

Full wwPDB X-ray Structure Validation Report (i)

Mar 6, 2023 – 12:29 pm GMT

PDB ID	:	8AYR							
Title	:	Sialidases and Fucosidases of Akkermansia muciniphila are key for rapid growth							
		on colonic mucin and nutrient sharing amongst mucin-associated human gut microbiota							
Authors	:	Sakanaka, H.; Nielsen, T.S.; Pichler, M.J.; Nordberg Karlsson, E.; Abou							
		Hachem, M.; Morth, J.P.							
Deposited on	:	2022-09-02							
Resolution	:	2.70 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
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
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)	:	2.32.1

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 2.70 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	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
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	704	^{2%} 74%	21%	•••		
1	В	704	4%	22%	•••		



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2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10626 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 Coagulation factor 5/8 type domain protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A 677		Total	С	Ν	0	\mathbf{S}	0	0	0
	011	5303	3366	949	974	14	0			
1	Р	676	Total	С	Ν	0	\mathbf{S}	0	0	0
	070	5299	3364	948	973	14	0	0	0	

• 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	6	Total O 6 6	0	0
3	В	14	Total O 14 14	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.

 \bullet Molecule 1: Coagulation factor 5/8 type domain protein





G657 F656 K672 K653 K673 K673 K673 K415 V408 K415 7660 K578 K663 K578 K47 A415 7660 K578 K678 K47 A423 7671 K593 K47 A423 7673 K593 K47 A436 7671 K583 E438 A433 7673 K678 K447 A436 7671 K678 K447 A436 7671 K678 K447 A436 7693 K683 K447 A436 7693 K683 K447 A436 7694 K691 K447 A432 7693 K691 K447 A432 7694 K691 K447 A432 7693 K691 K447 A432 7694 K691 K447 A432 7694 K691 K447 A432 7694 K691 K447 A432 7694 K616



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	76.19Å 76.45Å 84.50Å	Deperitor
a, b, c, α , β , γ	88.41° 89.08° 88.23°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	34.51 - 2.70	Depositor
Resolution (A)	34.51 - 2.70	EDS
% Data completeness	90.4 (34.51-2.70)	Depositor
(in resolution range)	90.6(34.51-2.70)	EDS
R _{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.06 (at 2.68 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
D D.	0.233 , 0.275	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.236 , 0.278	DCC
R_{free} test set	2453 reflections $(5.19%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	58.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.28, 43.1	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.34$	Xtriage
	0.000 for k,-h,l	
	0.000 for -k,h,l	
	0.000 for h,-k,-l	
Estimated twinning fraction	0.000 for -h,k,-l	Xtriage
	0.000 for -h,-k,l	
	0.000 for k,h,-l	
	0.000 for -k,-h,-l	
F_o, F_c correlation	0.94	EDS
Total number of atoms	10626	wwPDB-VP
Average B, all atoms $(Å^2)$	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.87% 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).

Mol	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.31	0/5453	0.60	2/7424~(0.0%)	
1	В	0.31	0/5449	0.61	3/7419~(0.0%)	
All	All	0.31	0/10902	0.60	5/14843~(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	В	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	340	ARG	CG-CD-NE	6.19	124.80	111.80
1	В	86	LEU	CA-CB-CG	5.89	128.84	115.30
1	А	86	LEU	CA-CB-CG	5.71	128.42	115.30
1	В	126	LYS	CA-CB-CG	-5.48	101.35	113.40
1	В	692	GLY	C-N-CA	-5.05	109.07	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	692	GLY	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	5303	0	5172	112	0
1	В	5299	0	5169	120	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
3	А	6	0	0	0	0
3	В	14	0	0	0	0
All	All	10626	0	10341	230	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 11.

All (230) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A + 1	A + 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:639:TYR:HE2	1:B:671:ILE:HG12	1.41	0.86
1:A:126:LYS:HG3	1:B:661:ASN:HD22	1.44	0.82
1:B:493:VAL:O	1:B:555:ARG:NH2	2.15	0.80
1:A:379:TRP:HB3	1:A:397:VAL:HG23	1.68	0.76
1:B:379:TRP:HB3	1:B:397:VAL:HG23	1.69	0.75
1:B:573:VAL:HG11	1:B:583:PRO:HB2	1.68	0.75
1:B:241:ARG:HD3	1:B:258:TYR:CG	2.22	0.74
1:B:689:VAL:HG21	1:B:693:SER:HA	1.71	0.73
1:B:658:GLU:OE2	1:B:688:ARG:NH2	2.20	0.73
1:B:408:VAL:HG22	1:B:471:ARG:HG2	1.71	0.73
1:A:408:VAL:HG22	1:A:471:ARG:HG2	1.72	0.72
1:B:74:GLU:HA	1:B:124:PRO:HD3	1.70	0.72
1:A:405:PRO:HG2	1:A:474:LEU:HB2	1.72	0.71
1:B:382:HIS:HB2	1:B:397:VAL:HG22	1.71	0.71
1:A:382:HIS:HB2	1:A:397:VAL:HG22	1.73	0.70
1:B:326:VAL:HG13	1:B:457:ARG:HH21	1.55	0.69
1:B:241:ARG:HD3	1:B:258:TYR:CD2	2.27	0.69
1:A:241:ARG:NH1	1:A:290:ILE:O	2.27	0.68
1:A:519:ARG:NH1	1:A:531:SER:O	2.27	0.68
1:A:573:VAL:HG11	1:A:583:PRO:HB2	1.76	0.67
1:A:42:GLN:HE21	1:A:239:ASP:HA	1.60	0.67



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Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:440:ARG:HE	1:A:443:GLY:HA2	1.59	0.66	
1:B:639:TYR:CE2	1:B:671:ILE:HG12	2.28	0.66	
1:B:42:GLN:HE21	1:B:239:ASP:HA	1.58	0.66	
1:A:59:ASN:HB2	1:A:303:PHE:CE2	2.31	0.66	
1:A:495:LEU:HB3	1:A:557:SER:HB3	1.77	0.66	
1:B:495:LEU:HD13	1:B:555:ARG:HH21	1.61	0.65	
1:A:361:GLU:OE1	1:A:555:ARG:NH1	2.20	0.64	
1:B:319:LEU:HD12	1:B:491:TYR:HE1	1.62	0.64	
1:A:62:THR:HG21	1:A:71:GLU:HG2	1.79	0.64	
1:B:495:LEU:HB3	1:B:557:SER:HB2	1.80	0.64	
1:B:58:ILE:HD12	1:B:76:PHE:HB2	1.80	0.63	
1:B:640:ALA:HB2	1:B:687:LYS:HD2	1.81	0.62	
1:A:58:ILE:HB	1:A:108:PHE:CD2	2.34	0.62	
1:A:57:THR:HG23	1:A:59:ASN:H	1.64	0.62	
1:A:85:ASP:OD2	1:A:343:ARG:NH1	2.32	0.62	
1:B:556:LYS:HG2	1:B:557:SER:H	1.64	0.62	
1:A:297:SER:HA	1:A:335:ASN:HB3	1.82	0.61	
1:B:250:ALA:O	1:B:328:ARG:NH1	2.32	0.61	
1:A:423:ALA:HB3	1:A:485:GLU:HB3	1.82	0.61	
1:B:595:TRP:CZ3	1:B:610:LEU:HD11	2.37	0.60	
1:B:31:LEU:HD12	1:B:428:LEU:HD13	1.83	0.60	
1:A:112:PRO:HG3	1:A:129:LYS:HD3	1.84	0.60	
1:A:159:ALA:HB2	1:A:200:GLY:HA3	1.82	0.59	
1:B:319:LEU:HD12	1:B:491:TYR:CE1	2.37	0.58	
1:A:47:ASP:OD2	1:A:392:ARG:NH2	2.30	0.58	
1:B:150:TYR:HE1	1:B:190:ASP:HB2	1.68	0.58	
1:B:57:THR:HG23	1:B:59:ASN:H	1.68	0.58	
1:A:659:PHE:HZ	1:A:671:ILE:HD11	1.69	0.57	
1:A:622:ALA:HB3	1:A:703:LEU:HB2	1.86	0.57	
1:A:504:ARG:NH2	1:A:568:THR:O	2.34	0.57	
1:A:626:THR:HB	1:A:699:GLU:HB2	1.86	0.57	
1:A:634:GLY:HA2	1:A:694:HIS:O	2.05	0.57	
1:B:405:PRO:HG2	1:B:474:LEU:HB2	1.86	0.56	
1:B:231:VAL:HG13	1:B:239:ASP:HB3	1.87	0.56	
1:A:31:LEU:HD11	1:A:431:ARG:HH12	1.70	0.56	
1:A:252:TYR:HB2	1:A:328:ARG:HH11	1.70	0.56	
1:A:326:VAL:HG13	1:A:457:ARG:HH11	1.71	0.56	
1:A:607:PRO:HA	1:A:686:GLY:O	2.05	0.56	
1:B:578:ARG:NH2	1:B:584:GLU:OE2	2.37	0.56	
1:A:65:GLU:OE2	1:A:305:HIS:NE2	2.30	0.56	
1:B:31:LEU:HD22	1:B:32:THR:H	1.69	0.55	



	lo uo pugo	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:58:ILE:HG22	1:B:106:ASP:OD2	2.06	0.55	
1:A:126:LYS:HG3	1:B:661:ASN:ND2	2.16	0.55	
1:B:293:GLU:OE2	1:B:333:ASN:ND2	2.33	0.55	
1:A:59:ASN:HB2	1:A:303:PHE:HE2	1.73	0.54	
1:B:361:GLU:OE1	1:B:555:ARG:NH1	2.41	0.54	
1:B:423:ALA:HB3	1:B:485:GLU:HB3	1.90	0.54	
1:A:505:ASN:OD1	1:A:569:ARG:HD3	2.08	0.53	
1:B:367:PHE:HD2	1:B:415:ALA:HB1	1.74	0.53	
1:A:556:LYS:HG2	1:A:557:SER:H	1.74	0.53	
1:B:103:LYS:HB3	1:B:151:LEU:HD12	1.91	0.53	
1:B:297:SER:HA	1:B:335:ASN:HB3	1.90	0.53	
1:A:620:VAL:HG23	1:A:702:VAL:HG13	1.91	0.53	
1:B:85:ASP:OD2	1:B:343:ARG:NH1	2.41	0.53	
1:A:324:ASP:HA	1:A:328:ARG:HE	1.74	0.52	
1:B:445:TRP:CH2	1:B:471:ARG:HG3	2.44	0.52	
1:A:575:ALA:HB3	1:A:611:GLU:HB2	1.91	0.52	
1:A:637:ASP:O	1:A:659:PHE:N	2.37	0.52	
1:B:150:TYR:CE1	1:B:190:ASP:HB2	2.43	0.52	
1:B:689:VAL:HG22	1:B:693:SER:HB2	1.92	0.52	
1:B:375:SER:HB3	1:B:384:ALA:HB2	1.92	0.52	
1:B:298:ILE:HG23	1:B:299:ARG:HG3	1.91	0.52	
1:B:575:ALA:HB3	1:B:611:GLU:HB2	1.92	0.51	
1:A:150:TYR:HE1	1:A:190:ASP:HB2	1.74	0.51	
1:A:236:VAL:HG13	1:A:260:PRO:HG2	1.92	0.51	
1:B:571:TRP:CD1	1:B:614:MET:HA	2.45	0.51	
1:A:193:ASN:HB3	1:A:210:ARG:HH21	1.74	0.51	
1:A:520:TYR:OH	1:A:535:ARG:NH1	2.42	0.51	
1:A:583:PRO:HA	1:A:595:TRP:CD1	2.46	0.51	
1:A:326:VAL:HG13	1:A:457:ARG:NH1	2.25	0.50	
1:A:580:ALA:HB2	1:A:599:ALA:HB2	1.93	0.50	
1:B:241:ARG:NE	1:B:290:ILE:O	2.37	0.50	
1:B:622:ALA:HA	1:B:671:ILE:O	2.11	0.50	
1:B:523:ASP:OD1	1:B:524:GLY:N	2.43	0.50	
1:B:241:ARG:HG3	1:B:290:ILE:HG22	1.94	0.50	
1:A:46:HIS:HA	1:A:331:ASN:HD21	1.77	0.50	
1:A:68:TYR:HA	1:A:156:ARG:HD2	1.92	0.50	
1:B:104:HIS:CD2	1:B:150:TYR:HE2	2.30	0.49	
1:B:689:VAL:HG23	1:B:690:VAL:N	2.25	0.49	
1:B:588:ASP:OD2	1:B:593:THR:OG1	2.29	0.49	
1:A:565:PRO:HA	1:A:703:LEU:HD23	1.94	0.49	
1:B:150:TYR:CD1	1:B:188:TRP:HE3	2.30	0.49	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:438:GLU:HG2	1:B:447:LYS:HA	1.94	0.49
1:A:298:ILE:HG23	1:A:299:ARG:HG3	1.94	0.49
1:A:55:HIS:ND1	1:A:101:THR:HG21	2.28	0.48
1:B:644:SER:O	1:B:679:ALA:HB1	2.12	0.48
1:A:126:LYS:O	1:A:128:GLY:N	2.45	0.48
1:A:571:TRP:CD1	1:A:614:MET:HA	2.48	0.48
1:B:491:TYR:CD1	1:B:492:PRO:HD2	2.48	0.48
1:B:606:PRO:HD2	1:B:693:SER:OG	2.13	0.48
1:A:535:ARG:HG2	1:A:536:ASN:N	2.28	0.48
1:B:251:GLY:O	1:B:254:CYS:HB2	2.14	0.48
1:A:61:PHE:CD1	1:A:61:PHE:N	2.81	0.48
1:A:55:HIS:HB3	1:A:303:PHE:CD1	2.49	0.48
1:A:61:PHE:N	1:A:61:PHE:HD1	2.10	0.48
1:B:595:TRP:O	1:B:696:ALA:HA	2.14	0.48
1:A:59:ASN:HB2	1:A:303:PHE:CD2	2.48	0.48
1:A:231:VAL:HG13	1:A:239:ASP:HB3	1.94	0.48
1:B:622:ALA:HB3	1:B:703:LEU:HB2	1.96	0.48
1:B:641:VAL:O	1:B:654:ALA:N	2.47	0.48
1:A:56:PHE:O	1:A:110:LEU:HD11	2.14	0.48
1:A:42:GLN:NE2	1:A:239:ASP:HA	2.27	0.47
1:A:58:ILE:HG22	1:A:106:ASP:OD2	2.14	0.47
1:B:111:TRP:O	1:B:113:THR:N	2.47	0.47
1:A:89:THR:HG21	1:A:349:LYS:HG2	1.96	0.47
1:A:118:HIS:CE1	1:A:157:ASN:HD22	2.32	0.47
1:B:296:VAL:HG11	1:B:321:LEU:HD11	1.96	0.47
1:A:474:LEU:HD13	1:A:481:PRO:HB2	1.96	0.47
1:A:379:TRP:HE3	1:A:397:VAL:HG21	1.80	0.47
1:A:46:HIS:O	1:A:457:ARG:NH2	2.46	0.47
1:A:397:VAL:HG12	1:A:482:ALA:HB2	1.95	0.47
1:B:193:ASN:HB3	1:B:210:ARG:NH2	2.30	0.47
1:B:367:PHE:N	1:B:367:PHE:CD1	2.82	0.47
1:B:490:LYS:NZ	1:B:491:TYR:O	2.47	0.47
1:A:125:TRP:CE2	1:A:126:LYS:HD3	2.50	0.46
1:B:659:PHE:CE1	1:B:669:GLN:HB3	2.49	0.46
1:A:251:GLY:O	1:A:254:CYS:HB2	2.15	0.46
1:A:51:TYR:O	1:A:333:ASN:HA	2.15	0.46
1:B:101:THR:HA	1:B:150:TYR:HB3	1.98	0.46
1:B:367:PHE:N	1:B:367:PHE:HD1	2.14	0.46
1:B:619:ASN:HA	1:B:678:LYS:HA	1.97	0.46
1:A:118:HIS:CG	1:A:157:ASN:ND2	2.83	0.46
1:A:625:TYR:HE1	1:A:697:VAL:HG22	1.81	0.46



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:253:PRO:HB3	1:A:452:ALA:HB3	1.97	0.46	
1:A:61:PHE:HZ	1:A:78:PRO:HB3	1.81	0.46	
1:A:375:SER:HB3	1:A:384:ALA:HB2	1.97	0.45	
1:B:637:ASP:OD1	1:B:638:ARG:N	2.50	0.45	
1:A:298:ILE:HG12	1:A:312:VAL:HG13	1.99	0.45	
1:A:440:ARG:HB2	1:A:445:TRP:CE2	2.51	0.45	
1:A:670:ARG:NE	1:A:672:ASP:OD1	2.50	0.45	
1:B:259:THR:HG22	1:B:287:LYS:H	1.81	0.45	
1:A:108:PHE:HE1	1:A:119:SER:C	2.20	0.44	
1:A:111:TRP:O	1:A:113:THR:N	2.50	0.44	
1:B:42:GLN:NE2	1:B:239:ASP:HA	2.28	0.44	
1:B:110:LEU:HB3	1:B:132:VAL:HB	1.99	0.44	
1:B:186:LEU:HA	1:B:231:VAL:O	2.17	0.44	
1:B:258:TYR:CE2	1:B:260:PRO:HG3	2.52	0.44	
1:B:105:HIS:CD2	1:B:154:TRP:HE3	2.35	0.44	
1:B:606:PRO:HG3	1:B:695:VAL:HG23	1.98	0.44	
1:B:51:TYR:O	1:B:333:ASN:HA	2.17	0.44	
1:A:31:LEU:HD22	1:A:32:THR:H	1.82	0.44	
1:B:67:GLY:O	1:B:156:ARG:NH1	2.51	0.44	
1:A:303:PHE:CD1	1:A:303:PHE:N	2.85	0.44	
1:A:523:ASP:OD1	1:A:524:GLY:N	2.49	0.44	
1:B:61:PHE:N	1:B:61:PHE:CD1	2.84	0.44	
1:B:118:HIS:CE1	1:B:157:ASN:HD22	2.36	0.44	
1:B:275:ARG:HH12	1:B:277:ARG:HD2	1.81	0.43	
1:B:399:ALA:O	1:B:401:GLU:N	2.48	0.43	
1:B:61:PHE:N	1:B:61:PHE:HD1	2.15	0.43	
1:B:474:LEU:HD13	1:B:481:PRO:HB2	2.01	0.43	
1:A:399:ALA:O	1:A:401:GLU:N	2.48	0.43	
1:A:38:PRO:HB3	1:A:289:TRP:CD1	2.53	0.43	
1:A:63:GLY:N	1:A:340:ARG:HH22	2.17	0.43	
1:A:595:TRP:CH2	1:A:610:LEU:HD11	2.53	0.43	
1:B:298:ILE:HG12	1:B:312:VAL:HG13	2.00	0.43	
1:B:645:MET:HG2	1:B:679:ALA:HA	2.00	0.43	
1:A:495:LEU:HD11	1:A:552:TYR:HB3	2.00	0.43	
1:B:234:SER:OG	1:B:237:GLY:N	2.48	0.43	
1:B:241:ARG:HG3	1:B:290:ILE:CG2	2.48	0.43	
1:B:638:ARG:HD3	1:B:687:LYS:HD3	2.01	0.43	
1:B:495:LEU:HD13	1:B:555:ARG:NH2	2.31	0.43	
1:B:500:VAL:HG22	1:B:510:LEU:HD22	1.99	0.43	
1:B:492:PRO:HB3	1:B:555:ARG:HH12	1.84	0.43	
1:B:626:THR:HB	1:B:699:GLU:HB2	2.01	0.43	



	lo us page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:118:HIS:CG	1:B:157:ASN:ND2	2.87	0.43	
1:B:159:ALA:HB2	1:B:200:GLY:HA3	2.01	0.43	
1.B.302.TRP.O	1.B.335.ASN.ND2	2.51	0.43	
1.A.422.LEU.HD22	1:A:435:PHE:CE2	2.54	0.42	
1:B:625:TYB:CE2	1:B:636:VAL:HG12	2.54	0.42	
1:B:689:VAL:CG2	1:B:693:SER:HB2	2.49	0.42	
1:A:639:TYB:CE2	1:A:671:ILE:HG12	2.54	0.42	
1:A:38:PRO:HB3	1:A:289:TRP:NE1	2.34	0.42	
1:A:326:VAL:O	1:A:457:ARG:HD3	2.20	0.42	
1:B:497:ALA:HB2	1:B:558:SEB:HB3	2.01	0.42	
1·B·636·VAL·HG23	1.B.688.ABG.O	2.19	0.42	
1.B:591.SEB.HA	1·B·699·GLU·HG2	2.02	0.42	
1:A:221:GLY:O	1:A:225:LYS:HG3	2.20	0.42	
1:B:56:PHE:O	1:B:110:LEU:HD11	2.19	0.42	
1·B·101·THR·HG22	1.B.150.TYB.HD2	1.85	0.42	
1:A:31:LEU:HD13	1:A:32:THR:N	2.35	0.42	
1.B:573:VAL:HG11	1.B.583.PBO.CB	2.33	0.42	
1:A:65:GLU:O	1.A.66.TRP.HD1	2.13	0.42	
1:A:527:PRO:O	1:A:556:LYS:NZ	2.26	0.12	
1:A:156:ABG:HG2	1:A:197:GLY:HA3	2.01	0.41	
1:B:233:PHE:HD1	1:B:240:VAL:HG12	1.85	0.41	
1:B:361:GLU:HG3	1:B:553:ABG:HE	1.85	0.41	
1.B.397.VAL:HG12	1.B.482.ALA.HB2	2.02	0.41	
1:A:641:VAL:CG1	1:A:655:ALA:HB3	2.50	0.41	
1:B:373:ALA:HB2	1:B:388:LEU:HD21	2.03	0.41	
1:A:125:TRP:O	1:A:126:LYS:HB2	2.20	0.41	
1:A:435:PHE:CZ	1:A:460:LEU:HD11	2.56	0.41	
1:B:574:VAL:HG21	1:B:613:ASP:HB2	2.02	0.41	
1:B:597:THR:OG1	1:B:694:HIS:HB2	2.21	0.41	
1:B:639:TYR:O	1:B:656:GLU:HA	2.20	0.41	
1:A:289:TRP:CD1	1:A:291:PRO:HD3	2.55	0.41	
1:A:234:SER:OG	1:A:237:GLY:N	2.52	0.41	
1:A:439:VAL:HG22	1:A:448:TRP:HB2	2.02	0.41	
1:A:637:ASP:OD1	1:A:638:ARG:N	2.54	0.41	
1:B:106:ASP:N	1:B:106:ASP:OD1	2.54	0.41	
1:B:703:LEU:HA	1:B:703:LEU:HD22	1.88	0.41	
1:A:302:TRP:C	1:A:303:PHE:HD1	2.24	0.41	
1:A:150:TYR:CE1	1:A:190:ASP:HB2	2.53	0.41	
1:B:45:TRP:CZ2	1:B:331:ASN:HB2	2.56	0.41	
1:B:146:ARG:HB3	1:B:185:PHE:CD1	2.56	0.41	
1:B:72:LYS:O	1:B:75:LEU:HG	2.21	0.41	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TYR:CD1	1:A:188:TRP:HE3	2.40	0.40
1:A:302:TRP:O	1:A:335:ASN:ND2	2.47	0.40
1:A:108:PHE:HB2	1:A:118:HIS:CE1	2.56	0.40
1:A:433:ARG:HH21	1:A:478:ARG:HD3	1.86	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	675/704~(96%)	617 (91%)	55 (8%)	3~(0%)	34	60
1	В	674/704~(96%)	617 (92%)	53 (8%)	4 (1%)	25	50
All	All	1349/1408~(96%)	1234 (92%)	108 (8%)	7(0%)	29	54

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	515	ASN
1	В	579	SER
1	А	237	GLY
1	В	513	ALA
1	А	127	GLN
1	А	284	MET
1	В	237	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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.



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	546/563~(97%)	540~(99%)	6 (1%)	73 90
1	В	546/563~(97%)	535~(98%)	11 (2%)	55 81
All	All	1092/1126~(97%)	1075 (98%)	17 (2%)	62 85

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

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	61	PHE
1	А	126	LYS
1	А	188	TRP
1	А	440	ARG
1	А	457	ARG
1	А	535	ARG
1	В	61	PHE
1	В	126	LYS
1	В	188	TRP
1	В	275	ARG
1	В	319	LEU
1	В	367	PHE
1	В	457	ARG
1	В	638	ARG
1	В	639	TYR
1	В	693	SER
1	В	703	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	157	ASN
1	В	157	ASN
1	В	661	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	$OWAB(Å^2)$	Q<0.9
1	А	677/704~(96%)	0.20	14 (2%) 63 65	58, 87, 135, 192	0
1	В	676/704~(96%)	0.29	28 (4%) 37 36	56, 79, 153, 192	0
All	All	1353/1408~(96%)	0.24	42 (3%) 49 49	56, 83, 144, 192	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	В	690	VAL	5.1	
1	В	693	SER	5.0	
1	В	607	PRO	4.9	
1	В	632	SER	4.8	
1	В	705	LYS	4.7	
1	В	633	THR	3.9	
1	В	696	ALA	3.7	
1	А	514	GLU	3.7	
1	В	704	GLY	3.7	
1	В	692	GLY	3.6	
1	В	691	GLU	3.5	
1	А	693	SER	3.3	
1	В	694	HIS	3.2	
1	В	659	PHE	3.1	
1	В	31	LEU	3.0	
1	В	601	GLN	2.9	
1	А	692	GLY	2.7	
1	А	607	PRO	2.7	
1	А	705	LYS	2.7	
1	В	666	PRO	2.6	
1	А	539	PHE	2.6	
1	А	515	ASN	2.6	
1	В	188	TRP	2.6	
1	В	564	ILE	2.5	



Mol	Chain	Res	Type	RSRZ
1	А	263	LEU	2.5
1	А	188	TRP	2.5
1	В	543	GLY	2.4
1	А	601	GLN	2.4
1	А	619	ASN	2.4
1	В	695	VAL	2.4
1	В	661	ASN	2.4
1	В	630	ASP	2.4
1	А	264	GLN	2.3
1	В	663	ARG	2.3
1	А	676	PRO	2.2
1	В	682	LEU	2.1
1	В	152	SER	2.1
1	В	569	ARG	2.1
1	В	617	PRO	2.0
1	В	624	ILE	2.0
1	А	629	ARG	2.0
1	В	400	PRO	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	$B-factors(Å^2)$	Q<0.9
2	CA	В	802	1/1	0.89	0.16	75,75,75,75	0
2	CA	А	801	1/1	0.94	0.06	98,98,98,98	0
2	CA	В	801	1/1	0.95	0.04	122,122,122,122	0
2	CA	А	802	1/1	0.96	0.08	88,88,88,88	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.

