

Full wwPDB X-ray Structure Validation Report (i)

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:	4HZH
:	Structure of recombinant Gla-domainless prothrombin mutant S525A
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:	2012-11-15
:	3.30 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	:	2.35.1
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)	:	2.35.1

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 3.30 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))		
Rfree	130704	1149 (3.34-3.26)		
Clashscore	141614	1205 (3.34-3.26)		
Ramachandran outliers	138981	1183 (3.34-3.26)		
Sidechain outliers	138945	1182 (3.34-3.26)		
RSRZ outliers	127900	1115 (3.34-3.26)		

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	533	% 53%	17% •	26%		
1	В	533	5%	30%	6% 12%		

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	В	703	-	-	-	Х



 $\mathbf{2}$

Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6940 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 Prothrombin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	392	Total 3141	C 1986	N 549	O 585	S 21	0	0	0
1	В	468	Total 3743	C 2353	N 663	0 701	S 26	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	525	ALA	SER	engineered mutation	UNP P00734
В	525	ALA	SER	engineered mutation	UNP P00734

• Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	А	1	Total 14	C 8	N 1	O 5	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
2	В	1	Total C N O	0	0	
		I	14 8 1 5	0	0	
0	D	1	Total C N O	0	0	
2 D	1	14 8 1 5	0	0		
0	D	1	Total C N O	0	0	
2	D	В І	14 8 1 5	0	U	



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: Prothrombin



ARG ALA ILE GLU GLU GLY ARG ARG ALA ALA S275 S275 S275 **Y**316 V336 V336 C338 C339 C340 X341 X341 X342 S342 S342 S343 S344 1334 1<mark>362</mark> E31 **S**31 V458 T459 G460 L379 L380 V381 B382 N415 L416 D417 <mark>D442</mark> R443 E444 T445 1373 7374 **D378** H436 P437 A421 1423 P441 K511 P512 D513 E514 G515 K516 R517 R517 G526 G527 P528 F529 V530 V530 M531 K532 S533 r467 1468 1468 1469 (498 (499 (500 (501 (502)503 N537 R538 1507 1508 *i*461 <mark>W539</mark> Y540



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	82.58Å 103.14Å 149.55Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	40.00 - 3.30	Depositor
Resolution (A)	32.88 - 3.30	EDS
% Data completeness	96.0 (40.00-3.30)	Depositor
(in resolution range)	96.2 (32.88-3.30)	EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.07 (at 3.32 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
B B.	0.295 , 0.329	Depositor
n, n_{free}	0.296 , 0.337	DCC
R_{free} test set	980 reflections (5.16%)	wwPDB-VP
Wilson B-factor $(Å^2)$	51.1	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.26 , 17.6	EDS
L-test for $twinning^2$	$ < L >=0.34, < L^2>=0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	6940	wwPDB-VP
Average B, all atoms $(Å^2)$	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.94% 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: NAG

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	Bo	nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.48	2/3220~(0.1%)	0.65	4/4353~(0.1%)	
1	В	0.38	0/3839	0.58	0/5198	
All	All	0.43	2/7059~(0.0%)	0.61	4/9551~(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
1	В	0	3
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	468	TRP	C-N	10.55	1.58	1.34
1	А	468	TRP	CB-CG	-5.48	1.40	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	А	468	TRP	O-C-N	10.95	140.21	122.70
1	А	468	TRP	N-CA-C	9.47	136.57	111.00
1	А	468	TRP	CA-C-N	-6.58	102.73	117.20
1	А	467	THR	CA-CB-CG2	-5.16	105.18	112.40

There are no chirality outliers.

All (4) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	469	THR	Peptide
1	В	123	GLY	Peptide
1	В	140	ILE	Peptide
1	В	284	ARG	Mainchain

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	3141	0	3024	78	0
1	В	3743	0	3580	119	0
2	А	14	0	13	0	0
2	В	42	0	39	4	0
All	All	6940	0	6656	197	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 14.

All (197) 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:A:468:TRP:CZ2	1:A:547:TRP:CD2	2.41	1.09
1:B:330:GLY:HA3	1:B:434:TYR:HD1	1.17	1.04
1:A:468:TRP:HZ2	1:A:547:TRP:CD2	1.75	1.00
1:B:459:THR:HG22	1:B:482:VAL:HB	1.56	0.87
1:B:330:GLY:HA3	1:B:434:TYR:CD1	2.08	0.85
1:A:468:TRP:HZ2	1:A:547:TRP:CG	1.95	0.84
1:B:551:CYS:HA	1:B:554:ASP:HB2	1.60	0.82
1:B:483:VAL:HG22	1:B:484:ASN:N	1.95	0.81
1:B:69:LEU:HD12	1:B:122:THR:HG23	1.62	0.80
1:B:340:ARG:O	1:B:344:GLN:HA	1.82	0.78
1:B:459:THR:HG22	1:B:482:VAL:CB	2.17	0.75
1:B:459:THR:HG22	1:B:482:VAL:CG2	2.17	0.75
1:A:541:GLN:O	1:A:563:VAL:HG21	1.90	0.71
1:B:473:GLY:O	1:B:474:LYS:HB2	1.89	0.71
1:B:76:HIS:CD2	2:B:703:NAG:C8	2.74	0.70
1:A:463:ASN:HB3	1:A:524:ASP:HA	1.73	0.69



		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:367:TYR:HD2	1:A:370:TRP:HB2	1.59	0.68		
1:A:468:TRP:CZ2	1:A:547:TRP:CE2	2.81	0.68		
1:A:468:TRP:CZ2	1:A:547:TRP:CE3	2.81	0.67		
1:B:551:CYS:HA	1:B:554:ASP:CB	2.24	0.67		
1:B:483:VAL:CG2	1:B:484:ASN:N	2.58	0.67		
1:A:468:TRP:CZ2	1:A:547:TRP:CG	2.78	0.66		
1:B:372:LYS:HD2	1:B:374:PHE:HE2	1.60	0.66		
1:B:415:ASN:HD21	1:B:500:ARG:H	1.43	0.65		
1:A:327:ALA:O	1:A:386:HIS:HE1	1.80	0.64		
1:B:483:VAL:CG2	1:B:484:ASN:H	2.11	0.64		
1:B:483:VAL:HG22	1:B:484:ASN:H	1.61	0.64		
1:A:351:SER:HB3	1:A:528:PRO:HG3	1.80	0.63		
1:B:536:ASN:H	1:B:536:ASN:HD22	1.47	0.62		
1:A:382:ARG:HD3	1:A:385:LYS:HD2	1.82	0.62		
1:A:468:TRP:C	1:A:470:ALA:H	2.03	0.62		
1:B:459:THR:CG2	1:B:482:VAL:CG2	2.78	0.62		
1:B:116:ASN:HB2	1:B:124:PRO:HA	1.83	0.61		
1:B:86:CYS:HB2	1:B:112:ASN:HD22	1.64	0.61		
1:A:467:THR:O	1:A:469:THR:N	2.31	0.60		
1:B:480:LEU:O	1:B:480:LEU:HG	2.01	0.60		
1:A:286:PHE:CE2	1:A:354:SER:HB3	2.35	0.60		
1:A:341:LYS:HE2	1:A:380:LEU:HD23	1.84	0.59		
1:B:382:ARG:HG2	1:B:398:ILE:HB	1.86	0.58		
1:B:479:VAL:O	1:B:481:GLN:N	2.36	0.58		
1:A:440:LEU:HB2	1:A:567:LYS:HE2	1.85	0.58		
1:B:76:HIS:CD2	2:B:703:NAG:H81	2.39	0.57		
1:B:308:THR:O	1:B:311:GLU:HB3	2.05	0.57		
1:B:563:VAL:HA	1:B:566:LEU:HD21	1.86	0.57		
1:A:550:GLY:HA3	1:A:559:PHE:CE2	2.40	0.57		
1:A:550:GLY:HA3	1:A:559:PHE:HE2	1.70	0.56		
1:A:370:TRP:O	1:A:371:ASP:HB2	2.04	0.56		
1:A:472:VAL:HG13	1:A:474:LYS:O	2.05	0.56		
1:A:186:THR:HG21	1:A:409:ARG:HG3	1.87	0.56		
1:B:340:ARG:HB3	1:B:343:PRO:O	2.05	0.56		
1:B:183:ALA:HB2	1:B:218:PHE:CD1	2.41	0.55		
1:B:520:ALA:O	1:B:521:CYS:HB2	2.06	0.55		
1:B:297:PRO:HA	1:B:301:LYS:HD3	1.88	0.55		
1:B:79:ILE:HD13	1:B:79:ILE:H	1.72	0.55		
1:A:458:VAL:HG23	1:A:529:PHE:HD1	1.69	0.55		
1:B:140:ILE:HB	1:B:141:PRO:HD3	1.87	0.55		
1:B:176:GLN:HA	1:B:221:ASN:HB3	1.87	0.55		



	,	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:573:VAL:O	1:A:576:GLN:HB3	2.06	0.54		
1:B:98:GLU:OE2	1:B:127:TYR:HE2	1.91	0.54		
1:A:325:SER:O	1:A:482:VAL:HG12	2.06	0.54		
1:A:464:LEU:HD23	1:A:521:CYS:HA	1.90	0.54		
1:A:548:GLY:O	1:A:551:CYS:HB2	2.07	0.54		
1:B:415:ASN:O	1:B:417:ASP:N	2.35	0.54		
1:B:194:TRP:HZ3	1:B:232:TYR:HD2	1.56	0.53		
1:A:553:ARG:HA	1:A:553:ARG:HE	1.72	0.53		
1:B:325:SER:O	1:B:481:GLN:OE1	2.27	0.53		
1:B:460:GLY:O	1:B:481:GLN:HB2	2.08	0.53		
1:A:466:GLU:HG3	1:A:476:GLN:NE2	2.24	0.52		
1:B:192:LEU:HD21	1:B:234:ALA:HB2	1.89	0.52		
1:B:98:GLU:OE1	1:B:135:ARG:NH1	2.42	0.52		
1:A:317:ILE:HD12	1:A:317:ILE:H	1.75	0.52		
1:B:497:THR:HG21	1:B:501:ILE:HD11	1.91	0.52		
1:B:469:THR:C	1:B:471:ASN:H	2.11	0.52		
1:A:308:THR:O	1:A:311:GLU:HB3	2.10	0.52		
1:A:361:ALA:HA	1:A:419:ASP:O	2.11	0.51		
1:B:81:ARG:O	1:B:82:SER:HB3	2.11	0.51		
1:B:436:HIS:CG	1:B:437:PRO:HD2	2.46	0.51		
1:B:536:ASN:O	1:B:538:ARG:N	2.44	0.51		
1:A:466:GLU:HG3	1:A:476:GLN:HE21	1.76	0.51		
1:A:490:ARG:HH22	1:A:502:THR:C	2.14	0.51		
1:B:326:ASP:CG	1:B:479:VAL:HG11	2.31	0.51		
1:B:466:GLU:C	1:B:468:TRP:H	2.15	0.50		
1:A:468:TRP:C	1:A:470:ALA:N	2.65	0.50		
1:A:473:GLY:O	1:A:474:LYS:HB2	2.11	0.50		
1:B:253:GLU:HB3	1:B:450:LEU:HD13	1.93	0.50		
1:B:459:THR:HG22	1:B:482:VAL:HG21	1.92	0.50		
1:B:445:THR:HA	1:B:448:SER:OG	2.10	0.50		
1:A:418:ARG:HG3	1:A:420:ILE:HD11	1.93	0.50		
1:A:340:ARG:N	1:A:345:GLU:O	2.40	0.50		
1:A:357:TRP:CZ3	1:A:424:LYS:HB2	2.47	0.50		
1:A:530:VAL:HG12	1:A:541:GLN:HA	1.94	0.49		
1:B:512:PRO:HA	1:B:516:LYS:HB3	1.94	0.49		
1:B:89:TRP:HE3	1:B:109:LEU:HB3	1.77	0.49		
1:B:340:ARG:HD3	1:B:343:PRO:HD2	1.94	0.49		
1:B:533:SER:O	1:B:537:ASN:HA	2.13	0.48		
1:B:339:PHE:O	1:B:379:LEU:HA	2.13	0.48		
1:A:531:MET:SD	1:A:542:MET:HG3	2.53	0.48		
1:B:459:THR:CG2	1:B:482:VAL:HG21	2.44	0.48		



		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:550:GLY:CA	1:A:559:PHE:HE2	2.26	0.48		
1:B:137:GLU:H	1:B:137:GLU:CD	2.18	0.48		
1:A:455:LYS:HA	1:A:486:PRO:HA	1.95	0.47		
1:A:309:GLU:OE1	1:A:532:LYS:NZ	2.44	0.47		
1:A:407:HIS:HB3	1:A:420:ILE:HG13	1.96	0.47		
1:B:82:SER:OG	1:B:136:GLN:NE2	2.48	0.47		
1:A:282:ASN:HD21	1:A:284:ARG:HB2	1.79	0.47		
1:A:336:VAL:HG22	1:A:383:ILE:HG23	1.97	0.47		
1:A:412:TRP:HA	1:A:416:LEU:HD23	1.97	0.47		
1:B:458:VAL:O	1:B:482:VAL:HG23	2.14	0.47		
1:B:69:LEU:CD1	1:B:122:THR:HG23	2.40	0.47		
1:A:468:TRP:CH2	1:A:547:TRP:CE2	3.04	0.46		
1:A:487:ILE:HD12	1:A:487:ILE:H	1.79	0.46		
1:B:388:ARG:HB2	1:B:461:TRP:CD1	2.50	0.46		
1:A:252:VAL:HA	1:A:443:ARG:HH12	1.81	0.46		
1:A:409:ARG:O	1:A:418:ARG:HB2	2.15	0.46		
1:A:385:LYS:HG3	1:A:396:GLU:HB3	1.97	0.46		
1:A:431:PHE:CE1	1:A:437:PRO:HD3	2.51	0.46		
1:B:125:TRP:CE3	1:B:135:ARG:HD2	2.51	0.46		
1:B:362:ALA:HA	1:B:421:ALA:HB2	1.97	0.46		
1:B:251:ALA:HB2	1:B:490:ARG:HD3	1.98	0.46		
1:B:482:VAL:HG13	1:B:482:VAL:O	2.15	0.46		
1:B:529:PHE:O	1:B:542:MET:N	2.39	0.46		
1:B:407:HIS:HB2	1:B:420:ILE:HB	1.96	0.46		
1:A:325:SER:HA	1:A:481:GLN:OE1	2.16	0.46		
1:B:511:LYS:O	1:B:516:LYS:HD2	2.15	0.46		
1:A:503:ASP:OD2	1:A:565:ARG:NH1	2.45	0.46		
1:B:108:ASP:O	1:B:115:ARG:HD2	2.15	0.46		
1:B:381:VAL:O	1:B:398:ILE:HA	2.16	0.46		
1:B:193:ALA:HB3	1:B:196:SER:HB3	1.98	0.45		
1:A:385:LYS:HG3	1:A:396:GLU:CB	2.47	0.45		
1:A:472:VAL:HG12	1:A:472:VAL:O	2.15	0.45		
1:B:93:TYR:CD1	1:B:94:PRO:HA	2.52	0.45		
1:B:420:ILE:HD13	1:B:566:LEU:HD22	1.98	0.45		
1:B:334:TRP:O	1:B:336:VAL:HG23	2.16	0.45		
1:B:424:LYS:HE3	1:B:577:PHE:CE2	2.52	0.45		
1:B:532:LYS:HE2	1:B:537:ASN:OD1	2.16	0.45		
1:A:445:THR:O	1:A:449:LEU:HG	2.16	0.45		
1:B:341:LYS:N	1:B:378:ASP:O	2.47	0.45		
1:B:227:GLU:HB3	1:B:242:TYR:CE2	2.52	0.44		
1:A:469:THR:C	1:A:471:ASN:N	2.70	0.44		



	lo uo pugom	Interatomic	Clash		
Atom-1	Atom-2	distance $(Å)$	overlap (Å)		
1:B:76:HIS:HD2	2:B:703:NAG:C8	2.27	0.44		
1:B:119:SER:O	1:B:120:SER:O	2.35	0.44		
1:B:529:PHE:CD1	1:B:542:MET:HB2	2.52	0.44		
1:B:128:THR:HG21	1:B:133:VAL:HG12	1.99	0.44		
1:B:441:PRO:HG3	1:B:540:TYR:HB3	1.99	0.44		
1:B:88:LEU:HG	1:B:111:GLU:HA	2.00	0.44		
1:B:191:CYS:HA	1:B:232:TYR:O	2.18	0.44		
1:A:415:ASN:O	1:A:416:LEU:HB2	2.18	0.43		
1:B:326:ASP:OD1	1:B:479:VAL:HG21	2.18	0.43		
1:B:366:LEU:HA	1:B:372:LYS:O	2.18	0.43		
1:A:468:TRP:CE2	1:A:547:TRP:CE3	3.06	0.43		
1:B:488:VAL:HB	1:B:507:CYS:HB3	2.00	0.43		
1:B:562:HIS:ND1	1:B:564:PHE:HE1	2.16	0.43		
1:A:349:GLY:HA3	1:A:524:ASP:HB3	2.01	0.43		
1:A:459:THR:HA	1:A:481:GLN:O	2.19	0.43		
1:B:536:ASN:HD22	1:B:536:ASN:N	2.12	0.43		
1:B:543:GLY:HA2	1:B:561:THR:O	2.19	0.43		
1:A:441:PRO:HD3	1:A:540:TYR:HB3	2.01	0.43		
1:A:298:LEU:HD12	1:A:330:GLY:HA3	2.01	0.43		
1:A:463:ASN:O	1:A:467:THR:HG23	2.18	0.43		
1:A:550:GLY:HA2	1:A:553:ARG:HG3	2.01	0.42		
1:B:92:ARG:HD3	1:B:96:LYS:HG3	2.01	0.42		
1:B:357:TRP:CZ3	1:B:424:LYS:HB2	2.54	0.42		
1:B:415:ASN:ND2	1:B:500:ARG:H	2.13	0.42		
1:B:465:LYS:HD3	1:B:521:CYS:HB3	2.02	0.42		
1:B:286:PHE:CE2	1:B:354:SER:HB3	2.55	0.42		
1:A:468:TRP:CE3	1:A:468:TRP:CA	3.03	0.42		
1:B:102:THR:HG23	2:B:702:NAG:H82	2.02	0.42		
1:B:183:ALA:HB2	1:B:218:PHE:HD1	1.82	0.42		
1:A:193:ALA:HA	1:A:217:ASN:CB	2.49	0.41		
1:B:456:GLY:HA2	1:B:531:MET:HG2	2.02	0.41		
1:A:460:GLY:O	1:A:480:LEU:HD12	2.19	0.41		
1:A:547:TRP:O	1:A:548:GLY:C	2.58	0.41		
1:B:81:ARG:O	1:B:82:SER:CB	2.68	0.41		
1:B:99:ILE:HG13	1:B:103:THR:CG2	2.50	0.41		
1:A:275:SER:OG	1:A:536:ASN:O	2.38	0.41		
1:A:213:GLN:H	1:A:213:GLN:HG2	1.74	0.41		
1:A:367:TYR:CD2	1:A:370:TRP:HB2	2.46	0.41		
1:A:464:LEU:HD23	1:A:521:CYS:CA	2.50	0.41		
1:A:471:ASN:O	1:A:473:GLY:N	2.51	0.41		
1:B:334:TRP:HA	1:B:352:LEU:HB3	2.02	0.41		



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:469:THR:C	1:B:471:ASN:N	2.74	0.41	
1:A:333:PRO:HD2	1:A:334:TRP:CZ3	2.56	0.41	
1:B:194:TRP:HZ3	1:B:232:TYR:CD2	2.36	0.41	
1:B:315:SER:O	1:B:316:TYR:C	2.59	0.41	
1:B:333:PRO:HD2	1:B:334:TRP:CE3	2.56	0.41	
1:B:520:ALA:O	1:B:521:CYS:CB	2.68	0.41	
1:B:99:ILE:HG23	1:B:104:HIS:HB2	2.02	0.41	
1:B:179:GLN:HE21	1:B:179:GLN:HB2	1.66	0.41	
1:B:342:SER:HA	1:B:343:PRO:HA	1.85	0.41	
1:B:193:ALA:HA	1:B:217:ASN:HB3	2.03	0.40	
1:B:426:LYS:O	1:B:428:PRO:HD3	2.21	0.40	
1:B:186:THR:HG21	1:B:409:ARG:NE	2.36	0.40	
1:B:473:GLY:O	1:B:474:LYS:CB	2.65	0.40	
1:B:490:ARG:HH21	1:B:503:ASP:HA	1.85	0.40	
1:B:130:ASP:HA	1:B:131:PRO:HD3	1.92	0.40	
1:B:221:ASN:HB2	1:B:229:VAL:HG12	2.04	0.40	
1:B:185:THR:HA	1:B:243:CYS:HA	2.02	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	Perc	centiles
1	А	388/533~(73%)	325~(84%)	51 (13%)	12 (3%)	4	23
1	В	462/533~(87%)	358~(78%)	72 (16%)	32~(7%)	1	8
All	All	850/1066~(80%)	683~(80%)	123 (14%)	44 (5%)	2	13

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type					
1	А	468	TRP					
Continued and and and								



Mol	Chain	Res	Type
1	А	474	LYS
1	А	548	GLY
1	В	69	LEU
1	В	82	SER
1	В	117	PRO
1	В	119	SER
1	В	120	SER
1	В	140	ILE
1	В	142	VAL
1	В	316	TYR
1	В	344	GLN
1	В	474	LYS
1	В	480	LEU
1	В	537	ASN
1	А	372	LYS
1	А	472	VAL
1	В	112	ASN
1	В	141	PRO
1	В	216	GLU
1	В	222	PRO
1	В	416	LEU
1	В	467	THR
1	В	482	VAL
1	А	204	LYS
1	А	311	GLU
1	А	555	GLY
1	В	481	GLN
1	А	205	HIS
1	А	469	THR
1	A	550	GLY
1	В	238	GLY
1	B	508	ALA
1	В	515	GLY
1	B	197	ALA
1	В	395	ILE
1	В	415	ASN
1	A	395	ILE
1	В	106	GLY
1	B	428	PRO
1	В	172	PRO
1	В	289	GLY
1	В	528	PRO



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Mol	Chain	Res	Type	
1	В	237	PRO	

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.

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

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	335/456~(74%)	314~(94%)	21~(6%)	18	47	
1	В	404/456~(89%)	365~(90%)	39 (10%)	8	29	
All	All	739/912~(81%)	679 (92%)	60 (8%)	11	36	

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	184	VAL
1	А	198	GLN
1	А	253	GLU
1	А	301	LYS
1	А	312	LEU
1	А	317	ILE
1	А	332	SER
1	А	340	ARG
1	А	372	LYS
1	А	383	ILE
1	А	385	LYS
1	А	396	GLU
1	А	440	LEU
1	А	443	ARG
1	А	469	THR
1	А	521	CYS
1	А	536	ASN
1	А	547	TRP
1	А	553	ARG
1	А	554	ASP
1	А	577	PHE
1	В	69	LEU



Mol	Chain	Res	Type
1	В	76	HIS
1	В	79	ILE
1	В	95	HIS
1	В	98	GLU
1	В	115	ARG
1	В	122	THR
1	В	128	THR
1	В	130	ASP
1	В	198	GLN
1	В	205	HIS
1	В	239	ASP
1	В	248	CYS
1	В	301	LYS
1	В	308	THR
1	В	321	ILE
1	В	325	SER
1	В	326	ASP
1	В	332	SER
1	В	338	LEU
1	В	340	ARG
1	В	347	LEU
1	В	392	GLU
1	В	398	ILE
1	В	414	GLU
1	В	423	MET
1	В	443	ARG
1	В	444	GLU
1	В	466	GLU
1	В	490	ARG
1	В	493	CYS
1	В	498	ARG
1	В	499	ILE
1	В	502	THR
1	В	514	GLU
1	В	530	VAL
1	В	536	ASN
1	В	553	ARG
1	В	566	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:



Mol	Chain	Res	Type
1	А	282	ASN
1	А	386	HIS
1	А	536	ASN
1	А	541	GLN
1	В	76	HIS
1	В	112	ASN
1	В	136	GLN
1	В	177	GLN
1	В	179	GLN
1	В	415	ASN
1	В	536	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)

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	Tink	Bo	ond leng	$_{\rm ths}$	В	ond ang	gles
	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	В	701	1	14,14,15	0.47	0	17,19,21	1.03	1 (5%)
2	NAG	А	701	1	14,14,15	0.54	0	17,19,21	1.27	1 (5%)
2	NAG	В	702	1	14,14,15	0.52	0	17,19,21	1.03	1 (5%)



Mal	Type	Chain	Dog	Link	Bo	ond leng	\mathbf{ths}	В	ond ang	les
	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	NAG	В	703	1	14,14,15	0.58	0	17,19,21	1.09	1 (5%)

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	NAG	В	701	1	-	2/6/23/26	0/1/1/1
2	NAG	А	701	1	-	2/6/23/26	0/1/1/1
2	NAG	В	702	1	-	0/6/23/26	0/1/1/1
2	NAG	В	703	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	701	NAG	C1-O5-C5	4.48	118.27	112.19
2	В	701	NAG	C1-O5-C5	3.01	116.27	112.19
2	В	703	NAG	O5-C1-C2	-2.68	107.06	111.29
2	В	702	NAG	C1-O5-C5	2.40	115.44	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	701	NAG	O5-C5-C6-O6
2	В	701	NAG	C4-C5-C6-O6
2	В	701	NAG	O5-C5-C6-O6
2	А	701	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	702	NAG	1	0
2	В	703	NAG	3	0



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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	392/533~(73%)	-0.07	3 (0%) 86 86	20, 38, 70, 82	0
1	В	468/533~(87%)	0.42	25 (5%) 26 24	48, 66, 105, 112	0
All	All	860/1066 (80%)	0.20	28 (3%) 46 44	20, 59, 101, 112	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	201	ALA	7.4
1	В	552	ASP	4.4
1	В	274	THR	4.1
1	В	579	GLU	3.8
1	В	473	GLY	3.4
1	В	205	HIS	3.4
1	В	181	ARG	3.3
1	В	275	SER	3.2
1	В	197	ALA	3.0
1	В	555	GLY	3.0
1	А	318	ASP	2.9
1	А	201	ALA	2.8
1	В	276	GLU	2.7
1	В	578	GLY	2.7
1	В	517	ARG	2.7
1	В	526	GLY	2.6
1	В	196	SER	2.6
1	В	206	GLN	2.4
1	В	83	GLY	2.3
1	В	512	PRO	2.3
1	В	194	TRP	2.3
1	В	514	GLU	2.2
1	В	198	GLN	2.2
1	В	554	ASP	2.2



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Mol	Chain	Res	Type	RSRZ
1	А	515	GLY	2.2
1	В	170	CYS	2.2
1	В	277	TYR	2.1
1	В	122	THR	2.1

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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	NAG	В	703	14/15	0.62	0.43	69,70,71,71	0
2	NAG	В	701	14/15	0.78	0.21	54,56,56,56	0
2	NAG	В	702	14/15	0.82	0.24	61,61,62,62	0
2	NAG	А	701	14/15	0.85	0.17	28,30,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.

