

Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 03:58 PM JST

PDB ID	:	7CX1
Title	:	Crystal structure of a tyrosine decarboxylase from Enterococcus faecalis in
		complex with the cofactor PLP and inhibitor methyl-tyrosine
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Deposited on	:	2020-09-01
Resolution	:	2.54 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 2.54 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	$1284 \ (2.56-2.52)$		
Clashscore	141614	$1332 \ (2.56-2.52)$		
Ramachandran outliers	138981	1315 (2.56-2.52)		
Sidechain outliers	138945	1315 (2.56-2.52)		
RSRZ outliers	127900	$1272 \ (2.56-2.52)$		

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	620	71%	25%	••
1	В	620	67%	29%	••
1	С	620	4% 68%	26%	• 5%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14498 atoms, of which 60 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	Atoms					ZeroOcc	AltConf	Trace	
1	Δ	602	Total	С	Ν	0	Р	\mathbf{S}	0	0	0
1	Π		4749	3030	786	911	1	21			
1	В	603	Total	С	Ν	Ο	Р	\mathbf{S}	0	0	0
1	D	005	4787	3058	792	915	1	21			
1	С	500	Total	С	Ν	0	Р	S	0	0	0
	590	4649	2969	770	888	1	21	0	0	0	

• Molecule 1 is a protein called Decarboxylase.

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	62	LYS	GLU	conflict	UNP Q8KXD2
В	62	LYS	GLU	conflict	UNP Q8KXD2
С	62	LYS	GLU	conflict	UNP Q8KXD2

• Molecule 2 is 4-[(2R)-2-(methylamino)propyl]phenol (three-letter code: GKU) (formula: $C_{10}H_{15}NO$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
9	Λ	1	Total	С	Η	Ν	Ο	0	0
	A	1	27	10	15	1	1	0	0
0	В	1	Total	С	Η	Ν	0	0	0
	1	27	10	15	1	1	0	0	
0	В	1	Total	С	Η	Ν	0	0	0
	D	1	27	10	15	1	1	0	0
0	C	1	Total	С	Η	Ν	0	0	0
		1	27	10	15	1	1	U	

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	78	Total O 78 78	0	0
3	В	62	$\begin{array}{cc} \text{Total} & \text{O} \\ 62 & 62 \end{array}$	0	0
3	С	65	$\begin{array}{cc} \text{Total} & \text{O} \\ 65 & 65 \end{array}$	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: Decarboxylase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	131.49Å 131.49Å 385.66Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Bosolution(A)	24.85 - 2.54	Depositor
Resolution (A)	24.85 - 2.54	EDS
% Data completeness	99.7 (24.85-2.54)	Depositor
(in resolution range)	99.7(24.85 - 2.54)	EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.96 (at 2.53 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
P. P.	0.210 , 0.253	Depositor
n, n_{free}	0.226 , 0.250	DCC
R_{free} test set	3283 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	44.6	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 32.9	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14498	wwPDB-VP
Average B, all atoms $(Å^2)$	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: LLP, GKU

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		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.51	0/4842	0.72	0/6580	
1	В	0.55	0/4880	0.75	0/6623	
1	С	0.49	0/4738	0.72	0/6436	
All	All	0.52	0/14460	0.73	0/19639	

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	4749	0	4503	124	0
1	В	4787	0	4592	145	0
1	С	4649	0	4415	162	0
2	А	12	15	0	1	0
2	В	24	30	0	1	0
2	С	12	15	0	0	0
3	А	78	0	0	2	0
3	В	62	0	0	1	0
3	С	65	0	0	2	0
All	All	14438	60	13510	406	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 15.

All (406) 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:B:160:LEU:HD21	1:C:438:GLU:HA	1.41	1.02
1:A:154:ILE:O	1:A:441:LYS:HE2	1.63	0.98
1:A:133:MET:CE	1:A:447:ALA:HA	1.95	0.96
1:C:531:TYR:HB3	1:C:612:LYS:HG3	1.47	0.94
1:C:233:LYS:HD2	1:C:259:ILE:HD11	1.54	0.89
1:B:547:SER:OG	1:B:584:ARG:HB2	1.75	0.85
1:C:207:LEU:HG	1:C:214:ILE:CD1	2.07	0.84
1:A:364:GLU:OE2	1:A:366:LYS:HD2	1.82	0.79
1:B:141:PHE:HB3	1:B:404:VAL:HG22	1.63	0.79
1:B:160:LEU:CD2	1:C:438:GLU:HA	2.12	0.78
1:A:297:SER:OG	1:A:300:GLU:HG2	1.83	0.77
1:B:96:TRP:O	1:B:546:THR:HG23	1.85	0.76
1:C:303:VAL:HG23	1:C:502:ASP:HB3	1.68	0.75
1:B:335:GLY:HA2	1:B:467:ILE:HD13	1.67	0.75
1:C:214:ILE:HG23	1:C:215:ASP:OD1	1.86	0.75
1:B:153:HIS:CE1	1:B:155:VAL:HG22	2.22	0.74
1:A:610:GLN:O	1:A:614:GLU:HG3	1.89	0.72
1:A:525:ASN:HA	1:A:528:VAL:HG22	1.69	0.72
1:B:240:LYS:HE3	1:B:245:LEU:HD21	1.72	0.72
1:B:573:GLU:HA	1:B:576:ARG:HG2	1.69	0.72
1:C:611:GLU:HG2	1:C:612:LYS:N	2.05	0.72
1:B:563:PHE:O	1:B:566:SER:HB3	1.90	0.71
1:C:191:SER:OG	1:C:194:GLU:HG3	1.91	0.71
1:A:233:LYS:HB3	1:A:259:ILE:HD12	1.72	0.71
1:C:173:LYS:HD2	1:C:289:LEU:HA	1.72	0.71
1:A:172:ILE:CD1	1:A:413:VAL:HG11	2.21	0.70
1:B:210:ALA:O	1:B:214:ILE:HG13	1.92	0.70
1:A:350:GLU:H	1:A:350:GLU:CD	1.94	0.70
1:B:85:HIS:HB3	1:C:128:PRO:HB2	1.73	0.70
1:B:145:MET:HE1	1:B:386:VAL:HG11	1.74	0.70
1:B:160:LEU:HD21	1:C:438:GLU:CA	2.21	0.69
1:B:602:ALA:HB3	1:B:603:PRO:HD3	1.75	0.69
1:C:172:ILE:HG13	1:C:413:VAL:HG11	1.75	0.69
1:C:335:GLY:HA2	1:C:467:ILE:HD13	1.73	0.69
1:B:544:PHE:HD2	1:B:605:ILE:HD12	1.58	0.69
1:C:531:TYR:HB3	1:C:612:LYS:CG	2.23	0.68
1:A:167:TRP:CH2	1:A:414:ILE:HG23	2.28	0.68



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:146:SER:OG	1:A:336:ARG:NH2	2.27	0.67
1:C:437:LEU:O	1:C:437:LEU:HD23	1.95	0.66
1:C:295:VAL:HG21	1:C:380:ILE:HD11	1.75	0.66
1:A:208:GLU:HG3	1:A:409:ARG:HD2	1.78	0.66
1:C:207:LEU:HG	1:C:214:ILE:HD11	1.76	0.66
1:C:94:ARG:NH2	1:C:604:LYS:HD2	2.11	0.66
1:A:172:ILE:HD13	1:A:413:VAL:HG11	1.79	0.65
1:C:615:GLN:O	1:C:615:GLN:HG2	1.96	0.65
1:C:544:PHE:CD2	1:C:605:ILE:HG23	2.32	0.65
1:C:153:HIS:CE1	1:C:155:VAL:HG22	2.32	0.65
1:C:484:LEU:HD23	1:C:495:VAL:HG21	1.79	0.65
1:B:53:VAL:HG21	1:C:92:ALA:CB	2.27	0.64
1:B:85:HIS:O	1:C:128:PRO:HD2	1.97	0.64
1:A:133:MET:HE2	1:A:447:ALA:HA	1.77	0.64
1:A:168:TYR:O	1:A:172:ILE:HG12	1.98	0.63
1:A:170:ARG:HE	1:A:251:ILE:HG13	1.63	0.63
1:A:364:GLU:OE2	1:A:366:LYS:CD	2.46	0.63
1:C:166:LEU:HD13	1:C:234:TRP:CE2	2.34	0.62
1:B:335:GLY:O	1:B:338:ILE:HG12	1.99	0.62
1:B:349:TYR:HA	1:B:352:LEU:HD13	1.82	0.62
1:C:546:THR:HG22	:546:THR:HG22 1:C:547:SER:N		0.62
1:A:413:VAL:HG23	1:A:414:ILE:HG13	1.83	0.61
1:A:153:HIS:CE1	1:A:155:VAL:HG22	2.35	0.61
1:B:171:ASN:HB3	1:B:413:VAL:HG13	1.81	0.61
1:C:531:TYR:CB	1:C:612:LYS:HG3	2.25	0.61
1:A:233:LYS:HD2	1:A:259:ILE:HD11	1.83	0.60
1:C:386:VAL:HB	1:C:404:VAL:CG1	2.31	0.60
1:C:277:ILE:O	1:C:281:LEU:HD13	2.00	0.60
1:A:229:GLN:NE2	3:A:801:HOH:O	2.33	0.60
1:B:559:SER:OG	1:B:560:PRO:HD3	2.01	0.60
1:C:303:VAL:HG23	1:C:502:ASP:CB	2.32	0.60
1:C:611:GLU:O	1:C:612:LYS:HB3	1.99	0.60
1:A:427:ASP:OD1	1:A:428:ILE:N	2.32	0.60
1:A:564:VAL:HG13	1:A:569:PHE:HB2	1.83	0.59
1:A:342:GLU:OE2	1:A:461:ALA:HB2	2.02	0.59
1:C:294:VAL:HG11	1:C:297:SER:HA	1.85	0.59
1:A:527:ASP:HB3	1:A:616:ILE:HD13	1.83	0.59
1:B:187:VAL:HB	1:B:195:LEU:HD21	1.85	0.59
1:B:546:THR:HG22	1:B:547:SER:N	2.19	0.58
1:C:237:PRO:HG2	1:C:294:VAL:HG23	1.84	0.58
1:C:432:LEU:O	1:C:432:LEU:HD12	2.03	0.58



	lo uo pugo	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:96:TRP:O	1:C:546:THR:HG23	2.03	0.58	
1:B:369:ILE:HG23	1:B:373:VAL:CG2	2.32	0.58	
1:C:207:LEU:CD2	1:C:214:ILE:HD11	2.33	0.58	
1:C:297:SER:OG	1:C:300:GLU:HG2	2.03	0.58	
1:A:233:LYS:CB	1:A:259:ILE:HD12	2.33	0.58	
1:B:410:MET:O	1:B:413:VAL:HB	2.03	0.58	
1:C:279:ARG:HG2	1:C:279:ARG:HH11	1.69	0.57	
1:B:546:THR:HG22	1:B:547:SER:H	1.69	0.57	
1:A:133:MET:HE1	1:A:447:ALA:HA	1.82	0.57	
1:B:32:LEU:HD11	1:B:112:ASN:HD22	1.70	0.57	
1:B:172:ILE:HD13	1:B:413:VAL:HG21	1.86	0.57	
1:B:46:TYR:CE2	1:C:91:THR:HG21	2.40	0.57	
1:C:176:PRO:HB3	1:C:195:LEU:HB3	1.87	0.56	
1:B:211:GLU:HA	1:B:214:ILE:HD11	1.85	0.56	
1:C:153:HIS:CD2	1:C:436:ILE:HG22	2.39	0.56	
1:C:124:TYR:CE1	R:CE1 1:C:428:ILE:HD13 2.40		0.56	
1:A:612:LYS:O	1:A:616:ILE:HG13	2.05	0.56	
1:B:170:ARG:HD3	1:B:251:ILE:HG13	1.86	0.56	
1:B:437:LEU:HD23	1:C:160:LEU:HD21	1.88	0.56	
1:B:153:HIS:CD2	1:B:436:ILE:HG22	2.41	0.56	
1:B:411:ARG:HG3	1:B:435:TYR:CD2	2.41	0.56	
1:C:531:TYR:HE1	1:C:536:LYS:HZ2	1.52	0.56	
1:C:542:ASN:O	1:C:543:GLU:HB2	2.05	0.56	
1:B:145:MET:CE	1:B:386:VAL:HG11	2.36	0.55	
1:C:437:LEU:HD23	1:C:437:LEU:C	2.27	0.55	
1:A:133:MET:CE	1:A:447:ALA:CA	2.77	0.55	
1:B:487:LYS:HG2	1:B:492:GLU:HG2	1.87	0.55	
1:C:336:ARG:HG3	1:C:377:TYR:HD2	1.71	0.55	
1:B:313:ARG:HD2	1:B:322:TYR:CE1	2.40	0.55	
1:B:250:ILE:O	0:ILE:O 1:C:251:ILE:HA		0.55	
1:A:336:ARG:HH12	1:A:378:LYS:HA	1.73	0.55	
1:B:46:TYR:HE2	1:B:46:TYR:HE2 1:C:91:THR:HG21		0.55	
1:B:369:ILE:HG23	1:B:373:VAL:HG23	1.89	0.54	
1:C:544:PHE:CE2	1:C:605:ILE:HG23	2.42	0.54	
1:B:147:TYR:CD2	1:B:406:GLN:HA	2.42	0.54	
1:B:411:ARG:HG3	1:B:435:TYR:HD2	1.72	0.54	
1:B:11:MET:HE3	1:B:456:LEU:HD23	1.89	0.54	
1:B:338:ILE:HD11	1:B:339:PHE:CZ	2.43	0.54	
1:C:477:PHE:CE2	1:C:481:LEU:HD11	2.42	0.54	
1:B:29:LYS:HG2	1:C:33:ILE:HD12	1.89	0.54	
1:C:325:VAL:HG13	1:C:383:ALA:HA	1.89	0.54	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:172:ILE:HD11	1:A:413:VAL:HG11	1.88	0.54	
1:B:168:TYR:O	1:B:172:ILE:HG12	2.08	0.54	
1:B:416:TYR:O	1:B:434:ALA:HB1	2.07	0.54	
1:C:207:LEU:CG	1:C:214:ILE:HD11	2.36	0.54	
1:B:270:ASP:HB3	1:B:273:GLU:HB2	1.89	0.54	
1:B:316:LEU:HB3	1:B:321:ILE:HB	1.91	0.53	
1:C:390:PRO:HB3	1:C:396:ILE:HD13	1.91	0.53	
1:B:335:GLY:HA2	1:B:467:ILE:HG21	1.89	0.53	
1:A:167:TRP:CE3	1:A:414:ILE:HD13	2.43	0.53	
1:C:72:LYS:HE2	3:C:859:HOH:O	2.07	0.53	
1:A:173:LYS:HG3	1:A:289:LEU:HD12	1.91	0.53	
1:B:522:ASN:O	1:B:526:HIS:HB2	2.09	0.53	
1:C:510:PHE:HZ	1:C:609:LEU:HD13	1.74	0.53	
1:A:182:VAL:HG11	1:A:216:GLU:HB3	1.90	0.53	
1:B:570:SER:HB2	1:B:573:GLU:H	1.73	0.53	
1:A:527:ASP:CB	1:A:616:ILE:HD13	2.39	0.52	
1:C:553:ILE:HD12	1:C:578:GLY:HA2	1.91	0.52	
1:A:25:GLY:O	1:A:29:LYS:HG3	2.08	0.52	
1:B:547:SER:HG	1:B:584:ARG:HB2	1.72	0.52	
1:A:416:TYR:O	1:A:434:ALA:HB1	2.10	0.52	
1:B:113:PHE:HE2	3:PHE:HE2 1:C:79:SER:HA		0.52	
1:B:592:MET:HB3	1:B:598:PHE:HD1	1.75	0.52	
1:C:143:HIS:HB3	1:C:344:ASN:ND2	2.25	0.52	
1:B:488:VAL:HG11	1:B:613:LEU:HB3	1.91	0.51	
1:C:279:ARG:HG2	1:C:279:ARG:NH1	2.23	0.51	
1:A:501:PRO:HB3	1:A:505:MET:O	2.11	0.51	
1:B:295:VAL:HG21	1:B:380:ILE:HD11	1.93	0.51	
1:C:595:LYS:HE2	1:C:599:ASP:OD1	2.09	0.51	
1:C:561:LEU:HA	1:C:564:VAL:HG22	1.93	0.51	
1:A:114:ALA:CB	1:A:444:ALA:HA	2.41	0.51	
1:A:389:ASP:OD2	1:A:392:LLP:HE2	2.10	0.51	
1:B:396:ILE:HG23	:B:396:ILE:HG23 1:B:397:PRO:HD2		0.51	
1:A:370:SER:HB3	1:A:372:GLU:OE2	2.11	0.51	
1:B:55:SER:O	1:B:59:ARG:HG3	2.10	0.51	
1:B:237:PRO:HG2	1:B:294:VAL:HG23	1.93	0.51	
1:B:389:ASP:OD2	1:B:392:LLP:HE3	2.11	0.51	
1:C:144:LEU:HD13	1:C:458:LEU:HB3	1.92	0.51	
1:C:166:LEU:HD13	1:C:234:TRP:CZ2	2.46 0.50		
1:C:482:ASN:OD1	1:C:497:THR:HG23	2.10	0.50	
1:C:498:LEU:HD21	1:C:551:PHE:HE2	1.76	0.50	
1:A:518:LEU:HD23	1:A:518:LEU:O	2.11	0.50	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:C:551:PHE:HB2	1:C:580:VAL:HG13	1.92	0.50	
1:B:298:THR:HG22	1:B:392:LLP:C3	2.42	0.50	
1:C:207:LEU:HG	1:C:214:ILE:HD12	1.90	0.50	
1:B:508:TYB:OH	1:B:546:THB:HG21	2.11	0.50	
1:B:561:LEU:HD12	1:B:564:VAL:CG2	2.41	0.50	
1:A:238:GLN:HG2	1:A:263:VAL:HG13	1.92	0.50	
1:A:336:ARG:NH1	1:A:377:TYR:O	2.45	0.50	
1:C:145:MET:HG3	1:C:404:VAL:HG11	1.94	0.50	
1:A:133:MET:HE2	1:A:447:ALA:CA	2.39	0.50	
1:A:542:ASN:OD1	1:A:612:LYS:NZ	2.33	0.50	
1:A:415:SER:HA	1:A:434:ALA:O	2.12	0.49	
1:B:166:LEU:HG	1:B:251:ILE:HG21	1.94	0.49	
1:C:458:LEU:HD23	1:C:463:TYR:CD2	2.46	0.49	
1:A:167:TRP:CZ3	1:A:414:ILE:CG2	2.96	0.49	
1:C:611:GLU:HG2	1:C:612:LYS:H	1.73	0.49	
1:A:167:TRP:CZ3	1:A:414:ILE:HG23	2.46 0.49		
1:A:330:ALA:O	1:A:389:ASP:HB2	2.11	0.49	
1:B:46:TYB:O	1:C:21:LYS:NZ	2.46	0.49	
1:B:141:PHE:HB3	1:B:404:VAL:CG2	2.40	0.49	
1:C:335:GLY:CA	1:C:467:ILE:HD13	2.42	0.49	
1:A:233:LYS:HB3	1:A:259:ILE:CD1	2.43	0.49	
1:A:544:PHE:CD1	1:A:605:ILE:HG23	2.48	0.49	
1:C:268:ARG:NH2	1:C:502:ASP:OD1	2.46	0.49	
1:B:33:ILE:HD12	1:C:29:LYS:HG2	1.94	0.48	
1:C:525:ASN:HA	1:C:528:VAL:HG22	1.94	0.48	
1:A:204:MET:CE	1:A:204:MET:HA	2.43	0.48	
1:B:78:ILE:O	1:B:82:MET:HG2	2.13	0.48	
1:B:295:VAL:HG23	1:B:327:VAL:HG13	1.93	0.48	
1:A:267:TYR:OH	1:A:498:LEU:HD11	2.13	0.48	
1:C:36:VAL:O	1:C:40:LEU:HG	2.13	0.48	
1:C:173:LYS:HE3	1:C:288:VAL:O	2.13	0.48	
1:C:611:GLU:CG	C:611:GLU:CG 1:C:612:LYS:N		0.48	
1:B:84:THR:HG22	1:B:85:HIS:CE1	2.48	0.48	
1:B:561:LEU:HA	1:B:564:VAL:HG22	1.94	0.48	
1:B:573:GLU:OE2	1:B:576:ARG:HD3	2.14	0.48	
1:C:170:ARG:HA	1:C:289:LEU:HD11	1.95	0.48	
1:A:168:TYR:OH	1:A:411:ARG:HA	2.14	0.48	
1:B:113:PHE:CE2	1:C:79:SER:HA	2.48	0.48	
1:B:472:GLU:HB3	1:B:593:ASN:HB2	1.96	0.48	
1:C:599:ASP:O	1:C:603:PRO:HD2	2.14	0.48	
1:A:550:ASP:OD2	1:A:579:LYS:HE2	2.13	0.48	



Interatomic Clash					
Atom-1	Atom-2	distance $(Å)$	overlap (Å)		
1:B:335:GLY:CA	1:B:467:ILE:HD13	2.40	0.48		
1:C:213:GLU:O	1:C:217:ILE:HG13	2.14	0.48		
1:C:483:ASP:OD1	1:C:483:ASP:N	2.47	0.48		
1:C:510:PHE:CZ	1:C:609:LEU:HD13	2.49	0.48		
1:A:528:VAL:CG2	1:A:583:LEU:HD11	2.44	0.47		
1:B:70:HIS:CG	1:C:6:LEU:HD11	2.50	0.47		
1:B:488:VAL:HG22	1:B:493:ILE:HG12	1.97	0.47		
1:C:166:LEU:HG	1:C:251:ILE:HG21	1.96	0.47		
1:A:135:GLU:OE2	1:A:139:HIS:NE2	2.46	0.47		
1:C:32:LEU:O	1:C:36:VAL:HG23	2.14	0.47		
1:C:546:THR:HG22	1:C:547:SER:O	2.14	0.47		
1:A:336:ARG:NH1	1:A:378:LYS:HA	2.29	0.47		
1:B:21:LYS:HD3	1:C:44:GLN:HA	1.96	0.47		
1:B:223:ARG:HB3	1:C:255:LEU:CD2	2.44	0.47		
1:B:371:ARG:HA	1:B:374:TYR:HB3	1.96	0.47		
1:A:170:ARG:HD2	1:A:228:LEU:HD22	1.96	0.47		
1:A:509:VAL:HG12	1:A:582:VAL:HA	1.97	0.47		
1:C:317:MET:HE2	1:C:317:MET:HB2	1.75	0.47		
1:A:608:ALA:O	1:A:612:LYS:HG3	2.14	0.47		
1:B:518:LEU:HD13	1:B:569:PHE:CE2	2.49	0.47		
1:B:336:ARG:NH1	1:B:377:TYR:O	2.47	0.47		
1:C:57:GLN:CD	1:C:57:GLN:H	2.18	0.46		
1:C:166:LEU:HD23	1:C:247:ALA:HB1	1.97	0.46		
1:C:221:SER:OG	1:C:223:ARG:HD3	2.14	0.46		
1:B:338:ILE:CD1	1:B:369:ILE:HD13	2.45	0.46		
1:B:546:THR:HG22	1:B:584:ARG:O	2.15	0.46		
1:A:277:ILE:HA	3:A:832:HOH:O	2.14	0.46		
1:C:221:SER:HG	1:C:223:ARG:HD3	1.80	0.46		
1:A:156:ALA:HB3	1:A:160:LEU:HD12	1.98	0.46		
1:A:237:PRO:HG2	37:PRO:HG2 1:A:294:VAL:HG13		0.46		
1:A:550:ASP:CG	1:A:579:LYS:HE2	2.36	0.46		
1:B:68:VAL:HG23	1:C:15:ALA:HB1	1.98	0.46		
1:B:391:HIS:HA	1:B:396:ILE:O	2.15	0.46		
1:C:531:TYR:HE1	1:C:536:LYS:NZ	2.13	0.46		
1:A:509:VAL:CG1	1:A:582:VAL:HG12	2.46	0.46		
1:A:528:VAL:HG21	1:A:583:LEU:HD11	1.98	0.46		
1:C:171:ASN:HB3	1:C:413:VAL:CG1	2.46	0.46		
1:B:395:TYR:CD2	1:B:466:LEU:HD21	2.50	0.46		
1:A:428:ILE:HG23	1:A:428:ILE:O	2.15	0.46		
1:B:143:HIS:HB3	1:B:344:ASN:ND2	2.31	0.46		
1:B:175:LEU:HD11	1:B:413:VAL:HG22	1.98	0.46		



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:267:TYR:CE2	1:C:498:LEU:HD21	2.51	0.46	
1:A:12:ASN:OD1	1:A:14:ASN:HB2	2.15	0.46	
1:C:542:ASN:O	1:C:543:GLU:CB	2.64	0.46	
1:C:199:PRO:HA	1:C:322:TYR:CD1	2.51	0.45	
1:C:271:ILE:CD1	1:C:309:ILE:HG12	2.46	0.45	
1:C:316:LEU:HB3	1:C:321:ILE:HB	1.97	0.45	
1:A:187:VAL:HB	1:A:195:LEU:HD21	1.98	0.45	
1:A:172:ILE:HG21	1:A:200:THR:HG23	1.98	0.45	
1:A:297:SER:HG	1:A:300:GLU:HG2	1.78	0.45	
1:C:143:HIS:HB3	1:C:344:ASN:HD21	1.81	0.45	
1:B:457:PRO:HD2	1:B:462:GLY:HA3	1.99	0.45	
1:A:141:PHE:HB3	1:A:404:VAL:HG22	1.98	0.45	
1:C:196:LEU:HD13	1:C:287:PRO:HG3	1.98	0.45	
1:C:452:ALA:HB1	1:C:463:TYR:OH	2.17	0.45	
1:A:197:ASN:OD1	1:A:321:ILE:HA	2.16	0.45	
1:A:416:TYR:O	1:A:417:PHE:CD1	2.70	0.45	
1:B:469:ALA:HA	1:B:593:ASN:CB	2.47	0.45	
1:A:348:PRO:CB	1:A:350:GLU:OE2	2.65	0.45	
1:A:611:GLU:O	1:A:615:GLN:HG3	2.17	0.45	
1:B:127:SER:HB3	1:B:130:THR:OG1	2.16	0.45	
1:C:96:TRP:CZ2	1:C:605:ILE:HD11	2.52	0.45	
1:C:154:ILE:CD1	1:C:446:ALA:HA	2.46	0.45	
1:C:237:PRO:O	1:C:240:LYS:HB3	2.16	0.45	
1:C:330:ALA:O	1:C:389:ASP:HB2	2.17	0.45	
1:A:166:LEU:HD21	1:A:234:TRP:CD2	2.52	0.44	
1:B:36:VAL:O	1:B:40:LEU:HG	2.16	0.44	
1:B:249:ASP:OD1	1:C:170:ARG:NH2	2.46	0.44	
1:C:303:VAL:CG2	1:C:502:ASP:HB3	2.42	0.44	
1:C:153:HIS:NE2	1:C:436:ILE:HG22	2.33	0.44	
1:A:191:SER:O	1:A:195:LEU:HG	2.18	0.44	
1:B:251:ILE:HA	1:C:250:ILE:O	2.17	0.44	
1:C:207:LEU:CG	:207:LEU:CG 1:C:214:ILE:CD1		0.44	
1:C:391:HIS:HA	1:C:396:ILE:O	2.18	0.44	
1:C:609:LEU:HD23	1:C:609:LEU:HA	1.74	0.44	
1:A:381:GLU:O	1:A:381:GLU:HG2	2.17	0.44	
1:B:47:MET:HG3	1:C:94:ARG:CD	2.47	0.44	
1:B:517:ASP:HB3	1:B:520:ALA:HB3	2.00	0.44	
1:C:335:GLY:HA2	1:C:467:ILE:HG21	1.98	0.44	
1:C:12:ASN:OD1	1:C:14:ASN:HB2	2.18	0.44	
1:C:266:ASN:HB3	1:C:268:ARG:HH11	1.82	0.44	
1:C:611:GLU:O	1:C:613:LEU:N	2.46	0.44	



	louo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:147:TYR:CG	1:B:406:GLN:HA	2.53	0.44
1:C:173:LYS:HD3	1:C:231:ILE:O	2.18	0.44
1:B:211:GLU:HA	1:B:214:ILE:CD1	2.46	0.44
1:B:474:SER:HA	1:B:587:VAL:HG21	1.99	0.44
1:B:39:HIS:CD2	1:B:116:LEU:HB3	2.52	0.43
1:C:564:VAL:O	1:C:565:ASN:C	2.57	0.43
1:A:105:MET:N	1:A:106:PRO:HD2	2.34	0.43
1:A:390:PRO:HB3	1:A:396:ILE:HD12	2.00	0.43
1:A:551:PHE:O	1:A:579:LYS:HA	2.18	0.43
1:B:251:ILE:HA	1:B:251:ILE:HD12	1.81	0.43
1:C:546:THR:CG2	1:C:547:SER:N	2.81	0.43
1:A:78:ILE:O	1:A:82:MET:HG2	2.18	0.43
1:B:441:LYS:HB2	1:B:441:LYS:HE3	1.51	0.43
1:A:133:MET:HE1	1:A:447:ALA:CB	2.49	0.43
1:B:310:ILE:HD13	1:B:325:VAL:HG21	1.98	0.43
1:A:147:TYR:CG	1:A:406:GLN:HA	A:406:GLN:HA 2.54	
1:B:396:ILE:HG21	1:B:449:VAL:HG22	2.01	0.43
1:A:36:VAL:O	1:A:40:LEU:HG	2.18	0.43
1:B:561:LEU:HD13	1:B:574:TRP:CD1	2.54	0.43
1:C:544:PHE:CE1	1:C:546:THR:OG1	2.71	0.43
1:B:32:LEU:HD11	1:B:112:ASN:ND2	2.33	0.43
1:A:144:LEU:HD13	1:A:458:LEU:HB3	2.01	0.43
1:C:105:MET:N	1:C:106:PRO:HD2	2.34	0.43
1:C:207:LEU:HD21	1:C:214:ILE:HD11	2.00	0.43
1:C:546:THR:HG22	1:C:547:SER:H	1.82	0.43
1:C:611:GLU:O	1:C:612:LYS:CB	2.64	0.43
1:A:370:SER:HB2	1:A:373:VAL:H	1.84	0.42
1:B:33:ILE:HD13	1:B:33:ILE:HA	1.83	0.42
1:C:270:ASP:HB3	1:C:273:GLU:HB2	2.00	0.42
1:C:398:TYR:HA	1:C:399:SER:HA	1.80	0.42
1:A:54:ILE:HG23	LE:HG23 1:A:58:GLU:HG2		0.42
1:A:146:SER:HB2	1:A:381:GLU:HB2	2.02	0.42
1:A:147:TYR:CD2	1:A:406:GLN:HA	2.54	0.42
1:A:348:PRO:HB3	1:A:350:GLU:OE2	2.20	0.42
1:A:531:TYR:CZ	1:A:536:LYS:HD3	2.53	0.42
1:B:348:PRO:HB2	1:B:351:ASP:OD2	2.19	0.42
1:B:398:TYR:CZ	1:C:120:ASN:HB2	2.54	0.42
1:C:187:VAL:HB	1:C:195:LEU:HD21	2.02 0.42	
1:C:482:ASN:OD1	1:C:497:THR:CG2	2.67	0.42
1:C:197:ASN:OD1	1:C:321:ILE:HA	2.20	0.42
1:C:531:TYR:CD1	1:C:536:LYS:HG3	2.53	0.42



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:347:ILE:HD13	1:A:355:VAL:HG11	2.00	0.42	
1:A:385:SER:HA	1:A:404:VAL:O	2.20	0.42	
1:A:457:PRO:HD2	1:A:462:GLY:HA3	2.02	0.42	
1:A:589:THR:O	1:A:589:THR:HG23	2.20	0.42	
1:B:109:LEU:HD12	1:B:109:LEU:HA	1.91	0.42	
1:B:122:VAL:HB	1:B:440:SER:HA	2.01	0.42	
1:B:595:LYS:O	1:B:595:LYS:HG3	2.19	0.42	
1:C:472:GLU:HG2	1:C:593:ASN:O	2.19	0.42	
1:B:238:GLN:HG2	1:B:263:VAL:HG13	2.02	0.42	
1:C:386:VAL:HB	1:C:404:VAL:HG12	2.02	0.42	
1:C:411:ARG:HG3	1:C:435:TYR:HD1	1.84	0.42	
1:A:218:LYS:HB3	1:A:218:LYS:HE3	1.83	0.42	
1:A:452:ALA:HB1	1:A:463:TYR:OH	2.20	0.42	
1:A:573:GLU:HA	1:A:573:GLU:OE1	2.20	0.42	
1:C:548:HIS:HB2	1:C:583:LEU:HD23	2.02	0.42	
1:A:100:ASN:ND2	1:A:398:TYR:OH	2.48	0.42	
1:A:298:THR:HG22	1:A:299:GLU:OE2	2.20	0.42	
1:B:381:GLU:HG3	1:B:382:LEU:HD22	2.02	0.42	
1:C:390:PRO:HB3	1:C:396:ILE:CD1	2.50	0.42	
1:A:153:HIS:ND1	1:A:154:ILE:O	2.50	0.42	
1:A:312:LEU:HG	1:A:316:LEU:HD22	2.02	0.42	
1:A:525:ASN:HA	1:A:528:VAL:CG2	2.44	0.42	
1:B:154:ILE:O	1:B:441:LYS:NZ	2.53	0.42	
1:B:369:ILE:CG2	1:B:373:VAL:HG23	2.50	0.42	
1:B:590:PRO:HD2	1:B:591:TYR:CD2	2.54	0.42	
1:A:338:ILE:HG12	1:A:356:HIS:CE1	2.55	0.41	
1:A:505:MET:HG3	1:A:586:ALA:HA	2.01	0.41	
1:B:143:HIS:HB3	1:B:344:ASN:HD21	1.84	0.41	
1:B:342:GLU:HG3	3:B:1210:HOH:O	2.20	0.41	
1:B:173:LYS:HG3	1:B:289:LEU:HD12	2.02	0.41	
1:B:488:VAL:O	1:B:488:VAL:HG23	2.19	0.41	
1:C:485:THR:HG22	1:C:494:GLU:HB2	2.02	0.41	
1:A:11:MET:SD	1:A:456:LEU:HD23	2.60	0.41	
1:C:170:ARG:NH2	1:C:171:ASN:OD1	2.49	0.41	
1:C:297:SER:HG	1:C:300:GLU:HG2	1.83	0.41	
1:C:307:ASP:HA	1:C:379:ALA:CB	2.50	0.41	
1:C:411:ARG:HG3	1:C:435:TYR:CD1	2.55	0.41	
1:A:371:ARG:O	1:A:371:ARG:HG2	2.19	0.41	
1:A:551:PHE:HB2	1:A:580:VAL:CG1	2.49	0.41	
1:A:553:ILE:HG12	1:A:574:TRP:CZ2	2.55	0.41	
1:B:561:LEU:HD13	1:B:574:TRP:CG	2.56	0.41	



	lo do pagom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:33:ILE:HD13	1:C:33:ILE:HA	1.90	0.41	
1:C:416:TYR:O	1:C:417:PHE:CD1	2.73	0.41	
1:B:86:SER:HB3	1:C:117:TRP:CD1	2.56	0.41	
1:B:415:SER:HA	1:B:434:ALA:O	2.21	0.41	
1:B:459:ASN:OD1	1:B:461:ALA:HB3	2.20	0.41	
1:B:544:PHE:CE1	1:B:546:THR:OG1	2.74	0.41	
1:C:313:ARG:NH1	1:C:325:VAL:HG12	2.35	0.41	
1:C:407:ASP:O	1:C:410:MET:HB2	2.20	0.41	
1:B:338:ILE:HD12	1:B:369:ILE:HD13	2.03	0.41	
1:A:99:MET:HE2	2:A:701:GKU:N	2.35	0.41	
1:A:166:LEU:HD12	1:A:247:ALA:HB1	2.03	0.41	
1:A:371:ARG:HA	1:A:374:TYR:HB3	2.02	0.41	
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.89	0.41	
1:B:265:HIS:CD2	1:B:265:HIS:H	2.39	0.41	
1:C:172:ILE:CG1	1:C:413:VAL:HG21	2.51	0.41	
1:A:146:SER:CB	1:A:336:ARG:NH2	2.84	0.41	
1:A:99:MET:SD	ET:SD 1:A:392:LLP:HD2 2		0.41	
1:A:410:MET:O	1:A:413:VAL:HG22	2.21	0.41	
1:A:564:VAL:HG11	1:A:574:TRP:HB2	2.02	0.41	
1:B:119:GLY:HA3	1:B:127:SER:HB2	2.03	0.41	
1:B:159:SER:HB3	3:C:840:HOH:O	2.21	0.41	
1:B:535:VAL:HG12	1:B:536:LYS:HG3	2.03	0.41	
1:A:396:ILE:HD13	1:A:449:VAL:HG22	2.03	0.40	
1:B:100:ASN:ND2	2:B:1101:GKU:OH	2.48	0.40	
1:B:163:LEU:HG	1:B:437:LEU:HD11	2.02	0.40	
1:B:254:GLY:HA3	1:C:224:SER:O	2.20	0.40	
1:C:614:GLU:O	1:C:615:GLN:C	2.58	0.40	
1:A:544:PHE:CE2	1:A:609:LEU:HD21	2.56	0.40	
1:B:390:PRO:HD2	1:B:400:ALA:O	2.21	0.40	
1:B:546:THR:CG2	1:B:584:ARG:O	2.69	0.40	
1:C:96:TRP:O	1:C:546:THR:HA	2.21	0.40	
1:C:498:LEU:HD13	1:C:582:VAL:HG11	2.04	0.40	
1:A:238:GLN:HG3	1:A:239:THR:HG23	2.03	0.40	
1:B:208:GLU:HG3	1:B:409:ARG:HD2	2.03	0.40	
1:B:510:PHE:N	1:B:525:ASN:OD1	2.34	0.40	
1:B:559:SER:N	1:B:560:PRO:CD	2.84	0.40	
1:A:307:ASP:OD1	1:A:307:ASP:N	2.54	0.40	
1:B:196:LEU:HD13	1:B:196:LEU:HA	1.92	0.40	
1:C:175:LEU:HD23	1:C:175:LEU:HA	1.90	0.40	
1:C:384:GLU:O	1:C:410:MET:HE1	2.21	0.40	
1:B:553:ILE:HB	1:B:554:PRO:HD3	2.04	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	597/620~(96%)	561 (94%)	36~(6%)	0	100	100
1	В	598/620~(96%)	572 (96%)	26 (4%)	0	100	100
1	С	581/620~(94%)	547 (94%)	34 (6%)	0	100	100
All	All	1776/1860~(96%)	1680 (95%)	96 (5%)	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 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	Percer	ntiles
1	А	493/524~(94%)	478 (97%)	15 (3%)	41	55
1	В	502/524~(96%)	486 (97%)	16 (3%)	39	53
1	С	481/524~(92%)	470 (98%)	11 (2%)	50	65
All	All	1476/1572 (94%)	1434 (97%)	42 (3%)	43	58

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	173	LYS
1	А	177	PHE



Mol	Chain	Res	Type
1	А	180	LYS
1	А	209	SER
1	А	221	SER
1	А	240	LYS
1	А	264	ASP
1	А	269	MET
1	А	310	ILE
1	А	316	LEU
1	А	483	ASP
1	А	484	LEU
1	А	555	ASP
1	А	564	VAL
1	А	584	ARG
1	В	66	LYS
1	В	103	THR
1	В	108	LEU
1	В	109	LEU
1	В	115	MET
1	В	131	SER
1	В	177	PHE
1	В	190	LYS
1	В	201	LYS
1	В	209	SER
1	В	231	ILE
1	В	318	LYS
1	В	365	LYS
1	В	367	GLU
1	В	441	LYS
1	В	605	ILE
1	C	176	PRO
1	С	190	LYS
1	С	240	LYS
1	С	317	MET
1	С	325	VAL
1	С	336	ARG
1	С	399	SER
1	C	483	ASP
1	С	518	LEU
1	С	519	VAL
1	C	521	MET

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm sths}$	Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	С	392	1	23,24,25	0.59	0	25,32,34	0.83	1 (4%)
1	LLP	А	392	1	23,24,25	0.73	0	25,32,34	0.91	1 (4%)
1	LLP	В	392	1	23,24,25	0.69	0	25,32,34	0.83	1 (4%)

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
1	LLP	С	392	1	-	2/16/17/19	0/1/1/1
1	LLP	А	392	1	-	6/16/17/19	0/1/1/1
1	LLP	В	392	1	-	6/16/17/19	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	392	LLP	OP4-C5'-C5	2.93	114.94	109.35
1	А	392	LLP	OP4-C5'-C5	2.80	114.68	109.35
1	В	392	LLP	OP4-C5'-C5	2.56	114.22	109.35

There are no chirality outliers.

All (14) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
1	А	392	LLP	C4-C4'-NZ-CE
1	А	392	LLP	N-CA-CB-CG
1	А	392	LLP	C-CA-CB-CG
1	А	392	LLP	O-C-CA-CB
1	В	392	LLP	C4-C4'-NZ-CE
1	В	392	LLP	O-C-CA-CB
1	С	392	LLP	O-C-CA-CB
1	С	392	LLP	C4-C4'-NZ-CE
1	А	392	LLP	CG-CD-CE-NZ
1	В	392	LLP	CE-CD-CG-CB
1	А	392	LLP	CE-CD-CG-CB
1	В	392	LLP	CA-CB-CG-CD
1	В	392	LLP	CG-CD-CE-NZ
1	В	392	LLP	C5'-OP4-P-OP2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	392	LLP	2	0
1	В	392	LLP	2	0

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	Turne	Chain	Dec	Tinle	Bo	ond leng	ths	Bond angles		
IVIOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GKU	С	701	-	12,12,12	0.89	1 (8%)	$14,\!15,\!15$	0.69	0
2	GKU	А	701	-	12,12,12	0.72	0	14,15,15	1.43	3 (21%)



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	Bond angles		
INIOI	туре	Unain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GKU	В	1102	-	12,12,12	1.02	1 (8%)	14,15,15	0.59	0
2	GKU	В	1101	-	12,12,12	1.07	1 (8%)	14,15,15	1.15	1 (7%)

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	GKU	С	701	-	-	2/6/6/6	0/1/1/1
2	GKU	А	701	-	-	2/6/6/6	0/1/1/1
2	GKU	В	1102	-	-	2/6/6/6	0/1/1/1
2	GKU	В	1101	-	-	2/6/6/6	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	1102	GKU	OH-CZ	2.60	1.43	1.37
2	В	1101	GKU	OH-CZ	2.28	1.42	1.37
2	С	701	GKU	OH-CZ	2.14	1.42	1.37

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	1101	GKU	C-CA-CB	-3.58	104.53	111.91
2	А	701	GKU	CB-CA-N	2.75	118.65	110.44
2	А	701	GKU	C-CA-CB	-2.50	106.75	111.91
2	А	701	GKU	CG-CB-CA	-2.11	109.62	113.39

All (4) bond angle outliers are listed below:

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	701	GKU	C-CA-N-C10
2	А	701	GKU	CB-CA-N-C10
2	В	1102	GKU	CB-CA-N-C10
2	С	701	GKU	CB-CA-N-C10
2	В	1102	GKU	C-CA-N-C10
2	С	701	GKU	C-CA-N-C10
2	В	1101	GKU	CB-CA-N-C10



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Mol	Chain	\mathbf{Res}	Type	Atoms
2	В	1101	GKU	C-CA-N-C10

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	701	GKU	1	0
2	В	1101	GKU	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 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	$\langle RSRZ \rangle$	#RSRZ>2 OWAB(Å ²)			Q<0.9	
1	А	601/620~(96%)	0.03	15 (2%)	57	63	25, 44, 71, 86	0
1	В	602/620~(97%)	0.19	28 (4%)	31	38	27, 50, 70, 87	0
1	С	589/620~(95%)	0.14	22 (3%)	41	48	27, 48, 81, 89	0
All	All	1792/1860~(96%)	0.12	65 (3%)	42	49	25, 48, 75, 89	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	6	LEU	4.2
1	В	519	VAL	4.0
1	С	189	GLY	4.0
1	В	583	LEU	3.6
1	В	509	VAL	3.6
1	С	483	ASP	3.5
1	С	508	TYR	3.0
1	В	290	GLY	3.0
1	В	315	GLU	2.9
1	В	510	PHE	2.8
1	С	496	HIS	2.8
1	С	322	TYR	2.8
1	С	583	LEU	2.7
1	А	366	LYS	2.7
1	В	325	VAL	2.6
1	В	289	LEU	2.6
1	С	519	VAL	2.6
1	В	265	HIS	2.6
1	А	583	LEU	2.6
1	С	417	PHE	2.5
1	А	427	ASP	2.5
1	С	5	LYS	2.5
1	В	188	ALA	2.5



Mol	Chain	Res	Type	RSRZ
1	А	265	HIS	2.5
1	А	574	TRP	2.5
1	В	177	PHE	2.5
1	С	514	GLY	2.5
1	С	265	HIS	2.4
1	В	169	ALA	2.4
1	В	485	THR	2.4
1	А	186	LEU	2.4
1	А	569	PHE	2.3
1	В	206	LEU	2.3
1	С	289	LEU	2.3
1	С	169	ALA	2.3
1	В	578	GLY	2.3
1	С	230	ALA	2.3
1	С	428	ILE	2.3
1	С	536	LYS	2.2
1	С	574	TRP	2.2
1	А	322	TYR	2.2
1	А	189	GLY	2.2
1	С	427	ASP	2.2
1	А	430	ALA	2.2
1	С	518	LEU	2.2
1	А	509	VAL	2.2
1	В	535	VAL	2.2
1	А	315	GLU	2.2
1	В	180	LYS	2.2
1	В	490	ASP	2.2
1	В	7	ALA	2.2
1	А	10	GLU	2.2
1	В	508	TYR	2.1
1	A	571	ASP	2.1
1	В	189	GLY	2.1
1	C	615	GLN	2.1
1	В	576	ARG	2.1
1	В	484	LEU	2.1
1	В	487	LYS	2.1
1	В	428	ILE	2.1
1	В	489	GLY	2.1
1	В	580	VAL	2.0
1	C	324	TYR	2.0
1	С	613	LEU	2.0
1	А	558	ASN	2.0

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6.2 Non-standard residues in protein, DNA, RNA chains (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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
1	LLP	В	392	24/25	0.94	0.14	33,40,45,46	0
1	LLP	С	392	24/25	0.94	0.15	34,41,46,48	0
1	LLP	А	392	24/25	0.96	0.12	32,40,43,43	0

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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	GKU	В	1101	12/12	0.75	0.37	45,55,60,65	0
2	GKU	А	701	12/12	0.80	0.37	41,51,59,70	0
2	GKU	В	1102	12/12	0.80	0.37	39,52,64,71	0
2	GKU	С	701	12/12	0.86	0.39	42,55,64,69	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.

