

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

#### Sep 30, 2024 - 04:09 PM EDT

:	9BQ0
:	Complex structure of protein crystal of Tri17 with ATP
:	Zhai, R.; Zhang, W.
:	2024-05-08
:	2.90  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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
$\mathrm{EDS}$	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

# 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 2.90 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>	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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	Δ	EC 4	16%								
L	A	304	56%	30%	• 14%						
			8%								
1	В	564	57%	27%	• 15%						
			15%								
1	С	564	52%	32%	15%						
			16%								
1	D	564	57%	27%	• 15%						

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	С	602	-	-	-	Х



#### 9BQ0

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 29878 atoms, of which 14521 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues			Atom	IS	ZeroOcc	AltConf	Trace		
1	Δ	487	Total	С	Η	Ν	0	$\mathbf{S}$	0	0	0
1	Л	401	7410	2385	3653	662	697	13	0	0	
1	В	470	Total	С	Η	Ν	0	S	0	0	0
1	Б	419	7300	2350	3599	652	686	13	0	0	0
1	С	480	Total	С	Η	Ν	0	S	0	0	0
1	U	400	7335	2361	3622	652	687	13	0	0	
1	П	489	Total	С	Н	Ν	0	S	0	0	0
	D	402	7333	2375	3599	657	689	13		0	

• Molecule 1 is a protein called AMP-binding protein.

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MET	-	initiating methionine	UNP A0A5H2UY12
А	557	LEU	-	expression tag	UNP A0A5H2UY12
А	558	GLU	-	expression tag	UNP A0A5H2UY12
А	559	HIS	-	expression tag	UNP A0A5H2UY12
А	560	HIS	-	expression tag	UNP A0A5H2UY12
А	561	HIS	-	expression tag	UNP A0A5H2UY12
А	562	HIS	-	expression tag	UNP A0A5H2UY12
А	563	HIS	-	expression tag	UNP A0A5H2UY12
А	564	HIS	-	expression tag	UNP A0A5H2UY12
В	1	MET	-	initiating methionine	UNP A0A5H2UY12
В	557	LEU	-	expression tag	UNP A0A5H2UY12
В	558	GLU	-	expression tag	UNP A0A5H2UY12
В	559	HIS	-	expression tag	UNP A0A5H2UY12
В	560	HIS	-	expression tag	UNP A0A5H2UY12
В	561	HIS	-	expression tag	UNP A0A5H2UY12
В	562	HIS	-	expression tag	UNP A0A5H2UY12
В	563	HIS	-	expression tag	UNP A0A5H2UY12
В	564	HIS	-	expression tag	UNP A0A5H2UY12
С	1	MET	-	initiating methionine	UNP A0A5H2UY12
С	557	LEU	-	expression tag	UNP A0A5H2UY12
С	558	GLU	-	expression tag	UNP A0A5H2UY12



Chain	Residue	Modelled	Actual	Comment	Reference
С	559	HIS	-	expression tag	UNP A0A5H2UY12
С	560	HIS	-	expression tag	UNP A0A5H2UY12
С	561	HIS	-	expression tag	UNP A0A5H2UY12
С	562	HIS	-	expression tag	UNP A0A5H2UY12
С	563	HIS	-	expression tag	UNP A0A5H2UY12
С	564	HIS	-	expression tag	UNP A0A5H2UY12
D	1	MET	-	initiating methionine	UNP A0A5H2UY12
D	557	LEU	-	expression tag	UNP A0A5H2UY12
D	558	GLU	-	expression tag	UNP A0A5H2UY12
D	559	HIS	-	expression tag	UNP A0A5H2UY12
D	560	HIS	-	expression tag	UNP A0A5H2UY12
D	561	HIS	-	expression tag	UNP A0A5H2UY12
D	562	HIS	-	expression tag	UNP A0A5H2UY12
D	563	HIS	-	expression tag	UNP A0A5H2UY12
D	564	HIS	-	expression tag	UNP A0A5H2UY12

• Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
0	Δ	1	Total	С	Η	Ν	Ο	Р	0	0
	A	1	43	10	12	5	13	3	0	0
0	D	1	Total	С	Η	Ν	0	Р	0	0
	D	1	43	10	12	5	13	3	0	0
0	С	1	Total	С	Η	Ν	Ο	Р	0	0
	U	1	43	10	12	5	13	3	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	D	1	Total 43	C 10	Н 12	N 5	O 13	Р 3	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
3	В	2	Total Mg 2 2	0	0
3	С	1	Total Mg 1 1	0	0
3	D	2	Total Mg 2 2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	118	Total O 118 118	0	0
4	В	74	Total O 74 74	0	0
4	С	68	Total O 68 68	0	0
4	D	62	$\begin{array}{cc} \text{Total} & \text{O} \\ 62 & 62 \end{array}$	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: AMP-binding protein













# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants	87.09Å 152.33Å 229.64Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	46.44 - 2.90	Depositor
Resolution (A)	46.44 - 2.90	EDS
% Data completeness	99.5 (46.44-2.90)	Depositor
(in resolution range)	99.9 (46.44 - 2.90)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.29 (at 2.91 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
B B.	0.278 , $0.330$	Depositor
II, II, <i>free</i>	0.278 , $0.327$	DCC
$R_{free}$ test set	3421 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	$0.35 \;,  57.7$	EDS
L-test for $twinning^2$	$ < L >=0.55, < L^2>=0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	29878	wwPDB-VP
Average B, all atoms $(Å^2)$	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 60.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4473e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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: ATP, 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).

Mal	Chain	Bond lengths		Bond angles	
Moi Chair	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.71	0/3841	0.88	0/5213
1	В	0.67	0/3786	0.83	0/5142
1	С	0.62	0/3801	0.84	0/5165
1	D	0.62	0/3821	0.83	0/5188
All	All	0.66	0/15249	0.85	0/20708

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3757	3653	3673	148	0
1	В	3701	3599	3626	121	0
1	С	3713	3622	3630	147	0
1	D	3734	3599	3658	130	0
2	А	31	12	12	0	0
2	В	31	12	12	0	0
2	С	31	12	12	0	0
2	D	31	12	12	1	0
3	А	1	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	2	0	0	0	0
3	С	1	0	0	0	0
3	D	2	0	0	0	0
4	А	118	0	0	9	0
4	В	74	0	0	1	0
4	С	68	0	0	2	0
4	D	62	0	0	0	0
All	All	15357	14521	14635	535	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 18.

All (535) 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:C:274:THR:HG21	1:C:301:ASP:HB2	1.54	0.89
1:C:39:TRP:HB2	1:C:248:VAL:HG22	1.54	0.87
1:C:343:MET:HA	1:C:397:LEU:HD23	1.58	0.86
1:C:39:TRP:CB	1:C:248:VAL:HG22	2.06	0.85
1:D:137:HIS:HD2	1:D:155:LEU:HG	1.40	0.84
1:C:365:ARG:HH21	1:C:428:ALA:HB1	1.43	0.84
1:B:199:THR:OG1	1:B:202:THR:HG23	1.77	0.83
1:B:284:ASP:OD1	1:B:285:LEU:N	2.13	0.82
1:D:137:HIS:CD2	1:D:155:LEU:HG	2.17	0.80
1:C:21:ASN:O	1:C:25:ARG:HG2	1.82	0.79
1:B:15:ALA:HB3	1:D:13:ALA:HA	1.66	0.77
1:C:329:VAL:HG12	1:C:330:PRO:HD2	1.64	0.77
1:C:89:ILE:HG23	1:C:249:HIS:ND1	2.01	0.74
1:C:329:VAL:HG12	1:C:330:PRO:CD	2.18	0.74
1:B:110:ASN:H	1:B:185:HIS:HE1	1.37	0.73
1:D:510:ASN:OD1	1:D:521:VAL:HG12	1.88	0.72
1:D:280:MET:HE3	1:D:311:LEU:HD22	1.73	0.70
1:A:79:LYS:HE3	4:A:741:HOH:O	1.92	0.70
1:A:132:THR:HG21	1:A:140:LEU:HD12	1.71	0.70
1:A:199:THR:OG1	1:A:202:THR:HG23	1.92	0.69
1:B:182:LEU:CD2	1:B:231:VAL:HG23	2.22	0.69
1:C:461:TYR:O	1:C:463:GLU:HG2	1.93	0.68
1:B:283:GLU:O	1:B:285:LEU:HD12	1.93	0.68
1:B:280:MET:O	1:B:285:LEU:HD11	1.94	0.68
1:A:33:LEU:HD23	1:A:57:LEU:HD23	1.76	0.68
1:A:15:ALA:HB3	1:C:13:ALA:HA	1.76	0.68



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:60:LEU:HD21	1:C:97:MET:SD	2.34	0.67
1:A:121:TYR:OH	1:A:185:HIS:HB3	1.94	0.67
1:B:457:LEU:HD21	1:B:513:LEU:CD1	2.24	0.67
1:C:223:LEU:HD12	1:C:248:VAL:CG1	2.25	0.67
1:D:113:MET:HE3	1:D:117:THR:HG22	1.76	0.67
1:B:305:ALA:HB1	1:B:308:ILE:HG21	1.75	0.67
1:C:86:SER:OG	1:C:87:THR:N	2.27	0.67
1:D:312:LEU:HD21	1:D:334:PHE:HB2	1.77	0.67
1:D:277:PHE:HD1	1:D:280:MET:HE2	1.59	0.66
1:B:185:HIS:C	1:B:341:THR:HG21	2.15	0.66
1:A:185:HIS:C	1:A:341:THR:HG21	2.16	0.66
1:D:39:TRP:HB2	1:D:248:VAL:HG22	1.79	0.65
1:D:453:THR:O	1:D:456:VAL:HG22	1.96	0.65
1:D:387:VAL:HG22	1:D:434:LEU:HD12	1.77	0.65
1:C:192:ILE:HD12	1:C:192:ILE:H	1.62	0.64
1:B:121:TYR:OH	1:B:185:HIS:HB3	1.97	0.64
1:C:77:ARG:O	1:C:80:ASP:HB2	1.98	0.64
1:C:89:ILE:HG13	1:C:233:ALA:HB1	1.78	0.64
1:D:120:GLU:OE1	1:D:120:GLU:HA	1.98	0.64
1:B:374:VAL:HG12	1:B:382:LEU:HD12	1.79	0.63
1:D:489:VAL:O	1:D:521:VAL:HG23	1.98	0.63
1:A:470:VAL:HG13	1:A:471:GLY:N	2.12	0.63
1:C:134:GLU:OE2	1:C:155:LEU:HD13	1.98	0.63
1:B:274:THR:HG23	1:B:305:ALA:HB2	1.81	0.63
1:C:39:TRP:HB2	1:C:248:VAL:CG2	2.28	0.63
1:C:22:VAL:HG21	1:C:238:LEU:HB3	1.81	0.62
1:C:223:LEU:HD12	1:C:248:VAL:HG12	1.80	0.62
1:C:349:ASP:HB2	1:C:367:MET:HE2	1.82	0.62
1:C:463:GLU:CB	1:C:465:LEU:N	2.63	0.62
1:C:67:TYR:CD1	1:C:159:VAL:HG11	2.35	0.61
1:C:72:THR:HG21	1:C:168:PRO:HD3	1.82	0.61
1:B:9:GLN:OE1	1:D:174:ARG:CD	2.49	0.61
1:C:460:GLU:OE1	1:C:515:ARG:CZ	2.48	0.61
1:C:470:VAL:HG12	1:C:471:GLY:N	2.15	0.61
1:A:470:VAL:HG13	1:A:471:GLY:H	1.65	0.61
1:D:88:SER:HB3	1:D:91:ASP:HB2	1.83	0.61
1:D:490:TYR:HA	1:D:521:VAL:CG2	2.31	0.61
1:A:155:LEU:HD13	1:A:158:GLU:OE2	2.00	0.61
1:A:19:ALA:HB3	1:A:181:ILE:HD13	1.83	0.60
1:A:155:LEU:CD1	1:A:158:GLU:OE2	2.49	0.60
1:B:393:ARG:HD2	1:B:415:GLY:O	2.01	0.60



	io ao pagoini	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:285:LEU:HD22	1:A:290:LEU:HD11	1.84	0.60
1:D:77:ARG:O	1:D:80:ASP:HB2	2.00	0.60
1:A:137:HIS:NE2	1:A:141:LEU:HD11	2.16	0.60
1:C:463:GLU:HB3	1:C:465:LEU:N	2.17	0.60
1:D:382:LEU:HD13	1:D:386:GLN:HG2	1.83	0.60
1:A:405:ASN:ND2	1:B:403:ASN:H	2.00	0.60
1:C:40:LEU:HD11	1:C:55:LEU:HD12	1.83	0.60
1:B:220:ARG:HD2	1:B:268:THR:HG21	1.84	0.60
1:D:375:VAL:HG22	1:D:379:GLY:HA2	1.84	0.60
1:B:491:ALA:C	1:B:492:LEU:HD23	2.22	0.59
1:D:280:MET:CE	1:D:311:LEU:HD22	2.32	0.59
1:B:113:MET:HB3	1:B:118:ARG:HG3	1.84	0.59
1:B:441:ILE:HD12	1:B:489:VAL:CG2	2.33	0.59
1:C:300:GLY:O	1:C:301:ASP:HB2	2.02	0.59
1:A:121:TYR:CZ	1:A:185:HIS:HB3	2.37	0.59
1:A:223:LEU:HD11	1:A:250:TYR:CD1	2.38	0.59
1:D:442:ARG:NH1	1:D:447:PHE:CZ	2.71	0.58
1:A:220:ARG:HD2	1:A:268:THR:HG21	1.84	0.58
1:B:339:GLY:HA2	1:B:343:MET:HG3	1.85	0.58
1:C:293:VAL:HG11	1:C:296:TYR:CZ	2.39	0.58
1:D:167:ARG:HD2	1:D:171:TYR:CG	2.38	0.58
1:A:480:GLY:H	1:A:483:ASP:HB2	1.69	0.58
1:C:375:VAL:HG23	1:C:389:ARG:HB2	1.85	0.58
1:B:110:ASN:H	1:B:185:HIS:CE1	2.22	0.58
1:D:375:VAL:CG2	1:D:379:GLY:HA2	2.34	0.58
1:A:337:MET:HB3	1:A:346:VAL:HG11	1.86	0.57
1:C:365:ARG:HH21	1:C:428:ALA:CB	2.14	0.57
1:B:323:ASP:OD2	1:B:325:LYS:HB2	2.04	0.57
1:D:23:ILE:HG21	1:D:97:MET:HE2	1.85	0.57
1:A:220:ARG:NH2	1:A:269:ILE:HG21	2.19	0.57
1:A:480:GLY:N	1:A:483:ASP:HB2	2.19	0.57
1:B:42:GLY:O	1:B:51:ARG:HD3	2.05	0.57
1:D:333:ILE:HG22	1:D:335:ILE:HG13	1.87	0.57
1:D:490:TYR:HA	1:D:521:VAL:HG23	1.87	0.57
1:A:39:TRP:HB2	1:A:248:VAL:HG22	1.86	0.57
1:C:273:PHE:O	1:C:276:THR:HG22	2.04	0.57
1:C:137:HIS:ND1	1:C:155:LEU:HG	2.20	0.57
1:A:359:ILE:HG22	1:A:359:ILE:O	2.05	0.56
1:A:202:THR:HG21	1:A:399:PRO:HD3	1.87	0.56
1:A:329:VAL:CG1	1:A:330:PRO:HD2	2.35	0.56
1:B:308:ILE:HD12	1:B:312:LEU:HD13	1.87	0.56



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:170:ALA:HA	4:A:747:HOH:O	2.04	0.56	
1:B:223:LEU:HD11	1:B:250:TYR:CD1	2.40	0.56	
1:A:184:SER:OG	1:A:341:THR:HG22	2.05	0.56	
1:A:280:MET:O	1:A:285:LEU:HD11	2.05	0.56	
1:B:110:ASN:HB2	1:B:229:HIS:CD2	2.41	0.56	
1:B:182:LEU:HD22	1:B:231:VAL:HG23	1.86	0.56	
1:B:9:GLN:OE1	1:D:174:ARG:NE	2.38	0.56	
1:A:305:ALA:HB1	1:A:308:ILE:CG2	2.36	0.56	
1:A:213:ASP:HB2	1:A:215:LEU:HD12	1.88	0.55	
1:D:443:THR:O	1:D:444:GLU:C	2.45	0.55	
1:B:185:HIS:O	1:B:341:THR:HG21	2.06	0.55	
1:B:340:SER:OG	1:B:343:MET:HG2	2.07	0.55	
1:D:118:ARG:NH1	1:D:140:LEU:HD21	2.21	0.55	
1:B:513:LEU:HD23	1:B:519:PRO:O	2.07	0.55	
1:C:84:ILE:HG22	1:C:92:PHE:CE1	2.42	0.55	
1:A:274:THR:HB	1:A:303:ALA:HB3	1.89	0.55	
1:A:374:VAL:HG12	1:A:382:LEU:HD12	1.89	0.55	
1:B:93:ALA:O	1:B:97:MET:HG3	2.07	0.55	
1:C:262:ILE:HD11	1:C:270:VAL:HG21	1.88	0.55	
1:D:26:LEU:HD21	1:D:242:THR:HA	1.88	0.55	
1:A:293:VAL:HG11	1:A:296:TYR:CZ	2.42	0.55	
1:A:339:GLY:HA3	4:A:751:HOH:O	2.06	0.55	
1:B:76:VAL:O	1:B:77:ARG:NH1	2.40	0.55	
1:B:489:VAL:C	1:B:490:TYR:HD1	2.09	0.55	
1:B:26:LEU:HD22	1:B:31:ARG:NH1	2.21	0.55	
1:A:44:TRP:CH2	1:A:63:VAL:HG11	2.41	0.54	
1:B:182:LEU:HD21	1:B:231:VAL:HG23	1.89	0.54	
1:D:96:LEU:O	1:D:100:THR:HG23	2.07	0.54	
1:D:448:VAL:HG11	1:D:489:VAL:HG21	1.90	0.54	
1:B:285:LEU:C	1:B:314:LYS:HE3	2.28	0.54	
1:A:34:ASP:O	1:A:56:THR:CG2	2.56	0.54	
1:C:300:GLY:O	1:C:301:ASP:CB	2.55	0.54	
1:A:33:LEU:HD22	1:A:58:GLY:HA2	1.89	0.54	
1:A:422:LEU:HD21	1:A:481:TRP:CE2	2.43	0.54	
1:B:227:PRO:HG2	1:B:230:HIS:CE1	2.42	0.54	
1:A:195:SER:O	1:A:401:PHE:HA	2.08	0.54	
1:B:441:ILE:HD12	1:B:489:VAL:HG22	1.90	0.54	
1:D:342:GLU:HG3	1:D:417:PHE:CZ	2.42	0.54	
1:A:329:VAL:HG13	1:A:330:PRO:HD2	1.88	0.54	
1:B:312:LEU:O	1:B:331:GLY:HA2	2.07	0.54	
1:C:489:VAL:HG13	1:C:521:VAL:HG23	1.89	0.54	



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:468:THR:HG22	1:B:470:VAL:HG13	1.90	0.54
1:C:41:ASP:OD1	1:C:43:THR:HG22	2.07	0.54
1:D:263:GLU:OE1	1:D:288:ARG:NH1	2.38	0.53
1:D:506:THR:O	1:D:510:ASN:HB2	2.08	0.53
1:C:123:ARG:HB3	4:C:715:HOH:O	2.07	0.53
1:D:72:THR:HG21	1:D:168:PRO:HG3	1.90	0.53
1:C:26:LEU:HD21	1:C:242:THR:HA	1.91	0.53
1:C:230:HIS:CD2	1:C:231:VAL:HG22	2.43	0.53
1:D:387:VAL:O	1:D:387:VAL:HG12	2.09	0.53
1:C:375:VAL:CG2	1:C:389:ARG:HB2	2.38	0.53
1:D:33:LEU:HD23	1:D:57:LEU:HG	1.90	0.53
1:D:290:LEU:HD13	1:D:311:LEU:HD21	1.90	0.53
1:A:375:VAL:HG13	1:A:379:GLY:HA2	1.89	0.53
1:C:405:ASN:O	1:C:409:HIS:HD2	1.92	0.53
1:C:43:THR:HG21	1:C:251:THR:HG21	1.90	0.53
1:C:338:PHE:HB2	1:C:363:ILE:HG23	1.89	0.53
1:A:230:HIS:CE1	1:A:273:PHE:CZ	2.97	0.52
1:A:494:ASN:C	1:A:495:LEU:HD23	2.28	0.52
1:C:460:GLU:OE2	1:C:515:ARG:NH1	2.43	0.52
1:A:297:TYR:CD1	1:A:335:ILE:HD13	2.44	0.52
1:D:366:PRO:CG	1:D:372:ALA:HB3	2.39	0.52
1:C:470:VAL:HG12	1:C:471:GLY:H	1.74	0.52
1:A:79:LYS:CE	4:A:741:HOH:O	2.51	0.52
1:A:363:ILE:HD11	1:A:431:PHE:HB3	1.90	0.52
1:C:185:HIS:O	1:C:341:THR:HG21	2.10	0.52
1:C:266:ARG:HG2	1:C:266:ARG:HH11	1.75	0.52
1:D:185:HIS:HD2	1:D:186:SER:O	1.93	0.52
1:D:189:THR:HB	2:D:601:ATP:O1G	2.10	0.52
1:A:39:TRP:CD1	1:A:54:VAL:HG22	2.44	0.52
1:D:230:HIS:ND1	1:D:231:VAL:N	2.58	0.52
1:A:34:ASP:O	1:A:56:THR:HG21	2.09	0.52
1:B:392:VAL:O	1:B:393:ARG:HG3	2.10	0.52
1:B:454:GLU:HG3	1:B:469:VAL:HG23	1.92	0.52
1:A:120:GLU:OE1	1:A:120:GLU:HA	2.11	0.51
1:A:302:ALA:O	1:A:303:ALA:C	2.48	0.51
1:C:39:TRP:HB3	1:C:248:VAL:HG22	1.89	0.51
1:A:339:GLY:CA	4:A:751:HOH:O	2.58	0.51
1:B:39:TRP:CG	1:B:54:VAL:HG23	2.45	0.51
1:B:489:VAL:C	1:B:490:TYR:CD1	2.84	0.51
1:A:86:SER:OG	1:A:87:THR:N	2.43	0.51
1:A:263:GLU:OE2	1:A:288:ARG:HA	2.10	0.51



	louo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:365:ARG:NH2	1:C:428:ALA:HB1	2.19	0.51
1:D:363:ILE:HD11	1:D:431:PHE:CB	2.41	0.51
1:D:182:LEU:C	1:D:182:LEU:HD23	2.31	0.51
1:D:137:HIS:CE1	1:D:141:LEU:HD11	2.46	0.51
1:D:468:THR:HB	1:D:492:LEU:HD12	1.93	0.51
1:C:297:TYR:CE2	1:C:335:ILE:HD12	2.46	0.51
1:D:277:PHE:CE2	1:D:298:ALA:HB2	2.46	0.51
1:D:293:VAL:HG11	1:D:296:TYR:CE1	2.46	0.51
1:B:181:ILE:HD11	1:B:203:LEU:HD23	1.93	0.50
1:C:137:HIS:NE2	1:C:141:LEU:HD11	2.25	0.50
1:B:434:LEU:HD13	1:C:324:LEU:HD13	1.93	0.50
1:A:39:TRP:CD1	1:A:54:VAL:CG2	2.95	0.50
1:A:280:MET:HB2	1:A:311:LEU:HD11	1.91	0.50
1:B:175:HIS:HE1	4:B:712:HOH:O	1.94	0.50
1:C:137:HIS:C	1:C:137:HIS:CD2	2.85	0.50
1:C:220:ARG:O	1:C:245:ALA:HB1	2.11	0.50
1:D:137:HIS:HE1	1:D:141:LEU:HD21	1.76	0.50
1:D:296:TYR:OH	1:D:311:LEU:HD23	2.11	0.50
1:B:113:MET:SD	1:B:118:ARG:HA	2.52	0.50
1:D:17:LEU:HD22	1:D:29:TYR:OH	2.12	0.50
1:A:393:ARG:HD2	1:A:415:GLY:O	2.12	0.50
1:C:155:LEU:O	1:C:158:GLU:HG3	2.11	0.50
1:C:262:ILE:CD1	1:C:270:VAL:HG21	2.41	0.50
1:A:34:ASP:HB2	4:A:744:HOH:O	2.11	0.50
1:A:434:LEU:O	1:A:451:ALA:HB3	2.11	0.50
1:B:268:THR:HG22	1:B:294:GLU:HG2	1.93	0.50
1:D:454:GLU:O	1:D:458:LEU:HD12	2.11	0.50
1:A:137:HIS:CD2	1:A:141:LEU:HD11	2.47	0.50
1:D:222:ARG:HB3	1:D:269:ILE:HD11	1.94	0.50
1:B:192:ILE:N	1:B:192:ILE:HD12	2.26	0.50
1:B:224:LEU:N	1:B:224:LEU:HD23	2.27	0.50
1:D:441:ILE:HD13	1:D:489:VAL:HG22	1.94	0.50
1:C:413:LEU:HB3	1:C:418:LEU:HD11	1.93	0.50
1:D:40:LEU:HD11	1:D:55:LEU:HD12	1.94	0.49
1:A:441:ILE:HG23	1:A:479:PHE:CD2	2.47	0.49
1:D:182:LEU:HD23	1:D:183:ILE:N	2.28	0.49
1:D:132:THR:OG1	1:D:133:ARG:N	2.44	0.49
1:D:202:THR:HG22	1:D:395:LYS:O	2.12	0.49
1:B:33:LEU:HB3	1:B:58:GLY:HA3	1.95	0.49
1:B:491:ALA:O	1:B:492:LEU:HD23	2.12	0.49
1:D:363:ILE:HD11	1:D:431:PHE:HB3	1.94	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:375:VAL:CG1	1:D:389:ARG:HB2	2.42	0.49
1:D:39:TRP:CD1	1:D:54:VAL:HG22	2.48	0.49
1:B:220:ARG:HH21	1:B:269:ILE:HG21	1.77	0.49
1:A:194:LYS:HD2	1:A:401:PHE:CE2	2.48	0.49
1:A:297:TYR:CE1	1:A:335:ILE:HD13	2.48	0.49
1:C:209:SER:OG	1:C:369:PHE:HB3	2.13	0.49
1:A:400:GLY:HA2	1:A:408:TRP:CD2	2.47	0.49
1:B:105:ILE:HG12	1:B:180:PRO:HB2	1.95	0.49
1:C:96:LEU:O	1:C:100:THR:HG23	2.13	0.49
1:C:129:GLY:HA3	1:C:152:PHE:CE1	2.47	0.49
1:D:258:VAL:O	1:D:262:ILE:HG13	2.12	0.49
1:D:289:ASP:C	1:D:290:LEU:HD23	2.33	0.49
1:C:433:HIS:CD2	1:C:435:ASP:N	2.81	0.48
1:D:23:ILE:CG2	1:D:97:MET:HE2	2.42	0.48
1:C:40:LEU:HD11	1:C:55:LEU:CD1	2.43	0.48
1:C:128:VAL:O	1:C:151:LEU:HB2	2.13	0.48
1:D:132:THR:HG21	1:D:140:LEU:HD12	1.95	0.48
1:A:132:THR:HG21	1:A:140:LEU:CD1	2.43	0.48
1:C:293:VAL:HG11	1:C:296:TYR:CE1	2.49	0.48
1:D:453:THR:HG22	1:D:469:VAL:HG21	1.96	0.48
1:C:263:GLU:CD	4:C:705:HOH:O	2.52	0.48
1:C:510:ASN:HD21	1:C:521:VAL:HG13	1.78	0.48
1:C:405:ASN:O	1:C:409:HIS:CD2	2.66	0.48
1:B:147:ASP:O	1:B:149:PRO:HD3	2.14	0.48
1:B:296:TYR:HB2	1:B:334:PHE:HD1	1.78	0.48
1:A:329:VAL:CG1	1:A:330:PRO:CD	2.92	0.48
1:B:230:HIS:CE1	1:B:273:PHE:CZ	3.02	0.48
1:C:93:ALA:O	1:C:97:MET:HG3	2.14	0.48
1:C:70:PHE:CG	1:C:159:VAL:HG22	2.49	0.48
1:C:84:ILE:CD1	1:C:95:ASN:HB3	2.44	0.48
1:D:398:THR:HG23	1:D:408:TRP:CH2	2.49	0.48
1:B:220:ARG:NH2	1:B:269:ILE:HG21	2.29	0.47
1:B:285:LEU:HD23	1:B:314:LYS:HD2	1.96	0.47
1:B:312:LEU:HG	1:B:332:ALA:O	2.14	0.47
1:C:375:VAL:HG22	1:C:389:ARG:O	2.14	0.47
1:A:91:ASP:O	1:A:95:ASN:ND2	2.47	0.47
1:D:254:SER:O	1:D:258:VAL:HG23	2.14	0.47
1:D:293:VAL:HG11	1:D:296:TYR:CZ	2.49	0.47
1:B:223:LEU:HB3	1:B:270:VAL:HG22	1.96	0.47
1:A:23:ILE:HG13	1:A:61:HIS:CE1	2.50	0.47
1:C:47:PRO:O	1:C:161:PRO:HD3	2.14	0.47



	io ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:62:GLU:O	1:C:66:GLU:HG2	2.14	0.47
1:C:346:VAL:HG13	1:C:367:MET:HE3	1.95	0.47
1:A:223:LEU:HB3	1:A:270:VAL:HG22	1.97	0.47
1:A:359:ILE:N	4:A:704:HOH:O	2.46	0.47
1:B:41:ASP:OD2	1:B:251:THR:OG1	2.26	0.47
1:A:108:LEU:N	1:A:108:LEU:HD23	2.30	0.47
1:B:101:GLY:O	1:B:173:PHE:HB2	2.15	0.47
1:D:120:GLU:OE1	1:D:120:GLU:CA	2.63	0.47
1:D:387:VAL:HG22	1:D:434:LEU:CD1	2.43	0.47
1:D:442:ARG:NH1	1:D:447:PHE:CE1	2.83	0.47
1:A:185:HIS:HA	1:A:194:LYS:O	2.15	0.47
1:C:66:GLU:OE1	1:C:164:ARG:HB3	2.15	0.47
1:A:456:VAL:HG11	1:A:518:LEU:HD13	1.97	0.47
1:C:72:THR:OG1	1:C:168:PRO:HD3	2.15	0.47
1:C:406:VAL:HG21	1:D:126:ARG:CZ	2.45	0.47
1:A:329:VAL:HG13	1:A:330:PRO:CD	2.44	0.46
1:C:490:TYR:HA	1:C:521:VAL:CG2	2.46	0.46
1:C:513:LEU:HD12	1:C:520:ARG:HA	1.97	0.46
1:D:113:MET:HE2	1:D:118:ARG:HA	1.97	0.46
1:D:182:LEU:HD23	1:D:183:ILE:CA	2.45	0.46
1:A:210:ARG:NH1	1:A:367:MET:HG2	2.31	0.46
1:B:26:LEU:HD21	1:B:242:THR:HA	1.97	0.46
1:C:441:ILE:HB	1:C:448:VAL:CG2	2.46	0.46
1:B:164:ARG:O	1:B:167:ARG:NH1	2.44	0.46
1:C:516:ALA:CB	1:C:518:LEU:CD1	2.94	0.46
1:A:184:SER:HB3	1:A:231:VAL:CG1	2.46	0.46
1:A:323:ASP:OD2	1:A:325:LYS:HB2	2.15	0.46
1:A:461:TYR:CE1	1:A:512:ALA:HB2	2.50	0.46
1:B:134:GLU:N	1:B:135:PRO:CD	2.78	0.46
1:C:110:ASN:HB2	1:C:229:HIS:ND1	2.29	0.46
1:D:290:LEU:HD23	1:D:290:LEU:N	2.30	0.46
1:A:72:THR:HG21	1:A:168:PRO:HG3	1.96	0.46
1:B:223:LEU:HD12	1:B:248:VAL:CG1	2.45	0.46
1:B:461:TYR:CZ	1:B:512:ALA:HB2	2.51	0.46
1:D:23:ILE:HA	1:D:26:LEU:HD12	1.98	0.46
1:B:84:ILE:HG22	1:B:92:PHE:CD1	2.51	0.46
1:D:435:ASP:HB2	1:D:449:TYR:HB3	1.98	0.46
1:B:160:GLU:H	1:B:163:ASN:ND2	2.14	0.46
1:B:185:HIS:O	1:B:341:THR:CG2	2.64	0.46
1:C:433:HIS:HD2	1:C:435:ASP:H	1.64	0.46
1:A:26:LEU:HD21	1:A:242:THR:HA	1.98	0.46



		Interatomic Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:188:GLY:O	1:A:189:THR:HB	2.16	0.46	
1:A:465:LEU:HG	1:A:495:LEU:HA	1.98	0.46	
1:B:137:HIS:HB2	1:B:155:LEU:HD21	1.97	0.46	
1:A:40:LEU:HD11	1:A:55:LEU:CD1	2.46	0.45	
1:A:367:MET:HE1	4:A:725:HOH:O	2.15	0.45	
1:C:88:SER:HB3	1:C:91:ASP:HB2	1.97	0.45	
1:C:286:THR:HG22	1:C:287:ASP:OD1	2.16	0.45	
1:C:108:LEU:N	1:C:108:LEU:HD23	2.31	0.45	
1:D:86:SER:OG	1:D:87:THR:N	2.49	0.45	
1:A:17:LEU:HD22	1:A:29:TYR:OH	2.17	0.45	
1:C:343:MET:HB3	1:C:343:MET:HE2	1.80	0.45	
1:D:286:THR:HG23	1:D:287:ASP:N	2.32	0.45	
1:B:133:ARG:HH11	1:B:133:ARG:HB3	1.80	0.45	
1:C:510:ASN:HD21	1:C:521:VAL:CG1	2.29	0.45	
1:D:502:PRO:HB2	1:D:505:PRO:N	2.31	0.45	
1:A:185:HIS:O	1:A:341:THR:CG2	2.64	0.45	
1:A:456:VAL:HG21	1:A:518:LEU:HD11	1.98	0.45	
1:B:121:TYR:CZ	1:B:185:HIS:HB3	2.52	0.45	
1:B:335:ILE:N	1:B:335:ILE:HD12	2.31	0.45	
1:C:290:LEU:N	1:C:290:LEU:HD23	2.31	0.45	
1:A:2:MET:SD	1:D:383:PRO:HA	2.57	0.45	
1:B:335:ILE:HG22	1:B:337:MET:HG3	1.98	0.45	
1:C:67:TYR:CD1	1:C:67:TYR:N	2.85	0.45	
1:D:296:TYR:CZ	1:D:311:LEU:HD23	2.51	0.45	
1:A:89:ILE:HA	1:A:228:GLY:HA3	1.97	0.45	
1:A:194:LYS:HD2	1:A:401:PHE:CZ	2.51	0.45	
1:C:453:THR:O	1:C:454:GLU:C	2.55	0.45	
1:D:160:GLU:O	1:D:163:ASN:OD1	2.34	0.45	
1:D:510:ASN:ND2	1:D:520:ARG:HB3	2.32	0.45	
1:A:137:HIS:CD2	1:A:137:HIS:C	2.91	0.45	
1:B:195:SER:O	1:B:401:PHE:HA	2.16	0.45	
1:D:39:TRP:CZ3	1:D:246:PRO:HB3	2.52	0.45	
1:B:223:LEU:HD11	1:B:250:TYR:CE1	2.52	0.45	
1:B:312:LEU:HD21	1:B:334:PHE:HB2	1.98	0.45	
1:D:250:TYR:CE2	1:D:261:GLY:HA3	2.52	0.45	
1:D:366:PRO:HG2	1:D:372:ALA:HB3	1.98	0.45	
1:A:99:LEU:HD12	1:A:106:ALA:HB2	1.99	0.44	
1:A:269:ILE:HD11	1:A:271:PHE:HE1	1.83	0.44	
1:C:67:TYR:N	1:C:67:TYR:HD1	2.15	0.44	
1:C:469:VAL:CG1	1:C:489:VAL:CG2	2.95	0.44	
1:D:230:HIS:CE1	1:D:231:VAL:HG22	2.52	0.44	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:375:VAL:HG11	1:D:418:LEU:CD2	2.47	0.44
1:B:389:ARG:HH11	1:B:418:LEU:HD13	1.83	0.44
1:A:220:ARG:HB3	1:A:268:THR:HB	1.99	0.44
1:B:297:TYR:CE1	1:B:335:ILE:HD13	2.52	0.44
1:B:454:GLU:OE2	1:B:468:THR:HA	2.18	0.44
1:C:60:LEU:O	1:C:64:VAL:HG23	2.17	0.44
1:C:382:LEU:HB3	1:C:383:PRO:HD2	2.00	0.44
1:A:120:GLU:HG2	4:A:770:HOH:O	2.17	0.44
1:A:210:ARG:HD3	1:A:216:ASP:OD2	2.18	0.44
1:C:39:TRP:CD1	1:C:54:VAL:HG22	2.53	0.44
1:A:400:GLY:HA2	1:A:408:TRP:CE2	2.52	0.44
1:A:421:ASP:OD1	1:A:436:ARG:HG2	2.18	0.44
1:A:141:LEU:HD23	1:A:153:VAL:HB	2.00	0.44
1:A:442:ARG:NH1	1:A:483:ASP:O	2.51	0.44
1:B:327:LYS:O	1:B:329:VAL:HG13	2.18	0.44
1:C:72:THR:HG21	1:C:168:PRO:CD	2.47	0.44
1:C:220:ARG:HB3	1:C:268:THR:HB	2.00	0.44
1:C:222:ARG:HB3	1:C:269:ILE:HD11	2.00	0.44
1:D:375:VAL:HG12	1:D:389:ARG:HB2	1.99	0.44
1:B:44:TRP:CH2	1:B:46:ALA:HA	2.53	0.44
1:B:340:SER:H	1:B:343:MET:HG3	1.83	0.44
1:C:405:ASN:ND2	1:D:197:PHE:CE1	2.85	0.44
1:D:510:ASN:OD1	1:D:521:VAL:CG1	2.63	0.44
1:A:221:LYS:HG3	1:A:246:PRO:HB2	2.00	0.44
1:A:477:VAL:HG22	1:A:479:PHE:HD1	1.83	0.44
1:B:26:LEU:HB2	1:B:27:PRO:HD3	2.00	0.44
1:A:134:GLU:OE1	1:A:134:GLU:N	2.26	0.43
1:A:135:PRO:HB2	1:A:136:TRP:CE2	2.53	0.43
1:B:374:VAL:CG1	1:B:382:LEU:HD12	2.48	0.43
1:C:489:VAL:C	1:C:521:VAL:HG23	2.38	0.43
1:A:465:LEU:HD12	1:A:495:LEU:H	1.83	0.43
1:C:518:LEU:N	1:C:518:LEU:HD12	2.33	0.43
1:D:366:PRO:HG3	1:D:372:ALA:HB3	1.99	0.43
1:A:258:VAL:HG12	1:A:262:ILE:CD1	2.49	0.43
1:B:39:TRP:CD1	1:B:54:VAL:HG23	2.54	0.43
1:C:33:LEU:HD23	1:C:57:LEU:HD23	2.00	0.43
1:D:386:GLN:HE21	1:D:386:GLN:HB2	1.62	0.43
1:C:283:GLU:O	1:C:284:ASP:C	2.55	0.43
1:D:404:ASP:OD1	1:D:404:ASP:O	2.36	0.43
1:A:202:THR:HG21	1:A:399:PRO:CD	2.48	0.43
1:A:266:ARG:N	1:A:267:PRO:CD	2.81	0.43



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:273:PHE:HB2	1:A:275:HIS:CE1	2.53	0.43	
1:B:222:ARG:HB3	1:B:269:ILE:HD11	1.99	0.43	
1:D:143:HIS:O	1:D:150:PRO:HD2	2.19	0.43	
1:D:433:HIS:HD2	1:D:435:ASP:N	2.17	0.43	
1:A:155:LEU:HD12	1:A:158:GLU:OE2	2.18	0.43	
1:A:255:GLY:HA2	1:A:280:MET:HG2	2.01	0.43	
1:A:285:LEU:HD22	1:A:290:LEU:CD1	2.47	0.43	
1:A:426:ASP:OD1	1:A:428:ALA:HB3	2.18	0.43	
1:A:479:PHE:CD1	1:A:487:ALA:HB2	2.54	0.43	
1:B:340:SER:N	1:B:343:MET:HG3	2.33	0.43	
1:D:89:ILE:HG13	1:D:233:ALA:HB1	2.00	0.43	
1:D:382:LEU:HB3	1:D:383:PRO:HD2	2.01	0.43	
1:A:92:PHE:CE2	1:A:229:HIS:HB3	2.54	0.43	
1:B:285:LEU:O	1:B:314:LYS:HE3	2.18	0.43	
1:C:23:ILE:HA	1:C:26:LEU:HD12	2.00	0.43	
1:C:80:ASP:O	1:C:104:ALA:HB1	2.19	0.43	
1:C:274:THR:HG23	1:C:299:SER:O	2.19	0.43	
1:C:504:ASP:HB3	1:C:507:ALA:HB3	2.00	0.43	
1:A:26:LEU:N	1:A:27:PRO:CD	2.81	0.43	
1:C:182:LEU:HD23	1:C:183:ILE:N	2.33	0.43	
1:D:53:GLU:O	1:D:54:VAL:HG23	2.19	0.43	
1:D:263:GLU:OE2	1:D:288:ARG:HA	2.19	0.43	
1:D:490:TYR:HA	1:D:521:VAL:HG21	2.01	0.43	
1:A:184:SER:CB	1:A:231:VAL:HG13	2.49	0.42	
1:B:259:LEU:HB3	1:B:288:ARG:CZ	2.48	0.42	
1:B:280:MET:HE2	1:B:311:LEU:HD11	2.01	0.42	
1:C:134:GLU:N	1:C:135:PRO:CD	2.82	0.42	
1:A:107:SER:OG	1:A:125:GLN:OE1	2.37	0.42	
1:C:82:VAL:HG21	1:C:99:LEU:HD21	2.01	0.42	
1:A:268:THR:HG23	1:A:294:GLU:HG3	2.00	0.42	
1:B:33:LEU:O	1:B:56:THR:HB	2.19	0.42	
1:C:5:GLU:OE2	1:C:9:GLN:NE2	2.51	0.42	
1:C:18:GLY:HA3	1:C:200:HIS:CE1	2.53	0.42	
1:D:424:TYR:HD2	1:D:434:LEU:HD11	1.84	0.42	
1:D:491:ALA:O	1:D:492:LEU:HD23	2.19	0.42	
1:B:388:GLY:O	1:B:422:LEU:HA	2.20	0.42	
1:C:72:THR:CG2	1:C:168:PRO:HD3	2.48	0.42	
1:C:98:ALA:O	1:C:102:ILE:HG23	2.19	0.42	
1:C:340:SER:OG	1:C:343:MET:HG3	2.19	0.42	
1:D:452:TYR:CE2	1:D:518:LEU:HD21	2.55	0.42	
1:A:33:LEU:HA	1:A:57:LEU:HB3	2.01	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:186:SER:O	1:B:193:PRO:HB3	2.19	0.42	
1:C:66:GLU:OE2	1:C:161:PRO:HA	2.18	0.42	
1:D:250:TYR:OH	1:D:261:GLY:HA2	2.20	0.42	
1:B:132:THR:HG21	1:B:140:LEU:HD12	2.02	0.42	
1:D:40:LEU:HD11	1:D:55:LEU:CD1	2.49	0.42	
1:A:26:LEU:HA	1:A:29:TYR:CD2	2.54	0.42	
1:A:36:GLU:HB3	1:A:39:TRP:CH2	2.55	0.42	
1:A:305:ALA:HB1	1:A:308:ILE:HG23	2.01	0.42	
1:B:77:ARG:O	1:B:80:ASP:HB2	2.20	0.42	
1:C:119:ARG:HB3	1:C:123:ARG:NH1	2.34	0.42	
1:D:113:MET:HE2	1:D:121:TYR:HB3	2.02	0.42	
1:A:143:HIS:O	1:A:150:PRO:HD2	2.20	0.42	
1:C:84:ILE:HG22	1:C:92:PHE:CD1	2.55	0.42	
1:C:316:TYR:HA	1:C:331:GLY:N	2.35	0.42	
1:C:374:VAL:HG12	1:C:382:LEU:HD12	2.02	0.42	
1:D:82:VAL:HG13	1:D:129:GLY:O	2.20	0.42	
1:D:406:VAL:HG12	1:D:407:ARG:N	2.34	0.42	
1:A:62:GLU:O	1:A:65:ALA:HB3	2.20	0.42	
1:A:176:ALA:O	1:A:177:PRO:C	2.57	0.42	
1:A:273:PHE:CE1	1:A:299:SER:HB2	2.54	0.42	
1:B:62:GLU:O	1:B:66:GLU:HG2	2.20	0.42	
1:B:425:ARG:O	1:B:425:ARG:HG3	2.19	0.42	
1:C:275:HIS:CG	1:C:276:THR:N	2.87	0.42	
1:D:220:ARG:O	1:D:245:ALA:HB1	2.19	0.42	
1:A:19:ALA:CB	1:A:181:ILE:CD1	2.98	0.42	
1:A:296:TYR:O	1:A:335:ILE:HD12	2.20	0.42	
1:A:495:LEU:HD23	1:A:495:LEU:N	2.35	0.42	
1:B:421:ASP:HA	1:B:436:ARG:HA	2.02	0.42	
1:C:433:HIS:HD2	1:C:435:ASP:N	2.18	0.42	
1:D:41:ASP:OD1	1:D:42:GLY:N	2.52	0.42	
1:D:176:ALA:O	1:D:177:PRO:C	2.57	0.42	
1:D:329:VAL:HG12	1:D:330:PRO:CD	2.50	0.42	
1:D:448:VAL:O	1:D:448:VAL:HG12	2.20	0.42	
1:A:33:LEU:HD23	1:A:57:LEU:CD2	2.48	0.41	
1:B:96:LEU:HD12	1:B:96:LEU:O	2.20	0.41	
1:B:343:MET:HA	1:B:397:LEU:HD23	2.01	0.41	
1:C:18:GLY:CA	1:C:200:HIS:CE1	3.03	0.41	
1:C:48:ASP:HA	1:C:161:PRO:CG	2.50	0.41	
1:D:110:ASN:H	1:D:185:HIS:HE1	1.68	0.41	
1:D:433:HIS:HD2	1:D:434:LEU:N	2.18	0.41	
1:B:210:ARG:NH1	1:B:367:MET:SD	2.93	0.41	



	le us pagem	Interatomic Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:400:GLY:HA2	1:B:408:TRP:CE2	2.54	0.41	
1:C:259:LEU:HB3	1:C:288:ARG:CZ	2.50	0.41	
1:D:5:GLU:O	1:D:5:GLU:HG3	2.20	0.41	
1:C:123:ARG:HG2	1:C:146:ASP:OD2	2.21	0.41	
1:C:199:THR:OG1	1:C:202:THR:HG23	2.19	0.41	
1:C:470:VAL:CG1	1:C:471:GLY:N	2.81	0.41	
1:D:312:LEU:HD11	1:D:334:PHE:HB2	2.02	0.41	
1:A:359:ILE:CD1	1:D:320:THR:O	2.68	0.41	
1:B:36:GLU:OE1	1:B:39:TRP:CZ2	2.73	0.41	
1:B:374:VAL:HG12	1:B:382:LEU:HB2	2.03	0.41	
1:C:433:HIS:CD2	1:C:434:LEU:N	2.89	0.41	
1:A:19:ALA:HB3	1:A:181:ILE:CD1	2.48	0.41	
1:A:184:SER:OG	1:A:341:THR:CG2	2.69	0.41	
1:A:479:PHE:CD2	1:A:479:PHE:O	2.73	0.41	
1:A:513:LEU:CD1	1:A:521:VAL:HG13	2.51	0.41	
1:C:130:ILE:HD12	1:C:153:VAL:HG22	2.01	0.41	
1:C:229:HIS:CD2	1:C:229:HIS:C	2.94	0.41	
1:C:433:HIS:HD2	1:C:434:LEU:N	2.17	0.41	
1:A:221:LYS:HE2	1:A:265:HIS:HB3	2.02	0.41	
1:A:285:LEU:CD2	1:A:290:LEU:HD11	2.48	0.41	
1:B:188:GLY:O	1:B:189:THR:CB	2.68	0.41	
1:C:89:ILE:HG23	1:C:249:HIS:CG	2.54	0.41	
1:C:479:PHE:CD1	1:C:479:PHE:C	2.94	0.41	
1:C:479:PHE:CD2	1:C:487:ALA:HB2	2.56	0.41	
1:D:133:ARG:C	1:D:155:LEU:HD23	2.41	0.41	
1:D:441:ILE:HD13	1:D:489:VAL:CG2	2.51	0.41	
1:A:224:LEU:CD2	1:A:271:PHE:CD1	3.04	0.41	
1:A:466:ASP:H	1:A:494:ASN:HB2	1.86	0.41	
1:A:470:VAL:CG1	1:A:471:GLY:N	2.80	0.41	
1:B:2:MET:SD	1:C:383:PRO:HA	2.60	0.41	
1:B:119:ARG:O	1:B:119:ARG:HG3	2.20	0.41	
1:C:113:MET:SD	1:C:118:ARG:HA	2.61	0.41	
1:C:489:VAL:O	1:C:521:VAL:HG23	2.21	0.41	
1:B:203:LEU:HD11	1:B:235:SER:HB3	2.03	0.41	
1:A:335:ILE:HA	1:A:350:PHE:CZ	2.55	0.40	
1:A:454:GLU:HG3	1:A:469:VAL:HG23	2.04	0.40	
1:A:513:LEU:HD22	1:A:518:LEU:HD22	2.02	0.40	
1:B:86:SER:OG	1:B:87:THR:N	2.53	0.40	
1:B:107:SER:HA	1:B:183:ILE:HB	2.03	0.40	
1:B:457:LEU:HD21	1:B:513:LEU:HD13	1.99	0.40	
1:C:513:LEU:CD1	1:C:520:ARG:HA	2.52	0.40	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:99:LEU:HD22	1:D:104:ALA:HB3	2.03	0.40
1:D:375:VAL:HG12	1:D:389:ARG:O	2.20	0.40
1:A:312:LEU:HD11	1:A:334:PHE:HB2	2.03	0.40
1:C:377:GLU:OE2	1:C:389:ARG:NE	2.54	0.40
1:A:471:GLY:HA2	1:A:489:VAL:HA	2.02	0.40
1:B:194:LYS:HD2	1:B:401:PHE:CE2	2.56	0.40
1:B:280:MET:HB2	1:B:311:LEU:HD11	2.02	0.40
1:B:426:ASP:OD1	1:B:428:ALA:N	2.51	0.40
1:D:101:GLY:O	1:D:173:PHE:HB2	2.21	0.40
1:A:239:LEU:O	1:A:239:LEU:HD12	2.22	0.40
1:C:123:ARG:HG3	1:C:143:HIS:CE1	2.56	0.40
1:D:134:GLU:N	1:D:135:PRO:CD	2.84	0.40
1:D:146:ASP:O	1:D:147:ASP:C	2.59	0.40
1:A:335:ILE:HD12	1:A:335:ILE:N	2.37	0.40
1:B:99:LEU:CD1	1:B:106:ALA:HB2	2.52	0.40
1:C:84:ILE:HD11	1:C:95:ASN:HB3	2.03	0.40
1:D:82:VAL:HG21	1:D:99:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	465/564~(82%)	443~(95%)	22~(5%)	0	100	100
1	В	461/564~(82%)	447~(97%)	14 (3%)	0	100	100
1	С	460/564~(82%)	442 (96%)	18 (4%)	0	100	100
1	D	461/564~(82%)	436~(95%)	25~(5%)	0	100	100
All	All	1847/2256~(82%)	1768 (96%)	79 (4%)	0	100	100

There are no Ramachandran outliers to report.



#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	387/447~(87%)	376~(97%)	11 (3%)	38 73
1	В	383/447~(86%)	373~(97%)	10 (3%)	41 74
1	С	385/447~(86%)	367~(95%)	18 (5%)	22 55
1	D	387/447~(87%)	375~(97%)	12 (3%)	35 70
All	All	1542/1788~(86%)	1491 (97%)	51 (3%)	33 68

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	34	ASP
1	А	48	ASP
1	А	50	SER
1	А	112	ASN
1	А	204	PHE
1	А	284	ASP
1	А	287	ASP
1	А	346	VAL
1	А	375	VAL
1	А	488	THR
1	А	495	LEU
1	В	79	LYS
1	В	119	ARG
1	В	139	ASP
1	В	182	LEU
1	В	189	THR
1	В	204	PHE
1	В	218	SER
1	В	$\overline{260}$	ASP
1	В	327	LYS
1	В	495	LEU
1	С	1	MET
1	С	102	ILE
1	С	131	MET



	0	-	1 0
Mol	Chain	Res	Type
1	С	136	TRP
1	С	184	SER
1	С	204	PHE
1	С	213	ASP
1	С	215	LEU
1	С	250	TYR
1	С	312	LEU
1	С	327	LYS
1	С	406	VAL
1	С	429	ASN
1	С	447	PHE
1	С	459	ARG
1	С	466	ASP
1	С	486	VAL
1	С	488	THR
1	D	31	ARG
1	D	192	ILE
1	D	204	PHE
1	D	223	LEU
1	D	230	HIS
1	D	256	LYS
1	D	275	HIS
1	D	387	VAL
1	D	411	GLN
1	D	436	ARG
1	D	481	TRP
1	D	489	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	9	GLN
1	А	110	ASN
1	А	137	HIS
1	А	230	HIS
1	А	405	ASN
1	А	409	HIS
1	В	185	HIS
1	В	198	HIS
1	В	229	HIS
1	В	230	HIS
1	С	21	ASN



Mol	Chain	Res	Type
1	С	166	HIS
1	С	230	HIS
1	С	409	HIS
1	С	433	HIS
1	D	9	GLN
1	D	137	HIS
1	D	163	ASN
1	D	185	HIS
1	D	205	HIS
1	D	317	HIS
1	D	386	GLN
1	D	405	ASN
1	D	433	HIS

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	Turne	Chain	Dec	Tiple	Bond lengths			Bond angles		
MOI	туре	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ATP	В	601	3	28,33,33	0.81	1 (3%)	34,52,52	0.81	1 (2%)



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm sths}$	B	ond ang	les
IVIOI	туре	Unain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ATP	С	601	3	28,33,33	0.85	1 (3%)	34,52,52	0.82	1 (2%)
2	ATP	А	601	3	28,33,33	0.80	0	34,52,52	0.85	1 (2%)
2	ATP	D	601	3	28,33,33	0.77	0	34,52,52	0.80	1 (2%)

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	ATP	В	601	3	-	8/18/38/38	0/3/3/3
2	ATP	С	601	3	-	8/18/38/38	0/3/3/3
2	ATP	А	601	3	-	7/18/38/38	0/3/3/3
2	ATP	D	601	3	-	6/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	С	601	ATP	C1'-N9	-2.14	1.44	1.49
2	В	601	ATP	C1'-N9	-2.06	1.44	1.49

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	601	ATP	C5-C6-N6	2.52	124.15	120.31
2	D	601	ATP	C5-C6-N6	2.34	123.88	120.31
2	В	601	ATP	C5-C6-N6	2.31	123.83	120.31
2	С	601	ATP	C5-C6-N6	2.05	123.44	120.31

All (4) bond angle outliers are listed below:

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	601	ATP	C5'-O5'-PA-O1A
2	А	601	ATP	C5'-O5'-PA-O2A
2	А	601	ATP	C5'-O5'-PA-O3A
2	В	601	ATP	C5'-O5'-PA-O1A
2	В	601	ATP	C5'-O5'-PA-O2A
2	В	601	ATP	C5'-O5'-PA-O3A
2	С	601	ATP	PB-O3A-PA-O5'



Mol	Chain	$\mathbf{Res}$	Type	Atoms
2	С	601	ATP	C5'-O5'-PA-O1A
2	С	601	ATP	C5'-O5'-PA-O2A
2	С	601	ATP	C5'-O5'-PA-O3A
2	D	601	ATP	C5'-O5'-PA-O2A
2	В	601	ATP	O4'-C4'-C5'-O5'
2	С	601	ATP	O4'-C4'-C5'-O5'
2	В	601	ATP	C3'-C4'-C5'-O5'
2	С	601	ATP	C3'-C4'-C5'-O5'
2	А	601	ATP	C3'-C4'-C5'-O5'
2	А	601	ATP	PB-O3A-PA-O1A
2	А	601	ATP	PB-O3A-PA-O5'
2	В	601	ATP	PB-O3A-PA-O5'
2	D	601	ATP	PB-O3A-PA-O5'
2	D	601	ATP	C5'-O5'-PA-O1A
2	D	601	ATP	C5'-O5'-PA-O3A
2	С	601	ATP	C4'-C5'-O5'-PA
2	С	601	ATP	PB-O3B-PG-O3G
2	В	601	ATP	PG-O3B-PB-O2B
2	D	601	ATP	PA-O3A-PB-O1B
2	D	601	ATP	PA-O3A-PB-O2B
2	А	601	ATP	O4'-C4'-C5'-O5'
2	В	601	ATP	PB-O3A-PA-O2A

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There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and 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		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	487/564~(86%)	1.07	92 (18%) 4	}	28,53,101,124	0
1	В	479/564~(84%)	0.63	47 (9%) 14 1	2	27, 50, 95, 116	0
1	С	480/564~(85%)	1.06	82 (17%) 5 4	ł	28,64,94,113	0
1	D	482/564~(85%)	1.14	91 (18%) 4 3	}	27,  64,  96,  118	0
All	All	1928/2256~(85%)	0.97	312 (16%) 5	5	27, 57, 96, 124	0

All (312) RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	В	350	PHE	9.9
1	А	455	GLU	9.2
1	А	299	SER	7.2
1	А	41	ASP	7.1
1	А	302	ALA	7.0
1	В	301	ASP	6.8
1	D	301	ASP	6.7
1	С	465	LEU	6.5
1	D	310	ARG	6.1
1	А	350	PHE	6.0
1	А	518	LEU	6.0
1	D	447	PHE	5.9
1	А	304	HIS	5.3
1	В	302	ALA	5.3
1	А	305	ALA	5.2
1	А	522	ALA	5.2
1	D	375	VAL	5.1
1	С	493	VAL	5.1
1	С	301	ASP	5.0
1	А	521	VAL	5.0
1	С	463	GLU	5.0



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Mol	Chain	Res	Type	RSRZ
1	D	45	ARG	4.9
1	А	303	ALA	4.9
1	С	447	PHE	4.8
1	D	188	GLY	4.8
1	С	21	ASN	4.7
1	С	62	GLU	4.6
1	А	456	VAL	4.6
1	В	344	GLY	4.6
1	А	516	ALA	4.5
1	А	290	LEU	4.4
1	А	328	LYS	4.4
1	D	467	CYS	4.3
1	D	350	PHE	4.3
1	В	516	ALA	4.3
1	В	308	ILE	4.3
1	В	458	LEU	4.3
1	А	298	ALA	4.2
1	А	232	SER	4.1
1	С	457	LEU	4.1
1	В	456	VAL	4.1
1	D	443	THR	4.1
1	В	305	ALA	4.1
1	В	442	ARG	4.1
1	В	303	ALA	4.1
1	D	189	THR	4.0
1	А	473	ALA	4.0
1	А	38	LEU	4.0
1	А	55	LEU	4.0
1	D	397	LEU	4.0
1	В	298	ALA	3.9
1	В	519	PRO	3.9
1	D	300	GLY	3.9
1	В	480	GLY	3.9
1	А	465	LEU	3.9
1	D	312	LEU	3.9
1	D	505	PRO	3.9
1	А	343	MET	3.9
1	С	300	GLY	3.9
1	D	109	VAL	3.8
1	В	467	CYS	3.8
1	D	388	GLY	3.8
1	А	273	PHE	3.8



Mol	Chain	Res	Type	RSRZ
1	А	495	LEU	3.8
1	С	45	ARG	3.7
1	В	448	VAL	3.7
1	А	513	LEU	3.7
1	D	374	VAL	3.7
1	С	443	THR	3.6
1	А	54	VAL	3.6
1	D	349	ASP	3.6
1	С	492	LEU	3.6
1	D	195	SER	3.5
1	В	189	THR	3.5
1	А	490	TYR	3.5
1	В	457	LEU	3.5
1	С	134	GLU	3.5
1	В	328	LYS	3.5
1	D	481	TRP	3.5
1	С	471	GLY	3.4
1	D	465	LEU	3.4
1	С	361	ARG	3.4
1	А	285	LEU	3.4
1	А	501	ALA	3.4
1	С	351	VAL	3.4
1	С	490	TYR	3.4
1	D	466	ASP	3.4
1	D	311	LEU	3.4
1	А	314	LYS	3.4
1	С	284	ASP	3.3
1	А	453	THR	3.3
1	D	493	VAL	3.3
1	С	405	ASN	3.3
1	В	495	LEU	3.3
1	D	490	TYR	3.3
1	А	278	THR	3.3
1	С	502	PRO	3.2
1	С	190	THR	3.2
1	D	367	MET	3.2
1	В	485	GLY	3.2
1	С	324	LEU	3.2
1	С	338	PHE	3.2
1	A	133	ARG	3.2
1	D	266	ARG	3.2
1	D	187	SER	3.2



Mol	Chain	Res	Type	RSRZ
1	А	174	ARG	3.2
1	С	263	GLU	3.2
1	В	443	THR	3.1
1	D	256	LYS	3.1
1	С	312	LEU	3.1
1	В	471	GLY	3.1
1	D	506	THR	3.1
1	А	338	PHE	3.1
1	D	286	THR	3.1
1	А	462	PRO	3.1
1	В	518	LEU	3.1
1	А	461	TYR	3.1
1	С	123	ARG	3.1
1	С	394	SER	3.1
1	А	337	MET	3.1
1	С	169	ALA	3.1
1	С	501	ALA	3.1
1	А	307	HIS	3.0
1	D	123	ARG	3.0
1	D	233	ALA	3.0
1	D	511	GLU	3.0
1	В	188	GLY	3.0
1	D	204	PHE	3.0
1	D	503	GLN	3.0
1	D	33	LEU	3.0
1	D	336	ASP	3.0
1	D	362	CYS	3.0
1	В	304	HIS	3.0
1	А	266	ARG	3.0
1	D	236	ASN	3.0
1	D	361	ARG	3.0
1	D	250	TYR	3.0
1	D	104	ALA	3.0
1	D	444	GLU	3.0
1	А	517	GLY	2.9
1	А	345	TYR	2.9
1	В	463	GLU	2.9
1	А	380	SER	2.9
1	С	407	ARG	2.9
1	А	344	GLY	2.9
1	В	461	TYR	2.9
1	D	299	SER	2.9



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Mol	Chain	Res	Type	RSRZ
1	А	515	ARG	2.9
1	С	102	ILE	2.9
1	С	337	MET	2.9
1	D	119	ARG	2.9
1	D	95	ASN	2.9
1	А	256	LYS	2.8
1	А	472	LEU	2.8
1	D	489	VAL	2.8
1	D	521	VAL	2.8
1	А	466	ASP	2.8
1	С	466	ASP	2.8
1	D	448	VAL	2.8
1	D	486	VAL	2.8
1	С	349	ASP	2.8
1	D	328	LYS	2.8
1	А	479	PHE	2.8
1	D	376	GLY	2.8
1	С	521	VAL	2.7
1	В	349	ASP	2.7
1	С	256	LYS	2.7
1	D	316	TYR	2.7
1	D	492	LEU	2.7
1	С	61	HIS	2.7
1	А	52	PRO	2.7
1	А	339	GLY	2.7
1	D	461	TYR	2.7
1	D	43	THR	2.7
1	А	123	ARG	2.7
1	А	407	ARG	2.7
1	D	124	ARG	2.7
1	D	410	LYS	2.7
1	С	350	PHE	2.7
1	D	385	GLY	2.7
1	А	469	VAL	2.6
1	С	250	TYR	2.6
1	С	459	ARG	2.6
1	А	334	PHE	2.6
1	D	166	HIS	2.6
1	С	316	TYR	2.6
1	D	436	ARG	2.6
1	В	510	ASN	2.6
1	D	330	PRO	2.6



Mol	Chain	Res	Type	RSRZ
1	D	292	SER	2.6
1	В	395	LYS	2.6
1	С	75	GLY	2.6
1	А	221	LYS	2.5
1	D	459	ARG	2.5
1	А	43	THR	2.5
1	А	291	THR	2.5
1	С	327	LYS	2.5
1	А	134	GLU	2.5
1	D	463	GLU	2.5
1	А	477	VAL	2.5
1	В	345	TYR	2.5
1	С	120	GLU	2.5
1	А	324	LEU	2.5
1	В	285	LEU	2.5
1	С	104	ALA	2.5
1	С	509	ILE	2.5
1	С	152	PHE	2.5
1	D	314	LYS	2.4
1	D	193	PRO	2.4
1	С	448	VAL	2.4
1	D	329	VAL	2.4
1	С	328	LYS	2.4
1	D	34	ASP	2.4
1	В	360	GLY	2.4
1	В	486	VAL	2.4
1	С	148	GLU	2.4
1	D	455	GLU	2.4
1	С	192	ILE	2.4
1	A	316	TYR	2.4
1	С	287	ASP	2.4
1	С	313	ASP	2.4
1	D	340	SER	2.4
1	С	508	TRP	2.4
1	D	281	ALA	2.4
1	В	125	GLN	2.4
1	A	189	THR	2.4
1	С	27	PRO	2.3
1	А	49	GLY	2.3
1	A	64	VAL	2.3
1	А	340	SER	2.3
1	С	232	SER	2.3



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Mol	Chain	Res	Type	RSRZ
1	D	313	ASP	2.3
1	В	455	GLU	2.3
1	D	499	ALA	2.3
1	D	237	THR	2.3
1	С	223	LEU	2.3
1	С	330	PRO	2.3
1	С	410	LYS	2.3
1	С	375	VAL	2.3
1	D	469	VAL	2.3
1	С	487	ALA	2.3
1	С	155	LEU	2.3
1	D	267	PRO	2.3
1	D	464	ILE	2.3
1	D	440	ALA	2.3
1	А	349	ASP	2.3
1	D	50	SER	2.3
1	С	462	PRO	2.3
1	А	250	TYR	2.2
1	А	470	VAL	2.2
1	С	345	TYR	2.2
1	А	277	PHE	2.2
1	А	222	ARG	2.2
1	А	499	ALA	2.2
1	С	135	PRO	2.2
1	А	268	THR	2.2
1	D	441	ILE	2.2
1	С	143	HIS	2.2
1	D	345	TYR	2.2
1	А	33	LEU	2.2
1	A	226	LEU	2.2
1	С	504	ASP	2.2
1	В	380	SER	2.2
1	С	346	VAL	2.2
1	С	485	GLY	2.2
1	D	273	PHE	2.2
1	С	440	ALA	2.2
1	А	202	THR	2.2
1	C	318	THR	2.2
1	D	192	ILE	2.2
1	А	485	GLY	2.2
1	А	275	HIS	2.2
1	В	275	HIS	2.2



Mol	Chain	Res	Type	RSRZ
1	В	449	TYR	2.2
1	А	327	LYS	2.2
1	D	395	LYS	2.2
1	D	406	VAL	2.2
1	В	272	GLY	2.1
1	А	31	ARG	2.1
1	А	410	LYS	2.1
1	В	196	ALA	2.1
1	С	363	ILE	2.1
1	С	406	VAL	2.1
1	D	186	SER	2.1
1	А	108	LEU	2.1
1	D	427	ALA	2.1
1	А	494	ASN	2.1
1	В	358	VAL	2.1
1	В	489	VAL	2.1
1	С	73	ARG	2.1
1	С	70	PHE	2.1
1	А	363	ILE	2.1
1	А	40	LEU	2.1
1	А	320	THR	2.1
1	С	286	THR	2.1
1	С	187	SER	2.1
1	D	298	ALA	2.1
1	С	165	GLU	2.1
1	А	467	CYS	2.1
1	В	61	HIS	2.1
1	С	43	THR	2.0
1	С	323	ASP	2.0
1	А	335	ILE	2.0
1	А	510	ASN	2.0
1	В	376	GLY	2.0
1	А	99	LEU	2.0
1	А	492	LEU	2.0
1	D	223	LEU	2.0
1	А	98	ALA	2.0
1	С	336	ASP	2.0
1	С	461	TYR	2.0
1	В	343	MET	2.0

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

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

### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
3	MG	D	603	1/1	0.42	0.17	30,30,30,30	0
3	MG	С	602	1/1	0.49	0.46	85,85,85,85	0
2	ATP	С	601	31/31	0.71	0.21	53,86,103,124	0
2	ATP	D	601	31/31	0.79	0.17	57,74,102,114	0
3	MG	В	602	1/1	0.87	0.37	50,50,50,50	0
2	ATP	А	601	31/31	0.87	0.14	45,70,90,109	0
2	ATP	В	601	31/31	0.87	0.14	45,64,81,83	0
3	MG	А	602	1/1	0.88	0.28	48,48,48,48	0
3	MG	В	603	1/1	0.89	0.12	30,30,30,30	0
3	MG	D	602	1/1	0.90	0.40	50,50,50,50	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.

