

Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2021 – 01:04 pm BST

PDB ID	:	6ZA2
Title	:	Crystal structure of dimeric latent PorU from Porphyromonas gingivalis
Authors	:	Gomis-Ruth, F.X.; Goulas, T.; Guevara, T.; Rodriguez-Banqueri, A.;
		Potempa, J.
Deposited on	:	2020-06-04
Resolution	:	3.35 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
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42 - 3.30)
Ramachandran outliers	138981	1599(3.42-3.30)
Sidechain outliers	138945	1598(3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	1156	3% 83%	10%	6%
1	В	1156	5% 85%	9%	• 6%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 31870 atoms, of which 15484 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 Por secretion system protein porU.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	А	1081	Total	C 5180	H 7891	N 1406	0 1508	S 24	7821	0	0
			10040	0109	1021	1400	1598	34			
1	В	1083	Total	С	Н	Ν	0	\mathbf{S}	7663	0	0
1	D	D 1003		5128	7663	1395	1595	33	1000		0

Chain	Residue	Modelled	Actual	Comment	Reference
А	3	GLY	-	expression tag	UNP B2RGP6
А	4	SER	-	expression tag	UNP B2RGP6
А	5	SER	-	expression tag	UNP B2RGP6
А	6	HIS	-	expression tag	UNP B2RGP6
А	7	HIS	-	expression tag	UNP B2RGP6
А	8	HIS	-	expression tag	UNP B2RGP6
А	9	HIS	-	expression tag	UNP B2RGP6
А	10	HIS	-	expression tag	UNP B2RGP6
А	11	HIS	-	expression tag	UNP B2RGP6
А	12	SER	-	expression tag	UNP B2RGP6
А	13	GLN	-	expression tag	UNP B2RGP6
А	14	ASP	-	expression tag	UNP B2RGP6
А	15	PRO	-	expression tag	UNP B2RGP6
А	16	ASN	-	expression tag	UNP B2RGP6
А	17	SER	-	expression tag	UNP B2RGP6
А	18	SER	-	expression tag	UNP B2RGP6
А	19	SER	-	expression tag	UNP B2RGP6
А	20	ALA	-	expression tag	UNP B2RGP6
А	21	ARG	-	expression tag	UNP B2RGP6
А	22	LEU	-	expression tag	UNP B2RGP6
А	23	GLN	-	expression tag	UNP B2RGP6
В	-21	GLY	-	expression tag	UNP B2RGP6
В	-20	SER	-	expression tag	UNP B2RGP6
В	-19	SER	-	expression tag	UNP B2RGP6
В	-18	HIS	-	expression tag	UNP B2RGP6

There are 42 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
В	-17	HIS	-	expression tag	UNP B2RGP6
В	-16	HIS	-	expression tag	UNP B2RGP6
В	-15	HIS	-	expression tag	UNP B2RGP6
В	-14	HIS	-	expression tag	UNP B2RGP6
В	-13	HIS	-	expression tag	UNP B2RGP6
В	-12	SER	-	expression tag	UNP B2RGP6
В	-11	GLN	-	expression tag	UNP B2RGP6
В	-10	ASP	-	expression tag	UNP B2RGP6
В	-9	PRO	-	expression tag	UNP B2RGP6
В	-8	ASN	-	expression tag	UNP B2RGP6
В	-7	SER	-	expression tag	UNP B2RGP6
В	-6	SER	-	expression tag	UNP B2RGP6
В	-5	SER	-	expression tag	UNP B2RGP6
В	-4	ALA	-	expression tag	UNP B2RGP6
В	-3	ARG	-	expression tag	UNP B2RGP6
В	-2	LEU	-	expression tag	UNP B2RGP6
В	-1	GLN	-	expression tag	UNP B2RGP6

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Ca 2 2	0	0
2	В	2	Total Ca 2 2	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total O 2 2	0	0
3	В	2	Total O 2 2	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: Por secretion system protein porU

• Molecule 1: Por secretion system protein porU









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	171.70Å 171.70Å 440.40Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution(A)	88.48 - 3.35	Depositor
Resolution (A)	88.48 - 3.35	EDS
% Data completeness	100.0 (88.48-3.35)	Depositor
(in resolution range)	$100.0 \ (88.48-3.35)$	EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.14 (at 3.33 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
P. P.	0.202 , 0.243	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.206 , 0.235	DCC
R_{free} test set	836 reflections $(1.49%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	125.7	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for $twinning^2$	$ L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31870	wwPDB-VP
Average B, all atoms $(Å^2)$	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.44% 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: CA

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

Mal	Chain	Bond	lengths	Bond angles		
Moi Chai	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.52	0/8404	0.70	1/11434~(0.0%)	
1	В	0.51	0/8323	0.71	1/11338~(0.0%)	
All	All	0.52	0/16727	0.70	2/22772~(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	2
1	В	0	2
All	All	0	4

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	В	571	ARG	CD-NE-CZ	11.93	140.31	123.60
1	А	571	ARG	CD-NE-CZ	6.36	132.50	123.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	614	MET	Mainchain
1	А	929	ILE	Mainchain
1	В	614	MET	Mainchain
1	В	929	ILE	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	8227	7821	7821	24	0
1	В	8151	7663	7665	23	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
3	А	2	0	0	0	0
3	В	2	0	0	0	0
All	All	16386	15484	15486	42	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 1.

All (42) 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:A:861:LEU:HD11	1:B:738:ARG:HG2	1.73	0.69	
1:A:985:ILE:HG23	1:A:1033:VAL:HG12	1.77	0.65	
1:A:738:ARG:HG2	1:B:861:LEU:HD11	1.80	0.62	
1:B:504:LEU:C	1:B:504:LEU:HD22	2.24	0.57	
1:A:333:VAL:HG21	1:A:361:ILE:HG12	1.87	0.57	
1:A:427:ARG:HB3	1:A:433:LEU:HD21	1.87	0.56	
1:A:563:ARG:HD2	1:B:663:TRP:CE2	2.43	0.54	
1:B:874:ALA:HB3	1:B:1008:THR:OG1	2.09	0.53	
1:B:241:PHE:CE1	1:B:264:LEU:HD22	2.45	0.52	
1:A:241:PHE:CE1	1:A:264:LEU:HD22	2.45	0.51	
1:A:499:TRP:CE3	1:A:504:LEU:HB3	2.47	0.50	
1:A:235:ALA:HB1	1:A:277:LEU:HD11	1.94	0.50	
1:A:1103:VAL:HB	1:A:1116:ILE:HD11	1.94	0.49	
1:A:563:ARG:HD2	1:B:663:TRP:CZ2	2.47	0.49	
1:B:235:ALA:HB1	1:B:277:LEU:HD11	1.95	0.49	
1:B:1103:VAL:HB	1:B:1116:ILE:HD11	1.94	0.49	
1:B:995:LEU:HD13	1:B:995:LEU:N	2.28	0.49	
1:A:860:ASP:C	1:A:861:LEU:HG	2.35	0.47	
1:A:907:ALA:HB3	1:A:916:ALA:HB3	1.97	0.47	
1:B:907:ALA:HB3	1:B:916:ALA:HB3	1.97	0.46	
1:B:782:ASP:HB3	1:B:785:VAL:HG23	1.98	0.45	



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:860:ASP:C	1:B:861:LEU:HG	2.37	0.44
1:B:769:PRO:HA	1:B:773:ASN:HB2	2.00	0.44
1:A:766:THR:O	1:A:766:THR:HG23	2.18	0.44
1:A:1114:ILE:HG23	1:B:249:SER:OG	2.18	0.44
1:A:544:TRP:CZ3	1:A:767:VAL:HG11	2.53	0.43
1:B:264:LEU:HD12	1:B:264:LEU:N	2.33	0.43
1:A:868:TYR:N	1:A:869:PRO:HD3	2.35	0.42
1:B:162:ILE:HD11	1:B:328:PHE:CE1	2.55	0.42
1:A:264:LEU:N	1:A:264:LEU:HD12	2.34	0.42
1:A:854:LEU:HD23	1:A:854:LEU:HA	1.96	0.42
1:A:720:THR:HG23	1:A:776:SER:O	2.20	0.41
1:B:724:VAL:HG21	1:B:775:LEU:HB3	2.01	0.41
1:A:493:ARG:CB	1:A:495:VAL:HG13	2.51	0.41
1:A:672:ASN:OD1	1:A:677:PHE:HB3	2.21	0.41
1:A:724:VAL:HG21	1:A:775:LEU:HB3	2.02	0.41
1:B:112:VAL:HG22	1:B:127:VAL:HG12	2.03	0.41
1:B:841:PHE:CD2	1:B:841:PHE:N	2.88	0.41
1:B:493:ARG:CB	1:B:495:VAL:HG13	2.51	0.41
1:B:766:THR:HB	1:B:769:PRO:HD2	2.02	0.41
1:B:493:ARG:HB3	1:B:495:VAL:HG13	2.02	0.40
1:A:493:ARG:HB3	1:A:495:VAL:HG13	2.03	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	1073/1156~(93%)	993~(92%)	64 (6%)	16 (2%)	10	39
1	В	1075/1156~(93%)	1004 (93%)	55 (5%)	16 (2%)	10	39
All	All	2148/2312 (93%)	1997 (93%)	119 (6%)	32 (2%)	10	39



Mol	Chain	Res	Type
1	А	712	SER
1	А	894	VAL
1	А	981	VAL
1	В	258	ALA
1	В	712	SER
1	В	894	VAL
1	В	900	GLU
1	В	981	VAL
1	А	25	ARG
1	А	203	ARG
1	А	258	ALA
1	А	678	ASN
1	В	203	ARG
1	В	506	GLN
1	В	729	ASN
1	В	930	PRO
1	А	615	PRO
1	А	661	ALA
1	А	679	TYR
1	В	102	ASN
1	В	661	ALA
1	А	683	PRO
1	А	729	ASN
1	В	771	SER
1	В	181	SER
1	В	683	PRO
1	А	181	SER
1	А	713	GLY
1	В	713	GLY
1	А	502	PRO
1	В	154	GLY
1	А	154	GLY

All (32) Ramachandran outliers are listed below:

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	Perce	entiles
1	А	859/978~(88%)	793~(92%)	66~(8%)	13	41
1	В	839/978~(86%)	778~(93%)	61 (7%)	14	43
All	All	1698/1956~(87%)	1571 (92%)	127 (8%)	13	42

All (127) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	27	MET
1	А	29	LYS
1	А	35	LEU
1	А	54	LEU
1	А	65	SER
1	А	99	ARG
1	А	126	THR
1	А	150	GLN
1	А	170	LEU
1	А	175	LEU
1	А	203	ARG
1	А	209	SER
1	А	229	ARG
1	А	239	LEU
1	А	248	THR
1	А	256	TYR
1	А	267	SER
1	А	268	THR
1	А	273	LEU
1	А	301	ASN
1	А	318	LEU
1	А	325	SER
1	А	341	GLN
1	А	355	THR
1	А	356	VAL
1	А	391	ILE
1	А	421	ASP
1	А	502	PRO
1	А	503	TYR
1	А	575	ASP
1	А	576	ARG
1	А	666	GLU
1	А	719	SER
1	А	764	LEU
1	А	787	MET



Mol	Chain	Res	Type
1	A	831	THR
1	A	856	GLU
1	A	859	ASN
1	A	861	LEU
1	A	893	ASP
1	A	899	HIS
1	A	900	GLU
1	A	906	TYR
1	A	934	THR
1	A	938	THR
1	A	959	ASN
1	A	971	LEU
1	A	981	VAL
1	A	994	ASP
1	A	995	LEU
1	A	1004	THR
1	A	1005	SER
1	А	1028	THR
1	A	1032	THR
1	А	1039	ASN
1	А	1070	SER
1	А	1072	THR
1	А	1082	SER
1	А	1083	ASP
1	А	1100	SER
1	А	1101	LEU
1	А	1105	THR
1	А	1107	SER
1	А	1132	PHE
1	А	1141	SER
1	А	1145	GLN
1	В	33	ARG
1	В	35	LEU
1	В	65	SER
1	В	98	LEU
1	В	102	ASN
1	В	126	THR
1	В	170	LEU
1	В	175	LEU
1	В	203	ARG
1	В	209	SER
1	В	229	ARG



Mol	Chain	Res	Type
1	B	234	SEB
1	B	239	LEU
1	B	248	THR
1	B	257	LEU
1	B	267	SEB
1	B	268	THR
1	B	273	LEU
1	B	318	LEU
1	B	325	SEB
1	B	341	GLN
1	B	355	THR
1	B	356	VAL
1	B	421	ASP
1	B	504	LEU
1	B	575	ASP
1	B	576	ARG
1	B	666	GLU
1	B	678	ASN
1	B	682	MET
1	B	719	SER
1	B	724	VAL
1	B	764	LEU
1	B	774	GLN
1	B	787	MET
1	В	831	THR
1	B	861	LEU
1	B	872	MET
1	В	889	ILE
1	В	893	ASP
1	В	906	TYR
1	В	938	THR
1	В	959	ASN
1	В	971	LEU
1	В	995	LEU
1	В	1004	THR
1	В	1005	SER
1	В	1014	THR
1	В	1022	LEU
1	В	1028	THR
1	В	1032	THR
1	В	1039	ASN
1	В	1070	SER
	1	1	



Continued from previous page						
Mol	Chain	Res	Type			
1	В	1072	THR			
1	В	1078	ASN			
1	В	1079	ARG			
1	В	1084	LEU			
1	В	1100	SER			
1	В	1101	LEU			
1	В	1132	PHE			
1	В	1141	SER			

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	282	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



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		>2	$OWAB(Å^2)$	Q<0.9
1	А	1081/1156~(93%)	0.35	34 (3%)	49	52	85, 127, 218, 290	0
1	В	1083/1156~(93%)	0.40	59 (5%)	25	28	85, 134, 257, 289	0
All	All	2164/2312~(93%)	0.38	93 (4%)	35	38	85, 130, 250, 290	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	690	CYS	11.3
1	В	703	GLY	9.9
1	А	621	ASP	5.6
1	А	704	GLU	5.1
1	В	981	VAL	4.9
1	В	929	ILE	4.8
1	А	588	ALA	4.5
1	В	930	PRO	4.4
1	А	587	PHE	4.0
1	В	100	GLN	4.0
1	В	638	LYS	3.9
1	В	987	LEU	3.8
1	В	872	MET	3.8
1	А	520	ASN	3.7
1	А	586	CYS	3.7
1	А	541	ASN	3.6
1	А	400	LEU	3.5
1	В	867	ASP	3.5
1	В	231	MET	3.3
1	В	1065	ASN	3.3
1	В	1022	LEU	3.3
1	А	412	SER	3.2
1	В	811	ILE	3.1
1	В	999	LEU	3.0



Mol	Chain	Res	Type	RSRZ	
1	А	544	TRP	3.0	
1	А	677	PHE	3.0	
1	А	287	GLY	3.0	
1	В	968	VAL	3.0	
1	В	947	LEU	2.9	
1	А	646	GLN	2.8	
1	А	363	PHE	2.8	
1	В	813	LEU	2.8	
1	А	216	PHE	2.8	
1	В	931	ASP	2.8	
1	А	212	LEU	2.7	
1	А	245	PHE	2.7	
1	В	934	THR	2.7	
1	В	503	TYR	2.6	
1	В	958	VAL	2.6	
1	А	638	LYS	2.6	
1	В	1033	VAL	2.6	
1	А	54	LEU	2.6	
1	В	735	PHE	2.6	
1	В	675	HIS	2.6	
1	А	485	PHE	2.5	
1	В	1073	PHE	2.5	
1	В	716	ILE	2.5	
1	В	485	PHE	2.5	
1	А	860	ASP	2.5	
1	В	1015	ILE	2.5	
1	В	423	LEU	2.4	
1	А	963	LEU	2.4	
1	В	258	ALA	2.4	
1	В	960	PRO	2.4	
1	А	222	ALA	2.4	
1	В	996	THR	2.4	
1	В	1054	ALA	2.4	
1	В	989	ILE	2.4	
1	В	923	ILE	2.4	
1	В	677	PHE	2.3	
1	В	1053	ILE	2.3	
1	В	530	PHE	2.3	
1	В	845	PHE	2.3	
1	В	569	THR	2.2	
1	В	1128	ILE	2.2	
1	А	934	THR	2.2	



Continued from previous page							
Mol	Chain	Res	Type	RSRZ			
1	В	993	ALA	2.2			
1	В	980	GLY	2.2			
1	А	958	VAL	2.1			
1	А	732	ILE	2.1			
1	А	504	LEU	2.1			
1	В	685	TRP	2.1			
1	В	925	VAL	2.1			
1	В	412	SER	2.1			
1	В	957	GLU	2.1			
1	В	660	PRO	2.1			
1	А	740	MET	2.1			
1	В	671	LEU	2.1			
1	В	1019	ILE	2.1			
1	В	614	MET	2.1			
1	В	1158	GLN	2.1			
1	В	1124	TYR	2.1			
1	В	554	PHE	2.1			
1	В	871	VAL	2.1			
1	А	519	THR	2.1			
1	А	1087	VAL	2.1			
1	В	775	LEU	2.0			
1	А	741	PHE	2.0			
1	В	400	LEU	2.0			
1	В	765	SER	2.0			
1	А	530	PHE	2.0			
1	В	1154	ILE	2.0			
1	А	435	VAL	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,



Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
2	CA	А	2002	1/1	0.63	0.11	169, 169, 169, 169, 169	0
2	CA	В	2002	1/1	0.76	0.10	213,213,213,213	0
2	CA	А	2001	1/1	0.97	0.21	106,106,106,106	0
2	CA	В	2001	1/1	0.98	0.23	103,103,103,103	0

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.

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.

