

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

#### Nov 19, 2023 – 09:33 PM JST

PDB ID	:	7BUQ
Title	:	mcGAS bound with 23-cGAMP
Authors	:	Wang, B.; Su, X.D.
Deposited on	:	2020-04-07
Resolution	:	3.09  Å(reported)

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

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

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

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

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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain						
1	А	507	43%	25%	••	29%			
1	В	507	43%	22%	5%	29%	_		

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	1SY	А	602	-	-	-	Х



#### $7\mathrm{BUQ}$

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6070 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 Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	362	Total 2993	C 1924	N 509	0 547	S 13	0	0	0
1	В	361	Total 2984	C 1919	N 508	O 544	S 13	0	0	0

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Zn 1 1	0	0
2	В	1	Total Zn 1 1	0	0

• Molecule 3 is cGAMP (three-letter code: 1SY) (formula:  $C_{20}H_{24}N_{10}O_{13}P_2$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	Δ	1	Total	С	Ν	Ο	Р	0	0
3	3 A	1	45	20	10	13	2	0	0
9	D	1	Total	С	Ν	0	Р	0	0
3	D	1	45	20	10	13	2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total O 1 1	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: Cyclic GMP-AMP synthase

# K484 E361 1270 K485 R364 R371 F487 R365 R364 F487 R365 R364 K491 R364 V274 K491 R365 R364 K491 R365 R364 K491 R372 V274 K491 R372 R375 K491 R372 R376 K492 R376 R376 K372 R376 R376 K376 R376 R386 K386 R386 R386 K396 R386 R396 K396 R386 R396 K396 R396 R396 K396 R396 R396 K396 R396 R396 K410 R361 R396



# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	47.65Å 109.81Å 75.64Å	Dopositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $94.13^{\circ}$ $90.00^{\circ}$	Depositor	
Bosolution (Å)	37.72 - 3.09	Depositor	
Itesolution (A)	37.72 - 3.09	EDS	
% Data completeness	97.2 (37.72-3.09)	Depositor	
(in resolution range)	97.2 (37.72-3.09)	EDS	
$R_{merge}$	0.25	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$2.19 (at 3.12 \text{\AA})$	Xtriage	
Refinement program	PHENIX 1.14	Depositor	
B B.	0.249 , $0.296$	Depositor	
II, II free	0.248 , $0.292$	DCC	
$R_{free}$ test set	1402  reflections  (10.10%)	wwPDB-VP	
Wilson B-factor $(Å^2)$	65.9	Xtriage	
Anisotropy	0.026	Xtriage	
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , $47.1$	EDS	
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
$F_o, F_c$ correlation	0.89	EDS	
Total number of atoms	6070	wwPDB-VP	
Average B, all atoms $(Å^2)$	67.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



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

# 5 Model quality (i)

# 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 1SY

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

Mal	Chain	Bo	nd lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.86	0/3058	0.77	4/4106~(0.1%)	
1	В	0.74	1/3049~(0.0%)	0.73	1/4093~(0.0%)	
All	All	0.80	1/6107~(0.0%)	0.75	5/8199~(0.1%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	463	GLU	CD-OE2	-5.22	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	201	TYR	N-CA-C	-5.63	95.80	111.00
1	А	222	ARG	N-CA-C	5.58	126.07	111.00
1	А	206	ILE	CB-CA-C	-5.31	100.99	111.60
1	А	210	ASN	N-CA-C	5.19	125.02	111.00
1	В	214	VAL	CB-CA-C	-5.04	101.81	111.40

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	2993	0	3039	214	0
1	В	2984	0	3034	214	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	45	0	22	14	0
3	В	45	0	22	13	0
4	А	1	0	0	0	0
All	All	6070	0	6117	431	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 35.

All (431) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:206:ILE:HG23	1:B:399:LYS:CG	1.47	1.42
1:B:164:ILE:CD1	1:B:202:GLU:HA	1.56	1.35
1:A:223:ILE:CD1	1:A:239:PHE:HE1	1.41	1.33
1:A:300:ASN:HB3	1:A:301:PRO:CD	1.55	1.33
1:A:300:ASN:CB	1:A:301:PRO:HD3	1.52	1.30
1:B:164:ILE:HD11	1:B:202:GLU:CG	1.66	1.25
1:B:198:GLY:CA	1:B:201:TYR:HE1	1.56	1.19
1:A:296:LEU:HB2	1:A:306:VAL:CG2	1.75	1.17
1:A:265:LYS:HG2	1:A:269:ILE:CD1	1.74	1.16
1:B:207:SER:CB	1:B:402:LYS:HG3	1.76	1.15
1:B:198:GLY:HA3	1:B:201:TYR:CE1	1.80	1.15
1:B:207:SER:HB3	1:B:402:LYS:HG3	1.26	1.14
1:A:205:LYS:O	1:A:402:LYS:HD2	1.47	1.14
1:A:243:PRO:HD2	1:A:246:ASN:HD22	1.11	1.14
1:B:285:GLU:CG	1:B:297:LEU:HD23	1.78	1.13
1:A:203:HIS:ND1	1:A:207:SER:HB2	1.62	1.13
3:A:602:1SY:H8	3:A:602:1SY:H18	1.13	1.12
1:B:463:GLU:HG2	1:B:486:LYS:HE3	1.19	1.12
1:B:206:ILE:CG2	1:B:399:LYS:HG2	1.81	1.09
1:B:181:ARG:HG2	1:B:273:GLU:OE2	1.52	1.09
1:A:223:ILE:CD1	1:A:239:PHE:CE1	2.34	1.09
1:B:164:ILE:CD1	1:B:202:GLU:HG3	1.83	1.08
1:B:198:GLY:CA	1:B:201:TYR:CE1	2.36	1.08
1:A:162:LYS:HG3	1:B:387:SER:OG	1.52	1.08
1:B:206:ILE:HG23	1:B:399:LYS:HG2	1.12	1.08
1:B:198:GLY:HA3	1:B:201:TYR:HE1	1.03	1.07
1:A:160:LYS:HD3	1:A:203:HIS:CB	1.85	1.06



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:207:SER:HB3	1:B:402:LYS:CG	1.84	1.06
1:B:171:VAL:O	1:B:175:VAL:HG23	1.55	1.06
3:B:602:1SY:H18	3:B:602:1SY:H8	1.13	1.06
1:B:206:ILE:CG2	1:B:399:LYS:CG	2.37	1.02
1:A:409:LYS:HE3	1:A:418:PHE:O	1.59	1.02
1:A:161:ARG:HH22	1:B:201:TYR:HE2	1.06	1.01
1:A:223:ILE:HD12	1:A:239:PHE:HE1	1.21	1.01
1:B:164:ILE:HG21	1:B:205:LYS:HG3	1.42	1.01
1:B:300:ASN:HB3	1:B:301:PRO:HD3	1.41	1.00
1:A:447:SER:O	1:A:451:LYS:HG3	1.60	1.00
1:A:221:PRO:HG3	1:A:246:ASN:HD21	1.23	1.00
1:B:164:ILE:HD13	1:B:202:GLU:HA	1.02	1.00
1:A:296:LEU:HB2	1:A:306:VAL:HG23	1.40	0.99
1:B:164:ILE:CD1	1:B:202:GLU:CA	2.41	0.98
1:A:206:ILE:HA	1:A:402:LYS:HD3	1.45	0.97
1:A:223:ILE:HD13	1:A:239:PHE:HE1	1.27	0.96
1:B:206:ILE:HG23	1:B:399:LYS:HG3	1.43	0.96
1:B:285:GLU:HG3	1:B:297:LEU:HD23	1.48	0.95
1:B:244:ARG:HE	1:B:244:ARG:HA	1.27	0.95
1:A:205:LYS:C	1:A:402:LYS:NZ	2.22	0.94
1:B:179:LEU:O	1:B:183:GLN:HG3	1.66	0.94
1:A:204:VAL:CG1	1:A:395:LYS:HE2	1.98	0.93
1:B:309:ILE:CD1	3:B:602:1SY:N42	2.31	0.93
1:A:203:HIS:CG	1:A:207:SER:HB2	2.04	0.92
3:B:602:1SY:H18	3:B:602:1SY:C3'	1.99	0.91
1:B:463:GLU:HG2	1:B:486:LYS:CE	2.00	0.91
1:A:146:GLU:HB2	1:A:147:PRO:HD2	1.52	0.91
1:A:223:ILE:HD12	1:A:239:PHE:CE1	2.01	0.91
1:B:164:ILE:HD11	1:B:202:GLU:HG3	0.91	0.90
1:B:164:ILE:O	1:B:168:ALA:HB3	1.70	0.90
1:B:164:ILE:HG12	1:B:205:LYS:HZ3	1.37	0.90
1:A:300:ASN:CB	1:A:301:PRO:CD	2.29	0.89
1:B:207:SER:HB3	1:B:402:LYS:CB	2.03	0.88
1:A:146:GLU:HB2	1:A:147:PRO:CD	2.03	0.88
1:A:172:ASN:HA	1:A:200:TYR:OH	1.74	0.87
1:B:158:ARG:O	1:B:158:ARG:NH2	2.07	0.87
1:B:201:TYR:CE2	1:B:203:HIS:ND1	2.42	0.87
1:B:201:TYR:CE2	1:B:203:HIS:CE1	2.63	0.86
1:A:265:LYS:HG2	1:A:269:ILE:HD11	1.55	0.86
1:A:160:LYS:HD3	1:A:203:HIS:HB2	1.57	0.86
3:B:602:1SY:O17	3:B:602:1SY:H4	1.76	0.86



		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:B:201:TYR:CZ	1:B:203:HIS:ND1	2.44	0.85	
1:B:244:ARG:HA	1:B:244:ARG:NE	1.87	0.85	
1:B:159:LEU:HD12	1:B:159:LEU:H	1.41	0.84	
1:A:205:LYS:O	1:A:402:LYS:CD	2.25	0.84	
1:A:160:LYS:CD	1:A:203:HIS:HB2	2.08	0.84	
1:A:223:ILE:HD13	1:A:239:PHE:CE1	2.05	0.83	
1:B:164:ILE:HG21	1:B:205:LYS:CG	2.08	0.83	
1:B:463:GLU:CG	1:B:486:LYS:HE3	2.07	0.83	
1:B:181:ARG:HH12	1:B:277:ILE:HG21	1.40	0.83	
3:A:602:1SY:H18	3:A:602:1SY:C3'	2.04	0.83	
1:A:149:LYS:O	1:A:153:VAL:HG23	1.80	0.82	
1:A:219:GLU:OE2	1:A:315:LYS:HD2	1.78	0.82	
1:A:219:GLU:OE2	1:A:315:LYS:HG3	1.79	0.82	
1:A:206:ILE:HA	1:A:402:LYS:CD	2.09	0.81	
1:A:203:HIS:ND1	1:A:207:SER:CB	2.44	0.81	
1:A:205:LYS:C	1:A:402:LYS:HZ3	1.81	0.81	
1:B:297:LEU:HA	1:B:304:ILE:O	1.80	0.80	
1:A:203:HIS:CE1	1:A:207:SER:CB	2.64	0.80	
1:A:243:PRO:HD2	1:A:246:ASN:ND2	1.94	0.80	
1:A:153:VAL:O	1:A:157:LEU:HG	1.82	0.80	
1:A:265:LYS:CG	1:A:269:ILE:CD1	2.58	0.79	
1:A:160:LYS:HD3	1:A:203:HIS:CG	2.17	0.79	
1:B:181:ARG:NH1	1:B:277:ILE:HG21	1.97	0.79	
1:B:181:ARG:NH1	1:B:277:ILE:CG2	2.47	0.78	
1:A:265:LYS:HG2	1:A:269:ILE:HD13	1.64	0.78	
1:B:285:GLU:HG2	1:B:297:LEU:HD23	1.63	0.78	
1:B:300:ASN:CB	1:B:301:PRO:HD3	2.13	0.78	
1:B:478:GLN:H	1:B:478:GLN:NE2	1.82	0.77	
1:B:171:VAL:O	1:B:175:VAL:CG2	2.32	0.77	
1:B:367:PHE:O	1:B:371:GLU:HG3	1.84	0.77	
1:B:164:ILE:HD11	1:B:202:GLU:CA	2.11	0.77	
1:B:203:HIS:NE2	1:B:376:ASN:ND2	2.33	0.76	
1:A:248:LEU:N	1:A:248:LEU:HD22	2.02	0.75	
3:A:602:1SY:H8	3:A:602:1SY:C25	2.06	0.75	
1:B:164:ILE:HG21	1:B:205:LYS:HB2	1.68	0.75	
1:B:414:GLU:HG3	1:B:414:GLU:O	1.84	0.75	
1:B:182:MET:CE	1:B:270:ILE:HG12	2.16	0.74	
1:A:219:GLU:OE2	1:A:315:LYS:CD	2.35	0.74	
1:A:300:ASN:HB3	1:A:301:PRO:HD3	0.77	0.74	
1:A:204:VAL:HG13	1:A:395:LYS:HE2	1.70	0.73	
1:A:171:VAL:HG12	1:A:200:TYR:CE1	2.23	0.73	



		Interatomic Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:203:HIS:CE1	1:A:207:SER:HB2	2.24	0.73	
1:B:187:SER:O	1:B:190:LYS:HG2	1.89	0.73	
1:B:203:HIS:CE1	1:B:376:ASN:HD21	2.06	0.73	
1:A:206:ILE:N	1:A:402:LYS:HZ3	1.86	0.72	
1:B:164:ILE:HG12	1:B:205:LYS:NZ	2.03	0.72	
1:B:220:VAL:HB	1:B:221:PRO:HD2	1.70	0.72	
1:B:164:ILE:HD11	1:B:202:GLU:CB	2.19	0.72	
1:B:195:LEU:HD21	1:B:346:TYR:OH	1.90	0.72	
1:B:207:SER:OG	1:B:402:LYS:HG3	1.89	0.71	
1:A:219:GLU:OE2	1:A:315:LYS:CG	2.38	0.71	
3:B:602:1SY:O29	3:B:602:1SY:O2'	2.04	0.71	
1:B:292:PRO:HB2	1:B:349:PRO:HG2	1.73	0.71	
1:B:276:GLU:HG3	1:B:276:GLU:O	1.89	0.71	
1:B:182:MET:HE3	1:B:270:ILE:HG12	1.73	0.71	
1:B:154:LEU:HD11	1:B:396:GLU:HB3	1.72	0.71	
1:A:402:LYS:O	1:A:406:GLU:HG3	1.90	0.70	
1:B:300:ASN:HB3	1:B:301:PRO:CD	2.21	0.70	
1:B:234:PHE:CD2	1:B:352:ALA:HB2	2.25	0.70	
3:B:602:1SY:H8	3:B:602:1SY:C25	2.07	0.70	
1:A:196:ASN:OD1	1:A:372:LYS:NZ	2.24	0.70	
1:A:203:HIS:CD2	1:A:207:SER:OG	2.45	0.70	
1:A:206:ILE:HG12	1:A:420:SER:CB	2.22	0.70	
1:A:160:LYS:CG	1:A:203:HIS:HD2	2.06	0.69	
1:B:198:GLY:HA2	1:B:201:TYR:CE1	2.26	0.69	
1:B:164:ILE:HG21	1:B:205:LYS:CB	2.23	0.69	
1:A:203:HIS:CG	1:A:207:SER:CB	2.76	0.68	
1:A:160:LYS:O	1:A:164:ILE:HG22	1.92	0.68	
1:B:206:ILE:HG23	1:B:399:LYS:CD	2.20	0.68	
1:A:171:VAL:CG1	1:A:200:TYR:CE1	2.76	0.68	
1:A:202:GLU:HG2	1:A:202:GLU:O	1.93	0.67	
1:A:223:ILE:HG21	1:A:237:VAL:HG22	1.76	0.67	
1:B:253:GLU:OE1	1:B:261:LYS:HE3	1.95	0.67	
1:A:188:GLU:HG2	1:A:250:HIS:HE1	1.60	0.67	
1:A:300:ASN:HB2	1:A:301:PRO:HD3	1.69	0.67	
1:A:222:ARG:HD3	1:A:222:ARG:N	2.10	0.66	
1:A:221:PRO:CG	1:A:246:ASN:HD21	2.06	0.66	
1:B:309:ILE:HD12	3:B:602:1SY:C40	2.26	0.66	
1:B:280:ILE:O	1:B:280:ILE:HD12	1.95	0.66	
1:A:274:VAL:HG22	1:A:282:VAL:O	1.96	0.66	
1:A:243:PRO:CD	1:A:246:ASN:HD22	2.00	0.66	
1:B:159:LEU:HD12	1:B:159:LEU:N	2.07	0.65	



	lo de page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:238:LYS:HD2	1:A:256:VAL:HG22	1.78	0.65	
1:B:483:ARG:HA	1:B:486:LYS:HG3	1.78	0.65	
1:A:205:LYS:C	1:A:402:LYS:HZ2	1.98	0.65	
1:A:409:LYS:HE2	1:A:415:LEU:O	1.96	0.65	
1:A:258:SER:HA	1:A:361:GLU:HG2	1.78	0.64	
1:B:274:VAL:CG2	1:B:282:VAL:CG1	2.74	0.64	
1:B:285:GLU:CG	1:B:297:LEU:CD2	2.67	0.64	
1:B:177:ARG:NH2	1:B:279:ASP:OD2	2.30	0.64	
1:A:210:ASN:HB2	1:A:211:GLU:OE2	1.97	0.64	
1:A:238:LYS:HD2	1:A:256:VAL:CG2	2.28	0.64	
1:A:287:GLU:O	1:A:287:GLU:HG3	1.98	0.64	
1:B:309:ILE:HD12	3:B:602:1SY:N42	2.12	0.64	
1:B:206:ILE:CG2	1:B:399:LYS:HG3	2.17	0.64	
1:A:284:VAL:HG12	1:A:296:LEU:HD23	1.80	0.64	
1:B:182:MET:HE1	1:B:270:ILE:CG1	2.28	0.64	
1:A:252:LEU:HD12	1:A:257:LEU:HA	1.79	0.63	
1:B:195:LEU:HG	1:B:217:LYS:HD3	1.80	0.63	
1:B:274:VAL:CG2	1:B:282:VAL:HG13	2.28	0.63	
1:B:164:ILE:O	1:B:168:ALA:CB	2.47	0.63	
1:A:160:LYS:CD	1:A:203:HIS:CB	2.66	0.62	
1:A:309:ILE:CD1	3:A:602:1SY:N42	2.62	0.62	
1:A:160:LYS:HD3	1:A:203:HIS:HB3	1.79	0.62	
1:A:503:ILE:O	1:A:503:ILE:HG12	1.98	0.62	
1:B:285:GLU:HG3	1:B:297:LEU:CD2	2.26	0.62	
1:B:297:LEU:CD1	1:B:303:GLU:HG3	2.30	0.62	
1:A:223:ILE:O	1:A:240:LYS:NZ	2.32	0.62	
1:A:168:ALA:HB1	1:A:200:TYR:CB	2.30	0.62	
1:A:274:VAL:HG13	1:A:275:LYS:HG2	1.81	0.61	
1:B:393:CYS:HA	1:B:396:GLU:OE1	2.00	0.61	
1:A:265:LYS:CG	1:A:269:ILE:HD11	2.25	0.61	
1:A:188:GLU:OE1	1:A:250:HIS:CE1	2.54	0.61	
1:A:298:ILE:HG22	1:A:298:ILE:O	1.99	0.61	
1:A:407:GLN:HB3	1:A:503:ILE:HD11	1.83	0.61	
1:A:203:HIS:HA	1:A:207:SER:HA	1.83	0.61	
1:A:188:GLU:N	1:A:188:GLU:OE2	2.31	0.61	
1:A:265:LYS:O	1:A:269:ILE:HD12	2.01	0.61	
1:B:195:LEU:HD21	1:B:346:TYR:CZ	2.36	0.61	
1:A:306:VAL:HG23	1:A:306:VAL:O	2.00	0.61	
1:B:478:GLN:H	1:B:478:GLN:CD	2.05	0.60	
1:A:409:LYS:CE	1:A:418:PHE:O	2.43	0.60	
1:B:228:TYR:HB3	1:B:234:PHE:O	2.02	0.60	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:246:ASN:OD1	1:A:247:PRO:HD2	2.01	0.60
1:A:160:LYS:HD3	1:A:203:HIS:CD2	2.37	0.60
1:A:205:LYS:CA	1:A:402:LYS:HZ2	2.15	0.59
1:A:309:ILE:HD11	3:A:602:1SY:H20	1.84	0.59
1:A:206:ILE:CA	1:A:402:LYS:HD3	2.28	0.59
1:B:297:LEU:HD12	1:B:303:GLU:HG3	1.84	0.59
1:A:160:LYS:HG3	1:A:203:HIS:HD2	1.68	0.59
1:B:164:ILE:CG2	1:B:205:LYS:HB2	2.32	0.59
1:A:160:LYS:HD2	1:A:203:HIS:HB2	1.84	0.59
1:B:309:ILE:CD1	3:B:602:1SY:H24	2.13	0.59
1:B:351:ASN:HD22	1:B:351:ASN:C	2.05	0.59
1:A:309:ILE:HD12	3:A:602:1SY:N42	2.18	0.59
1:B:181:ARG:CZ	1:B:277:ILE:HG23	2.34	0.58
1:A:319:PRO:HG2	1:A:365:LEU:HD11	1.84	0.58
1:B:274:VAL:HG22	1:B:282:VAL:HG13	1.86	0.58
1:B:161:ARG:HA	1:B:165:SER:CB	2.34	0.58
1:B:181:ARG:NH1	1:B:277:ILE:HG23	2.18	0.58
1:B:181:ARG:CZ	1:B:277:ILE:CG2	2.82	0.58
1:A:231:THR:O	1:A:473:PHE:HD2	1.87	0.58
1:A:223:ILE:HG23	1:A:237:VAL:HG13	1.86	0.58
3:A:602:1SY:H13	3:A:602:1SY:H10	1.86	0.58
1:A:161:ARG:NH2	1:B:203:HIS:HE1	2.02	0.58
3:A:602:1SY:O29	3:A:602:1SY:O2'	2.15	0.58
1:A:274:VAL:CG2	1:A:282:VAL:O	2.51	0.57
1:B:182:MET:HE1	1:B:270:ILE:HG12	1.86	0.57
1:B:220:VAL:HB	1:B:221:PRO:CD	2.33	0.57
1:A:168:ALA:HB1	1:A:200:TYR:HB3	1.85	0.57
1:B:309:ILE:HD13	3:B:602:1SY:N42	2.18	0.57
1:B:487:GLU:O	1:B:491:LYS:HG2	2.04	0.57
1:B:184:LYS:HE3	1:B:273:GLU:OE1	2.05	0.57
1:A:328:ILE:HB	1:A:332:LEU:HB2	1.86	0.57
1:A:158:ARG:NH1	1:B:386:GLU:O	2.31	0.57
1:B:181:ARG:CG	1:B:273:GLU:OE2	2.40	0.57
1:B:203:HIS:CE1	1:B:376:ASN:ND2	2.72	0.56
1:B:207:SER:HB3	1:B:402:LYS:HB3	1.86	0.56
1:A:161:ARG:NH2	1:B:201:TYR:CE2	2.66	0.56
1:B:198:GLY:C	1:B:201:TYR:HE1	2.08	0.56
1:B:358:PHE:N	1:B:358:PHE:CD1	2.72	0.56
1:A:188:GLU:CG	1:A:250:HIS:HE1	2.17	0.56
1:A:222:ARG:HD3	1:A:222:ARG:H	1.71	0.56
1:B:348:VAL:HG21	1:B:364:ARG:NH2	2.20	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:146:GLU:CB	1:A:147:PRO:CD	2.77	0.56
1:B:315:LYS:HG2	1:B:344:PRO:HG3	1.88	0.56
1:B:164:ILE:CD1	1:B:202:GLU:CG	2.59	0.55
1:B:201:TYR:CZ	1:B:203:HIS:CE1	2.91	0.55
1:A:172:ASN:HA	1:A:200:TYR:CZ	2.40	0.55
1:A:205:LYS:O	1:A:402:LYS:CE	2.54	0.55
1:B:274:VAL:CG2	1:B:282:VAL:HG11	2.37	0.55
1:B:298:ILE:H	1:B:304:ILE:HG22	1.72	0.55
1:A:220:VAL:HB	1:A:223:ILE:HD11	1.89	0.55
1:B:161:ARG:HA	1:B:165:SER:HB2	1.88	0.55
1:A:381:GLU:HB2	1:A:437:ASP:OD2	2.06	0.55
1:A:211:GLU:HG2	1:A:305:SER:OG	2.07	0.54
1:A:206:ILE:HG12	1:A:420:SER:HB2	1.88	0.54
1:B:309:ILE:HD13	3:B:602:1SY:C36	2.38	0.54
1:B:378:HIS:CD2	1:B:394:ARG:HD2	2.43	0.54
1:A:265:LYS:O	1:A:269:ILE:CD1	2.55	0.54
1:A:160:LYS:CG	1:A:203:HIS:CD2	2.87	0.54
1:A:171:VAL:CG1	1:A:200:TYR:HE1	2.20	0.54
1:A:203:HIS:CD2	1:A:207:SER:HG	2.25	0.54
1:B:161:ARG:HG2	1:B:165:SER:HB3	1.90	0.54
1:B:200:TYR:OH	1:B:214:VAL:CG2	2.55	0.54
1:B:231:THR:HG21	1:B:234:PHE:HB2	1.90	0.53
1:A:309:ILE:HD13	3:A:602:1SY:C36	2.39	0.53
1:A:210:ASN:ND2	1:A:211:GLU:H	2.07	0.53
1:B:182:MET:HE1	1:B:270:ILE:HG13	1.90	0.52
1:A:210:ASN:HD22	1:A:211:GLU:H	1.54	0.52
1:A:160:LYS:HG3	1:A:203:HIS:CD2	2.44	0.52
1:A:252:LEU:CD1	1:A:257:LEU:HA	2.39	0.52
1:B:265:LYS:O	1:B:265:LYS:HD3	2.09	0.52
1:A:266:PHE:O	1:A:270:ILE:HG13	2.09	0.52
1:A:309:ILE:CD1	3:A:602:1SY:H20	2.38	0.52
1:B:175:VAL:HG21	1:B:200:TYR:OH	2.10	0.52
1:A:180:ARG:HA	1:A:183:GLN:HG3	1.91	0.52
1:A:270:ILE:HG22	1:A:270:ILE:O	2.10	0.52
1:B:412:PHE:CE2	1:B:492:LYS:HE3	2.45	0.52
1:A:267:ARG:O	1:A:271:LYS:HD3	2.10	0.51
1:B:309:ILE:HD11	3:B:602:1SY:H24	1.76	0.51
1:A:223:ILE:C	1:A:240:LYS:HZ2	2.14	0.51
1:B:358:PHE:HD1	1:B:358:PHE:H	1.56	0.51
1:A:161:ARG:NH1	1:B:201:TYR:CD2	2.77	0.51
1:A:274:VAL:HG22	1:A:274:VAL:O	2.10	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:351:ASN:CG	1:B:359:GLN:O	2.50	0.50
1:A:155:ASP:O	1:A:158:ARG:HG2	2.11	0.50
1:B:200:TYR:N	1:B:200:TYR:CD1	2.79	0.50
1:A:149:LYS:O	1:A:149:LYS:HG3	2.11	0.50
1:A:296:LEU:HB2	1:A:306:VAL:HG22	1.84	0.50
1:B:300:ASN:CB	1:B:301:PRO:CD	2.85	0.50
1:A:198:GLY:O	1:B:166:GLU:OE2	2.30	0.50
1:A:203:HIS:CE1	1:A:207:SER:HG	2.29	0.49
3:A:602:1SY:H1	3:A:602:1SY:O19	2.12	0.49
1:B:303:GLU:O	1:B:303:GLU:HG2	2.13	0.49
1:B:347:LEU:HA	1:B:364:ARG:O	2.13	0.49
1:B:206:ILE:O	1:B:399:LYS:HG2	2.12	0.49
1:B:394:ARG:HB3	1:B:431:TRP:CZ2	2.48	0.49
3:A:602:1SY:H10	3:A:602:1SY:C21	2.42	0.49
1:B:494:GLU:O	1:B:498:ASN:ND2	2.45	0.49
1:B:158:ARG:HH21	1:B:159:LEU:HA	1.77	0.48
1:B:231:THR:HG23	1:B:232:GLY:N	2.28	0.48
1:A:172:ASN:CB	1:A:200:TYR:CE2	2.96	0.48
1:A:239:PHE:CD2	1:A:242:ILE:CD1	2.96	0.48
1:B:285:GLU:CD	1:B:297:LEU:HD23	2.33	0.48
1:A:213:ASP:N	1:A:213:ASP:OD1	2.46	0.48
1:B:280:ILE:HD12	1:B:280:ILE:C	2.34	0.48
1:B:295:THR:HG22	1:B:307:ASP:HA	1.95	0.48
1:A:224:GLU:HB2	1:A:240:LYS:HD2	1.95	0.48
1:B:344:PRO:O	1:B:369:HIS:NE2	2.47	0.48
1:A:178:LEU:HD13	1:A:182:MET:HE3	1.96	0.48
1:A:210:ASN:HD22	1:A:211:GLU:N	2.12	0.48
1:A:322:THR:O	1:A:341:ARG:NH2	2.46	0.47
1:A:211:GLU:CG	1:A:305:SER:OG	2.61	0.47
1:A:223:ILE:CG2	1:A:237:VAL:HG13	2.44	0.47
1:B:223:ILE:HD12	1:B:238:LYS:O	2.14	0.47
1:A:267:ARG:HB2	1:A:267:ARG:CZ	2.44	0.47
1:B:178:LEU:O	1:B:182:MET:HB3	2.15	0.47
1:A:252:LEU:HD13	1:A:257:LEU:HD12	1.96	0.47
1:B:274:VAL:HG22	1:B:282:VAL:CG1	2.43	0.47
1:A:201:TYR:CE2	1:B:202:GLU:OE2	2.68	0.47
1:A:217:LYS:HA	1:A:311:ALA:O	2.15	0.47
1:A:453:LEU:CD1	1:A:501:PHE:HZ	2.28	0.47
1:A:453:LEU:HD11	1:A:501:PHE:CZ	2.50	0.47
1:B:200:TYR:OH	1:B:214:VAL:HG21	2.14	0.47
1:B:304:ILE:HD12	1:B:304:ILE:HA	1.76	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:328:ILE:HD12	1:B:332:LEU:HB2	1.96	0.47
1:A:164:ILE:HD11	1:A:212:PHE:CE1	2.49	0.47
1:B:181:ARG:O	1:B:184:LYS:HD2	2.15	0.47
1:B:378:HIS:HD2	1:B:394:ARG:HD2	1.80	0.47
1:B:274:VAL:HG23	1:B:282:VAL:HG11	1.97	0.46
1:B:309:ILE:HD11	3:B:602:1SY:N42	2.27	0.46
1:B:188:GLU:HG3	1:B:247:PRO:HB2	1.96	0.46
1:B:159:LEU:CD1	1:B:159:LEU:C	2.84	0.46
1:B:214:VAL:HG12	1:B:215:MET:N	2.31	0.46
1:B:158:ARG:O	1:B:158:ARG:CD	2.64	0.46
1:B:178:LEU:O	1:B:182:MET:CB	2.64	0.46
1:B:181:ARG:HG2	1:B:181:ARG:O	2.15	0.46
1:A:172:ASN:CG	1:A:200:TYR:HE2	2.20	0.46
1:A:391:LYS:HE3	1:A:391:LYS:HB3	1.78	0.46
1:B:358:PHE:HB3	1:B:361:GLU:HB2	1.97	0.46
1:A:412:PHE:HB3	1:A:414:GLU:OE1	2.16	0.46
1:B:249:SER:HA	1:B:252:LEU:HD13	1.98	0.45
1:A:395:LYS:O	1:A:399:LYS:HG3	2.15	0.45
1:A:206:ILE:HG12	1:A:420:SER:OG	2.16	0.45
1:A:265:LYS:CG	1:A:269:ILE:HD12	2.46	0.45
1:B:159:LEU:HD13	1:B:159:LEU:O	2.16	0.45
1:B:200:TYR:OH	1:B:214:VAL:HG22	2.15	0.45
1:A:205:LYS:O	1:A:402:LYS:NZ	2.49	0.45
1:A:242:ILE:O	1:A:242:ILE:CG2	2.65	0.45
1:A:470:ILE:HG22	1:A:473:PHE:H	1.81	0.45
1:B:407:GLN:HE21	1:B:407:GLN:HA	1.81	0.45
1:B:401:MET:HG2	1:B:449:PHE:HE1	1.82	0.45
1:B:412:PHE:CD2	1:B:488:PHE:HZ	2.35	0.45
1:A:227:GLU:HA	1:A:235:TYR:CD2	2.52	0.45
1:B:228:TYR:CB	1:B:234:PHE:O	2.65	0.45
1:B:358:PHE:HD2	1:B:361:GLU:HB2	1.82	0.45
1:A:354:ASP:O	1:A:359:GLN:HG2	2.16	0.44
1:A:478:GLN:HG3	1:A:479:GLU:OE1	2.17	0.44
1:B:201:TYR:CG	1:B:201:TYR:O	2.70	0.44
1:B:285:GLU:CD	1:B:297:LEU:CD2	2.85	0.44
1:B:346:TYR:HD1	1:B:369:HIS:CE1	2.36	0.44
1:A:214:VAL:CG1	1:A:308:ILE:HD13	2.48	0.44
1:B:201:TYR:HD1	1:B:201:TYR:H	1.65	0.44
1:B:231:THR:HG23	1:B:232:GLY:H	1.82	0.44
1:B:204:VAL:HG22	1:B:204:VAL:O	2.17	0.44
1:A:202:GLU:OE2	1:A:212:PHE:HD1	2.00	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:164:ILE:CG2	1:B:205:LYS:HG3	2.31	0.44
1:B:168:ALA:HA	1:B:171:VAL:HG23	2.00	0.44
1:A:205:LYS:C	1:A:402:LYS:HD2	2.29	0.44
1:A:172:ASN:HB2	1:A:200:TYR:CE2	2.53	0.44
1:A:507:LEU:N	1:A:507:LEU:HD22	2.33	0.44
1:A:206:ILE:HA	1:A:402:LYS:HD2	1.97	0.43
1:B:351:ASN:ND2	1:B:359:GLN:O	2.51	0.43
1:B:358:PHE:N	1:B:358:PHE:HD1	2.11	0.43
1:A:149:LYS:O	1:A:153:VAL:CG2	2.61	0.43
1:B:195:LEU:HD11	1:B:346:TYR:CZ	2.53	0.43
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.54	0.43
1:B:292:PRO:HB3	1:B:349:PRO:O	2.19	0.43
1:A:403:TYR:OH	1:A:506:LYS:HD3	2.18	0.43
1:A:162:LYS:CG	1:B:387:SER:OG	2.43	0.43
1:A:205:LYS:C	1:A:402:LYS:CD	2.85	0.43
1:A:273:GLU:OE2	1:A:273:GLU:N	2.52	0.43
1:B:168:ALA:HA	1:B:171:VAL:CG2	2.48	0.43
1:A:408:LEU:HD23	1:A:408:LEU:HA	1.82	0.43
1:B:292:PRO:CB	1:B:349:PRO:HG2	2.46	0.43
1:A:205:LYS:CA	1:A:402:LYS:NZ	2.76	0.43
1:B:158:ARG:NH2	1:B:159:LEU:HA	2.33	0.42
1:B:322:THR:HG22	1:B:470:ILE:HG12	2.00	0.42
1:B:479:GLU:N	1:B:479:GLU:CD	2.72	0.42
1:A:453:LEU:CD1	1:A:501:PHE:CZ	3.03	0.42
1:B:178:LEU:O	1:B:178:LEU:HD12	2.18	0.42
1:B:398:LEU:HD13	1:B:427:ILE:HG21	2.01	0.42
1:A:171:VAL:HG11	1:A:200:TYR:CE1	2.55	0.42
1:A:182:MET:HE3	1:A:182:MET:HB2	1.87	0.42
1:A:359:GLN:H	1:A:359:GLN:HG3	1.41	0.42
1:B:270:ILE:O	1:B:270:ILE:HG22	2.20	0.42
1:A:309:ILE:CD1	3:A:602:1SY:H24	2.30	0.42
1:B:478:GLN:NE2	1:B:478:GLN:N	2.60	0.42
1:A:354:ASP:C	1:A:356:ASN:N	2.73	0.42
1:B:412:PHE:CD1	1:B:412:PHE:N	2.88	0.42
1:A:215:MET:SD	3:A:602:1SY:N39	2.93	0.41
1:A:221:PRO:HG3	1:A:246:ASN:ND2	2.08	0.41
1:A:457:LEU:HD21	1:A:493:ILE:HB	2.02	0.41
1:B:159:LEU:O	1:B:162:LYS:O	2.37	0.41
1:B:179:LEU:HD11	1:B:192:VAL:HG13	2.02	0.41
1:B:375:LEU:O	1:B:395:LYS:HE3	2.20	0.41
1:A:196:ASN:HD21	1:A:372:LYS:HZ1	1.67	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:196:ASN:CG	1:A:372:LYS:NZ	2.72	0.41
1:A:214:VAL:HG12	1:A:308:ILE:HD13	2.02	0.41
1:B:385:CYS:HA	1:B:391:LYS:HD2	2.02	0.41
1:A:168:ALA:HB1	1:A:200:TYR:HB2	2.01	0.41
1:A:196:ASN:CG	1:A:372:LYS:HZ3	2.24	0.41
1:B:227:GLU:HA	1:B:235:TYR:CD2	2.55	0.41
1:B:155:ASP:O	1:B:158:ARG:HG3	2.21	0.41
1:B:280:ILE:C	1:B:280:ILE:CD1	2.89	0.41
1:B:331:TRP:HH2	1:B:431:TRP:HE3	1.68	0.41
1:A:205:LYS:HA	1:A:402:LYS:HZ2	1.86	0.41
1:A:252:LEU:HD12	1:A:257:LEU:CA	2.47	0.41
1:A:296:LEU:HB2	1:A:306:VAL:HG21	1.86	0.41
1:A:304:ILE:HG23	1:A:304:ILE:HD12	1.75	0.41
1:B:205:LYS:CG	1:B:205:LYS:O	2.69	0.41
1:A:172:ASN:CA	1:A:200:TYR:CZ	3.04	0.41
1:A:354:ASP:C	1:A:356:ASN:H	2.22	0.41
1:B:326:LEU:HD13	1:B:469:PHE:CE2	2.56	0.41
1:B:195:LEU:HD11	1:B:346:TYR:CE2	2.56	0.40
1:B:415:LEU:HD12	1:B:415:LEU:HA	1.85	0.40
1:A:160:LYS:HB3	1:A:160:LYS:HE2	1.81	0.40
1:A:203:HIS:CE1	1:A:207:SER:OG	2.75	0.40
1:A:298:ILE:HB	1:A:304:ILE:HB	2.03	0.40
1:A:323:LYS:O	1:A:323:LYS:HG2	2.20	0.40
1:A:470:ILE:HG22	1:A:470:ILE:O	2.21	0.40
1:B:346:TYR:CD1	1:B:369:HIS:CE1	3.10	0.40
1:A:156:LYS:C	1:A:158:ARG:H	2.24	0.40
1:A:198:GLY:N	1:A:372:LYS:HD2	2.36	0.40
1:A:288:LYS:HA	1:A:289:PRO:HD3	1.87	0.40
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.77	0.40
1:B:412:PHE:HD2	1:B:488:PHE:HZ	1.69	0.40
1:A:393:CYS:HA	1:A:396:GLU:HB2	2.02	0.40
1:A:403:TYR:HD2	1:A:504:PHE:CE1	2.39	0.40
1:B:351:ASN:C	1:B:351:ASN:ND2	2.73	0.40
1:A:203:HIS:NE2	1:A:207:SER:OG	2.45	0.40
1:B:348:VAL:HG13	1:B:366:SER:HB2	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	Percentiles
1	А	360/507~(71%)	317 (88%)	38 (11%)	5 (1%)	11 40
1	В	359/507~(71%)	314 (88%)	41 (11%)	4 (1%)	14 46
All	All	719/1014 (71%)	631 (88%)	79 (11%)	9 (1%)	12 42

All (9) Ramachandran outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	А	278	LYS
1	А	300	ASN
1	В	160	LYS
1	А	302	GLU
1	В	357	SER
1	А	205	LYS
1	В	292	PRO
1	В	301	PRO
1	А	221	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	335/447~(75%)	309~(92%)	26~(8%)		12	40
1	В	334/447~(75%)	301~(90%)	33~(10%)		8	29
All	All	669/894~(75%)	610 (91%)	59(9%)		10	36



All	(59)	residues	with a	non-rotameric	sidechain	are listed	below:
-----	------	----------	--------	---------------	-----------	------------	--------

Mol	Chain	Res	Type
1	А	158	ARG
1	А	161	ARG
1	А	181	ARG
1	А	201	TYR
1	А	202	GLU
1	А	205	LYS
1	А	206	ILE
1	А	210	ASN
1	А	212	PHE
1	А	222	ARG
1	А	226	GLN
1	А	229	TYR
1	А	238	LYS
1	А	240	LYS
1	А	241	ARG
1	А	246	ASN
1	А	261	LYS
1	А	299	ARG
1	А	300	ASN
1	А	303	GLU
1	А	305	SER
1	А	353	LYS
1	А	359	GLN
1	А	411	GLU
1	А	412	PHE
1	А	494	GLU
1	В	158	ARG
1	В	159	LEU
1	В	162	LYS
1	В	163	ASP
1	В	164	ILE
1	В	165	SER
1	В	180	ARG
1	В	184	LYS
1	В	185	ARG
1	В	187	SER
1	В	190	LYS
1	В	212	PHE
1	В	213	ASP
1	В	215	MET
1	В	244	ARG
1	В	249	SER



Mol	Chain	Res	Type
1	В	265	LYS
1	В	276	GLU
1	В	298	ILE
1	В	302	GLU
1	В	304	ILE
1	В	351	ASN
1	В	372	LYS
1	В	391	LYS
1	В	410	LYS
1	В	413	GLN
1	В	414	GLU
1	В	415	LEU
1	В	478	GLN
1	В	479	GLU
1	В	483	ARG
1	В	484	LYS
1	В	486	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	183	GLN
1	А	194	GLN
1	А	210	ASN
1	А	246	ASN
1	А	250	HIS
1	А	376	ASN
1	А	422	HIS
1	А	439	GLN
1	В	172	ASN
1	В	210	ASN
1	В	351	ASN
1	В	376	ASN
1	В	407	GLN
1	В	439	GLN
1	В	478	GLN
1	В	498	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 4 ligands modelled in this entry, 2 are 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	Mol Tuno Chain D		noin Dog Link		Bond lengths			Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	1SY	В	602	-	41,51,51	2.80	13 (31%)	51,80,80	1.81	14 (27%)
3	1SY	А	602	-	41,51,51	3.20	16 (39%)	51,80,80	2.01	11 (21%)

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
3	1SY	В	602	-	-	11/22/62/62	0/6/7/7
3	1SY	А	602	-	-	12/22/62/62	0/6/7/7

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
3	А	602	1SY	C4-N3	11.28	1.51	1.35
3	А	602	1SY	C2-N3	9.72	1.47	1.32
3	В	602	1SY	C4-N3	9.61	1.48	1.35
3	В	602	1SY	C2-N3	8.25	1.45	1.32
3	В	602	1SY	C2-N1	5.35	1.43	1.33
3	А	602	1SY	C40-N41	4.81	1.45	1.34



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
3	В	602	1SY	O43-C38	-4.43	1.15	1.23
3	А	602	1SY	C2-N1	4.38	1.42	1.33
3	А	602	1SY	O31-C32	4.00	1.46	1.41
3	А	602	1SY	C40-N39	3.90	1.42	1.33
3	В	602	1SY	C40-N41	3.76	1.43	1.34
3	В	602	1SY	O31-C32	3.72	1.46	1.41
3	А	602	1SY	O4'-C1'	3.72	1.46	1.41
3	А	602	1SY	C6-C5	3.46	1.56	1.43
3	А	602	1SY	O43-C38	-3.45	1.17	1.23
3	В	602	1SY	C40-N39	3.29	1.41	1.33
3	А	602	1SY	C5-C4	-3.23	1.32	1.40
3	А	602	1SY	C6-N01	3.23	1.45	1.34
3	А	602	1SY	P18-O20	3.20	1.68	1.60
3	В	602	1SY	O4'-C1'	3.20	1.45	1.41
3	А	602	1SY	C3'-C4'	-3.18	1.44	1.52
3	А	602	1SY	P27-O26	3.04	1.71	1.59
3	В	602	1SY	C3'-C4'	-2.81	1.45	1.52
3	В	602	1SY	C6-N01	2.72	1.44	1.34
3	В	602	1SY	C5-C4	-2.68	1.33	1.40
3	А	602	1SY	C40-N42	2.54	1.43	1.37
3	А	602	1SY	C37-C38	2.21	1.51	1.47
3	В	602	1SY	P27-O26	2.17	1.68	1.59
3	В	602	1SY	C5-N7	-2.05	1.32	1.39

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All (	(25)	bond	angle	outliers	are	listed	below:
,	- /		. 0 .				

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	602	1SY	N3-C2-N1	-8.02	116.14	128.68
3	В	602	1SY	N3-C2-N1	-5.80	119.61	128.68
3	А	602	1SY	O31-C24-C22	-5.64	93.96	105.11
3	В	602	1SY	O31-C24-C22	-4.99	95.24	105.11
3	А	602	1SY	N42-C40-N39	-3.22	117.31	123.32
3	В	602	1SY	O20-P18-O44	3.13	121.22	109.47
3	В	602	1SY	C5-C6-N01	-3.01	115.78	120.35
3	А	602	1SY	C22-C21-C32	-2.95	97.34	102.89
3	А	602	1SY	O20-P18-O44	2.89	120.30	109.47
3	В	602	1SY	C22-C21-C32	-2.76	97.70	102.89
3	В	602	1SY	N42-C40-N39	-2.65	118.38	123.32
3	В	602	1SY	N01-C6-N1	2.51	123.79	118.57
3	А	602	1SY	O28-P27-O29	-2.50	100.09	109.47
3	B	602	1SY	C2'-C3'-C4'	2.38	107.45	103.22
3	В	602	1SY	C3'-C2'-C1'	2.30	104.99	99.89



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
3	В	602	1SY	O26-C25-C24	2.24	116.70	108.99
3	А	602	1SY	O19-P18-O44	-2.18	101.44	112.24
3	А	602	1SY	O26-C25-C24	2.17	116.45	108.99
3	В	602	1SY	O4'-C4'-C3'	2.14	109.45	104.87
3	А	602	1SY	C16-C4'-C3'	-2.13	107.35	114.40
3	В	602	1SY	O19-P18-O44	-2.07	102.00	112.24
3	А	602	1SY	O20-C21-C32	2.07	117.56	110.10
3	В	602	1SY	C34-N35-C37	2.06	106.92	102.99
3	В	602	1SY	O28-P27-O29	-2.01	101.92	109.47
3	А	602	1SY	O4'-C1'-C2'	-2.00	104.00	106.93

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	602	1SY	O17-C16-C4'-C3'
3	А	602	1SY	O17-C16-C4'-O4'
3	А	602	1SY	C16-O17-P18-O44
3	А	602	1SY	C21-O20-P18-O17
3	А	602	1SY	C25-O26-P27-O29
3	В	602	1SY	C21-O20-P18-O17
3	В	602	1SY	C25-O26-P27-O29
3	А	602	1SY	C22-C24-C25-O26
3	А	602	1SY	O31-C24-C25-O26
3	В	602	1SY	O17-C16-C4'-C3'
3	В	602	1SY	C22-C24-C25-O26
3	В	602	1SY	O31-C24-C25-O26
3	В	602	1SY	O17-C16-C4'-O4'
3	А	602	1SY	C2'-C3'-O28-P27
3	В	602	1SY	C2'-C3'-O28-P27
3	А	602	1SY	C16-O17-P18-O20
3	А	602	1SY	C25-O26-P27-O28
3	А	602	1SY	C4'-C3'-O28-P27
3	В	602	1SY	C4'-C3'-O28-P27
3	В	602	1SY	C25-O26-P27-O28
3	В	602	1SY	C21-O20-P18-O44
3	A	602	1SY	C16-O17-P18-O19
3	В	602	1SY	C3'-O28-P27-O26

There are no ring outliers.

2 monomers are involved in 27 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	602	1SY	13	0
3	А	602	1SY	14	0

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







# 5.7 Other polymers (i)

There are no such residues in this entry.

# 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

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

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

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2		$OWAB(Å^2)$	Q<0.9	
1	А	362/507~(71%)	0.22	17 (4%)	31	15	26, 55, 122, 284	0
1	В	361/507~(71%)	0.36	31 (8%)	10	4	27, 54, 138, 259	0
All	All	723/1014 (71%)	0.29	48 (6%)	18	7	26, 55, 131, 284	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	303	GLU	7.2
1	В	305	SER	6.7
1	В	302	GLU	6.7
1	В	507	LEU	6.6
1	В	206	ILE	6.5
1	В	304	ILE	5.5
1	А	203	HIS	5.4
1	А	163	ASP	5.0
1	А	357	SER	4.8
1	В	207	SER	4.7
1	В	301	PRO	4.1
1	В	202	GLU	3.9
1	А	206	ILE	3.8
1	В	283	SER	3.6
1	В	356	ASN	3.6
1	А	200	TYR	3.5
1	А	283	SER	3.4
1	В	208	ALA	3.4
1	В	211	GLU	3.4
1	В	297	LEU	3.3
1	В	203	HIS	3.3
1	A	211	GLU	3.2
1	A	358	PHE	3.2
1	В	185	ARG	3.1



Mol	Chain	Res	Type	RSRZ
1	В	274	VAL	2.9
1	А	229	TYR	2.9
1	В	275	LYS	2.8
1	А	240	LYS	2.7
1	В	200	TYR	2.6
1	В	438	SER	2.6
1	В	231	THR	2.6
1	В	280	ILE	2.5
1	В	198	GLY	2.5
1	В	282	VAL	2.5
1	А	239	PHE	2.4
1	В	298	ILE	2.4
1	А	245	GLY	2.4
1	А	303	GLU	2.3
1	В	230	GLU	2.3
1	В	197	THR	2.2
1	А	207	SER	2.2
1	А	302	GLU	2.1
1	A	356	ASN	2.1
1	В	163	ASP	2.1
1	В	267	ARG	2.1
1	А	284	VAL	2.1
1	В	201	TYR	2.0
1	В	277	ILE	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	1SY	А	602	45/45	0.54	0.45	158,160,160,161	0
3	1SY	В	602	45/45	0.69	0.32	100,101,102,103	0
2	ZN	А	601	1/1	0.99	0.11	46,46,46,46	0
2	ZN	В	601	1/1	0.99	0.07	45,45,45,45	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.

