

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

#### Dec 3, 2023 - 03:29 pm GMT

PDB ID	:	2JHR
Title	:	Crystal structure of myosin-2 motor domain in complex with ADP- metavana-
		date and pentabromopseudilin
Authors	:	Fedorov, R.; Boehl, M.; Tsiavaliaris, G.; Hartmann, F.K.; Baruch, P.; Brenner,
		B.; Martin, R.; Knoelker, H.J.; Gutzeit, H.O.; Manstein, D.J.
Deposited on	:	2008-03-25
Resolution	:	2.80  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 (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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.



Matria	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
R <sub>free</sub>	130704	3140 (2.80-2.80)
Clashscore	141614	3569(2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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

Mol	Chain	Length	Quali	ty of chain	
1	А	788	47%	41%	7% ••

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PBQ	А	1780	-	-	Х	-



#### 2JHR

# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6761 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.

• Molecule 1 is a protein called MYOSIN-2 HEAVY CHAIN.

Mol	Chain	Residues		Α	toms			ZeroOcc	AltConf	Trace
1	А	776	Total 6239	C 3961	N 1076	0 1185	S 17	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	-10	MET	-	expression tag	UNP P08799
А	-9	HIS	-	expression tag	UNP P08799
А	-8	HIS	-	expression tag	UNP P08799
А	-7	HIS	-	expression tag	UNP P08799
А	-6	HIS	-	expression tag	UNP P08799
А	-5	HIS	-	expression tag	UNP P08799
А	-4	HIS	-	expression tag	UNP P08799
А	-3	HIS	-	expression tag	UNP P08799
А	-2	ASP	-	expression tag	UNP P08799
А	-1	GLY	-	expression tag	UNP P08799
А	0	THR	-	expression tag	UNP P08799
А	1	GLU	-	expression tag	UNP P08799
А	762	LEU	-	expression tag	UNP P08799
А	763	GLU	-	expression tag	UNP P08799
А	764	SER	-	expression tag	UNP P08799
А	765	ASN	-	expression tag	UNP P08799
А	766	GLU	-	expression tag	UNP P08799
А	767	PRO	-	expression tag	UNP P08799
А	768	PRO	-	expression tag	UNP P08799
А	769	MET	-	expression tag	UNP P08799
А	770	ASP	-	expression tag	UNP P08799
А	771	PHE	-	expression tag	UNP P08799
А	772	ASP	-	expression tag	UNP P08799
А	773	ASP	-	expression tag	UNP P08799
А	774	ASP	-	expression tag	UNP P08799
А	775	ILE	-	expression tag	UNP P08799
А	776	PRO	-	expression tag	UNP P08799

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	777	PHE	-	expression tag	UNP P08799

• Molecule 2 is ADP METAVANADATE (three-letter code: AD9) (formula:  $C_{10}H_{16}N_5O_{13}P_2V$ ).



Mol	Chain	Residues		A	ton	ns			ZeroOcc	AltConf
2	А	1	Total 31	C 10	N 5	O 13	Р 2	V 1	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Mg 1 1	0	0

• Molecule 4 is PENTABROMOPSEUDILIN (three-letter code: PBQ) (formula:  $C_{10}H_4Br_5NO$ ).





Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
4	Δ	1	Total	Br	С	Ν	Ο	0	0
4 4	A	A 1	17	5	10	1	1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	473	Total         O           473         473	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. 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. 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.

Chain	A:					47 <sup>0</sup>	%							•						41%	6						7	'%	·	•			
MET HIS HIS HIS HIS	SIH SIH	ASP GLY THR	GLU N2 P3	14 14	H5 D6	R/ T8	V11	H12	K13 V14	L15	CC2	770	F25 1776	L27	T28 V29	<b>S</b> 30	D31	135	W36 V27	13/ N38	07.4	E43	R44 D45		Vb3	T56	S57 D58	<b>S59</b>	K63	T64	COV D66	090	RTO
Q71 V72 K73 N75	D76 079	183 K84	G87	000	892 892	E93 L94	895 Voe	L90	N98 F99		F103 H104	N105	L106	V108	R109	Q112	D113 L114	1115	V110	S119	G120	L123	F1 29	K130	Y135	T136	Q137	D141	K144	G145	R147	R148 N149	E150
V151 A152 P153 A157	1158 8159 0160	V161 R164	R170	N172	41/3 S174		G182	K185	T186	K190	K191 V192	1193	0194 V105	0.00	S198 V199	A200	G201 R202	N203	0204 ADOE	N206	G207	6209	V210 1.211	E212	u213 0214	1215	L216 0217	, a	<b>F.2.2</b>	F225	K229	T230 T231	R232
N233 N234 R238 F239	E244 1245	Q246 F247 N248	S249 A250	1253	A256	5257 1258	VD61	1201 L262	L263 F264	K265	S266 R267		E273 T074	E275	R276 N277	Y278	H279 1280	F281	Y282	4203 L284	1000	A288	T289 A290	E291	E292 K293	K294	A295 1.296	H297	P.788	P301	<b>5303</b>	F304 N305	
N308 V313 K316	6317 V318 S319	D320 <mark>S321</mark> E322	E323 F324 V305	1326 1326	132/ R328	4329 A330	M331	1333	V334 G335	F336	S337	E340	Q341 M340	5343 S343	1344 F345	K346	1347 1348		1351 1350		N356 T267	K358	K361	<mark>G362</mark>	E365	<b>G366</b>	A367 V368	L369	K370 D371	K372	13/3 A374	L375 N376	
T380 N385 P386 S387	L389 E390	K391 <mark>A392</mark> L393	M394 E395 P306	R397	1398 L399	R402	D403	V405	A406 0407	H408	L409 N410	V411	E412	R418	D419	V422	K423 A424		F430 1 434	N432	L433 V424	K435	K436 T437	N438	N439 V440	L441	C442 0443	E444	K445 K446	A447	1440 F449	1.453	D454
1455 8456 6457 F458 F458	1460 F461	N464 S465 F466	E467 Q468 1460	C470		F482 N483	H484 UABE	M486	F487 K488	L489	V494	L495	K496	K498	I499 N500		F506	L516	I517 De10	G519	R520	P522	T525		D530	<mark>8533</mark>	V534 F535	P536	K557	200	ZQQN	K565 T566	E567
F568 G569 Y573	M578 Y579 E580	1581 0582 0583	E586	D590	E597	F600	K601	S603	V607		K610	D614	P615 Wete	1617 1617	A618 S619		K622 K623		N626 F627	r 02/	0633 V634	103 <del>1</del> K635	E636	S640	L641 M642	A643	E.646	T647	1648 N649	P650	TCOH	1657	K661
Q662 K666 L667	D669 K670 V671	V672 L673 D674	0675	N679	16 <mark>87</mark>	F692	P693	R695	1696 1697	¥698	A699 D700	F701	V702	R704	Y705 V706	L707	L708 A709	P710	117N	P7 13	R714 D715	A716	E717 D718	S719	ц//20 К721	A7 22	T723 D724	A7 25	V726 L727	K7 28	L730	N731 1732	D733
P734 E735 Q736 Y737 R738	F739 G740 I741	T742 K743 1744	F745 F746 b777	A748	G749 Q750	L751 A752	R753	E755	E756 A757	R758	E759 0760	R761	L762 E763	S764	N765 F766	P767	P768 M769	D770	F771	D773	D774	P776	F777										

• Molecule 1: MYOSIN-2 HEAVY CHAIN



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	89.76Å 150.46Å 154.55Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	8.00 - 2.80	Depositor
Resolution (A)	77.08 - 2.20	EDS
% Data completeness	(Not available) $(8.00-2.80)$	Depositor
(in resolution range)	76.5(77.08-2.20)	EDS
R <sub>merge</sub>	0.09	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.84 (at 2.20 \text{\AA})$	Xtriage
Refinement program	CNS 1.0	Depositor
D D	0.217 , $0.265$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.231 , $0.269$	DCC
$R_{free}$ test set	9883 reflections (4.97%)	wwPDB-VP
Wilson B-factor $(Å^2)$	22.9	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, $155.4$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.011  for  1/2 *h-1/2 *k,-3/2 *h-1/2 *k,-l	Vtriago
Estimated twinning fraction	0.027  for  1/2 *h + 1/2 *k, 3/2 *h - 1/2 *k, -1	Attrage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	6761	wwPDB-VP
Average B, all atoms $(Å^2)$	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.61% 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: PBQ, AD9, MG

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

Mol	Chain	Bo	nd lengths	Bond angles				
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5			
1	А	0.57	5/6364~(0.1%)	0.97	44/8590~(0.5%)			

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	10

Chain  $\mathbf{Z}$ Mol Res Type Atoms Observed(A)Ideal(Å) PRO А 713 N-CD 19.30 1.741 1.471 А 747 ARG C-N -7.761.161.34 $\overline{7}10$ 1 А PRO N-CD 7.021.571.47PRO N-CD 1 А 767 6.391.561.47ASP C-N 1 А 718-5.101.221.34

All (5) bond length outliers are listed below:

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	203	ASN	CB-CA-C	-15.77	78.87	110.40
1	А	739	PHE	CB-CA-C	-15.21	79.97	110.40
1	А	708	LEU	CB-CA-C	14.16	137.10	110.20
1	А	757	ALA	CB-CA-C	13.91	130.97	110.10
1	А	722	ALA	CB-CA-C	-13.73	89.50	110.10
1	А	741	ILE	N-CA-C	13.59	147.70	111.00
1	А	711	ASN	N-CA-C	13.05	146.24	111.00
1	А	748	ALA	N-CA-CB	12.30	127.31	110.10



Mol	Chain	Res	Type	Atoms	$\mathbf{Z} = \mathbf{Observed}(^{o})$		$Ideal(^{o})$
1	А	741	ILE	N-CA-CB	-12.20	82.75	110.80
1	А	741	ILE	CB-CA-C	-10.90	89.80	111.60
1	А	708	LEU	N-CA-C	-10.17	83.54	111.00
1	А	204	GLN	N-CA-C	10.06	138.18	111.00
1	А	747	ARG	CB-CA-C	-9.73	90.93	110.40
1	А	712	VAL	C-N-CD	-9.13	100.52	120.60
1	А	711	ASN	CB-CA-C	-9.04	92.32	110.40
1	А	713	PRO	CA-N-CD	-8.95	98.97	111.50
1	А	758	ARG	N-CA-CB	-8.59	95.14	110.60
1	А	718	ASP	CB-CA-C	8.44	127.27	110.40
1	А	495	LEU	N-CA-C	8.39	133.64	111.00
1	А	713	PRO	N-CA-CB	8.14	113.06	103.30
1	А	719	SER	N-CA-CB	8.06	122.58	110.50
1	А	742	THR	N-CA-C	-8.05	89.27	111.00
1	А	365	GLU	CB-CA-C	-7.94	94.52	110.40
1	А	208	SER	N-CA-CB	-7.55	99.17	110.50
1	А	747	ARG	O-C-N	-7.53	110.65	122.70
1	А	718	ASP	N-CA-C	-7.34	91.17	111.00
1	А	713	PRO	N-CA-C	-7.03	93.83	112.10
1	А	719	SER	N-CA-C	-6.90	92.38	111.00
1	А	718	ASP	O-C-N	-6.84	111.75	122.70
1	А	494	TYR	CB-CA-C	-6.63	97.14	110.40
1	А	742	THR	N-CA-CB	6.50	122.66	110.30
1	А	709	ALA	N-CA-CB	-6.05	101.63	110.10
1	А	365	GLU	N-CA-C	5.91	126.95	111.00
1	А	590	ASP	CB-CG-OD2	5.86	123.58	118.30
1	А	712	VAL	N-CA-C	-5.82	95.29	111.00
1	А	772	ASP	CB-CG-OD2	5.79	123.51	118.30
1	А	261	TYR	CB-CA-C	-5.75	98.90	110.40
1	А	262	LEU	CA-CB-CG	5.41	127.73	115.30
1	А	709	ALA	CB-CA-C	5.40	118.19	110.10
1	А	709	ALA	N-CA-C	5.38	125.54	111.00
1	А	204	GLN	N-CA-CB	-5.37	100.93	110.60
1	А	205	ALA	CB-CA-C	5.09	117.74	110.10
1	А	773	ASP	CB-CG-OD2	5.08	122.87	118.30
1	А	774	ASP	CB-CG-OD2	5.03	122.83	118.30

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There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group				
1	А	711	ASN	Peptide				
Continued on next nage								



Mol	Chain	Res	Type	Group
1	А	712	VAL	Peptide
1	А	718	ASP	Mainchain
1	А	747	ARG	Mainchain
1	А	767	PRO	Peptide
1	А	768	PRO	Peptide
1	А	769	MET	Peptide
1	А	773	ASP	Peptide
1	А	775	ILE	Peptide
1	А	776	PRO	Peptide

## 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	6239	0	6175	471	0
2	А	31	0	14	2	0
3	А	1	0	0	0	0
4	А	17	0	3	11	0
5	А	473	0	0	35	0
All	All	6761	0	6192	474	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (474) 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:A:713:PRO:N	1:A:713:PRO:CD	1.74	1.44
1:A:431:LEU:HD13	4:A:1780:PBQ:BR18	1.95	1.20
1:A:773:ASP:H	1:A:775:ILE:HG22	1.10	1.16
1:A:496:LYS:O	1:A:498:LYS:HG2	1.47	1.12
1:A:739:PHE:HA	1:A:744:ILE:HG13	1.31	1.12
1:A:202:ARG:HB2	1:A:208:SER:HB3	1.34	1.09
1:A:424:ALA:HB2	4:A:1780:PBQ:BR14	2.07	1.09
1:A:767:PRO:HD2	1:A:768:PRO:CD	1.83	1.08
1:A:204:GLN:HA	1:A:209:GLY:HA3	1.25	1.07



	A L	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:767:PRO:HD2	1:A:768:PRO:HD2	1.03	1.02		
1:A:204:GLN:CA	1:A:209:GLY:HA3	1.88	1.01		
1:A:499:ILE:HD12	1:A:740:GLY:HA3	1.42	1.00		
1:A:206:ASN:HA	1:A:210:VAL:HB	1.43	1.00		
1:A:736:GLN:OE1	1:A:747:ARG:HB2	1.62	0.98		
1:A:756:GLU:HA	1:A:759:GLU:HB3	1.41	0.97		
1:A:766:GLU:H	1:A:767:PRO:HD3	1.30	0.94		
1:A:767:PRO:CD	1:A:768:PRO:HD2	1.95	0.93		
1:A:173:GLN:HE22	1:A:649:ASN:HD22	1.00	0.93		
1:A:766:GLU:N	1:A:767:PRO:HD3	1.82	0.92		
1:A:712:VAL:C	1:A:713:PRO:CD	2.38	0.92		
1:A:204:GLN:HA	1:A:209:GLY:CA	1.99	0.92		
1:A:277:ASN:HD22	1:A:278:TYR:H	1.18	0.92		
1:A:740:GLY:O	1:A:743:LYS:O	1.90	0.90		
1:A:366:GLY:HA3	1:A:408:HIS:ND1	1.89	0.87		
1:A:366:GLY:HA3	1:A:408:HIS:CE1	2.09	0.86		
1:A:712:VAL:CG1	1:A:712:VAL:O	2.25	0.85		
1:A:773:ASP:N	1:A:775:ILE:HG22	1.92	0.85		
1:A:712:VAL:N	1:A:713:PRO:HD3	1.91	0.85		
1:A:741:ILE:HG23	1:A:741:ILE:O	1.77	0.84		
1:A:325:LYS:O	1:A:329:GLN:HG2	1.78	0.84		
1:A:610:LYS:HE3	1:A:614:ASP:HB2	1.59	0.83		
1:A:262:LEU:HD11	1:A:470:CYS:HB3	1.60	0.83		
1:A:712:VAL:CA	1:A:713:PRO:HD3	2.09	0.83		
1:A:461:PHE:H	1:A:464:ASN:HD21	1.27	0.82		
1:A:712:VAL:O	1:A:712:VAL:HG13	1.80	0.81		
1:A:712:VAL:CA	1:A:713:PRO:CD	2.59	0.81		
1:A:764:SER:HA	1:A:768:PRO:HD3	1.62	0.81		
1:A:727:LEU:HD12	1:A:732:ILE:HD11	1.62	0.81		
1:A:741:ILE:O	1:A:741:ILE:CG2	2.23	0.80		
1:A:53:VAL:HG21	1:A:63:LYS:HG3	1.61	0.80		
1:A:497:GLU:HG2	1:A:745:PHE:HE2	1.47	0.79		
1:A:766:GLU:N	1:A:767:PRO:CD	2.46	0.79		
1:A:697:ILE:HD12	1:A:697:ILE:H	1.47	0.79		
1:A:750:GLN:HA	1:A:753:ARG:HH11	1.47	0.79		
1:A:719:SER:O	1:A:723:THR:HG23	1.84	0.78		
1:A:329:GLN:HE21	1:A:329:GLN:HA	1.49	0.78		
1:A:707:LEU:O	1:A:708:LEU:C	2.22	0.77		
1:A:173:GLN:HE22	1:A:649:ASN:ND2	1.80	0.77		
1:A:746:PHE:HD2	1:A:751:LEU:HB2	1.51	0.76		
1:A:760:GLN:HG3	5:A:2209:HOH:O	1.84	0.76		



	t i c	Interatomic	Clash		
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)		
1:A:465:SER:H	1:A:468:GLN:NE2	1.82	0.76		
1:A:761:ARG:O	1:A:765:ASN:HB2	1.85	0.76		
1:A:239:PHE:HB3	1:A:263:LEU:HD12	1.68	0.75		
1:A:424:ALA:HA	4:A:1780:PBQ:O	1.85	0.75		
1:A:695:ARG:HH11	1:A:695:ARG:HB3	1.51	0.75		
1:A:707:LEU:C	1:A:708:LEU:O	2.06	0.75		
1:A:262:LEU:HD23	1:A:262:LEU:O	1.86	0.75		
1:A:773:ASP:H	1:A:775:ILE:CG2	1.96	0.74		
1:A:431:LEU:CD1	4:A:1780:PBQ:BR18	2.86	0.74		
4:A:1780:PBQ:BR17	4:A:1780:PBQ:HD2	2.43	0.74		
1:A:145:GLY:H	1:A:164:ARG:HH21	1.37	0.73		
1:A:617:ILE:O	4:A:1780:PBQ:BR17	2.61	0.73		
1:A:718:ASP:O	1:A:721:LYS:HE2	1.89	0.73		
1:A:424:ALA:CB	4:A:1780:PBQ:BR14	2.91	0.72		
1:A:693:PRO:HA	1:A:695:ARG:HH22	1.55	0.72		
1:A:246:GLN:HG2	1:A:446:LYS:HB3	1.72	0.71		
1:A:706:TYR:H	1:A:706:TYR:HD2	1.38	0.71		
1:A:706:TYR:N	1:A:706:TYR:CD2	2.58	0.71		
1:A:706:TYR:O	1:A:712:VAL:HG13	1.91	0.71		
1:A:461:PHE:N	1:A:464:ASN:HD21	1.88	0.71		
1:A:453:LEU:HD13	1:A:641:LEU:HD21	1.73	0.70		
1:A:25:PHE:O	1:A:29:VAL:HG22	1.92	0.70		
1:A:755:GLU:O	1:A:758:ARG:HG3	1.90	0.70		
1:A:762:LEU:O	1:A:767:PRO:HG3	1.92	0.69		
1:A:118:TYR:CD2	1:A:153:PRO:HG3	2.27	0.69		
1:A:753:ARG:HA	1:A:756:GLU:OE1	1.92	0.69		
1:A:694:ASN:HB2	1:A:746:PHE:HB2	1.73	0.69		
1:A:186:THR:O	1:A:190:LYS:HG3	1.92	0.69		
1:A:741:ILE:HG22	1:A:742:THR:N	2.02	0.69		
1:A:305:ASN:H	1:A:356:ASN:HD21	1.41	0.69		
1:A:736:GLN:OE1	1:A:750:GLN:HB2	1.92	0.68		
1:A:695:ARG:HB2	1:A:743:LYS:HD2	1.75	0.68		
1:A:347:ILE:O	1:A:351:ILE:HG13	1.93	0.68		
1:A:291:GLU:O	1:A:294:LYS:HG3	1.93	0.68		
1:A:265:LYS:HD3	4:A:1780:PBQ:BR19	2.48	0.68		
1:A:499:ILE:HD12	1:A:740:GLY:CA	2.23	0.68		
1:A:615:PRO:O	1:A:619:SER:HB2	1.93	0.68		
1:A:727:LEU:HD23	1:A:728:LYS:N	2.09	0.68		
1:A:395:GLU:HA	1:A:407:GLN:O	1.94	0.67		
1:A:14:TYR:HA	5:A:2024:HOH:O	1.94	0.67		
1:A:204:GLN:HG3	1:A:209:GLY:HA3	1.77	0.67		



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:693:PRO:HA	1:A:695:ARG:NH2	2.09	0.67	
1:A:741:ILE:HG22	1:A:742:THR:HG22	1.77	0.67	
1:A:329:GLN:O	1:A:333:ILE:HD13	1.95	0.67	
1:A:499:ILE:HD11	1:A:740:GLY:H	1.59	0.67	
1:A:773:ASP:O	1:A:776:PRO:CG	2.43	0.67	
1:A:775:ILE:HG23	1:A:776:PRO:CD	2.25	0.66	
1:A:170:ARG:HG2	1:A:170:ARG:HH21	1.59	0.66	
1:A:497:GLU:HG2	1:A:745:PHE:CE2	2.31	0.66	
1:A:769:MET:HG2	1:A:770:ASP:OD1	1.94	0.66	
1:A:773:ASP:HB2	1:A:775:ILE:H	1.60	0.66	
1:A:775:ILE:HG23	1:A:776:PRO:HD3	1.78	0.66	
1:A:767:PRO:CD	1:A:768:PRO:CD	2.65	0.65	
1:A:206:ASN:CA	1:A:210:VAL:HB	2.23	0.65	
1:A:773:ASP:O	1:A:776:PRO:HG2	1.97	0.65	
1:A:764:SER:HA	1:A:768:PRO:CD	2.26	0.65	
1:A:716:ALA:HB1	1:A:721:LYS:HE2	1.79	0.65	
1:A:316:LYS:HB3	5:A:2200:HOH:O	1.97	0.65	
1:A:704:ARG:O	1:A:758:ARG:NH1	2.29	0.65	
1:A:736:GLN:CD	1:A:747:ARG:HB2	2.17	0.64	
1:A:708:LEU:HD21	1:A:758:ARG:HD2	1.78	0.64	
1:A:375:LEU:HD12	1:A:389:LEU:HD23	1.80	0.64	
1:A:706:TYR:O	1:A:712:VAL:O	2.15	0.64	
1:A:580:GLU:HG3	5:A:2394:HOH:O	1.98	0.64	
1:A:257:SER:HB3	1:A:442:CYS:SG	2.38	0.63	
2:A:1778:AD9:O2A	5:A:2472:HOH:O	2.16	0.63	
1:A:144:LYS:HG3	1:A:199:VAL:HG22	1.81	0.63	
1:A:465:SER:H	1:A:468:GLN:HE21	1.46	0.63	
1:A:597:GLU:O	1:A:601:LYS:HG3	1.99	0.63	
1:A:337:SER:HB2	1:A:340:GLU:HG3	1.81	0.62	
1:A:323:GLU:OE1	1:A:326:ILE:HD12	1.98	0.62	
1:A:145:GLY:N	1:A:164:ARG:HH21	1.97	0.62	
1:A:761:ARG:O	1:A:761:ARG:HD2	1.99	0.62	
1:A:697:ILE:HD12	1:A:697:ILE:N	2.14	0.62	
1:A:144:LYS:HA	1:A:195:TYR:OH	2.00	0.61	
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.80	0.61	
1:A:727:LEU:HB2	1:A:732:ILE:HG12	1.83	0.61	
1:A:202:ARG:HB3	5:A:2184:HOH:O	2.00	0.61	
1:A:657:ILE:HG22	1:A:675:GLN:NE2	2.15	0.61	
1:A:496:LYS:O	1:A:498:LYS:CG	2.37	0.61	
1:A:723:THR:O	1:A:727:LEU:HD22	2.00	0.61	
1:A:273:GLU:O	1:A:274:THR:OG1	2.10	0.61	



			Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:727:LEU:HD23	1:A:728:LYS:H	1.64	0.61	
1:A:724:ASP:HA	1:A:727:LEU:HD21	1.83	0.60	
1:A:721:LYS:HG2	1:A:722:ALA:N	2.14	0.60	
1:A:210:VAL:O	1:A:214:GLN:HG3	2.01	0.60	
1:A:305:ASN:H	1:A:356:ASN:ND2	1.99	0.60	
1:A:193:ILE:HD12	1:A:245:ILE:HD11	1.83	0.60	
1:A:239:PHE:HB3	1:A:263:LEU:CD1	2.30	0.60	
1:A:761:ARG:HH11	1:A:765:ASN:HA	1.66	0.60	
1:A:412:GLU:HB2	5:A:2284:HOH:O	2.02	0.60	
1:A:4:ILE:HD12	1:A:146:ARG:NH2	2.17	0.59	
1:A:211:LEU:O	1:A:215:ILE:HG13	2.00	0.59	
1:A:708:LEU:HD11	1:A:758:ARG:CB	2.32	0.59	
2:A:1778:AD9:O1G	2:A:1778:AD9:VG	1.59	0.59	
1:A:273:GLU:HG2	1:A:274:THR:HG23	1.84	0.59	
1:A:246:GLN:HG2	1:A:446:LYS:HD2	1.85	0.59	
1:A:329:GLN:HE21	1:A:329:GLN:CA	2.16	0.58	
1:A:458:PHE:HE1	1:A:460:ILE:HD11	1.67	0.58	
1:A:430:PHE:O	1:A:434:VAL:HG23	2.02	0.58	
1:A:302:GLU:HA	1:A:308:ASN:HB3	1.85	0.58	
1:A:45:ASP:OD1	1:A:670:LYS:HD2	2.02	0.58	
1:A:696:ILE:HD11	1:A:746:PHE:CE2	2.39	0.58	
1:A:202:ARG:HB2	1:A:208:SER:CB	2.22	0.58	
1:A:361:LYS:HE3	1:A:362:GLY:O	2.04	0.58	
1:A:438:ASN:O	1:A:442:CYS:HB2	2.03	0.58	
1:A:565:LYS:HB2	1:A:565:LYS:NZ	2.19	0.58	
1:A:397:ARG:HG2	1:A:397:ARG:HH11	1.69	0.57	
1:A:499:ILE:CD1	1:A:740:GLY:HA3	2.27	0.57	
1:A:93:GLU:HB3	5:A:2098:HOH:O	2.04	0.57	
1:A:170:ARG:HG2	1:A:170:ARG:NH2	2.16	0.57	
1:A:217:GLN:O	1:A:330:ALA:HB1	2.03	0.57	
1:A:262:LEU:HD11	1:A:470:CYS:CB	2.34	0.57	
1:A:728:LYS:C	1:A:731:ASN:H	2.08	0.57	
1:A:753:ARG:HB2	5:A:2465:HOH:O	2.05	0.57	
1:A:775:ILE:CG2	1:A:776:PRO:CD	2.81	0.57	
1:A:766:GLU:O	1:A:766:GLU:HG3	2.04	0.57	
1:A:375:LEU:CD1	1:A:389:LEU:HD23	2.35	0.57	
1:A:720:GLN:O	1:A:720:GLN:HG3	2.05	0.57	
1:A:708:LEU:HD11	1:A:758:ARG:HB3	1.86	0.56	
1:A:281:PHE:CD1	1:A:352:LEU:HD21	2.40	0.56	
1:A:496:LYS:C	1:A:498:LYS:N	2.56	0.56	
1:A:761:ARG:HD2	1:A:765:ASN:HB2	1.88	0.56	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:701:PHE:CE2	1:A:723:THR:HG22	2.41	0.56	
1:A:736:GLN:O	1:A:747:ARG:HG3	2.06	0.56	
1:A:761:ARG:O	1:A:765:ASN:CB	2.53	0.56	
1:A:341:GLN:O	1:A:344:ILE:HB	2.06	0.55	
1:A:497:GLU:CD	1:A:742:THR:HG23	2.27	0.55	
1:A:231:THR:HG23	1:A:275:GLU:OE2	2.06	0.55	
1:A:495:LEU:N	1:A:495:LEU:CD1	2.67	0.55	
1:A:432:TRP:NE1	1:A:436:LYS:HD3	2.22	0.55	
1:A:495:LEU:N	1:A:495:LEU:HD13	2.22	0.55	
1:A:697:ILE:HG13	1:A:743:LYS:HB3	1.88	0.55	
1:A:775:ILE:O	1:A:775:ILE:HG13	2.06	0.55	
1:A:79:GLN:HG2	1:A:96:TYR:CE2	2.41	0.55	
1:A:728:LYS:HA	5:A:2462:HOH:O	2.05	0.55	
1:A:135:TYR:CG	1:A:191:LYS:HD2	2.41	0.55	
1:A:173:GLN:NE2	1:A:649:ASN:HB3	2.21	0.55	
1:A:342:MET:HG3	1:A:346:LYS:HE3	1.89	0.55	
1:A:499:ILE:O	1:A:500:ASN:HB2	2.05	0.55	
1:A:697:ILE:HG23	1:A:742:THR:O	2.06	0.55	
1:A:702:VAL:CG2	1:A:714:ARG:HG3	2.36	0.55	
1:A:495:LEU:C	1:A:496:LYS:HE2	2.27	0.55	
1:A:697:ILE:HG22	1:A:698:TYR:N	2.22	0.55	
1:A:707:LEU:O	1:A:708:LEU:O	2.24	0.55	
1:A:724:ASP:O	1:A:728:LYS:HB3	2.06	0.55	
1:A:633:GLN:O	1:A:636:GLU:HB3	2.07	0.55	
1:A:708:LEU:HD21	1:A:758:ARG:HB2	1.88	0.54	
1:A:63:LYS:HG2	1:A:69:ASP:CG	2.28	0.54	
1:A:230:THR:HA	1:A:275:GLU:CD	2.27	0.54	
1:A:646:GLU:OE1	1:A:646:GLU:HA	2.06	0.54	
1:A:746:PHE:CD2	1:A:751:LEU:HB2	2.36	0.54	
1:A:157:ALA:O	1:A:161:VAL:HG23	2.07	0.54	
1:A:402:ARG:HG2	1:A:402:ARG:HH11	1.73	0.54	
1:A:497:GLU:OE2	1:A:742:THR:HG23	2.07	0.54	
1:A:761:ARG:HB2	5:A:2466:HOH:O	2.07	0.54	
1:A:701:PHE:CE2	1:A:723:THR:HA	2.43	0.54	
1:A:758:ARG:HE	1:A:758:ARG:C	2.11	0.54	
1:A:107:ARG:HD3	5:A:2109:HOH:O	2.07	0.54	
1:A:324:PHE:HE2	1:A:328:ARG:HH21	1.56	0.54	
1:A:137:GLN:NE2	1:A:141:ASP:OD1	2.41	0.54	
1:A:766:GLU:H	1:A:767:PRO:CD	2.08	0.54	
1:A:657:ILE:HG22	1:A:675:GLN:HE22	1.74	0.53	
1:A:399:LEU:HA	1:A:403:ASP:O	2.08	0.53	



	the pagetti	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:129:PHE:CZ	1:A:662:GLN:HA	2.43	0.53	
1:A:63:LYS:HG2	1:A:69:ASP:OD1	2.08	0.53	
1:A:118:TYR:CE2	1:A:153:PRO:HG3	2.43	0.53	
1:A:500:ASN:HB3	5:A:2324:HOH:O	2.06	0.53	
1:A:455:ILE:HG12	5:A:2162:HOH:O	2.09	0.53	
1:A:741:ILE:HG22	1:A:742:THR:CG2	2.39	0.53	
1:A:11:TYR:CD2	1:A:15:LEU:HD12	2.44	0.53	
1:A:326:ILE:HG23	5:A:2247:HOH:O	2.08	0.53	
1:A:371:ASP:OD2	1:A:373:THR:HG23	2.09	0.53	
1:A:758:ARG:O	1:A:761:ARG:HB3	2.09	0.53	
1:A:6:ASP:OD1	1:A:8:THR:HB	2.09	0.53	
1:A:727:LEU:HA	1:A:730:LEU:CD1	2.39	0.53	
1:A:262:LEU:CD1	1:A:470:CYS:HB3	2.36	0.52	
1:A:204:GLN:HG3	1:A:209:GLY:CA	2.39	0.52	
1:A:397:ARG:HB3	1:A:404:LEU:HD11	1.91	0.52	
1:A:357:ILE:HB	1:A:418:ARG:NH1	2.24	0.52	
1:A:706:TYR:CD2	1:A:707:LEU:N	2.74	0.52	
1:A:484:HIS:CE1	1:A:489:LEU:HD21	2.44	0.52	
1:A:497:GLU:OE1	1:A:742:THR:HG23	2.09	0.52	
1:A:112:GLN:O	1:A:113:ASP:HB2	2.10	0.52	
1:A:694:ASN:CB	1:A:746:PHE:HB2	2.39	0.52	
1:A:695:ARG:HH11	1:A:695:ARG:CB	2.22	0.52	
1:A:225:PHE:CE2	1:A:280:ILE:HG12	2.44	0.52	
1:A:200:ALA:O	1:A:253:ILE:HG12	2.09	0.52	
1:A:419:ASP:O	1:A:423:LYS:HG3	2.10	0.52	
1:A:714:ARG:O	1:A:714:ARG:HG2	2.10	0.52	
1:A:175:LEU:HD12	1:A:651:HIS:HB2	1.91	0.52	
1:A:367:ALA:HB2	1:A:411:VAL:N	2.25	0.52	
1:A:635:LYS:HE2	5:A:2340:HOH:O	2.09	0.52	
1:A:461:PHE:H	1:A:464:ASN:ND2	2.04	0.51	
1:A:622:LYS:HA	1:A:627:PHE:HA	1.90	0.51	
1:A:144:LYS:HG3	1:A:199:VAL:CG2	2.40	0.51	
1:A:147:ARG:HB2	1:A:150:GLU:CG	2.41	0.51	
1:A:750:GLN:HG2	1:A:754:ILE:HD12	1.93	0.51	
1:A:764:SER:C	1:A:767:PRO:HD2	2.31	0.51	
1:A:291:GLU:O	1:A:294:LYS:HE2	2.11	0.51	
1:A:330:ALA:O	1:A:334:VAL:HG23	2.11	0.51	
1:A:674:ASP:HB2	5:A:2448:HOH:O	2.11	0.51	
1:A:699:ALA:O	1:A:702:VAL:HG13	2.11	0.51	
1:A:715:ASP:O	1:A:716:ALA:HB2	2.09	0.51	
1:A:698:TYR:HE1	1:A:744:ILE:HB	1.75	0.51	



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:56:THR:O	1:A:74:LYS:HE3	2.11	0.51
1:A:765:ASN:OD1	1:A:765:ASN:C	2.49	0.51
1:A:289:THR:OG1	1:A:292:GLU:HG3	2.11	0.51
1:A:79:GLN:HG2	1:A:96:TYR:CZ	2.46	0.50
1:A:244:GLU:HG3	1:A:449:PHE:CD2	2.47	0.50
1:A:506:PHE:CZ	1:A:687:ILE:HD13	2.47	0.50
1:A:764:SER:O	1:A:768:PRO:HD2	2.12	0.50
1:A:8:THR:HA	5:A:2007:HOH:O	2.10	0.50
1:A:135:TYR:CD1	1:A:191:LYS:HD2	2.47	0.50
1:A:516:LEU:O	1:A:525:ILE:HG13	2.12	0.50
1:A:727:LEU:HB2	1:A:732:ILE:CG1	2.41	0.50
1:A:751:LEU:O	1:A:755:GLU:HB2	2.11	0.50
1:A:773:ASP:C	1:A:776:PRO:HD2	2.32	0.50
1:A:701:PHE:HE2	1:A:723:THR:HG22	1.76	0.50
1:A:773:ASP:CB	1:A:775:ILE:H	2.24	0.50
1:A:53:VAL:CG2	1:A:63:LYS:HG3	2.38	0.50
1:A:280:ILE:HG13	1:A:348:ILE:HD13	1.92	0.50
1:A:601:LYS:HD3	5:A:2414:HOH:O	2.11	0.50
1:A:499:ILE:O	1:A:499:ILE:HG23	2.10	0.50
1:A:535:PHE:HD2	1:A:536:PRO:HD2	1.77	0.50
1:A:245:ILE:O	1:A:449:PHE:HA	2.12	0.49
1:A:334:VAL:HG12	1:A:440:VAL:HG21	1.93	0.49
1:A:369:LEU:HD23	1:A:375:LEU:HD22	1.94	0.49
1:A:76:ASP:HB3	5:A:2082:HOH:O	2.12	0.49
1:A:225:PHE:CE2	1:A:348:ILE:HD11	2.47	0.49
1:A:622:LYS:HG2	1:A:626:ASN:O	2.12	0.49
1:A:697:ILE:H	1:A:697:ILE:CD1	2.20	0.49
1:A:700:ASP:HA	1:A:703:LYS:HG2	1.93	0.49
1:A:701:PHE:HE2	1:A:723:THR:HA	1.78	0.49
1:A:708:LEU:HD13	5:A:2469:HOH:O	2.13	0.49
1:A:718:ASP:HB3	1:A:721:LYS:HD3	1.93	0.49
1:A:244:GLU:O	1:A:256:ALA:HA	2.12	0.49
1:A:323:GLU:OE1	1:A:323:GLU:HA	2.12	0.49
1:A:84:LYS:HG2	5:A:2095:HOH:O	2.13	0.49
1:A:120:GLY:HA3	5:A:2456:HOH:O	2.12	0.49
1:A:720:GLN:O	1:A:723:THR:OG1	2.30	0.49
1:A:22:SER:O	1:A:26:LYS:HG2	2.13	0.49
1:A:173:GLN:NE2	1:A:649:ASN:HD22	1.85	0.49
1:A:482:PHE:CE1	1:A:486:MET:HG3	2.48	0.49
1:A:712:VAL:N	1:A:713:PRO:CD	2.72	0.49
1:A:319:SER:HB3	1:A:322:GLU:HB2	1.94	0.49



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:557:LYS:HE3	5:A:2336:HOH:O	2.13	0.49	
1:A:774:ASP:O	1:A:776:PRO:O	2.30	0.49	
1:A:147:ARG:HB2	1:A:150:GLU:CD	2.33	0.48	
1:A:737:TYR:HB3	1:A:750:GLN:OE1	2.13	0.48	
1:A:567:GLU:HA	1:A:579:TYR:O	2.13	0.48	
1:A:737:TYR:HB2	1:A:745:PHE:O	2.13	0.48	
1:A:752:ALA:HA	1:A:755:GLU:HB2	1.94	0.48	
1:A:770:ASP:O	1:A:773:ASP:OD1	2.31	0.48	
1:A:37:TYR:OH	1:A:65:VAL:HG22	2.13	0.48	
1:A:482:PHE:CZ	1:A:486:MET:HG3	2.48	0.48	
1:A:698:TYR:CE1	1:A:744:ILE:HB	2.47	0.48	
1:A:44:ARG:NH1	1:A:99:GLU:OE2	2.47	0.48	
1:A:518:ASP:HB2	1:A:635:LYS:HD2	1.95	0.48	
1:A:692:PHE:HB2	1:A:745:PHE:HB3	1.94	0.48	
1:A:277:ASN:ND2	1:A:278:TYR:H	1.99	0.48	
1:A:432:TRP:CE2	1:A:436:LYS:HD3	2.49	0.48	
1:A:569:GLY:HA3	1:A:578:MET:CE	2.44	0.48	
1:A:204:GLN:HA	1:A:209:GLY:N	2.29	0.48	
1:A:732:ILE:O	1:A:732:ILE:HG13	2.14	0.48	
1:A:712:VAL:O	1:A:712:VAL:HG12	2.11	0.48	
1:A:734:PRO:HA	1:A:737:TYR:CE2	2.49	0.47	
1:A:736:GLN:OE1	1:A:750:GLN:CB	2.61	0.47	
1:A:206:ASN:OD1	1:A:206:ASN:O	2.32	0.47	
1:A:728:LYS:O	1:A:731:ASN:ND2	2.47	0.47	
1:A:222:LEU:HD11	1:A:258:ILE:HD13	1.96	0.47	
1:A:98:ASN:HB3	5:A:2100:HOH:O	2.14	0.47	
1:A:246:GLN:HG2	1:A:446:LYS:CD	2.44	0.47	
1:A:372:LYS:HB2	1:A:376:ASN:HD21	1.79	0.47	
1:A:698:TYR:HB3	1:A:719:SER:HB2	1.96	0.47	
1:A:700:ASP:CA	1:A:703:LYS:HG2	2.44	0.47	
1:A:327:THR:HG22	1:A:331:MET:HE2	1.96	0.46	
1:A:700:ASP:O	1:A:703:LYS:HG2	2.15	0.46	
1:A:724:ASP:HA	1:A:727:LEU:CD2	2.45	0.46	
1:A:171:GLN:HE22	1:A:649:ASN:N	2.13	0.46	
1:A:318:VAL:HG11	5:A:2083:HOH:O	2.15	0.46	
1:A:573:TYR:O	1:A:678:CYS:HB2	2.15	0.46	
1:A:582:GLN:O	1:A:583:ASP:HB2	2.15	0.46	
1:A:160:ASP:OD1	5:A:2151:HOH:O	2.21	0.46	
1:A:465:SER:N	1:A:468:GLN:HE21	2.11	0.46	
1:A:736:GLN:CD	1:A:750:GLN:HB2	2.36	0.46	
1:A:225:PHE:CD2	1:A:280:ILE:HG12	2.51	0.46	



	t i c	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:248:ASN:HD21	1:A:250:ALA:HB3	1.81	0.46	
1:A:264:GLU:O	1:A:278:TYR:OH	2.29	0.46	
1:A:366:GLY:CA	1:A:408:HIS:CE1	2.91	0.46	
1:A:385:ASN:HA	1:A:386:PRO:HD2	1.74	0.46	
1:A:397:ARG:HA	1:A:406:ALA:HA	1.97	0.46	
1:A:610:LYS:HE3	1:A:614:ASP:CB	2.38	0.46	
1:A:705:TYR:CZ	1:A:754:ILE:HG22	2.50	0.46	
1:A:702:VAL:HG23	1:A:714:ARG:HG3	1.98	0.46	
1:A:679:ASN:HD22	1:A:679:ASN:N	2.13	0.46	
1:A:238:ARG:O	1:A:263:LEU:HD12	2.16	0.46	
1:A:773:ASP:O	1:A:776:PRO:HD2	2.16	0.46	
1:A:118:TYR:CE1	1:A:123:LEU:HD13	2.51	0.45	
1:A:170:ARG:O	1:A:448:TYR:HE1	1.99	0.45	
1:A:202:ARG:O	1:A:204:GLN:N	2.47	0.45	
1:A:667:LEU:HD11	1:A:672:VAL:HG21	1.97	0.45	
1:A:708:LEU:HD11	1:A:758:ARG:HB2	1.98	0.45	
1:A:580:GLU:OE2	1:A:582:GLN:HB2	2.16	0.45	
1:A:521:GLN:HA	1:A:522:PRO:HA	1.60	0.45	
1:A:495:LEU:HA	1:A:495:LEU:HD12	1.62	0.45	
1:A:496:LYS:C	1:A:498:LYS:H	2.20	0.45	
1:A:727:LEU:HB2	1:A:732:ILE:CD1	2.46	0.45	
1:A:301:PRO:HG2	1:A:302:GLU:OE1	2.16	0.45	
1:A:709:ALA:HB3	1:A:712:VAL:HG11	1.97	0.45	
1:A:7:ARG:HA	1:A:12:HIS:CG	2.52	0.45	
1:A:26:LYS:NZ	5:A:2036:HOH:O	2.49	0.45	
1:A:458:PHE:CE1	1:A:460:ILE:HD11	2.50	0.45	
1:A:773:ASP:HB2	1:A:775:ILE:HG22	1.98	0.45	
1:A:397:ARG:HG2	1:A:397:ARG:NH1	2.32	0.45	
1:A:675:GLN:O	1:A:679:ASN:HB2	2.16	0.44	
1:A:115:ILE:O	5:A:2120:HOH:O	2.21	0.44	
1:A:207:GLY:O	1:A:211:LEU:HB2	2.17	0.44	
1:A:258:ILE:HB	1:A:438:ASN:HD21	1.81	0.44	
1:A:762:LEU:N	1:A:762:LEU:HD13	2.33	0.44	
1:A:91:MET:CE	1:A:105:ASN:HB3	2.47	0.44	
1:A:499:ILE:HD11	1:A:740:GLY:N	2.29	0.44	
1:A:343:SER:HB2	1:A:607:VAL:HG21	1.99	0.44	
1:A:754:ILE:HG13	5:A:2465:HOH:O	2.18	0.44	
1:A:304:PHE:HA	1:A:356:ASN:HD21	1.83	0.44	
1:A:212:GLU:OE2	1:A:212:GLU:N	2.46	0.44	
1:A:643:ALA:O	1:A:647:THR:HG23	2.17	0.44	
1:A:671:VAL:O	1:A:675:GLN:HG3	2.17	0.44	



	h h	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:765:ASN:N	1:A:767:PRO:HD3	2.33	0.44	
1:A:283:GLN:HG2	1:A:320:ASP:O	2.18	0.44	
1:A:468:GLN:NE2	1:A:468:GLN:H	2.16	0.43	
1:A:745:PHE:N	1:A:745:PHE:CD2	2.86	0.43	
1:A:207:GLY:O	1:A:211:LEU:CB	2.67	0.43	
1:A:234:ASN:ND2	5:A:2201:HOH:O	2.50	0.43	
1:A:562:ARG:NH1	5:A:2373:HOH:O	2.50	0.43	
1:A:150:GLU:H	1:A:150:GLU:HG2	1.39	0.43	
1:A:246:GLN:CG	1:A:446:LYS:HD2	2.47	0.43	
1:A:393:LEU:O	1:A:409:LEU:HD12	2.18	0.43	
1:A:600:PHE:O	1:A:603:SER:HB3	2.19	0.43	
1:A:391:LYS:HD2	1:A:391:LYS:HA	1.72	0.43	
1:A:291:GLU:HA	1:A:294:LYS:HZ3	1.84	0.43	
1:A:336:PHE:CE2	1:A:433:LEU:HD23	2.54	0.43	
1:A:764:SER:C	1:A:768:PRO:HD2	2.39	0.43	
1:A:773:ASP:O	1:A:776:PRO:CD	2.67	0.43	
1:A:56:THR:HG23	1:A:59:SER:OG	2.19	0.43	
1:A:402:ARG:HG2	1:A:402:ARG:NH1	2.33	0.43	
1:A:640:SER:O	1:A:643:ALA:HB3	2.19	0.43	
1:A:705:TYR:OH	1:A:755:GLU:HA	2.18	0.43	
1:A:728:LYS:O	1:A:731:ASN:N	2.48	0.43	
1:A:741:ILE:CG2	1:A:742:THR:HG22	2.46	0.43	
1:A:262:LEU:HD12	1:A:634:TYR:CG	2.54	0.43	
1:A:296:LEU:HB2	1:A:298:LEU:HG	2.00	0.43	
1:A:702:VAL:HG23	1:A:702:VAL:O	2.18	0.43	
1:A:776:PRO:O	1:A:777:PHE:C	2.57	0.43	
1:A:149:ASN:OD1	1:A:149:ASN:N	2.40	0.42	
1:A:750:GLN:HG2	1:A:754:ILE:CD1	2.49	0.42	
1:A:284:LEU:HD13	1:A:345:PHE:HB3	2.00	0.42	
1:A:431:LEU:HD22	4:A:1780:PBQ:BR18	2.74	0.42	
1:A:732:ILE:HD12	1:A:754:ILE:CD1	2.49	0.42	
1:A:171:GLN:NE2	1:A:649:ASN:HB2	2.33	0.42	
1:A:173:GLN:HE21	1:A:173:GLN:HB3	1.68	0.42	
1:A:775:ILE:N	1:A:776:PRO:HD2	2.33	0.42	
1:A:305:ASN:HA	1:A:308:ASN:OD1	2.19	0.42	
1:A:661:LYS:NZ	1:A:666:LYS:NZ	2.68	0.42	
1:A:704:ARG:HB3	5:A:2460:HOH:O	2.18	0.42	
1:A:267:ARG:HB3	1:A:278:TYR:CE2	2.55	0.42	
1:A:657:ILE:O	1:A:675:GLN:NE2	2.50	0.42	
1:A:431:LEU:HD22	4:A:1780:PBQ:BR17	2.75	0.42	
1:A:459:GLU:OE2	1:A:468:GLN:HG3	2.19	0.42	



	A h	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:717:GLU:O	1:A:718:ASP:HB2	2.20	0.42	
1:A:56:THR:OG1	1:A:57:SER:N	2.52	0.42	
1:A:147:ARG:NH1	1:A:759:GLU:OE2	2.52	0.42	
1:A:266:SER:HA	1:A:423:LYS:HD2	2.02	0.42	
1:A:376:ASN:O	1:A:380:THR:OG1	2.30	0.42	
1:A:258:ILE:N	1:A:438:ASN:OD1	2.47	0.42	
1:A:280:ILE:HG23	1:A:281:PHE:N	2.34	0.42	
1:A:291:GLU:HB3	5:A:2229:HOH:O	2.20	0.42	
1:A:705:TYR:HE2	1:A:758:ARG:HD3	1.85	0.42	
1:A:182:GLY:HA2	1:A:233:ASN:ND2	2.35	0.42	
1:A:623:LYS:N	1:A:626:ASN:O	2.52	0.42	
1:A:713:PRO:HB2	1:A:715:ASP:H	1.85	0.42	
1:A:265:LYS:HE2	4:A:1780:PBQ:H11	1.84	0.41	
1:A:422:VAL:HG12	1:A:423:LYS:N	2.34	0.41	
1:A:495:LEU:HB3	1:A:496:LYS:CE	2.50	0.41	
1:A:586:GLU:HB3	5:A:2399:HOH:O	2.19	0.41	
1:A:695:ARG:HB2	1:A:743:LYS:CD	2.47	0.41	
1:A:697:ILE:HA	1:A:743:LYS:CB	2.50	0.41	
1:A:565:LYS:HB2	1:A:565:LYS:HZ2	1.85	0.41	
1:A:210:VAL:HG12	1:A:211:LEU:N	2.35	0.41	
1:A:727:LEU:O	1:A:731:ASN:N	2.53	0.41	
1:A:773:ASP:N	1:A:776:PRO:HD2	2.35	0.41	
1:A:72:VAL:HG22	1:A:73:LYS:O	2.18	0.41	
1:A:137:GLN:HE21	1:A:141:ASP:CG	2.24	0.41	
1:A:313:VAL:O	1:A:313:VAL:HG12	2.21	0.41	
1:A:319:SER:O	1:A:323:GLU:HG2	2.19	0.41	
1:A:614:ASP:HA	1:A:615:PRO:HD3	1.91	0.41	
1:A:752:ALA:O	1:A:755:GLU:N	2.53	0.41	
1:A:109:ARG:O	1:A:114:LEU:HB2	2.20	0.41	
1:A:497:GLU:OE1	1:A:497:GLU:HA	2.21	0.41	
1:A:205:ALA:O	1:A:208:SER:N	2.52	0.41	
1:A:289:THR:O	1:A:292:GLU:N	2.54	0.41	
1:A:749:GLY:O	1:A:753:ARG:HD2	2.21	0.41	
1:A:2:ASN:HA	1:A:3:PRO:HD3	1.84	0.41	
1:A:225:PHE:HE2	1:A:348:ILE:HD11	1.84	0.41	
1:A:229:LYS:O	1:A:275:GLU:HB3	2.21	0.41	
1:A:283:GLN:HB3	1:A:324:PHE:HB2	2.03	0.41	
1:A:499:ILE:CD1	1:A:740:GLY:H	2.32	0.41	
1:A:530:ASP:O	1:A:533:SER:HB2	2.20	0.41	
1:A:755:GLU:O	1:A:759:GLU:N	2.46	0.41	
1:A:496:LYS:O	1:A:498:LYS:N	2.54	0.41	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:ILE:O	1:A:733:ASP:C	2.58	0.41
1:A:741:ILE:HG22	1:A:742:THR:CA	2.50	0.41
1:A:775:ILE:CG2	1:A:776:PRO:HD2	2.51	0.41
1:A:727:LEU:HG	1:A:732:ILE:HG12	2.03	0.40
1:A:753:ARG:O	1:A:756:GLU:HG2	2.21	0.40
1:A:467:GLU:O	1:A:471:ILE:HG13	2.21	0.40
1:A:766:GLU:O	1:A:766:GLU:CG	2.69	0.40
1:A:103:PHE:CE2	1:A:669:ASP:HB3	2.57	0.40
1:A:185:LYS:NZ	1:A:457:GLY:HA3	2.36	0.40
1:A:87:GLY:O	1:A:88:VAL:C	2.60	0.40
1:A:484:HIS:CD2	1:A:488:LYS:HB3	2.57	0.40
1:A:499:ILE:CD1	1:A:740:GLY:N	2.84	0.40
1:A:569:GLY:HA3	1:A:578:MET:HE2	2.04	0.40
1:A:716:ALA:HB1	1:A:721:LYS:CE	2.50	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	774/788~(98%)	692~(89%)	72 (9%)	10 (1%)	12 36

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	497	GLU
1	А	713	PRO
1	А	709	ALA
1	А	710	PRO
1	А	766	GLU
1	А	287	GLY
1	А	708	LEU



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Mol	Chain	Res	Type
1	А	712	VAL
1	А	716	ALA
1	А	768	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	680/691~(98%)	597~(88%)	83 (12%)	5 15		

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	27	LEU
1	А	31	ASP
1	А	35	ILE
1	А	38	ASN
1	А	42	LYS
1	А	44	ARG
1	А	56	THR
1	А	65	VAL
1	А	66	ASP
1	А	71	GLN
1	А	75	ASP
1	А	79	GLN
1	А	83	ILE
1	А	91	MET
1	А	95	SER
1	А	130	LYS
1	А	150	GLU
1	А	151	VAL
1	А	158	ILE
1	А	171	GLN
1	А	198	SER
1	А	199	VAL
1	А	204	GLN



Mol	Chain	Res	Type
1	А	210	VAL
1	А	277	ASN
1	А	284	LEU
1	А	291	GLU
1	А	294	LYS
1	А	329	GLN
1	А	358	LYS
1	А	361	LYS
1	А	387	SER
1	А	397	ARG
1	А	402	ARG
1	А	435	LYS
1	А	444	GLU
1	А	445	ARG
1	А	446	LYS
1	А	468	GLN
1	А	495	LEU
1	А	497	GLU
1	А	498	LYS
1	А	499	ILE
1	А	520	ARG
1	А	603	SER
1	А	633	GLN
1	А	646	GLU
1	А	666	LYS
1	А	679	ASN
1	А	692	PHE
1	А	695	ARG
1	А	696	ILE
1	A	700	ASP
1	А	701	PHE
1	А	702	VAL
1	A	704	ARG
1	А	706	TYR
1	А	707	LEU
1	А	708	LEU
1	А	710	PRO
1	A	719	SER
1	A	720	GLN
1	А	721	LYS
1	А	726	VAL
1	А	727	LEU



Mol	Chain	Res	Type
1	А	728	LYS
1	А	730	LEU
1	А	736	GLN
1	А	742	THR
1	А	745	PHE
1	А	753	ARG
1	А	755	GLU
1	А	756	GLU
1	А	758	ARG
1	А	762	LEU
1	А	764	SER
1	А	766	GLU
1	A	767	PRO
1	A	769	MET
1	А	771	PHE
1	A	773	ASP
1	А	774	ASP
1	А	777	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	38	ASN
1	А	137	GLN
1	А	171	GLN
1	А	173	GLN
1	А	206	ASN
1	А	234	ASN
1	А	271	GLN
1	А	277	ASN
1	А	329	GLN
1	А	356	ASN
1	А	376	ASN
1	А	407	GLN
1	А	408	HIS
1	А	443	GLN
1	А	464	ASN
1	А	468	GLN
1	A	484	HIS
1	А	500	ASN
1	А	613	ASN
1	А	616	ASN



Continued from previous page...

Mol	Chain	Res	Type
1	А	633	GLN
1	А	679	ASN
1	А	731	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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 True	Turne	Chain	Dog	Dog	Dog	Dog	Dec	Dec	Dag	Dec	Dog	Dog	Dec	Dag	Dec	Dec	Dog	Dec	Dec	Dec	Dec	Dec	Tinle	Bo	ond leng	ths	B	ond ang	les
INIOI	туре	Chain	nes	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2																			
4	PBQ	А	1780	-	14,18,18	1.06	1 (7%)	16,27,27	1.52	3 (18%)																			
2	AD9	А	1778	3	24,33,33	1.98	6 (25%)	26,52,52	1.09	1 (3%)																			

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	$\mathbf{Res}$	Link	Chirals	Torsions	Rings
4	PBQ	А	1780	-	_	0/0/4/4	0/2/2/2



Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AD9	А	1778	3	-	4/12/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	1778	AD9	PB-O1B	5.49	1.70	1.50
2	А	1778	AD9	O4'-C1'	4.60	1.47	1.41
2	А	1778	AD9	PA-O2A	3.52	1.71	1.55
2	А	1778	AD9	C2-N3	2.51	1.36	1.32
4	А	1780	PBQ	CD2-CE2	2.42	1.40	1.36
2	А	1778	AD9	C4-N3	2.34	1.38	1.35
2	А	1778	AD9	C2'-C1'	2.05	1.56	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	1780	PBQ	C7-C8-C9	3.76	107.59	104.48
2	А	1778	AD9	O2B-PB-O3B	2.88	117.60	107.52
4	А	1780	PBQ	CD2-CE2-C3	-2.43	119.65	122.62
4	А	1780	PBQ	O-CR-CG	2.00	120.89	116.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	1778	AD9	PA-O3A-PB-O1B
2	А	1778	AD9	O4'-C4'-C5'-O5'
2	А	1778	AD9	C5'-O5'-PA-O1A
2	А	1778	AD9	C5'-O5'-PA-O2A

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	1780	PBQ	11	0
2	А	1778	AD9	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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks	
1	А	1	

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	747:ARG	C	748:ALA	N	1.16



# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

