

Full wwPDB X-ray Structure Validation Report (i)

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:	7VUA
:	Anaerobic hydroxyproline degradation involving C-N cleavage by a glycyl rad-
	ical enzyme
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:	2021-11-01
:	2.69 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity		4 02b-467
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Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
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)	:	2.28.1

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 2.69 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	$2808 \ (2.70-2.70)$
Clashscore	141614	$3122 \ (2.70-2.70)$
Ramachandran outliers	138981	3069(2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	785	76%	24%	•
1	В	785	5% 71%	27%	••



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12681 atoms, of which 125 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	А	785	Total C H N O S 6253 3879 109 1046 1176 43	0	0	0
1	В	785	Total C N O S 6042 3819 1028 1153 42	0	0	0

• Molecule 1 is a protein called HplG.

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	106	ALA	GLU	engineered mutation	UNP A0A316Q2B4
А	107	ALA	GLU	engineered mutation	UNP A0A316Q2B4
А	108	ALA	GLU	engineered mutation	UNP A0A316Q2B4
В	106	ALA	GLU	engineered mutation	UNP A0A316Q2B4
В	107	ALA	GLU	engineered mutation	UNP A0A316Q2B4
В	108	ALA	GLU	engineered mutation	UNP A0A316Q2B4

• Molecule 2 is (4S)-4-hydroxy-D-proline (three-letter code: UY7) (formula: C₅H₉NO₃) (labeled as "Ligand of Interest" by depositor).







Mol	Chain	Residues	Atoms				ZeroOcc	AltConf				
0	2 1	٨	Δ		1	Total	С	Η	Ν	Ο	0	0
Z A	1	17	5	8	1	3	0	0				
0	Р	1	Total	С	Η	Ν	0	0	0			
2 D	L	17	5	8	1	3	0	0				

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	187	Total O 187 187	0	0
3	В	165	Total O 165 165	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: HplG

F438 Q439 S440 N441 2397 4398 <mark>5399</mark> 7400 1401 423 424 .428 :429 433 V444 D481 D482 V483 M484 Y459 0460 V546 E49 F51 T580 N581 F582 E583 G584 K585 E586 E586 N585 M587 K598 F599 G600 N601 A547 G548 1569 1570 1571 V563 F564 Q693 S694 G695 L696 L697 F724 A725 Q726 N727 G728 F729 G659 T660 P661 L662 <mark>A663</mark> D664 N665 A666 <mark>Q732</mark> 1733 N734 V735 L736 V674 N675 G676 q700 R701 I716 E717 S718 S718 L/ 41 R7 42



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	117.84Å 218.21Å 168.17Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(Å)	32.14 - 2.69	Depositor
Resolution (A)	33.63 - 2.69	EDS
% Data completeness	95.9 (32.14-2.69)	Depositor
(in resolution range)	95.3 (33.63 - 2.69)	EDS
R _{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.23 (at 2.68 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.14_3247	Depositor
D D .	0.174 , 0.243	Depositor
n, n_{free}	0.174 , 0.243	DCC
R_{free} test set	2015 reflections $(3.37%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	49.1	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.34 , 44.5	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12681	wwPDB-VP
Average B, all atoms $(Å^2)$	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.80% 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: $\rm UY7$

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		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.43	0/6279	0.58	0/8515	
1	В	0.44	0/6175	0.57	1/8381~(0.0%)	
All	All	0.43	0/12454	0.57	1/16896~(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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	395	GLY	C-N-CA	-6.39	105.72	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	106	ALA	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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	6144	109	5832	151	0
1	В	6042	0	5674	189	0
2	А	9	8	0	1	0
2	В	9	8	0	0	0
3	А	187	0	0	1	0
3	В	165	0	0	3	0
All	All	12556	125	11506	333	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 14.

All (333) 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	$distance ({ m \AA})$	overlap (Å)
1:B:107:ALA:HA	1:B:110:GLU:CB	1.85	1.06
1:B:109:LYS:HD2	1:B:113:ARG:HD2	1.39	1.02
1:A:113:ARG:O	1:A:115:ILE:N	1.94	0.98
1:B:136:MET:HA	1:B:139:MET:HE2	1.53	0.90
1:B:656:ARG:NH1	1:B:660:THR:O	2.08	0.86
1:A:423:GLY:HA3	1:A:433:LEU:HD21	1.57	0.86
1:B:638:THR:H	1:B:665:ASN:HA	1.39	0.85
1:B:371:THR:HB	1:B:400:TYR:CE1	2.15	0.82
1:B:693:GLN:O	1:B:694:SER:HB2	1.79	0.81
1:A:343:GLU:HG2	1:A:417:LYS:HG2	1.63	0.81
1:A:698:LEU:HD23	1:A:731:ILE:HD13	1.62	0.80
1:B:576:ARG:NH1	1:B:580:THR:HG21	1.97	0.80
1:B:393:SER:O	1:B:395:GLY:N	2.16	0.79
1:A:244:VAL:HG21	1:A:258:LEU:HB2	1.68	0.74
1:B:227:ASP:OD1	1:B:229:LYS:HG2	1.87	0.74
1:B:392:ASP:O	1:B:393:SER:HB2	1.85	0.74
1:B:477:PHE:CD2	1:B:483:VAL:HG22	2.22	0.74
1:B:326:ALA:O	1:B:640:ALA:HB3	1.87	0.73
1:A:638:THR:HG23	1:A:665:ASN:HA	1.70	0.73
1:A:511:PHE:CE1	1:B:191:MET:HB3	2.23	0.73
1:B:312:VAL:HG13	1:B:315:MET:CE	2.20	0.72
1:A:244:VAL:CG2	1:A:258:LEU:HB2	2.19	0.72
1:B:549:ILE:HG23	1:B:613:LEU:HD23	1.73	0.70
1:B:481:ASP:HA	1:B:484:MET:HE2	1.73	0.70
1:B:5:ARG:NH2	1:B:233:GLU:OE2	2.22	0.70
1:B:394:GLY:HA3	1:B:755:LEU:HB3	1.72	0.69



	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:549:ILE:O	1:A:553:ILE:HG13	1.92	0.69	
1:A:244:VAL:HG22	1:A:245:PRO:HA	1.75	0.69	
1:B:540:HIS:O	1:B:630:GLY:HA3	1.91	0.68	
1:A:731:ILE:HD12	1:A:732:GLN:H	1.59	0.68	
1:B:315:MET:HE1	1:B:334:MET:SD	2.33	0.68	
1:B:721:ARG:HG2	1:B:721:ARG:HH11	1.59	0.67	
1:A:87:TYR:CE2	1:A:120:LYS:HG3	2.30	0.67	
1:A:296:LYS:HD3	1:A:300:TYR:CD2	2.30	0.67	
1:A:312:VAL:HA	1:A:315:MET:HE2	1.77	0.67	
1:B:76:VAL:HG21	1:B:101:LEU:HD22	1.77	0.67	
1:B:677:PRO:HD3	1:B:782:GLN:HB3	1.77	0.67	
1:B:773:GLN:O	1:B:777:ILE:HG13	1.95	0.67	
1:A:87:TYR:CZ	1:A:120:LYS:HE3	2.30	0.66	
1:B:774:ASN:O	1:B:778:GLU:HG3	1.95	0.66	
1:B:167:ARG:HD3	1:B:171:TYR:CD1	2.31	0.66	
1:B:99:ASP:O	1:B:100:ASN:HB3	1.96	0.66	
1:A:737:ASP:HB3	1:A:740:THR:H	1.60	0.65	
1:A:113:ARG:C	1:A:115:ILE:H	1.98	0.65	
1:B:2:ILE:HD12	1:B:3:SER:O	1.95	0.65	
1:B:732:GLN:OE1	1:B:757:ARG:NH1	2.30	0.65	
1:B:738:ASP:HB2	1:B:781:ILE:HD11	1.80	0.64	
1:A:312:VAL:HG13	1:A:315:MET:HE1	1.78	0.64	
1:B:139:MET:HE3	1:B:145:PHE:CZ	2.33	0.63	
1:B:564:PHE:CE2	1:B:571:MET:HE1	2.34	0.63	
1:B:549:ILE:O	1:B:553:ILE:HG13	1.99	0.63	
1:A:244:VAL:CG2	1:A:258:LEU:HD12	2.29	0.63	
1:B:563:VAL:HG22	1:B:569:LEU:CD1	2.30	0.62	
1:A:153:SER:O	1:A:155:MET:HG3	2.00	0.62	
1:B:312:VAL:HG13	1:B:315:MET:HE3	1.81	0.61	
1:A:326:ALA:HA	1:A:640:ALA:HB3	1.82	0.61	
1:A:142:VAL:HG12	1:A:463:ILE:HG21	1.84	0.60	
1:A:698:LEU:CD2	1:A:731:ILE:HD13	2.30	0.60	
1:B:775:ASN:HA	1:B:778:GLU:OE1	2.01	0.60	
1:A:18:PRO:HG2	1:A:100:ASN:O	2.00	0.60	
1:B:481:ASP:HA	1:B:484:MET:CE	2.32	0.60	
1:A:448:LEU:HD23	1:A:649:VAL:HG11	1.84	0.59	
1:A:244:VAL:HG22	1:A:258:LEU:HD12	1.83	0.59	
1:B:396:HIS:H	1:B:397:PRO:HD2	1.66	0.59	
1:B:576:ARG:HG3	1:B:576:ARG:HH11	1.66	0.59	
1:B:396:HIS:O	1:B:398:ALA:N	2.36	0.59	
1:B:564:PHE:CZ	1:B:571:MET:HE1	2.37	0.59	



	louo pugom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:547:ALA:HB3	1:A:645:MET:HE1	1.84	0.59	
1:A:547:ALA:CB	1:A:645:MET:HE2	2.33	0.59	
1:B:598:LYS:O	1:B:606:VAL:HG11	2.03	0.59	
1:B:109:LYS:HD2	1:B:113:ARG:HH11	1.65	0.59	
1:A:454:MET:HE3	1:A:487:TYR:HB2	1.83	0.59	
1:A:312:VAL:HG13	1:A:315:MET:CE	2.33	0.58	
1:B:633:THR:HB	1:B:693:GLN:O	2.02	0.58	
1:A:547:ALA:HB3	1:A:645:MET:CE	2.33	0.58	
1:A:568:TYR:CD2	1:A:591:LEU:HD21	2.39	0.58	
1:A:367:GLU:HB3	1:A:368:PRO:HA	1.84	0.58	
1:B:360:MET:CE	1:B:397:PRO:HD3	2.34	0.57	
1:A:79:HIS:O	1:A:83:THR:HG23	2.04	0.57	
1:B:22:LEU:O	1:B:26:ARG:HB2	2.04	0.57	
1:A:142:VAL:HG12	1:A:463:ILE:CG2	2.34	0.57	
1:A:326:ALA:O	1:A:640:ALA:HB3	2.05	0.57	
1:B:55:ARG:NH2	1:B:70:GLY:O	2.38	0.57	
1:A:343:GLU:CG	1:A:417:LYS:HG2	2.32	0.57	
1:A:496:GLU:HG3	1:A:624:PHE:CZ	2.40	0.57	
1:A:430:PRO:HG3	1:A:729:PHE:CZ	2.41	0.56	
1:B:712:GLY:O	1:B:716:ILE:N	2.37	0.56	
1:A:315:MET:HE3	1:A:334:MET:SD	2.45	0.56	
1:A:331:PRO:HB3	1:A:761:TYR:CG	2.39	0.56	
1:B:344:ASN:OD1	1:B:346:LYS:HG3	2.05	0.56	
1:B:466:LYS:HG2	1:B:466:LYS:O	2.06	0.56	
1:A:547:ALA:CB	1:A:645:MET:CE	2.84	0.56	
1:A:530:LYS:HE3	1:A:534:GLN:O	2.05	0.56	
1:B:454:MET:HG3	1:B:487:TYR:HA	1.88	0.56	
1:A:323:GLU:O	1:A:327:ASP:HB2	2.05	0.56	
1:B:755:LEU:HD13	1:B:764:TYR:CE1	2.41	0.56	
1:A:555:SER:CB	1:A:653:PRO:HD2	2.36	0.55	
1:A:638:THR:O	1:A:641:TYR:HB2	2.06	0.55	
1:B:430:PRO:HG3	1:B:729:PHE:CZ	2.41	0.55	
1:A:555:SER:HB2	1:A:653:PRO:HD2	1.87	0.55	
1:A:732:GLN:CD	1:A:757:ARG:HD2	2.28	0.55	
1:B:732:GLN:HE22	1:B:760:GLY:H	1.54	0.54	
1:B:471:SER:OG	1:B:490:GLN:NE2	2.40	0.54	
1:B:312:VAL:HG22	1:B:315:MET:HE2	1.90	0.54	
1:B:146:THR:HB	1:B:444:TYR:H	1.73	0.54	
1:B:335:HIS:ND1	1:B:371:THR:CG2	2.71	0.54	
1:B:341:GLN:HE21	1:B:345:GLY:HA2	1.71	0.54	
1:B:726:GLN:O	1:B:727:ASN:HB2	2.09	0.53	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:A:384:ARG:NH2	1:A:713:ILE:HB	2.24	0.53	
1:B:312:VAL:HA	1:B:315:MET:CE	2.38	0.53	
1:A:351:GLU:OE1	1:A:351:GLU:HA	2.08	0.53	
1:B:666:ALA:HB3	1.B.697.LEU.O	2.08	0.53	
1:A:70:GLY:HA3	1:A:75:ALA:CB	2.39	0.53	
1:B:217:LEU:O	1:B:221:GLN:HG3	2.09	0.53	
1:B:109:LYS:O	1:B:111:GLU:N	2.43	0.52	
1:A:87:TYB:OH	1:A:120:LYS:HE3	2.09	0.52	
1:A:755:LEU:HD13	1:A:764:TYR:CE1	2.45	0.52	
1:B:369:CYS:HA	1:B:396:HIS:CE1	2.45	0.52	
1:B:638:THB:O	1:B:641:TYB:HB2	2.09	0.52	
1:A:70:GLY:HA3	1:A:75:ALA:HB3	1.91	0.52	
1:A:684:LEU:HD11	1:A:698:LEU:HD13	1.92	0.52	
1:B:69:GLN:HG3	3:B:912:HOH:O	2.09	0.52	
1:B:777:ILE:HG22	1:B:777:ILE:O	2.09	0.51	
1:B:13:VAL:HG23	1:B:73:TRP:CZ3	2.45	0.51	
1:A:732:GLN:HE22	1:A:760:GLY:HA2	1.76	0.51	
1:B:285:LEU:HD13	1:B:350:ASN:ND2	2.25	0.51	
1:A:191:MET:HB3	1:B:511:PHE:CE1	2.45	0.51	
1:B:312:VAL:HA	1:B:315:MET:HE3	1.91	0.51	
1:B:647:LYS:HA	1:B:659:GLY:HA2	1.93	0.51	
1:B:601:ASN:HB2	1:B:603:ILE:HD12	1.93	0.51	
1:B:732:GLN:OE1	1:B:757:ARG:HD2	2.10	0.51	
1:A:371:THR:HG23	1:A:400:TYR:CD1	2.46	0.51	
1:A:455:LEU:HD21	1:A:559:MET:CE	2.41	0.51	
1:B:693:GLN:O	1:B:694:SER:CB	2.55	0.50	
1:A:720:PHE:CE1	1:A:733:ILE:HD11	2.46	0.50	
1:B:85:TRP:CG	1:B:320:CYS:HB3	2.47	0.50	
1:B:285:LEU:HD13	1:B:350:ASN:CG	2.31	0.50	
1:A:109:LYS:NZ	1:A:112:LEU:HD22	2.26	0.50	
1:B:721:ARG:HG2	1:B:721:ARG:NH1	2.24	0.50	
1:A:576:ARG:O	1:A:580:THR:HG23	2.11	0.50	
1:A:17:GLN:NE2	1:A:100:ASN:OD1	2.44	0.50	
1:B:87:TYR:HD1	1:B:116:VAL:HG12	1.76	0.50	
1:A:396:HIS:HD2	1:A:757:ARG:HH21	1.59	0.50	
1:A:574:LEU:HD21	1:A:653:PRO:HB3	1.93	0.50	
1:A:627:ALA:O	1:B:188:VAL:HG13	2.12	0.50	
1:B:136:MET:HA	1:B:139:MET:CE	2.34	0.50	
1:B:109:LYS:CD	1:B:113:ARG:HH11	2.25	0.50	
1:B:496:GLU:HG3	1:B:624:PHE:CZ	2.47	0.49	
1:A:155:MET:HG2	1:A:272:GLY:HA3	1.94	0.49	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:109:LYS:CD	1:B:113:ARG:HD2	2.28	0.49	
1:A:84:LYS:HD2	1:A:126:ASP:OD1	2.12	0.49	
1:A:720:PHE:HE1	1:A:733:ILE:HD11	1.76	0.49	
1:B:369:CYS:HA	1:B:396:HIS:HE1	1.78	0.49	
1:B:588:MET:HE3	1:B:588:MET:HA	1.94	0.49	
1:A:449:LYS:O	1:A:453:VAL:HG23	2.13	0.49	
1:A:83:THR:HB	1:A:85:TRP:NE1	2.28	0.49	
1:B:563:VAL:HG11	1:B:571:MET:CE	2.42	0.49	
1:A:364:GLN:HG3	1:A:393:SER:HB2	1.95	0.49	
1:B:582:PHE:HD2	1:B:657:MET:HE2	1.78	0.48	
1:B:76:VAL:HG21	1:B:101:LEU:CD2	2.44	0.48	
1:B:563:VAL:HG12	1:B:564:PHE:CD2	2.48	0.48	
1:B:569:LEU:C	1:B:569:LEU:HD12	2.33	0.48	
1:B:335:HIS:HA	1:B:369:CYS:O	2.13	0.48	
1:A:260:TRP:CZ2	1:A:311:LYS:HB3	2.49	0.48	
1:A:446:ASN:CG	1:A:645:MET:HE3	2.34	0.48	
1:B:660:THR:HG23	1:B:661:PRO:HD2	1.95	0.48	
1:B:2:ILE:HD11	1:B:7:ALA:HB2	1.94	0.48	
1:B:335:HIS:ND1	1:B:371:THR:HG21	2.29	0.48	
1:B:364:GLN:HG3	1:B:393:SER:OG	2.14	0.48	
1:B:396:HIS:N	1:B:397:PRO:HD2	2.29	0.48	
1:A:280:TYR:CZ	1:A:284:MET:HG3	2.49	0.48	
1:B:260:TRP:CE2	1:B:311:LYS:HD2	2.49	0.48	
1:B:549:ILE:HG22	1:B:553:ILE:CD1	2.44	0.48	
1:A:76:VAL:HG12	1:A:78:MET:HE3	1.95	0.47	
1:A:401:ASN:HB2	1:A:724:PHE:CD1	2.49	0.47	
1:A:562:CYS:O	1:A:569:LEU:HD23	2.14	0.47	
1:B:103:PHE:CE1	1:B:108:ALA:HA	2.49	0.47	
1:B:766:VAL:O	1:B:766:VAL:HG23	2.13	0.47	
1:A:36:SER:HA	1:B:122:GLN:HB3	1.96	0.47	
1:A:81:ASP:OD1	1:A:81:ASP:N	2.46	0.47	
1:A:462:VAL:HG12	1:A:463:ILE:HG23	1.95	0.47	
1:B:584:GLY:O	1:B:585:LYS:HG3	2.15	0.47	
1:B:646:GLY:HA2	1:B:662:LEU:CD1	2.44	0.47	
1:A:326:ALA:C	1:A:640:ALA:HB3	2.33	0.47	
1:B:401:ASN:HB2	1:B:724:PHE:CD1	2.49	0.47	
1:B:563:VAL:HG22	1:B:569:LEU:HD12	1.95	0.47	
1:B:735:VAL:HG12	1:B:735:VAL:O	2.14	0.47	
1:B:22:LEU:CD2	1:B:112:LEU:HD13	2.44	0.47	
1:A:384:ARG:NH1	1:A:713:ILE:HG22	2.30	0.47	
1:A:396:HIS:HD2	1:A:757:ARG:NH2	2.12	0.47	



Interstomic Clash					
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:B:546:VAL:HG21	1:B:617:LEU:HD13	1.97	0.47		
1:B:754:ILE:O	1:B:764:TYR:HA	2.15	0.47		
1:A:154:THR:O	1:A:156:ASN:ND2	2.48	0.47		
1:A:384:ARG:HG2	1:A:713:ILE:HG21	1.97	0.47		
1:A:326:ALA:CA	1:A:640:ALA:HB3	2.45	0.46		
1:B:230:ARG:NH2	1:B:234:LEU:HD21	2.30	0.46		
1:B:341:GLN:HE22	1:B:420:ARG:HE	1.63	0.46		
1:A:258:LEU:HD23	1:A:258:LEU:C	2.36	0.46		
1:A:342:LEU:HD23	1:A:348:ALA:HB2	1.96	0.46		
1:A:454:MET:HE3	1:A:487:TYR:CA	2.46	0.46		
1:A:454:MET:CE	1:A:487:TYR:HB2	2.45	0.46		
1:A:732:GLN:C	1:A:733:ILE:HD12	2.35	0.46		
1:A:643:VAL:O	1:A:647:LYS:HG3	2.15	0.46		
1:B:232:GLU:O	1:B:236:ILE:HD12	2.14	0.46		
1:A:463:ILE:O	1:A:463:ILE:HD12	2.15	0.46		
1:A:244:VAL:HG22	1:A:258:LEU:HB2	1.95	0.46		
1:B:639:GLN:HB3	1:B:640:ALA:H	1.63	0.46		
1:B:548:GLY:O	1:B:549:ILE:HG12	2.16	0.46		
1:A:21:ASP:OD1	1:A:23:ASP:HB2	2.16	0.46		
1:B:106:ALA:O	1:B:110:GLU:CB	2.64	0.45		
1:A:349:CYS:SG	1:A:378:ILE:HD11	2.56	0.45		
1:B:109:LYS:O	1:B:110:GLU:C	2.54	0.45		
1:A:338:LEU:O	1:A:339:ALA:HB3	2.16	0.45		
1:B:438:PHE:CE2	1:B:440:SER:HB3	2.52	0.45		
1:B:67:GLY:O	1:B:311:LYS:HE3	2.16	0.45		
1:B:423:GLY:HA3	1:B:433:LEU:HD21	1.98	0.45		
1:B:570:THR:HB	3:B:946:HOH:O	2.17	0.45		
1:B:86:LEU:HG	1:B:116:VAL:HG21	1.97	0.45		
1:A:578:LEU:HD13	1:A:651:ALA:O	2.16	0.45		
1:B:478:THR:N	1:B:482:ASP:OD2	2.49	0.45		
1:B:593:LEU:HD23	1:B:593:LEU:HA	1.85	0.45		
1:B:81:ASP:OD1	1:B:81:ASP:N	2.50	0.45		
1:A:332:LEU:HB3	1:A:334:MET:SD	2.56	0.45		
1:B:586:GLU:HG3	1:B:586:GLU:O	2.17	0.45		
1:B:424:ILE:HD13	1:B:428:ILE:HA	1.99	0.45		
1:B:109:LYS:HB3	1:B:109:LYS:HE2	1.53	0.44		
1:B:240:ASN:HD21	1:B:253:LEU:HD23	1.82	0.44		
1:B:357:LEU:HD11	1:B:386:ALA:HB2	1.98	0.44		
1:B:478:THR:HB	1:B:482:ASP:OD2	2.17	0.44		
1:A:455:LEU:HD21	1:A:559:MET:HE3	1.98	0.44		
1:A:726:GLN:O	1:A:727:ASN:HB2	2.17	0.44		



		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:B:549:ILE:HD12	1:B:613:LEU:CD2	2.47	0.44	
1:B:588:MET:HE3	1:B:588:MET:CA	2.47	0.44	
1:A:167:ARG:HB3	1:A:171:TYR:CB	2.47	0.44	
1:A:558:ALA:O	1:A:562:CYS:HB2	2.18	0.44	
1:A:677:PRO:HD3	1:A:782:GLN:HB3	2.00	0.44	
1:B:384:ARG:HA	1:B:387:ILE:HD12	1.99	0.44	
1:A:349:CYS:SG	1:A:378:ILE:CD1	3.05	0.44	
1:B:91:ASP:OD1	1:B:113:ARG:NH2	2.50	0.44	
1:B:110:GLU:O	1:B:111:GLU:CB	2.65	0.44	
1:B:139:MET:HE2	1:B:139:MET:HB2	1.80	0.44	
1:B:167:ARG:HB3	1:B:171:TYR:CB	2.48	0.44	
1:B:639:GLN:HA	1:B:759:ALA:HB1	1.98	0.44	
1:A:280:TYR:O	1:A:284:MET:HB2	2.18	0.44	
1:A:524:GLY:O	1:A:528:LYS:HD3	2.17	0.44	
1:B:733:ILE:HD13	1:B:735:VAL:HG23	2.00	0.44	
1:A:85:TRP:CD2	1:A:320:CYS:HA	2.53	0.44	
1:A:57:ILE:HG13	1:A:57:ILE:O	2.17	0.43	
1:A:608:LYS:HB3	1:A:608:LYS:HE3	1.87	0.43	
1:A:677:PRO:HD2	1:A:785:LEU:CB	2.47	0.43	
1:B:142:VAL:HG11	1:B:460:ASP:OD2	2.18	0.43	
1:B:352:LEU:HD12	1:B:352:LEU:O	2.18	0.43	
1:B:622:LYS:HE3	1:B:632:TYR:O	2.18	0.43	
1:A:35:PRO:CG	1:B:118:THR:HG22	2.48	0.43	
1:A:145:PHE:HA	1:A:444:TYR:O	2.18	0.43	
1:A:540:HIS:ND1	1:A:626:ASP:OD2	2.49	0.43	
1:B:22:LEU:HD11	1:B:107:ALA:HB1	1.99	0.43	
1:A:774:ASN:O	1:A:778:GLU:HG3	2.18	0.43	
1:B:255:ALA:O	1:B:259:VAL:HG23	2.17	0.43	
1:B:347:ASP:OD1	1:B:378:ILE:HA	2.19	0.43	
1:B:227:ASP:OD1	1:B:228:PRO:HD2	2.19	0.43	
1:B:371:THR:HB	1:B:400:TYR:CD1	2.51	0.43	
1:B:22:LEU:HD22	1:B:112:LEU:HD13	2.01	0.43	
1:B:354:ASN:HB3	1:B:358:ARG:NH2	2.33	0.43	
1:B:549:ILE:HG22	1:B:553:ILE:HD11	2.00	0.43	
1:B:554:ASP:OD1	1:B:598:LYS:HA	2.18	0.43	
1:B:761:TYR:O	1:B:762:SER:CB	2.66	0.43	
1:A:541:TYR:HB3	1:A:631:PRO:HD2	2.00	0.43	
1:B:59:ILE:HG13	1:B:217:LEU:HD23	1.99	0.43	
1:B:152:GLN:OE1	1:B:272:GLY:HA2	2.19	0.43	
1:B:247:ASN:HB3	1:B:248:PRO:HD2	2.00	0.43	
1:B:394:GLY:O	1:B:395:GLY:C	2.57	0.43	



	lo uo pugom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:534:GLN:O	1:B:535:LYS:HB2	2.19	0.43	
1:A:547:ALA:HB1	1:A:645:MET:HE2	2.00	0.43	
1:A:37:MET:HG3	1:B:81:ASP:O	2.18	0.42	
1:A:145:PHE:CD2	1:A:498:PHE:HB2	2.54	0.42	
1:B:372:PHE:CZ	1:B:378:ILE:HD11	2.54	0.42	
1:A:111:GLU:O	1:A:112:LEU:C	2.56	0.42	
1:A:173:ILE:O	1:A:177:LYS:HG3	2.19	0.42	
1:A:405:ALA:HB2	1:A:729:PHE:HE1	1.84	0.42	
1:A:555:SER:N	1:A:654:ASP:HB3	2.34	0.42	
1:A:604:GLU:HA	1:A:607:ASP:HB2	2.00	0.42	
1:B:258:LEU:C	1:B:258:LEU:HD23	2.39	0.42	
1:B:277:LEU:HB2	1:B:336:ILE:HG12	2.01	0.42	
1:B:701:ARG:HA	1:B:734:ASN:O	2.18	0.42	
1:B:756:VAL:O	1:B:762:SER:HA	2.19	0.42	
1:A:408:TYR:HD2	1:A:430:PRO:HG2	1.83	0.42	
1:A:454:MET:HE3	1:A:487:TYR:CB	2.48	0.42	
1:B:457:ASN:HB3	3:B:984:HOH:O	2.20	0.42	
1:B:657:MET:O	1:B:660:THR:HB	2.20	0.42	
1:B:700:GLN:O	1:B:733:ILE:HA	2.19	0.42	
1:A:457:ASN:OD1	1:A:470:GLU:HA	2.19	0.42	
1:B:588:MET:HE2	1:B:588:MET:HB3	1.86	0.42	
1:B:710:GLU:C	1:B:712:GLY:H	2.23	0.42	
1:A:429:GLU:OE2	2:A:801:UY7:O09	2.36	0.42	
1:A:81:ASP:O	1:B:37:MET:HG3	2.19	0.42	
1:A:641:TYR:O	1:A:645:MET:HB2	2.19	0.42	
1:A:165:ILE:O	1:A:249:PRO:HD2	2.20	0.42	
1:B:732:GLN:CD	1:B:757:ARG:HD2	2.40	0.42	
1:A:76:VAL:HG12	1:A:78:MET:CE	2.49	0.42	
1:A:563:VAL:HG11	1:A:571:MET:HG2	2.01	0.41	
1:A:563:VAL:HG13	1:A:569:LEU:O	2.19	0.41	
1:A:638:THR:HG23	1:A:665:ASN:CA	2.46	0.41	
1:A:597:PRO:CB	1:A:603:ILE:HG21	2.50	0.41	
1:B:148:GLY:O	1:B:149:ILE:C	2.58	0.41	
1:A:336:ILE:HD12	1:A:368:PRO:HG2	2.02	0.41	
1:B:227:ASP:CG	1:B:229:LYS:HG2	2.41	0.41	
1:A:454:MET:HE2	1:A:483:VAL:O	2.20	0.41	
1:B:263:HIS:HE2	1:B:315:MET:HE1	1.85	0.41	
1:A:691:VAL:HB	1:A:692:PRO:HD3	2.02	0.41	
1:B:285:LEU:HB3	1:B:286:PRO:HD3	2.03	0.41	
1:A:552:MET:HE2	1:A:613:LEU:HD13	2.02	0.41	
1:B:23:ASP:OD2	1:B:56:GLU:N	2.47	0.41	



A + 1	A + 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:103:PHE:CE1	1:A:108:ALA:HA	2.55	0.41	
1:A:559:MET:CE	1:A:571:MET:HE3	2.51	0.41	
1:A:731:ILE:HD12	1:A:732:GLN:N	2.32	0.41	
1:B:459:TYR:CZ	1:B:466:LYS:HB2	2.56	0.41	
1:B:639:GLN:HA	1:B:759:ALA:CB	2.50	0.41	
1:B:752:ARG:HA	1:B:766:VAL:HG21	2.02	0.41	
1:A:135:ASP:OD1	1:A:135:ASP:N	2.53	0.41	
1:A:247:ASN:HB3	1:A:248:PRO:HD2	2.01	0.41	
1:A:378:ILE:O	1:A:378:ILE:HG23	2.21	0.40	
1:A:737:ASP:CB	1:A:740:THR:OG1	2.69	0.40	
1:B:351:GLU:HA	1:B:351:GLU:OE1	2.21	0.40	
1:A:766:VAL:HG22	3:A:1019:HOH:O	2.20	0.40	
1:B:149:ILE:H	1:B:441:ASN:ND2	2.19	0.40	
1:B:755:LEU:HD13	1:B:764:TYR:CD1	2.56	0.40	
1:A:48:PHE:CZ	1:A:52:LEU:HD11	2.57	0.40	
1:A:559:MET:CE	1:A:571:MET:CE	3.00	0.40	
1:B:14:ARG:HG3	1:B:14:ARG:O	2.21	0.40	
1:B:392:ASP:O	1:B:393:SER:CB	2.60	0.40	
1:B:716:ILE:O	1:B:717:GLU:C	2.59	0.40	
1:B:569:LEU:CD1	1:B:569:LEU:C	2.90	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	\mathbf{ntiles}
1	А	783/785~(100%)	730~(93%)	46 (6%)	7 (1%)	17	40
1	В	783/785~(100%)	719~(92%)	51 (6%)	13 (2%)	9	23
All	All	1566/1570~(100%)	1449 (92%)	97~(6%)	20 (1%)	12	30

All (20) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	114	GLN
1	В	394	GLY
1	А	464	GLY
1	В	393	SER
1	В	395	GLY
1	А	339	ALA
1	В	110	GLU
1	В	718	SER
1	А	98	SER
1	А	105	SER
1	А	392	ASP
1	В	108	ALA
1	В	694	SER
1	В	396	HIS
1	В	549	ILE
1	В	762	SER
1	В	766	VAL
1	А	149	ILE
1	В	397	PRO
1	В	707	VAL

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	Analysed Rotameric Outliers		Percentiles		
1	А	641/669~(96%)	629~(98%)	12 (2%)	57 82		
1	В	614/669~(92%)	603~(98%)	11 (2%)	59 83		
All	All	1255/1338~(94%)	1232~(98%)	23~(2%)	59 83		

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	3	SER
1	А	274	ASP
1	А	324	SER
1	А	337	MET



Mol	Chain	Res	Type
1	А	459	TYR
1	А	588	MET
1	А	608	LYS
1	А	656	ARG
1	А	664	ASP
1	А	732	GLN
1	А	737	ASP
1	А	738	ASP
1	В	23	ASP
1	В	88	ASP
1	В	220	LYS
1	В	261	PHE
1	В	274	ASP
1	В	393	SER
1	В	396	HIS
1	В	569	LEU
1	В	664	ASP
1	В	710	GLU
1	В	762	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	396	HIS
1	А	699	ASN
1	А	732	GLN
1	В	341	GLN
1	В	377	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)

2 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	Trune	Chain	Dec	Tinle	B	ond leng	gths	B	ond ang	gles
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	UY7	В	801	-	6,9,9	6.12	4 (66%)	5,12,12	0.99	0
2	UY7	А	801	-	6,9,9	5.99	4 (66%)	5,12,12	1.85	1 (20%)

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	UY7	В	801	-	-	0/0/13/13	0/1/1/1
2	UY7	А	801	-	-	0/0/13/13	0/1/1/1

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	В	801	UY7	CD-CG	-9.42	1.30	1.53
2	А	801	UY7	CB-CA	-8.99	1.35	1.54
2	А	801	UY7	CD-CG	-8.92	1.32	1.53
2	В	801	UY7	CB-CA	-8.86	1.35	1.54
2	В	801	UY7	CB-CG	6.51	1.65	1.52
2	А	801	UY7	CB-CG	6.39	1.64	1.52
2	В	801	UY7	CD-N	3.75	1.60	1.47
2	А	801	UY7	CD-N	3.63	1.60	1.47

All (8) bond length outliers are listed below:

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	801	UY7	CB-CG-CD	3.72	107.83	103.27

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	801	UY7	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	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	785/785~(100%)	-0.06	25 (3%) 47 48	26, 44, 70, 84	0
1	В	785/785~(100%)	0.03	43 (5%) 25 24	24, 44, 80, 111	0
All	All	1570/1570~(100%)	-0.02	68 (4%) 35 33	24, 44, 75, 111	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	114	GLN	5.8
1	В	751	HIS	5.0
1	В	743	ALA	4.9
1	В	774	ASN	4.5
1	В	674	VAL	4.0
1	В	744	ALA	3.9
1	В	747	ASN	3.8
1	В	675	ASN	3.6
1	В	748	PRO	3.5
1	В	784	GLY	3.3
1	В	772	ILE	3.2
1	В	745	GLN	3.2
1	А	715	ILE	3.2
1	В	750	ASP	3.1
1	В	326	ALA	3.1
1	А	745	GLN	3.0
1	А	587	ASN	2.9
1	А	583	GLU	2.9
1	В	773	GLN	2.9
1	В	671	GLY	2.9
1	A	749	ASP	2.9
1	А	547	ALA	2.9
1	В	696	LEU	2.8
1	А	462	VAL	2.8



Mol	Chain	Res	Type	RSRZ	
1	А	703 ASP		2.7	
1	А	747 ASN		2.7	
1	В	746 LYS		2.7	
1	В	777 ILE		2.7	
1	В	568	TYR	2.7	
1	В	267	SER	2.7	
1	В	741	LEU	2.6	
1	В	599	PHE	2.6	
1	А	463	ILE	2.5	
1	А	293	ALA	2.5	
1	А	638	THR	2.5	
1	В	737	ASP	2.5	
1	В	265	ALA	2.5	
1	А	665	ASN	2.5	
1	А	766	VAL	2.4	
1	В	781	ILE	2.4	
1	В	98	SER	2.4	
1	А	737	ASP	2.3	
1	А	741	LEU	2.3	
1	В	636	VAL	2.3	
1	В	707	VAL	2.3	
1	В	766	VAL	2.3	
1	А	427	CYS	2.3	
1	А	697	LEU	2.3	
1	В	686	CYS	2.3	
1	В	780	THR	2.2	
1	В	749	ASP	2.2	
1	В	738	ASP	2.2	
1	А	751	HIS	2.2	
1	А	698	LEU	2.1	
1	А	548	GLY	2.1	
1	В	427	CYS	2.1	
1	В	602	ASP	2.1	
1	В	742	ARG	2.1	
1	А	637	ALA	2.1	
1	В	676	GLY	2.1	
1	В	266	ILE	2.1	
1	В	770	GLU	2.0	
1	А	742	ARG	2.0	
1	В	263	HIS	2.0	
1	В	778	GLU	2.0	
1	В	322	ASN	2.0	



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Mol	Chain	Res	Type	RSRZ
1	А	278	GLY	2.0
1	В	783	ARG	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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	UY7	А	801	9/9	0.96	0.17	$38,\!48,\!57,\!58$	0
2	UY7	В	801	9/9	0.97	0.14	$50,\!54,\!64,\!64$	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.

