN
1	Н	49	ASN
1	Н	121	HIS
1	Н	289	GLN
1	Н	312	ASN

### 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 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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



Mal	Mol Type Chain Bes		Dec	Tiple	В	Bond lengths			Bond angles		
	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2	
2	NAD	Н	401	-	42,48,48	4.80	14 (33%)	50,73,73	2.04	10 (20%)	
2	NAD	А	401	-	42,48,48	4.91	15 (35%)	50,73,73	1.72	7 (14%)	
2	NAD	С	401	-	42,48,48	4.80	13 (30%)	50,73,73	1.72	6 (12%)	
2	NAD	F	401	-	42,48,48	4.83	15 (35%)	50,73,73	1.68	8 (16%)	
2	NAD	Е	401	-	42,48,48	<b>5.03</b>	15 (35%)	50,73,73	1.70	6 (12%)	
2	NAD	В	401	-	42,48,48	4.87	16 (38%)	50,73,73	1.65	5 (10%)	
2	NAD	D	401	-	42,48,48	4.81	13 (30%)	50,73,73	1.65	7 (14%)	
2	NAD	G	401	-	42,48,48	4.77	12 (28%)	50,73,73	1.83	10 (20%)	

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).

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	NAD	Н	401	-	-	11/26/62/62	0/5/5/5
2	NAD	А	401	-	-	5/26/62/62	0/5/5/5
2	NAD	С	401	-	-	10/26/62/62	0/5/5/5
2	NAD	F	401	-	-	8/26/62/62	0/5/5/5
2	NAD	Е	401	-	-	8/26/62/62	0/5/5/5
2	NAD	В	401	-	-	5/26/62/62	0/5/5/5
2	NAD	D	401	-	-	16/26/62/62	0/5/5/5
2	NAD	G	401	-	-	7/26/62/62	0/5/5/5

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Н	401	NAD	O4D-C1D	15.31	1.62	1.41
2	Е	401	NAD	O4D-C1D	15.26	1.62	1.41
2	D	401	NAD	O4D-C1D	14.97	1.62	1.41
2	А	401	NAD	O4D-C1D	14.74	1.61	1.41
2	F	401	NAD	O4D-C1D	14.73	1.61	1.41
2	В	401	NAD	O4D-C1D	14.72	1.61	1.41
2	С	401	NAD	O4D-C1D	14.70	1.61	1.41
2	Е	401	NAD	O4B-C1B	14.61	1.61	1.41
2	G	401	NAD	O4D-C1D	14.35	1.61	1.41



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	401	NAD	O4B-C1B	14.33	1.61	1.41
2	Е	401	NAD	C2B-C1B	-14.27	1.32	1.53
2	А	401	NAD	C2B-C1B	-14.09	1.32	1.53
2	D	401	NAD	O4B-C1B	13.95	1.60	1.41
2	С	401	NAD	O4B-C1B	13.92	1.60	1.41
2	F	401	NAD	O4B-C1B	13.79	1.60	1.41
2	В	401	NAD	O4B-C1B	13.73	1.60	1.41
2	В	401	NAD	C2B-C1B	-13.72	1.32	1.53
2	G	401	NAD	C2B-C1B	-13.66	1.33	1.53
2	Н	401	NAD	O4B-C1B	13.65	1.60	1.41
2	F	401	NAD	C2D-C1D	-13.33	1.33	1.53
2	F	401	NAD	C2B-C1B	-13.30	1.33	1.53
2	С	401	NAD	C2B-C1B	-13.16	1.33	1.53
2	G	401	NAD	O4B-C1B	13.07	1.59	1.41
2	D	401	NAD	C2B-C1B	-13.05	1.34	1.53
2	G	401	NAD	C2D-C1D	-13.00	1.34	1.53
2	В	401	NAD	C2D-C1D	-12.94	1.34	1.53
2	Н	401	NAD	C2D-C1D	-12.71	1.34	1.53
2	Е	401	NAD	C2D-C1D	-12.62	1.34	1.53
2	Н	401	NAD	C2B-C1B	-12.61	1.34	1.53
2	D	401	NAD	C2D-C1D	-12.50	1.34	1.53
2	С	401	NAD	C2D-C1D	-12.29	1.35	1.53
2	А	401	NAD	C2D-C1D	-12.03	1.35	1.53
2	Е	401	NAD	C7N-N7N	8.95	1.50	1.33
2	D	401	NAD	C7N-N7N	8.34	1.48	1.33
2	А	401	NAD	C7N-N7N	8.34	1.48	1.33
2	С	401	NAD	C7N-N7N	7.93	1.48	1.33
2	Н	401	NAD	C7N-N7N	7.84	1.47	1.33
2	В	401	NAD	C7N-N7N	7.82	1.47	1.33
2	G	401	NAD	C7N-N7N	7.70	1.47	1.33
2	F	401	NAD	C7N-N7N	7.62	1.47	1.33
2	С	401	NAD	O4B-C4B	-6.58	1.30	1.45
2	G	401	NAD	O4B-C4B	-6.56	1.30	1.45
2	А	401	NAD	O4B-C4B	-6.53	1.30	1.45
2	В	401	NAD	O4D-C4D	-6.50	1.30	1.45
2	H	401	NAD	O4B-C4B	-6.25	1.31	1.45
2	C	401	NAD	O4D-C4D	-6.18	1.31	1.45
2	E	401	NAD	O4B-C4B	-6.15	1.31	1.45
2	E	401	NAD	O4D-C4D	-6.12	1.31	1.45
2	В	401	NAD	O4B-C4B	-6.11	1.31	1.45
2	F	401	NAD	O4B-C4B	-6.10	1.31	1.45
2	G	401	NAD	O4D-C4D	-5.96	1.31	1.45



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAD	O4B-C4B	-5.93	1.31	1.45
2	D	401	NAD	O4D-C4D	-5.92	1.31	1.45
2	F	401	NAD	O4D-C4D	-5.90	1.31	1.45
2	А	401	NAD	O4D-C4D	-5.87	1.31	1.45
2	Н	401	NAD	O4D-C4D	-5.39	1.32	1.45
2	В	401	NAD	C4N-C3N	-4.12	1.32	1.39
2	А	401	NAD	C4N-C3N	-4.02	1.32	1.39
2	Н	401	NAD	C2N-C3N	3.86	1.45	1.39
2	F	401	NAD	C4N-C3N	-3.82	1.32	1.39
2	D	401	NAD	C4N-C3N	-3.71	1.32	1.39
2	С	401	NAD	C4N-C3N	-3.62	1.33	1.39
2	А	401	NAD	C2N-C3N	3.62	1.44	1.39
2	G	401	NAD	C4N-C3N	-3.61	1.33	1.39
2	Е	401	NAD	C2N-C3N	3.57	1.44	1.39
2	Е	401	NAD	C4N-C3N	-3.39	1.33	1.39
2	G	401	NAD	C2N-C3N	3.26	1.44	1.39
2	Н	401	NAD	C4N-C3N	-3.21	1.33	1.39
2	С	401	NAD	C2N-C3N	3.17	1.43	1.39
2	D	401	NAD	C2N-C3N	2.94	1.43	1.39
2	Ε	401	NAD	PA-O5B	2.93	1.71	1.59
2	В	401	NAD	C5A-C4A	-2.93	1.33	1.40
2	Е	401	NAD	C5A-C4A	-2.93	1.33	1.40
2	Н	401	NAD	C6N-C5N	2.92	1.45	1.38
2	В	401	NAD	PA-O5B	2.89	1.71	1.59
2	F	401	NAD	C2N-C3N	2.86	1.43	1.39
2	С	401	NAD	O2D-C2D	2.86	1.49	1.43
2	G	401	NAD	C5A-C4A	-2.84	1.33	1.40
2	F	401	NAD	C5A-C4A	-2.77	1.33	1.40
2	D	401	NAD	PA-O5B	2.67	1.70	1.59
2	A	401	NAD	PA-O5B	2.61	1.69	1.59
2	D	401	NAD	C5A-C4A	-2.60	1.34	1.40
2	Н	401	NAD	C5A-C4A	-2.59	1.34	1.40
2	A	401	NAD	C5A-C4A	-2.56	1.34	1.40
2	F	401	NAD	O2B-C2B	2.50	1.48	1.43
2	G	401	NAD	PA-O5B	2.45	1.69	1.59
2	B	401	NAD	C2N-C3N	2.44	1.42	1.39
2	E	401	NAD	O2B-C2B	2.44	1.48	1.43
2	C	401	NAD	PA-O5B	2.41	1.69	1.59
2	D	401	NAD	C6N-C5N	2.40	1.43	1.38
2	C	401	NAD	C5A-C4A	-2.38	1.34	1.40
2	H	401	NAD	PA-O5B	2.35	1.68	1.59
2	В	401	NAD	O3B-C3B	-2.33	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Н	401	NAD	O7N-C7N	-2.30	1.19	1.24
2	F	401	NAD	O3B-C3B	-2.29	1.37	1.43
2	Е	401	NAD	C6N-C5N	2.26	1.43	1.38
2	G	401	NAD	O7N-C7N	-2.23	1.19	1.24
2	А	401	NAD	O2D-C2D	2.23	1.48	1.43
2	А	401	NAD	O3D-C3D	-2.22	1.37	1.43
2	А	401	NAD	C6N-C5N	2.22	1.43	1.38
2	F	401	NAD	C6N-C5N	2.21	1.43	1.38
2	F	401	NAD	PA-O5B	2.15	1.68	1.59
2	А	401	NAD	O2B-C2B	2.13	1.48	1.43
2	D	401	NAD	O3D-C3D	-2.13	1.38	1.43
2	В	401	NAD	O2B-C2B	2.11	1.47	1.43
2	В	401	NAD	O3D-C3D	-2.10	1.38	1.43
2	Ε	401	NAD	C3B-C4B	2.07	1.58	1.53
2	F	401	NAD	O3D-C3D	-2.05	1.38	1.43
2	В	401	NAD	O2D-C2D	2.05	1.47	1.43
2	В	401	NAD	C6A-C5A	-2.04	1.35	1.43
2	Н	401	NAD	O2B-C2B	2.04	1.47	1.43
2	С	401	NAD	O3B-C3B	-2.02	1.38	1.43
2	E	401	NAD	O3D-C3D	-2.02	1.38	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	401	NAD	C5A-C6A-N6A	7.15	131.21	120.35
2	G	401	NAD	C5A-C6A-N6A	7.08	131.11	120.35
2	А	401	NAD	C5A-C6A-N6A	6.51	130.24	120.35
2	Н	401	NAD	C5A-C6A-N6A	6.49	130.22	120.35
2	В	401	NAD	C5A-C6A-N6A	6.15	129.70	120.35
2	D	401	NAD	C5A-C6A-N6A	5.93	129.36	120.35
2	В	401	NAD	N3A-C2A-N1A	-5.90	119.46	128.68
2	Е	401	NAD	N3A-C2A-N1A	-5.88	119.49	128.68
2	F	401	NAD	C5A-C6A-N6A	5.54	128.77	120.35
2	А	401	NAD	N3A-C2A-N1A	-5.46	120.14	128.68
2	D	401	NAD	N3A-C2A-N1A	-5.40	120.24	128.68
2	Е	401	NAD	C5A-C6A-N6A	5.30	128.41	120.35
2	F	401	NAD	N3A-C2A-N1A	-5.26	120.46	128.68
2	G	401	NAD	N3A-C2A-N1A	-5.21	120.53	128.68
2	Н	401	NAD	N3A-C2A-N1A	-4.98	120.90	128.68
2	С	401	NAD	N3A-C2A-N1A	-4.93	120.97	128.68
2	G	401	NAD	N6A-C6A-N1A	-4.70	108.81	118.57
2	Н	401	NAD	N6A-C6A-N1A	-4.69	108.85	118.57



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	Н	401	NAD	C6N-N1N-C2N	-4.68	117.71	121.97
2	Н	401	NAD	PN-O3-PA	-4.32	118.02	132.83
2	Е	401	NAD	PN-O3-PA	-4.17	118.52	132.83
2	А	401	NAD	O4B-C1B-C2B	-4.15	100.86	106.93
2	F	401	NAD	N6A-C6A-N1A	-4.15	109.95	118.57
2	С	401	NAD	N6A-C6A-N1A	-4.05	110.17	118.57
2	В	401	NAD	N6A-C6A-N1A	-4.04	110.19	118.57
2	D	401	NAD	N6A-C6A-N1A	-3.99	110.30	118.57
2	D	401	NAD	PN-O3-PA	-3.92	119.38	132.83
2	Е	401	NAD	N6A-C6A-N1A	-3.84	110.60	118.57
2	А	401	NAD	N6A-C6A-N1A	-3.71	110.87	118.57
2	Н	401	NAD	C3B-C2B-C1B	3.67	106.51	100.98
2	С	401	NAD	C3B-C2B-C1B	3.62	106.43	100.98
2	G	401	NAD	PN-O3-PA	-3.55	120.65	132.83
2	С	401	NAD	PN-O3-PA	-3.33	121.40	132.83
2	Е	401	NAD	C1B-N9A-C4A	-3.27	120.89	126.64
2	F	401	NAD	O7N-C7N-C3N	3.13	123.38	119.63
2	F	401	NAD	C6N-N1N-C2N	-3.13	119.12	121.97
2	В	401	NAD	PN-O3-PA	-2.84	123.07	132.83
2	Н	401	NAD	C2N-C3N-C4N	2.64	121.26	118.26
2	Н	401	NAD	C5N-C4N-C3N	-2.63	117.23	120.34
2	F	401	NAD	C1B-N9A-C4A	-2.58	122.11	126.64
2	D	401	NAD	C6N-N1N-C2N	-2.52	119.68	121.97
2	D	401	NAD	O4B-C1B-C2B	-2.45	103.35	106.93
2	Н	401	NAD	O7N-C7N-N7N	-2.41	119.16	122.58
2	Е	401	NAD	O7N-C7N-N7N	-2.39	119.18	122.58
2	С	401	NAD	O7N-C7N-C3N	2.36	122.45	119.63
2	G	401	NAD	O4B-C1B-C2B	-2.35	103.49	106.93
2	F	401	NAD	O4B-C1B-C2B	-2.29	103.58	106.93
2	G	401	NAD	C5B-C4B-C3B	-2.29	106.61	115.18
2	G	401	NAD	O3D-C3D-C4D	-2.26	104.51	111.05
2	Н	401	NAD	O2B-C2B-C3B	-2.26	104.53	111.82
2	D	401	NAD	C5B-C4B-C3B	-2.25	106.75	115.18
2	F	401	NAD	PN-O3-PA	-2.24	125.14	132.83
2	В	401	NAD	O3B-C3B-C2B	-2.21	104.69	111.82
2	А	401	NAD	O3D-C3D-C4D	-2.19	104.71	111.05
2	А	401	NAD	O7N-C7N-N7N	-2.16	119.50	122.58
2	G	401	NAD	C2N-C3N-C4N	2.15	120.70	118.26
2	А	401	NAD	PN-O3-PA	-2.11	125.57	132.83
2	G	401	NAD	C6N-N1N-C2N	-2.02	120.14	121.97
2	G	401	NAD	C4A-C5A-N7A	-2.02	107.30	109.40

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There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
2	А	401	NAD	O4D-C1D-N1N-C2N
2	А	401	NAD	O4D-C1D-N1N-C6N
2	А	401	NAD	C2D-C1D-N1N-C2N
2	А	401	NAD	C2D-C1D-N1N-C6N
2	В	401	NAD	O4D-C1D-N1N-C2N
2	В	401	NAD	O4D-C1D-N1N-C6N
2	В	401	NAD	C2D-C1D-N1N-C2N
2	В	401	NAD	C2D-C1D-N1N-C6N
2	С	401	NAD	C5B-O5B-PA-O1A
2	С	401	NAD	O4D-C1D-N1N-C2N
2	С	401	NAD	O4D-C1D-N1N-C6N
2	С	401	NAD	C2D-C1D-N1N-C2N
2	С	401	NAD	C2D-C1D-N1N-C6N
2	D	401	NAD	C5B-O5B-PA-O1A
2	D	401	NAD	O4B-C4B-C5B-O5B
2	D	401	NAD	C5D-O5D-PN-O3
2	D	401	NAD	O4D-C4D-C5D-O5D
2	D	401	NAD	O4D-C1D-N1N-C2N
2	D	401	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	C2D-C1D-N1N-C2N
2	D	401	NAD	C2D-C1D-N1N-C6N
2	Е	401	NAD	O4D-C1D-N1N-C2N
2	Е	401	NAD	O4D-C1D-N1N-C6N
2	Е	401	NAD	C2D-C1D-N1N-C2N
2	F	401	NAD	O4D-C1D-N1N-C2N
2	F	401	NAD	O4D-C1D-N1N-C6N
2	F	401	NAD	C2D-C1D-N1N-C2N
2	F	401	NAD	C2D-C1D-N1N-C6N
2	G	401	NAD	C5D-O5D-PN-O3
2	G	401	NAD	O4D-C1D-N1N-C2N
2	G	401	NAD	O4D-C1D-N1N-C6N
2	G	401	NAD	C2D-C1D-N1N-C2N
2	G	401	NAD	C2D-C1D-N1N-C6N
2	Н	401	NAD	C5B-O5B-PA-O1A
2	Н	401	NAD	O4B-C4B-C5B-O5B
2	Н	401	NAD	O4D-C1D-N1N-C2N
2	Н	401	NAD	O4D-C1D-N1N-C6N
2	Н	401	NAD	C2D-C1D-N1N-C2N
2	Н	401	NAD	C2D-C1D-N1N-C6N
2	С	401	NAD	O4B-C4B-C5B-O5B
2	С	401	NAD	$C3B-C4B-C5B-O5\overline{B}$
2	D	401	NAD	$C3D-C4D-C5\overline{D-O5D}$

All (70) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	Е	401	NAD	O4B-C4B-C5B-O5B
2	D	401	NAD	C3B-C4B-C5B-O5B
2	Н	401	NAD	C3B-C4B-C5B-O5B
2	Е	401	NAD	C3B-C4B-C5B-O5B
2	D	401	NAD	PN-O3-PA-O5B
2	Е	401	NAD	PN-O3-PA-O5B
2	С	401	NAD	C5B-O5B-PA-O3
2	D	401	NAD	C5B-O5B-PA-O3
2	F	401	NAD	C5D-O5D-PN-O3
2	Н	401	NAD	C5B-O5B-PA-O3
2	С	401	NAD	C5B-O5B-PA-O2A
2	D	401	NAD	C5B-O5B-PA-O2A
2	D	401	NAD	C5D-O5D-PN-O1N
2	Н	401	NAD	C5B-O5B-PA-O2A
2	Н	401	NAD	PA-O3-PN-O2N
2	В	401	NAD	O4B-C4B-C5B-O5B
2	С	401	NAD	PA-O3-PN-O2N
2	D	401	NAD	PA-O3-PN-O1N
2	D	401	NAD	PA-O3-PN-O2N
2	Е	401	NAD	C5B-O5B-PA-O3
2	А	401	NAD	O4B-C4B-C5B-O5B
2	F	401	NAD	O4B-C4B-C5B-O5B
2	Е	401	NAD	PA-O3-PN-O2N
2	Н	401	NAD	PA-O3-PN-O1N
2	F	401	NAD	C5D-O5D-PN-O2N
2	G	401	NAD	C5D-O5D-PN-O1N
2	F	401	NAD	O4D-C4D-C5D-O5D
2	G	401	NAD	O4B-C4B-C5B-O5B

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There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Н	401	NAD	4	0
2	А	401	NAD	5	0
2	С	401	NAD	3	0
2	F	401	NAD	2	0
2	Е	401	NAD	6	0
2	В	401	NAD	2	0
2	D	401	NAD	4	0
2	G	401	NAD	3	0





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































# 5.7 Other polymers (i)

There are no such residues in this entry.

# 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

# 6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2		$OWAB(Å^2)$	Q < 0.9
1	А	366/370~(98%)	-0.03	1 (0%) 94	94	33, 46, 62, 76	0
1	В	366/370~(98%)	-0.03	3 (0%) 86	87	31, 43, 58, 74	0
1	С	363/370~(98%)	0.17	8 (2%) 62	65	35, 53, 72, 83	0
1	D	364/370~(98%)	0.20	10 (2%) 54	58	36, 51, 75, 90	0
1	Ε	364/370~(98%)	-0.01	4 (1%) 80	82	33, 46, 61, 73	0
1	F	362/370~(97%)	0.40	25 (6%) 16	17	35, 55, 84, 91	0
1	G	365/370~(98%)	0.09	4 (1%) 80	82	32, 46, 61, 75	0
1	Н	356/370~(96%)	0.20	11 (3%) 49	52	35, 53, 79, 88	0
All	All	2906/2960 (98%)	0.12	66 (2%) 60	63	31, 48, 74, 91	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	355	PHE	5.4
1	F	18	ILE	4.7
1	F	364	ALA	4.7
1	F	50	TRP	4.6
1	Н	85	ALA	4.4
1	D	122	LEU	4.3
1	С	60	GLY	4.0
1	D	147	VAL	3.9
1	Н	129	ASP	3.8
1	Н	16	PHE	3.8
1	В	241	ASN	3.7
1	D	342	ILE	3.7
1	F	33	VAL	3.4
1	F	16	PHE	3.2
1	Н	306	TRP	3.1
1	F	141	LEU	3.1



Mol	Chain	Res	Type	RSRZ
1	Н	18	ILE	3.1
1	С	63	PHE	3.1
1	F	40	LEU	3.1
1	D	79	TYR	3.0
1	С	358	MET	3.0
1	Н	79	TYR	3.0
1	F	74	LEU	2.9
1	Н	49	ASN	2.9
1	С	162	PRO	2.9
1	F	348	LEU	2.9
1	D	341	MET	2.9
1	В	54	ILE	2.9
1	F	79	TYR	2.8
1	D	162	PRO	2.8
1	Е	74	LEU	2.7
1	F	63	PHE	2.7
1	D	360	THR	2.7
1	В	238	ALA	2.7
1	С	61	ALA	2.7
1	Н	366	GLY	2.7
1	F	132	ILE	2.6
1	F	370	PHE	2.6
1	F	344	ARG	2.6
1	G	92	PHE	2.6
1	F	67	VAL	2.5
1	Е	82	LEU	2.5
1	D	158	ASN	2.5
1	С	74	LEU	2.5
1	F	72	THR	2.5
1	D	351	LEU	2.4
1	Е	245	LEU	2.4
1	F	43	THR	2.4
1	А	122	LEU	2.3
1	G	6	LYS	2.3
1	G	8	ALA	2.3
1	С	97	GLY	2.3
1	Е	155	ILE	2.3
1	Н	23	VAL	2.3
1	F	36	LYS	2.3
1	F	52	LYS	2.2
1	D	45	HIS	2.2
1	F	306	TRP	2.2



Mol	Chain	Res	Type	RSRZ
1	F	5	SER	2.2
1	С	243	ILE	2.2
1	G	130	THR	2.2
1	Н	231	GLY	2.1
1	F	146	LEU	2.0
1	Н	370	PHE	2.0
1	F	61	ALA	2.0
1	F	359	LEU	2.0

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

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

### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
3	ZN	D	402	1/1	0.66	0.10	71,71,71,71	0
3	ZN	Н	402	1/1	0.71	0.08	83,83,83,83	0
3	ZN	А	402	1/1	0.89	0.07	83,83,83,83	0
3	ZN	С	402	1/1	0.90	0.07	71,71,71,71	0
2	NAD	С	401	44/44	0.92	0.14	$36,\!53,\!58,\!66$	0
2	NAD	D	401	44/44	0.92	0.16	34,50,59,62	0
2	NAD	Н	401	44/44	0.94	0.14	39,52,60,64	0
2	NAD	Е	401	44/44	0.94	0.15	40,48,54,61	0
3	ZN	F	402	1/1	0.94	0.08	89,89,89,89	0
3	ZN	G	402	1/1	0.94	0.07	62,62,62,62	0
3	ZN	В	402	1/1	0.94	0.06	$68,\!68,\!68,\!68$	0
2	NAD	F	401	44/44	0.95	0.14	44,54,59,61	0
3	ZN	F	403	1/1	0.95	0.14	60,60,60,60	0
2	NAD	В	401	44/44	0.95	0.15	35,44,49,54	0
2	NAD	A	401	44/44	0.95	0.13	29,43,49,57	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	NAD	G	401	44/44	0.96	0.14	$38,\!45,\!52,\!54$	0
3	ZN	Е	402	1/1	0.96	0.04	78, 78, 78, 78, 78	0
3	ZN	G	403	1/1	0.97	0.06	62,62,62,62	0
3	ZN	D	403	1/1	0.97	0.07	$53,\!53,\!53,\!53$	0
3	ZN	Н	403	1/1	0.97	0.06	$57,\!57,\!57,\!57$	0
3	ZN	В	403	1/1	0.98	0.08	56, 56, 56, 56	0
3	ZN	А	403	1/1	0.98	0.11	61,61,61,61	0
3	ZN	С	403	1/1	0.98	0.09	57,57,57,57	0
3	ZN	Е	403	1/1	0.99	0.11	$53,\!53,\!53,\!53$	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.

