

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

#### Mar 13, 2024 - 06:12 PM EDT

Title : PI3Ka H1047R co-crystal structure with inhibitor in cryptic	pocket near	r
H1047R (compound 12).		
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Deposited on : $2023-12-06$		
Resolution : $2.93$ Å(reported)		

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

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

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

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

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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.93 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	$\begin{array}{c} {\rm Whole \ archive} \\ (\#{\rm Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122(2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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		1050	7%		_
	A	1072	80%	17%	••
			10%		
1	С	1072	78%	17%	•
			52%		-
2	В	279	67%	31%	
			27%		
2	D	279	78%	21%	•



#### 8V8U

# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21913 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	А	1054	Total 8612	C 5507	N 1480	O 1555	S 70	0	0	0
1	С	1033	Total 8434	C 5391	N 1447	O 1527	S 69	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	-3	ALA	-	expression tag	UNP P42336
А	-2	MET	-	expression tag	UNP P42336
А	-1	GLY	-	expression tag	UNP P42336
А	0	SER	-	expression tag	UNP P42336
А	1047	ARG	HIS	engineered mutation	UNP P42336
С	-3	ALA	-	expression tag	UNP P42336
С	-2	MET	-	expression tag	UNP P42336
С	-1	GLY	-	expression tag	UNP P42336
С	0	SER	-	expression tag	UNP P42336
С	1047	ARG	HIS	engineered mutation	UNP P42336

There are 10 discrepancies between the modelled and reference sequences:

• Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	270	Total	C N O S O		0	0			
	D	219	2366	1480	423	455	8	0	0	0
0	Л	270	Total	С	Ν	0	S	0	0	0
	D	219	2366	1480	423	455	8	0		

• Molecule 3 is (2S)-N 1 -{4-methyl-5-[2-(1,1,1-trifluoro-2-methylpropan-2-yl)pyridin-4-yl]-1,3-thiazol-2-yl}pyrrolidine-1,2-dicarboxamide (three-letter code: 1LT) (formula:  $C_{19}H_{22}F_3N_5O_2S$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf			
2	Δ	Δ	Δ	1	Total	С	F	Ν	0	S	0	0
5	A	L	30	19	3	5	2	1	0	0		
3	C	1	Total	С	F	Ν	0	$\mathbf{S}$	0	0		
3		1	30	19	3	5	2	1	0	U		

• Molecule 4 is (3S)-9-[(1R)-1-(2-carboxyanilino)ethyl]-3-cyano-7-methyl-4-oxo-2-(pipe ridin-1-yl)-3,4-dihydropyrido[1,2-a]pyrimidin-5-ium (three-letter code: YQB) (formula:  $C_{24}H_{25}N_5O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	А	1	Total 32	С 24	N 5	O 3	0	0



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	С	1	Total 32	C 24	N 5	O 3	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	11	Total         O           11         11	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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform



Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform
 Chain C: 78% 17% .







• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	84.63Å 121.86Å 163.88Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $91.69^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	84.60 - 2.93	Depositor
Resolution (A)	84.60 - 2.93	EDS
% Data completeness	90.0 (84.60-2.93)	Depositor
(in resolution range)	89.7(84.60-2.93)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.03 (at 2.91 \text{\AA})$	Xtriage
Refinement program		Depositor
D D	0.203 , $0.255$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.213 , $0.268$	DCC
$R_{free}$ test set	2000 reflections $(2.81%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	79.9	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , $85.6$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21913	wwPDB-VP
Average B, all atoms $(Å^2)$	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.

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



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

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

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		Bond lengths		Bond angles	
1VIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.25	0/8809	0.50	1/11903~(0.0%)
1	С	0.25	0/8622	0.48	1/11647~(0.0%)
2	В	0.24	0/2406	0.48	0/3223
2	D	0.24	0/2406	0.47	0/3223
All	All	0.25	0/22243	0.49	2/29996~(0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	866	LEU	N-CA-CB	14.91	140.22	110.40
1	С	233	LEU	CA-CB-CG	5.96	129.00	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	199	SER	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	8612	0	8638	104	0
1	С	8434	0	8469	124	0
2	В	2366	0	2339	69	0
2	D	2366	0	2339	40	0
3	А	30	0	22	1	0
3	С	30	0	22	0	0
4	А	32	0	0	1	0
4	С	32	0	0	2	0
5	А	11	0	0	0	0
All	All	21913	0	21829	313	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 7.

All (313) 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:C:966:LYS:HG2	1:C:967:GLY:HA2	1.62	0.82
2:B:372:LEU:HD23	2:B:420:LEU:HB3	1.65	0.78
1:C:232:MET:O	1:C:234:LEU:N	2.17	0.78
2:B:333:TRP:HB2	2:B:357:VAL:HG23	1.64	0.77
2:B:372:LEU:HB3	2:B:420:LEU:HD13	1.69	0.74
1:A:704:ARG:NH2	1:A:749:GLN:O	2.22	0.73
1:C:155:ASP:OD1	1:C:158:SER:OG	2.06	0.73
2:B:372:LEU:HD22	2:B:413:LEU:HD13	1.71	0.72
1:C:366:PRO:HD2	2:D:377:ASN:HD22	1.56	0.71
2:B:370:LEU:HD21	2:B:413:LEU:HD11	1.73	0.70
1:A:401:ARG:HH11	1:A:462:THR:HG22	1.57	0.69
1:A:1063:LYS:HG2	1:A:1064:GLN:HG2	1.75	0.69
2:B:370:LEU:HB2	2:B:405:ILE:HG23	1.76	0.68
2:B:347:LEU:HD13	2:B:371:THR:HG21	1.76	0.68
1:C:328:TRP:HA	1:C:394:PRO:HB3	1.76	0.68
1:A:336:ILE:HD13	1:A:402:LEU:HD22	1.76	0.67
1:A:213:HIS:HB2	1:A:268:SER:HB3	1.76	0.67
1:C:418:GLU:OE2	2:D:572:GLN:NE2	2.28	0.67



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:D:350:THR:HB	2:D:354:THR:HG21	1.77	0.66
1:C:410:LYS:NZ	2:D:569:ASP:OD1	2.28	0.66
1:A:199:SER:HB3	1:A:202:ASN:H	1.61	0.64
1:A:546:GLN:O	1:A:550:PHE:N	2.27	0.64
1:A:4:ARG:NH1	1:A:710:GLU:OE1	2.31	0.63
1:C:791:GLU:HA	1:C:795:GLN:HG2	1.80	0.63
1:C:9:GLU:OE2	1:C:38:ARG:NH2	2.28	0.63
2:B:402:VAL:HA	2:B:406:ASN:HB2	1.80	0.63
1:C:402:LEU:HD23	1:C:427:ILE:HD11	1.80	0.63
2:B:360:ALA:HB2	2:B:367:ASP:HB2	1.80	0.62
2:D:335:TRP:NE1	2:D:428:VAL:O	2.24	0.62
2:B:322:MET:SD	2:B:322:MET:N	2.72	0.62
1:A:328:TRP:HA	1:A:394:PRO:HB3	1.81	0.62
1:C:172:GLU:HG3	1:C:274:ARG:HD2	1.82	0.62
1:C:336:ILE:HD13	1:C:402:LEU:HD22	1.82	0.61
1:C:31:ILE:H	2:D:527:ASN:HD21	1.48	0.61
1:C:516:ARG:NH1	1:C:549:ASP:OD1	2.33	0.61
2:B:386:ARG:HH12	2:B:395:PRO:HA	1.65	0.61
1:A:9:GLU:OE2	1:A:38:ARG:NH2	2.34	0.60
2:B:436:VAL:O	2:B:580:TYR:OH	2.18	0.60
1:C:715:LEU:HD21	1:C:735:LEU:HD12	1.83	0.60
1:C:213:HIS:HB2	1:C:268:SER:HB3	1.84	0.60
2:B:511:LYS:HA	2:B:514:ARG:HE	1.67	0.60
1:C:861:GLN:HB3	1:C:872:PHE:HB2	1.83	0.59
1:A:871:GLN:HG3	1:A:1054:LYS:HB3	1.84	0.59
2:D:328:LEU:HD13	2:D:401:VAL:HB	1.84	0.59
1:A:226:ARG:HG3	1:A:243:VAL:HG21	1.84	0.59
2:D:409:ARG:HA	2:D:424:LEU:HB2	1.84	0.59
2:B:411:GLU:OE2	2:B:415:GLN:NE2	2.36	0.59
2:B:357:VAL:HG22	2:B:369:THR:H	1.67	0.59
1:C:4:ARG:HG3	1:C:76:GLU:HG3	1.85	0.59
1:C:544:THR:HG21	2:D:382:LYS:HB2	1.85	0.58
1:A:163:ALA:HB2	1:A:297:LEU:HD11	1.84	0.58
2:B:506:LYS:HA	2:B:509:ILE:HG12	1.84	0.58
1:A:279:LEU:HD13	1:A:281:ARG:HH21	1.70	0.57
1:C:344:VAL:HG11	1:C:406:ILE:HG21	1.86	0.57
2:B:404:LEU:HD23	2:B:405:ILE:HG12	1.87	0.57
2:B:343:VAL:HG22	2:B:356:LEU:HD11	1.86	0.56
1:C:966:LYS:NZ	1:C:968:ALA:O	2.36	0.56
1:A:540:LEU:O	2:B:340:ARG:NH2	2.38	0.56
1:C:204:LYS:NZ	1:C:791:GLU:OE2	2.36	0.56



			Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:C:412:ARG:NH2	2:D:569:ASP:OD1	2.37	0.56
1:C:358:THR:HB	1:C:402:LEU:HD11	1.88	0.55
1:C:398:ARG:NH2	1:C:434:ASP:OD1	2.34	0.55
1:C:628:LEU:HD23	1:C:663:ILE:HD13	1.87	0.55
1:A:131:VAL:HG21	1:A:136:VAL:HG11	1.89	0.55
2:B:386:ARG:NH2	1:C:214:ASP:OD2	2.39	0.55
1:A:38:ARG:HD3	1:A:741:ARG:NH1	2.22	0.55
1:C:237:GLU:HA	1:C:240:LYS:HE2	1.89	0.55
1:C:540:LEU:HB2	1:C:1023:ARG:HD2	1.88	0.55
1:C:1044:ASN:OD1	1:C:1047:ARG:NH1	2.39	0.55
1:C:517:LEU:HD13	1:C:555:ARG:HH22	1.72	0.54
1:A:791:GLU:HA	1:A:795:GLN:HG2	1.87	0.54
1:C:904:TYR:CE2	1:C:930:PHE:HA	2.42	0.54
2:B:386:ARG:HH21	2:B:387:ASP:HB2	1.72	0.54
1:A:542:GLU:HB3	2:B:380:LEU:HD13	1.90	0.54
1:A:544:THR:HG21	2:B:382:LYS:HB2	1.90	0.53
2:B:353:GLY:HA2	2:B:424:LEU:HD23	1.89	0.53
1:C:157:ASN:HB3	1:C:161:SER:HB2	1.88	0.53
2:B:409:ARG:HA	2:B:424:LEU:HD13	1.89	0.53
1:A:360:ILE:HG22	1:A:367:LEU:HD12	1.89	0.53
2:D:409:ARG:HG3	2:D:424:LEU:O	2.07	0.53
1:A:732:MET:HE1	1:A:771:ILE:H	1.74	0.53
1:C:250:TYR:CD2	1:C:287:LEU:HD21	2.44	0.53
1:A:1056:ASP:HB3	1:A:1061:THR:H	1.74	0.53
1:C:163:ALA:HB2	1:C:297:LEU:HD11	1.90	0.53
1:C:181:ILE:HD11	1:C:825:GLN:NE2	2.24	0.53
1:A:545:GLU:N	2:B:380:LEU:O	2.41	0.52
2:D:590:ARG:HB2	2:D:593:LYS:HG3	1.91	0.52
1:A:508:TYR:HD2	1:A:519:ARG:HH11	1.57	0.52
1:A:916:ARG:HH11	1:A:931:HIS:CD2	2.28	0.52
2:D:480:LYS:HB2	2:D:549:LEU:HD13	1.91	0.52
1:A:238:GLN:O	1:A:242:CYS:N	2.41	0.52
2:B:355:PHE:HB3	2:B:371:THR:O	2.10	0.52
2:B:433:GLN:O	2:B:437:VAL:N	2.38	0.52
1:A:508:TYR:HD2	1:A:519:ARG:NH1	2.09	0.51
1:A:869:ALA:O	1:A:871:GLN:N	2.37	0.51
1:A:809:GLN:NE2	1:A:1012:GLU:OE1	2.44	0.51
2:B:333:TRP:CD1	2:B:355:PHE:HE2	2.29	0.51
2:B:345:GLU:HA	2:B:348:ARG:HH12	1.75	0.51
1:C:5:PRO:HB3	2:D:479:MET:HG2	1.92	0.51
1:C:1047:ARG:NE	4:C:1101:YQB:O12	2.44	0.51



	A L	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:157:ASN:HB3	1:A:161:SER:HB2	1.93	0.51
1:A:328:TRP:CE2	1:A:577:ARG:HD2	2.46	0.51
1:A:453:GLU:OE2	2:B:574:ARG:NH1	2.43	0.51
2:B:407:HIS:O	2:B:407:HIS:ND1	2.44	0.51
1:A:337:LYS:HB3	1:A:476:GLU:HB3	1.93	0.50
1:A:363:GLY:N	1:A:607:PRO:HG3	2.26	0.50
2:D:335:TRP:HH2	2:D:433:GLN:HE21	1.57	0.50
2:B:449:LEU:HB2	2:B:583:TRP:HZ3	1.77	0.50
1:C:375:ARG:NH2	1:C:417:GLU:OE2	2.44	0.50
2:D:354:THR:HA	2:D:426:TYR:O	2.12	0.50
1:A:851:VAL:HG23	3:A:1100:1LT:H10	1.94	0.50
1:A:1050:GLY:O	1:A:1052:THR:N	2.45	0.50
1:C:941:LYS:NZ	1:C:942:LYS:HE2	2.27	0.50
2:B:366:GLY:HA2	2:B:390:TYR:CE2	2.47	0.49
1:C:895:ASP:OD2	1:C:899:ARG:NE	2.43	0.49
1:A:532:LYS:HD2	1:A:561:ILE:HD12	1.94	0.49
1:A:26:LEU:O	2:B:497:GLN:NE2	2.44	0.49
2:B:448:LYS:HD2	2:B:452:TYR:CE2	2.47	0.49
1:A:901:CYS:HA	1:A:929:LEU:HD22	1.94	0.49
1:A:268:SER:O	1:A:274:ARG:HB2	2.12	0.49
1:C:38:ARG:HD3	1:C:741:ARG:NH1	2.28	0.49
2:D:379:LYS:HG3	2:D:420:LEU:HD21	1.94	0.49
1:A:637:GLN:NE2	1:A:674:GLU:OE2	2.26	0.49
1:C:4:ARG:NH1	1:C:93:ARG:HG2	2.28	0.49
1:C:517:LEU:HD13	1:C:555:ARG:NH2	2.27	0.49
1:C:614:PHE:HA	1:C:617:ARG:HD3	1.94	0.49
2:B:379:LYS:HZ3	2:B:419:LYS:HB3	1.78	0.48
1:C:996:ASN:O	1:C:1000:ASN:ND2	2.46	0.48
1:A:865:GLY:O	1:A:866:LEU:HG	2.12	0.48
1:C:154:ARG:HD2	1:C:165:TYR:CG	2.48	0.48
1:A:23:GLU:HB2	1:A:98:PHE:HB2	1.95	0.48
1:A:124:PRO:HD2	1:A:127:GLU:OE2	2.13	0.48
1:A:634:GLN:HE22	1:A:815:GLN:HE22	1.60	0.48
1:A:492:ILE:HG21	1:A:584:TYR:HD2	1.79	0.48
1:A:305:PRO:HB3	1:A:693:ARG:HD3	1.96	0.48
1:C:221:ILE:O	1:C:225:ILE:HG12	2.14	0.48
1:C:518:ALA:HB1	1:C:522:GLU:HG3	1.94	0.48
1:C:360:ILE:HG22	1:C:367:LEU:HD12	1.95	0.48
1:A:1047:ARG:NE	4:A:1101:YQB:O12	2.47	0.48
2:B:351:ALA:HB3	2:B:426:TYR:HB2	1.95	0.48
2:D:441:ASN:OD1	2:D:442:ILE:N	2.47	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:B:335:TRP:HB2	2:B:357:VAL:O	2.13	0.47
1:C:124:PRO:HD2	1:C:127:GLU:OE2	2.13	0.47
1:C:735:LEU:HD22	1:C:771:ILE:HG13	1.96	0.47
2:D:392:PHE:CE1	2:D:404:LEU:HD21	2.50	0.47
1:C:401:ARG:HD2	1:C:462:THR:HG21	1.97	0.47
1:C:337:LYS:HD2	1:C:386:TRP:CE2	2.49	0.47
1:C:941:LYS:HZ3	1:C:942:LYS:HE2	1.79	0.47
1:A:116:GLU:OE1	1:A:700:LYS:NZ	2.43	0.47
1:C:949:ARG:C	1:C:951:ARG:H	2.17	0.47
1:C:117:ILE:O	1:C:121:ILE:HG13	2.14	0.47
1:C:856:THR:HA	1:C:922:MET:HG2	1.97	0.47
1:A:2:PRO:HG3	2:B:482:THR:OG1	2.14	0.47
1:A:667:PHE:CZ	1:A:671:LEU:HD11	2.50	0.47
1:C:233:LEU:HD12	1:C:234:LEU:N	2.30	0.47
1:C:985:TYR:CE1	1:C:1040:MET:HG2	2.49	0.47
2:D:494:PHE:HB3	2:D:535:ILE:HG12	1.95	0.47
1:A:657:ALA:HB1	1:A:664:GLY:HA2	1.96	0.47
2:B:526:HIS:O	2:B:530:LYS:HG3	2.15	0.47
1:C:38:ARG:NH1	1:C:741:ARG:HD3	2.31	0.46
1:A:953:PRO:HB3	1:A:1047:ARG:O	2.15	0.46
2:D:462:GLU:O	2:D:466:LEU:HB2	2.15	0.46
2:D:394:ASP:OD1	2:D:394:ASP:N	2.49	0.46
1:A:495:HIS:NE2	1:A:578:ASP:OD1	2.31	0.46
1:A:507:SER:HA	1:A:519:ARG:HH21	1.80	0.46
2:B:408:TYR:HB3	2:B:413:LEU:HD12	1.97	0.46
1:C:776:LYS:HD2	1:C:804:GLY:HA3	1.98	0.46
1:C:555:ARG:NH2	1:C:582:GLN:OE1	2.44	0.46
2:D:445:VAL:HG11	2:D:583:TRP:CE3	2.51	0.46
1:C:630:GLN:O	1:C:815:GLN:NE2	2.42	0.46
1:A:100:LYS:HD2	2:B:493:ILE:HG23	1.97	0.45
1:A:676:HIS:O	1:A:678:LYS:HD3	2.15	0.45
1:C:337:LYS:HB2	1:C:386:TRP:CE3	2.51	0.45
1:A:641:TYR:OH	1:A:1007:GLY:N	2.48	0.45
2:B:390:TYR:C	2:B:396:LEU:HB3	2.36	0.45
1:C:860:ILE:HG23	1:C:880:TRP:CG	2.51	0.45
2:B:510:GLU:O	2:B:514:ARG:NE	2.48	0.45
1:A:572:VAL:HG21	1:A:583:MET:HG2	1.99	0.45
2:B:409:ARG:HG3	2:B:424:LEU:HD22	1.98	0.45
2:B:475:GLN:O	2:B:479:MET:HG3	2.17	0.45
1:A:538:ASP:HA	1:A:996:ASN:OD1	2.17	0.45
1:C:42:LEU:HD21	1:C:92:LEU:HD11	1.98	0.45



	A	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:765:ARG:NH1	1:C:796:ASN:OD1	2.50	0.45
1:A:58:LEU:HB3	1:A:61:LEU:HD22	1.98	0.45
1:C:977:PHE:HZ	1:C:1047:ARG:HH21	1.65	0.45
2:B:447:LYS:HE3	2:B:450:HIS:ND1	2.32	0.45
1:A:421:PRO:HG3	1:A:454:ASP:O	2.17	0.44
1:A:809:GLN:HE21	1:A:1010:MET:HB3	1.82	0.44
1:C:522:GLU:O	1:C:524:ARG:N	2.50	0.44
1:C:817:ILE:HD13	1:C:904:TYR:HE1	1.81	0.44
1:C:951:ARG:HB3	1:C:1045:ASP:HB3	1.98	0.44
1:A:836:TYR:CE2	1:A:932:ILE:HG22	2.52	0.44
1:A:4:ARG:CZ	1:A:93:ARG:HG2	2.46	0.44
2:B:593:LYS:HG2	2:B:597:TRP:HB2	2.00	0.44
1:C:678:LYS:HB2	1:C:678:LYS:HE2	1.79	0.44
1:C:279:LEU:HD12	1:C:281:ARG:HH21	1.82	0.44
1:C:939:ASP:HB2	1:C:1021:TYR:CD1	2.51	0.44
2:D:355:PHE:CG	2:D:424:LEU:HD23	2.52	0.44
1:A:970:GLU:HB3	1:A:973:LYS:NZ	2.32	0.44
1:C:233:LEU:HD12	1:C:234:LEU:H	1.82	0.44
2:B:528:TYR:HE2	2:B:532:LYS:HE2	1.82	0.44
2:B:593:LYS:HE2	2:B:597:TRP:CD1	2.52	0.44
2:D:325:ASN:O	2:D:326:MET:HG3	2.18	0.44
1:A:136:VAL:HG13	1:A:686:LEU:HD11	2.00	0.44
1:C:337:LYS:HB3	1:C:476:GLU:HB3	2.00	0.44
2:D:355:PHE:CE1	2:D:424:LEU:HB3	2.53	0.44
1:C:50:PHE:O	1:C:54:ARG:HG2	2.18	0.44
1:C:689:GLU:OE2	1:C:693:ARG:NH2	2.49	0.44
1:A:957:THR:OG1	1:A:1048:HIS:HB3	2.18	0.44
1:A:446:TRP:CZ2	1:A:465:ASN:HA	2.53	0.43
1:A:940:HIS:NE2	1:A:1012:GLU:O	2.51	0.43
2:B:512:PHE:CZ	2:B:520:GLU:HG2	2.52	0.43
1:C:394:PRO:HB2	1:C:577:ARG:HD3	2.00	0.43
1:A:634:GLN:NE2	1:A:815:GLN:HE22	2.16	0.43
2:B:343:VAL:HG13	2:B:356:LEU:HD21	1.99	0.43
2:D:394:ASP:HA	2:D:395:PRO:HA	1.86	0.43
1:A:592:PRO:HB2	1:A:622:TYR:HE1	1.83	0.43
1:A:1027:ALA:HB1	1:A:1030:LYS:HD2	1.99	0.43
2:D:343:VAL:HG13	2:D:356:LEU:HD21	2.00	0.43
1:A:514:SER:O	1:A:516:ARG:N	2.51	0.43
2:B:385:HIS:HA	2:B:396:LEU:HD11	2.00	0.43
2:B:449:LEU:HD23	2:B:584:LEU:HD22	2.00	0.43
1:C:253:LYS:HD2	1:C:260:TYR:CE2	2.53	0.43



			Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:941:LYS:HD2	1:C:942:LYS:N	2.33	0.43
2:D:528:TYR:OH	2:D:532:LYS:HE3	2.18	0.43
1:A:148:LYS:HB2	1:A:304:MET:HE1	2.01	0.43
1:C:941:LYS:HD2	1:C:942:LYS:H	1.83	0.43
1:C:949:ARG:O	1:C:951:ARG:N	2.45	0.43
1:C:1043:MET:HB3	4:C:1101:YQB:C9	2.49	0.43
1:A:831:LEU:HD11	1:A:987:ALA:HB2	2.01	0.43
1:C:274:ARG:O	1:C:278:MET:HG2	2.18	0.43
1:C:266:PRO:HG2	1:C:269:GLN:HB2	2.01	0.43
1:C:339:LEU:HB2	1:C:474:GLU:HB2	2.01	0.43
1:C:938:LEU:C	1:C:940:HIS:H	2.22	0.43
1:A:357:ARG:O	1:A:404:LEU:HA	2.19	0.42
2:B:389:LYS:HB3	2:B:396:LEU:O	2.19	0.42
1:C:424:TRP:HE1	1:C:449:PRO:HD3	1.84	0.42
2:B:333:TRP:HD1	2:B:355:PHE:HE2	1.66	0.42
1:C:506:PHE:HB2	1:C:510:HIS:HB3	2.01	0.42
1:C:506:PHE:HE2	1:C:513:LEU:HB2	1.84	0.42
1:C:559:VAL:HG13	1:C:591:PRO:HD3	2.02	0.42
2:D:491:ILE:HD13	2:D:539:ILE:HG12	2.01	0.42
1:A:128:PHE:O	1:A:131:VAL:HG22	2.20	0.42
2:B:386:ARG:NH1	2:B:395:PRO:HA	2.34	0.42
1:A:525:GLU:HG3	1:C:828:GLY:HA3	2.01	0.42
2:B:381:ILE:HD12	2:B:416:TYR:CZ	2.55	0.42
1:C:250:TYR:CD1	1:C:289:ALA:HA	2.55	0.42
1:C:769:CYS:HA	1:C:780:TRP:O	2.19	0.42
1:A:701:HIS:O	1:A:705:GLN:HG3	2.20	0.42
2:B:335:TRP:CD1	2:B:356:LEU:HB2	2.54	0.42
2:B:381:ILE:HB	2:B:416:TYR:OH	2.20	0.42
2:B:494:PHE:HB3	2:B:535:ILE:HG12	2.00	0.42
1:C:401:ARG:HH11	1:C:462:THR:HG22	1.84	0.42
2:D:483:ALA:HB3	2:D:545:LEU:HD21	2.02	0.42
1:A:172:GLU:HG3	1:A:274:ARG:HD2	2.02	0.42
1:A:908:THR:HG21	1:A:931:HIS:HD2	1.85	0.42
2:B:445:VAL:C	2:B:447:LYS:H	2.23	0.42
1:C:446:TRP:CZ2	1:C:465:ASN:HA	2.55	0.42
1:C:510:HIS:CE1	1:C:513:LEU:HG	2.55	0.42
1:A:105:VAL:O	1:A:111:LYS:NZ	2.43	0.41
1:C:195:TRP:CZ3	1:C:206:LYS:HB2	2.55	0.41
1:C:633:ILE:HD12	1:C:633:ILE:H	1.85	0.41
1:A:61:LEU:HD23	2:B:504:TYR:CD2	2.55	0.41
1:A:420:CYS:HB2	2:B:568:PRO:HB3	2.03	0.41



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:601:LEU:HA	1:A:606:TYR:CD2	2.55	0.41
1:A:785:ASN:HB3	1:A:790:SER:HB2	2.02	0.41
1:C:151:VAL:HG11	1:C:302:PHE:HB3	2.02	0.41
1:C:337:LYS:HB2	1:C:386:TRP:CD2	2.55	0.41
2:D:446:GLY:HA3	2:D:597:TRP:CZ2	2.56	0.41
1:A:61:LEU:HD23	2:B:504:TYR:HD2	1.84	0.41
1:C:180:HIS:CE1	1:C:828:GLY:HA2	2.55	0.41
1:C:518:ALA:H	1:C:553:SER:HB2	1.86	0.41
1:A:634:GLN:HE22	1:A:815:GLN:NE2	2.18	0.41
1:A:135:GLU:OE2	1:A:644:TYR:HB3	2.21	0.41
1:A:1047:ARG:O	1:A:1048:HIS:HB2	2.19	0.41
1:C:545:GLU:HB3	2:D:381:ILE:HD13	2.02	0.41
1:A:904:TYR:CE2	1:A:930:PHE:HA	2.56	0.41
1:A:87:ARG:NH1	1:A:115:ARG:HD2	2.35	0.41
2:B:452:TYR:HE2	2:B:580:TYR:CZ	2.38	0.41
1:C:324:THR:HB	1:C:485:LYS:HG3	2.03	0.41
1:C:401:ARG:HH11	1:C:462:THR:CG2	2.34	0.41
1:A:464:SER:OG	1:A:468:LYS:NZ	2.53	0.41
1:A:615:ALA:O	1:A:619:LEU:HG	2.21	0.41
1:A:678:LYS:HE2	1:A:678:LYS:HB2	1.63	0.41
1:A:858:MET:N	1:A:918:ASN:HB2	2.36	0.41
1:C:519:ARG:HB2	1:C:522:GLU:HG2	2.03	0.41
1:C:523:LEU:H	1:C:523:LEU:HG	1.72	0.41
2:D:339:SER:O	2:D:343:VAL:HG23	2.21	0.41
1:A:446:TRP:CZ3	1:A:679:THR:HG22	2.55	0.41
1:C:700:LYS:HD3	1:C:700:LYS:HA	1.80	0.41
1:C:914:GLY:O	1:C:916:ARG:HG2	2.20	0.41
2:D:509:ILE:HG13	2:D:510:GLU:N	2.35	0.41
1:A:992:ARG:NH2	1:A:1027:ALA:O	2.37	0.40
1:C:450:HIS:HB2	2:D:467:TYR:CE2	2.56	0.40
1:C:602:LEU:O	1:C:612:ARG:NH2	2.47	0.40
1:C:413:LYS:N	1:C:413:LYS:HD2	2.37	0.40
1:A:178:PRO:HB2	1:A:181:ILE:HD12	2.04	0.40
1:C:7:SER:HB3	1:C:714:ASN:HB2	2.02	0.40
1:C:171:VAL:HG11	1:C:265:TYR:CD2	2.56	0.40
1:C:335:ARG:HG2	1:C:386:TRP:CE3	2.57	0.40
1:C:923:VAL:HG12	1:C:924:LYS:O	2.21	0.40
1:C:949:ARG:HD3	1:C:952:VAL:HA	2.02	0.40
1:A:169:PRO:HB3	1:A:270:TYR:CE1	2.57	0.40
2:B:445:VAL:O	2:B:447:LYS:N	2.52	0.40
1:C:96:GLN:HE21	2:D:487:PHE:HE1	1.70	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:914:GLY:O	1:C:916:ARG:N	2.54	0.40
1:A:136:VAL:HG13	1:A:686:LEU:CD1	2.51	0.40
1:A:325:LYS:HE2	1:A:482:SER:HB3	2.03	0.40
2:B:448:LYS:HD3	2:B:448:LYS:HA	1.79	0.40
1:C:419:HIS:HB2	2:D:349:ASP:OD2	2.21	0.40
1:C:1036:LEU:O	1:C:1040:MET:HG3	2.21	0.40
2:D:423:LYS:HE2	2:D:423:LYS:HB3	1.98	0.40
2:D:520:GLU:OE2	2:D:523:ARG:NH2	2.41	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	entiles
1	А	1050/1072~(98%)	988 (94%)	48 (5%)	14 (1%)	12	35
1	С	1027/1072~(96%)	956 (93%)	62 (6%)	9 (1%)	17	46
2	В	277/279~(99%)	254 (92%)	21 (8%)	2 (1%)	22	52
2	D	277/279~(99%)	264 (95%)	11 (4%)	2 (1%)	22	52
All	All	2631/2702 (97%)	2462 (94%)	142 (5%)	27 (1%)	15	43

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	866	LEU
1	С	233	LEU
1	С	234	LEU
1	С	871	GLN
1	С	915	ASP
1	А	522	GLU
1	А	1064	GLN



Mol	Chain	Res	Type
2	В	588	GLY
1	С	2	PRO
1	С	523	LEU
1	А	2	PRO
1	А	515	ASN
1	А	843	ASP
1	А	1051	TRP
1	С	509	SER
1	С	947	TYR
1	С	952	VAL
1	А	3	PRO
1	А	506	PHE
1	А	864	GLY
2	D	324	ASN
1	А	505	GLY
1	А	1048	HIS
2	D	596	GLU
2	В	446	GLY
1	А	865	GLY
1	А	935	GLY

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	962/976~(99%)	937~(97%)	25~(3%)	46 75
1	$\mathbf{C}$	944/976~(97%)	928~(98%)	16~(2%)	60 83
2	В	259/259~(100%)	247~(95%)	12~(5%)	27 57
2	D	259/259~(100%)	253~(98%)	6~(2%)	50 78
All	All	2424/2470~(98%)	2365~(98%)	59(2%)	49 77

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

Mol	Chain	Res	Type
1	А	14	HIS
	~	-	



Mol	Chain	Res	Type
1	А	115	ARG
1	А	148	LYS
1	А	199	SER
1	А	201	ASN
1	А	237	GLU
1	А	259	GLU
1	А	279	LEU
1	А	413	LYS
1	А	434	ASP
1	А	498	TRP
1	А	537	ARG
1	А	587	VAL
1	А	678	LYS
1	А	748	LEU
1	А	774	SER
1	А	829	LEU
1	А	852	ARG
1	А	931	HIS
1	А	937	PHE
1	А	951	ARG
1	А	952	VAL
1	А	969	GLN
1	А	979	ARG
1	А	1047	ARG
2	В	322	MET
2	В	326	MET
2	В	364	MET
2	В	386	ARG
2	В	413	LEU
2	В	425	LEU
2	В	443	GLU
2	В	466	LEU
2	В	583	TRP
2	В	592	LYS
2	В	594	LEU
2	В	598	LEU
1	С	98	PHE
1	С	244	LEU
1	С	413	LYS
1	С	478	ASP
1	С	523	LEU
1	С	587	VAL



Mol	Chain	Res	Type
1	С	594	LYS
1	С	630	GLN
1	С	774	SER
1	С	870	LEU
1	С	881	LEU
1	С	883	ASP
1	С	937	PHE
1	С	941	LYS
1	С	945	PHE
1	С	952	VAL
2	D	397	THR
2	D	404	LEU
2	D	425	LEU
2	D	466	LEU
2	D	575	LYS
2	D	597	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	634	GLN
1	А	809	GLN
1	А	931	HIS
1	С	825	GLN
2	D	527	ASN
2	D	572	GLN

#### 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)

4 ligands are modelled in this entry.

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	Iol Type Chain Beg		Tink	Bond lengths			Bond angles			
Moi Type Cha	Unam		Res Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2	
4	YQB	А	1101	-	32,35,35	1.24	2 (6%)	35,50,50	1.42	5 (14%)
3	1LT	А	1100	-	26,32,32	4.20	12 (46%)	29,49,49	1.69	7 (24%)
3	1LT	С	1100	-	26,32,32	4.18	11 (42%)	29,49,49	1.53	8 (27%)
4	YQB	С	1101	-	32,35,35	1.23	2 (6%)	35,50,50	1.66	8 (22%)

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
4	YQB	А	1101	-	-	3/13/26/26	0/4/4/4
3	1LT	А	1100	-	-	5/27/41/41	0/3/3/3
3	1LT	С	1100	-	-	7/27/41/41	0/3/3/3
4	YQB	С	1101	-	-	2/13/26/26	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
3	С	1100	1LT	C6-C7	-9.12	1.31	1.53
3	А	1100	1LT	C6-C7	-9.04	1.32	1.53
3	А	1100	1LT	C4-N2	-8.68	1.30	1.47
3	А	1100	1LT	C3-N1	8.57	1.52	1.37
3	А	1100	1LT	C7-N2	8.34	1.63	1.47
3	С	1100	1LT	C10-C9	8.33	1.56	1.48
3	С	1100	1LT	C4-N2	-8.26	1.31	1.47
3	С	1100	1LT	C7-N2	8.25	1.63	1.47
3	С	1100	1LT	C3-N1	8.04	1.51	1.37
3	А	1100	1LT	C10-C9	7.58	1.55	1.48



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	1100	1LT	C8-N3	4.96	1.45	1.32
3	С	1100	1LT	C8-N3	4.92	1.45	1.32
3	А	1100	1LT	C2-N1	4.62	1.44	1.36
3	С	1100	1LT	C2-N1	4.41	1.44	1.36
4	А	1101	YQB	O12-C10	4.15	1.34	1.22
4	С	1101	YQB	O12-C10	4.12	1.34	1.22
3	А	1100	1LT	C3-N2	3.58	1.49	1.37
3	С	1100	1LT	C3-N2	3.54	1.49	1.37
3	А	1100	1LT	C15-C13	3.22	1.59	1.53
3	С	1100	1LT	C15-C13	3.13	1.59	1.53
3	С	1100	1LT	C13-N4	-3.02	1.27	1.34
3	А	1100	1LT	C13-N4	-2.95	1.28	1.34
4	А	1101	YQB	O11-C10	-2.58	1.22	1.30
4	С	1101	YQB	O11-C10	-2.58	1.22	1.30
3	С	1100	1LT	C-C1	-2.17	1.46	1.50
3	А	1100	1LT	C-C1	-2.11	1.46	1.50
3	А	1100	1LT	C14-C10	-2.04	1.36	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	С	1101	YQB	C30-C20-C21	4.62	129.78	120.88
4	С	1101	YQB	N17-C23-N22	-4.34	118.84	123.67
4	А	1101	YQB	N17-C23-N22	-4.11	119.10	123.67
3	А	1100	1LT	C6-C7-N2	3.75	108.60	103.03
3	А	1100	1LT	C14-C13-C15	-3.38	118.78	122.68
4	А	1101	YQB	C30-C20-C21	3.23	127.09	120.88
4	С	1101	YQB	O11-C10-O12	-3.14	116.37	123.35
3	А	1100	1LT	C12-N4-C13	3.11	121.75	117.49
3	С	1100	1LT	C11-C12-N4	-2.94	120.30	123.96
3	С	1100	1LT	C12-N4-C13	2.93	121.49	117.49
4	А	1101	YQB	O11-C10-O12	-2.91	116.89	123.35
4	С	1101	YQB	O11-C10-C9	2.79	123.35	115.31
4	А	1101	YQB	O11-C10-C9	2.73	123.16	115.31
3	С	1100	1LT	C4-N2-C7	-2.72	107.68	112.00
3	А	1100	1LT	C8-C7-N2	-2.66	108.01	112.29
3	А	1100	1LT	C4-N2-C7	-2.60	107.88	112.00
3	С	1100	1LT	C6-C7-N2	2.53	106.78	103.03
3	А	1100	1LT	F1-C18-C15	-2.42	107.27	112.33
3	A	1100	1LT	C11-C12-N4	-2.41	120.96	123.96
3	С	1100	1LT	F1-C18-C15	-2.34	107.43	112.33
4	С	1101	YQB	C4-C9-C10	2.33	124.47	121.72



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	С	1101	YQB	C30-C20-C18	-2.31	112.28	115.23
3	С	1100	1LT	C14-C13-C15	-2.28	120.05	122.68
3	С	1100	1LT	C8-C7-N2	-2.20	108.75	112.29
3	С	1100	1LT	C5-C4-N2	2.17	107.06	103.25
4	С	1101	YQB	C25-N24-C21	2.15	125.75	119.72
4	С	1101	YQB	C16-C15-C14	2.04	120.17	118.16
4	A	1101	YQB	C4-C9-C10	2.02	124.10	121.72

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
3	С	1100	1LT	N2-C7-C8-N3
3	С	1100	1LT	C6-C7-C8-O1
3	С	1100	1LT	C6-C7-C8-N3
4	С	1101	YQB	C20-C21-N24-C25
4	С	1101	YQB	C20-C21-N24-C29
3	А	1100	1LT	С11-С10-С9-С1
3	А	1100	1LT	C14-C10-C9-C1
3	С	1100	1LT	С11-С10-С9-С1
3	С	1100	1LT	C14-C10-C9-C1
3	А	1100	1LT	C14-C13-C15-C17
3	С	1100	1LT	C14-C13-C15-C17
3	А	1100	1LT	N2-C7-C8-O1
3	А	1100	1LT	N2-C7-C8-N3
3	С	1100	1LT	N2-C7-C8-O1
4	А	1101	YQB	O11-C10-C9-C4
4	A	1101	YQB	O12-C10-C9-C4
4	А	1101	YQB	N22-C21-N24-C25

All (17) torsion outliers are listed below:

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	1101	YQB	1	0
3	А	1100	1LT	1	0
4	С	1101	YQB	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 similar 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	С	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	С	966:LYS	С	967:GLY	N	4.46



# 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	< <b>RSRZ</b> >	#RSR2	Z>2	2	$OWAB(Å^2)$	Q<0.9
1	А	1054/1072~(98%)	0.71	72 (6%) 17	7	15	47, 93, 181, 266	0
1	С	1033/1072~(96%)	0.92	111 (10%)	6	5	60, 105, 195, 387	0
2	В	279/279~(100%)	3.43	144 (51%)	0	0	87, 209, 332, 465	0
2	D	279/279~(100%)	1.37	74 (26%)	0	0	63, 151, 221, 273	0
All	All	2645/2702~(97%)	1.15	401 (15%)	2	1	47, 106, 240, 465	0

All (401) RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
2	В	369	THR	31.1
1	С	947	TYR	22.7
2	В	583	TRP	22.3
2	В	370	LEU	22.0
2	В	372	LEU	21.5
2	В	406	ASN	20.9
2	В	445	VAL	20.5
2	В	422	VAL	19.4
2	В	588	GLY	17.5
1	С	504	ALA	15.4
2	В	408	TYR	14.9
2	В	351	ALA	14.6
2	В	335	TRP	14.3
2	В	416	TYR	14.1
2	В	368	TYR	11.6
2	В	429	SER	11.5
1	С	507	SER	11.4
2	В	342	GLU	11.2
2	В	397	THR	11.1
1	С	872	PHE	10.4
2	В	446	GLY	10.4



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Mol	Chain	Res	Type	RSRZ
2	В	359	ASP	10.3
1	С	512	GLY	10.2
2	В	354	THR	10.1
2	В	379	LYS	9.4
1	С	517	LEU	9.3
1	С	509	SER	9.3
2	В	398	PHE	9.3
1	С	300	ASP	9.2
2	В	409	ARG	9.0
2	В	405	ILE	9.0
2	В	366	GLY	8.9
2	В	350	THR	8.9
1	А	512	GLY	8.9
2	В	589	VAL	8.8
2	В	393	SER	8.8
1	С	506	PHE	8.7
2	В	420	LEU	8.6
2	D	323	ASN	8.6
2	D	392	PHE	8.6
1	С	503	GLU	8.5
2	В	580	TYR	8.3
1	С	502	ARG	8.2
1	С	946	GLY	8.1
1	С	557	TYR	8.1
2	В	444	ALA	7.8
1	С	950	GLU	7.8
2	В	509	ILE	7.7
2	В	399	SER	7.6
1	С	200	PRO	7.6
2	В	371	THR	7.6
2	D	326	MET	7.5
2	В	343	VAL	7.4
2	В	439	GLU	7.3
2	В	407	HIS	7.2
2	В	413	LEU	7.2
2	В	401	VAL	7.2
2	В	358	ARG	7.1
2	В	425	LEU	7.0
2	В	331	ALA	6.9
2	В	382	LYS	6.9
2	В	402	VAL	6.9
2	В	380	LEU	6.9

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Mol	Chain	Res	Type	RSRZ
2	В	392	PHE	6.9
2	D	589	VAL	6.8
2	В	424	LEU	6.8
2	В	585	THR	6.8
2	D	416	TYR	6.8
2	В	442	ILE	6.6
1	А	1	MET	6.6
2	В	394	ASP	6.4
1	С	542	GLU	6.4
2	D	361	SER	6.3
1	А	504	ALA	6.3
2	D	437	VAL	6.2
1	С	520	ASP	6.2
2	В	440	ASP	6.2
2	В	333	TRP	6.2
2	В	417	ASN	6.1
1	С	942	LYS	6.1
1	А	940	HIS	6.1
1	С	505	GLY	6.1
2	В	381	ILE	6.1
1	А	513	LEU	6.1
2	В	356	LEU	6.0
2	D	584	LEU	6.0
1	С	519	ARG	5.9
1	С	948	LYS	5.9
1	С	940	HIS	5.9
2	D	420	LEU	5.8
2	В	355	PHE	5.8
2	В	327	SER	5.8
1	А	948	LYS	5.7
2	D	366	GLY	5.7
2	В	332	GLU	5.7
1	A	944	LYS	5.6
2	В	367	ASP	5.5
2	D	370	LEU	5.5
2	В	430	LYS	5.5
1	С	489	MET	5.4
2	В	334	TYR	5.4
1	A	503	GLU	5.4
2	В	437	VAL	5.4
2	В	357	VAL	5.3
1	С	949	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
2	D	413	LEU	5.3
1	А	946	GLY	5.2
2	В	505	SER	5.2
2	В	421	ASP	5.2
2	D	369	THR	5.2
1	С	514	SER	5.1
2	В	426	TYR	5.1
2	D	449	LEU	5.1
2	В	396	LEU	5.1
2	В	361	SER	5.0
1	С	871	GLN	5.0
1	С	513	LEU	5.0
1	A	519	ARG	5.0
2	D	365	HIS	4.9
2	В	341	GLU	4.9
2	В	600	ASN	4.8
2	В	512	PHE	4.8
2	D	381	ILE	4.8
2	В	345	GLU	4.8
2	В	423	LYS	4.7
2	В	441	ASN	4.7
2	В	346	LYS	4.7
2	В	328	LEU	4.7
2	В	584	LEU	4.7
1	А	232	MET	4.7
2	В	410	ASN	4.6
2	В	598	LEU	4.6
1	А	517	LEU	4.6
2	D	337	ASP	4.6
2	В	336	GLY	4.6
1	С	945	PHE	4.5
2	В	385	HIS	4.5
1	А	410	LYS	4.5
2	В	378	ASN	4.5
2	В	329	GLN	4.4
2	D	362	THR	4.4
2	В	390	TYR	4.4
1	С	499	SER	4.4
1	А	281	ARG	4.4
2	D	368	TYR	4.4
1	С	500	VAL	4.3
1	А	1062	ILE	4.3



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Mol	Chain	Res	Type	RSRZ
2	В	376	GLY	4.3
2	В	579	GLN	4.3
1	А	2	PRO	4.3
2	D	343	VAL	4.2
2	В	337	ASP	4.2
2	D	594	LEU	4.2
2	В	456	PHE	4.2
1	С	199	SER	4.2
1	С	866	LEU	4.2
2	В	418	PRO	4.2
2	В	400	SER	4.1
2	В	352	ASP	4.1
1	С	865	GLY	4.1
1	С	246	TYR	4.1
2	D	338	ILE	4.1
2	В	325	ASN	4.0
2	В	404	LEU	4.0
2	D	324	ASN	3.9
2	D	372	LEU	3.9
2	В	447	LYS	3.9
1	С	1013	LEU	3.9
1	С	941	LYS	3.9
1	А	302	PHE	3.9
2	D	431	TYR	3.8
1	С	328	TRP	3.8
2	В	498	CYS	3.8
2	В	452	TYR	3.8
1	А	499	SER	3.8
2	В	391	GLY	3.8
2	В	340	ARG	3.8
1	А	199	SER	3.7
1	А	872	PHE	3.7
1	С	297	LEU	3.7
1	C	938	LEU	3.7
2	D	380	LEU	3.7
1	A	300	ASP	3.7
1	A	28	ASN	3.7
1	С	1	MET	3.6
1	С	1046	ALA	3.6
1	A	177	LEU	3.6
2	D	581	LEU	3.6
2	D	590	ARG	3.6



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Mol	Chain	Res	Type	RSRZ
1	С	480	PHE	3.6
2	В	403	GLU	3.5
1	А	1063	LYS	3.5
1	А	506	PHE	3.5
2	В	383	ILE	3.5
2	D	375	GLY	3.5
1	С	510	HIS	3.5
1	С	508	TYR	3.5
2	D	333	TRP	3.5
2	D	363	LYS	3.5
1	С	516	ARG	3.5
2	D	436	VAL	3.4
1	С	396	LEU	3.4
1	A	3	PRO	3.4
2	D	435	GLN	3.4
2	В	436	VAL	3.4
1	А	505	GLY	3.4
1	С	864	GLY	3.4
1	А	1059	PHE	3.4
1	С	939	ASP	3.4
2	D	386	ARG	3.4
2	D	383	ILE	3.3
2	D	352	ASP	3.3
2	В	520	GLU	3.3
2	В	330	ASP	3.3
1	А	500	VAL	3.3
2	В	494	PHE	3.3
2	В	365	HIS	3.3
1	С	521	ASN	3.2
1	С	367	LEU	3.2
1	A	515	ASN	3.2
2	В	339	SER	3.2
2	D	384	PHE	3.2
2	В	504	TYR	3.2
1	С	531	LEU	3.2
1	С	128	PHE	3.2
2	В	493	ILE	3.2
2	D	433	GLN	3.2
1	А	947	TYR	3.2
1	C	831	LEU	3.2
1	С	944	LYS	3.1
2	D	445	VAL	3.1



Mol	Chain	Res	Type	RSRZ
2	D	322	MET	3.1
1	С	971	CYS	3.1
1	С	330	ILE	3.1
2	В	434	ASP	3.1
1	А	415	ALA	3.1
1	С	543	ILE	3.1
1	А	62	LEU	3.0
1	С	593	ILE	3.0
2	D	332	GLU	3.0
2	В	431	TYR	3.0
2	D	441	ASN	3.0
1	С	968	ALA	3.0
2	D	391	GLY	3.0
1	A	452	LEU	3.0
1	С	551	LEU	3.0
1	А	179	LYS	2.9
2	В	538	ILE	2.9
2	В	523	ARG	2.9
2	D	426	TYR	2.9
2	В	448	LYS	2.9
1	А	514	SER	2.9
2	В	597	TRP	2.9
1	С	484	VAL	2.9
1	С	980	PHE	2.9
1	С	794	PHE	2.9
1	А	30	MET	2.9
2	В	443	GLU	2.8
1	А	501	SER	2.8
1	А	1055	MET	2.8
1	C	493	GLU	2.8
2	D	405	ILE	2.8
1	A	518	ALA	2.8
2	D	359	ASP	2.8
2	D	583	TRP	2.8
1	С	991	ILE	2.7
1	А	23	GLU	2.7
1	А	980	PHE	2.7
2	D	371	THR	2.7
1	С	964	ILE	2.7
2	D	356	LEU	2.7
2	D	401	VAL	2.7
1	С	568	LEU	2.7



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Mol	Chain	Res	Type	RSRZ
1	С	643	GLN	2.7
2	В	518	GLU	2.7
1	А	234	LEU	2.7
1	С	523	LEU	2.7
2	В	455	GLN	2.7
1	С	818	ARG	2.7
1	А	1054	LYS	2.6
1	С	816	ILE	2.6
1	С	354	ILE	2.6
1	А	58	LEU	2.6
1	С	956	LEU	2.6
1	А	984	CYS	2.6
2	В	433	GLN	2.6
2	В	347	LEU	2.6
2	В	577	ARG	2.6
1	С	965	SER	2.6
2	В	586	GLN	2.6
1	С	323	SER	2.6
2	В	593	LYS	2.6
2	В	415	GLN	2.5
1	С	680	VAL	2.5
1	А	31	ILE	2.5
2	В	438	LYS	2.5
2	В	510	GLU	2.5
1	А	108	ARG	2.5
1	А	100	LYS	2.5
1	С	886	LYS	2.5
1	С	392	TYR	2.5
1	С	587	VAL	2.5
1	С	430	PHE	2.5
1	С	305	PRO	2.5
2	В	419	LYS	2.5
1	А	104	PRO	2.4
2	D	325	ASN	2.4
1	С	473	LEU	2.4
1	А	11	TRP	2.4
2	В	508	TYR	2.4
1	С	832	ARG	2.4
1	С	702	LEU	2.4
1	С	298	PRO	2.4
2	В	432	GLN	2.4
2	D	448	LYS	2.4



Mol	Chain	Res	Type	RSRZ
2	D	442	ILE	2.4
1	С	413	LYS	2.4
1	С	902	ALA	2.4
1	С	540	LEU	2.4
2	D	374	LYS	2.4
1	С	967	GLY	2.4
1	А	252	LEU	2.4
2	В	412	SER	2.3
2	D	410	ASN	2.3
1	А	68	TYR	2.3
2	D	346	LYS	2.3
2	В	460	SER	2.3
2	В	322	MET	2.3
1	С	889	ILE	2.3
1	С	999	ILE	2.3
1	С	146	VAL	2.3
1	С	951	ARG	2.3
1	А	640	LYS	2.3
1	А	881	LEU	2.3
1	С	511	ALA	2.3
2	В	353	GLY	2.3
1	С	149	GLU	2.3
1	С	185	LEU	2.3
2	В	525	MET	2.3
1	С	291	GLU	2.3
1	А	587	VAL	2.2
1	С	571	SER	2.2
2	D	347	LEU	2.2
2	D	444	ALA	2.2
1	С	823	ILE	2.2
1	С	597	GLN	2.2
1	А	937	PHE	2.2
1	А	413	LYS	2.2
1	С	429	LEU	2.2
1	А	557	TYR	2.2
2	D	592	LYS	2.2
1	А	4	ARG	2.2
1	А	200	PRO	2.2
1	А	1051	TRP	2.2
2	В	570	LEU	2.2
2	D	531	LEU	2.2
2	D	385	HIS	2.2



8V8U	8V	'8U
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Mol	Chain	Res	Type	RSRZ	
2	D	382	LYS	2.2	
1	А	26	LEU	2.2	
2	D	598	LEU	2.2	
2	В	491	ILE	2.2	
2	D	432	432 GLN		
1	А	509	SER	2.2	
2	В	373	ARG	2.2	
1	С	518	ALA	2.1	
2	D	579	GLN	2.1	
2	В	449	LEU	2.1	
2	D	424	LEU	2.1	
2	В	587	LYS	2.1	
2	D	339	SER	2.1	
1	А	239	LEU	2.1	
1	А	969	GLN	2.1	
1	С	304	MET	2.1	
1	С	943	LYS	2.1	
1	А	508	TYR	2.1	
1	А	204	LYS	2.1	
1	С	961	LEU	2.1	
1	С	307	TYR	2.1	
2	D	422	VAL	2.1	
1	А	408	SER	2.1	
2	D	425	LEU	2.1	
1	С	205	GLN	2.1	
2	D	351	ALA	2.1	
2	D	340	ARG	2.0	
2	В	374	LYS	2.0	
1	С	807	LEU	2.0	
2	В	569	ASP	2.0	
2	В	375	GLY	2.0	
1	С	599	MET	2.0	
2	D	498	CYS	2.0	
2	В	324	ASN	2.0	
2	В	395	PRO	2.0	
2	D	447	LYS	2.0	
1	А	120	ALA	2.0	
2	В	500	THR	2.0	
1	С	177	LEU	2.0	
1	С	327	LEU	2.0	
2	D	595	ASN	2.0	
1	А	614	PHE	2.0	



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Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	А	861	GLN	2.0
2	В	564	ASN	2.0

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
4	YQB	С	1101	32/32	0.89	0.39	105,124,158,241	0
3	1LT	С	1100	30/30	0.93	0.26	54,72,87,100	0
4	YQB	А	1101	32/32	0.95	0.33	87,99,130,153	0
3	1LT	А	1100	30/30	0.96	0.25	57,75,88,94	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.

