



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:20 PM GMT

PDB ID : 4HZH
Title : Structure of recombinant Gla-domainless prothrombin mutant S525A
Authors : Pozzi, N.; Niu, W.; Gohara, D.W.; Chen, Z.; Di Cera, E.
Deposited on : 2012-11-15
Resolution : 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

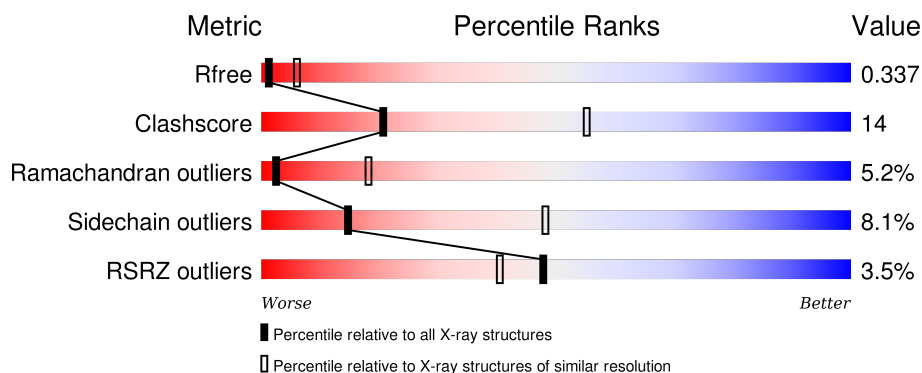
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-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))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	A	533	<div> <div></div> <div>53% 17% • 26%</div> </div>
1	B	533	<div> <div>5%</div> <div>51% 30% 6% 12%</div> </div>

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	B	703	-	-	-	X

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.

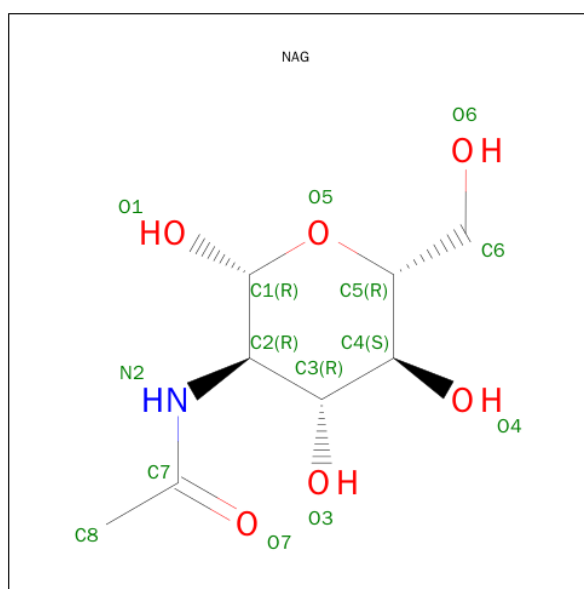
- Molecule 1 is a protein called Prothrombin.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	525	ALA	SER	ENGINEERED MUTATION	UNP P00734
B	525	ALA	SER	ENGINEERED MUTATION	UNP P00734

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

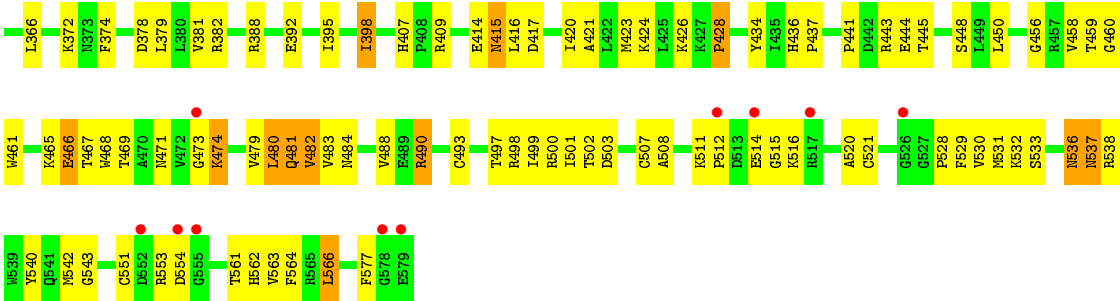


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.58Å 103.14Å 149.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 32.88 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (40.00-3.30) 96.2 (32.88-3.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.295 , 0.329 0.296 , 0.337	Depositor DCC
R_{free} test set	1011 reflections (5.61%)	DCC
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 , 17.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 18991 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	2/3220 (0.1%)	0.65	4/4353 (0.1%)
1	B	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	A	0	1
1	B	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	A	468	TRP	C-N	10.55	1.58	1.34
1	A	468	TRP	CB-CG	-5.48	1.40	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	468	TRP	O-C-N	10.95	140.21	122.70
1	A	468	TRP	N-CA-C	9.47	136.57	111.00
1	A	468	TRP	CA-C-N	-6.58	102.73	117.20
1	A	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	A	469	THR	Peptide
1	B	123	GLY	Peptide
1	B	140	ILE	Peptide
1	B	284	ARG	Mainchain

5.2 Too-close contacts ⓘ

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	A	3141	0	3024	78	0
1	B	3743	0	3580	119	0
2	A	14	0	13	0	0
2	B	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 distance (Å)	Clash 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:HG	1:B:480:LEU:O	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:472:VAL:HG13	1:A:474:LYS:O	2.05	0.56
1:A:370:TRP:O	1:A:371:ASP:HB2	2.04	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:H	1:B:79:ILE:HD13	1.72	0.55
1:B:176:GLN:HA	1:B:221:ASN:HB3	1.87	0.55
1:B:140:ILE:HB	1:B:141:PRO:HD3	1.87	0.55
1:A:458:VAL:HG23	1:A:529:PHE:HD1	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:B:192:LEU:HD21	1:B:234:ALA:HB2	1.89	0.52
1:A:466:GLU:HG3	1:A:476:GLN:NE2	2.24	0.52
1:B:98:GLU:OE1	1:B:135:ARG:NH1	2.42	0.52
1:A:317:ILE:H	1:A:317:ILE:HD12	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:536:ASN:O	1:B:538:ARG:N	2.44	0.51
1:B:436:HIS:CG	1:B:437:PRO:HD2	2.46	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:B:459:THR:HG22	1:B:482:VAL:HG21	1.92	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: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:357:TRP:CZ3	1:A:424:LYS:HB2	2.47	0.50
1:A:340:ARG:N	1:A:345:GLU:O	2.40	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:340:ARG:HD3	1:B:343:PRO:HD2	1.94	0.49
1:B:89:TRP:HE3	1:B:109:LEU:HB3	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:GLY:CA	1:A:559:PHE:HE2	2.26	0.48
1:B:137:GLU:CD	1:B:137:GLU:H	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:336:VAL:HG22	1:A:383:ILE:HG23	1.97	0.47
1:A:282:ASN:HD21	1:A:284:ARG:HB2	1.79	0.47
1:B:458:VAL:O	1:B:482:VAL:HG23	2.14	0.47
1:A:412:TRP:HA	1:A:416:LEU:HD23	1.97	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:409:ARG:O	1:A:418:ARG:HB2	2.15	0.46
1:A:252:VAL:HA	1:A:443:ARG:HH12	1.81	0.46
1:A:385:LYS:HG3	1:A:396:GLU:HB3	1.97	0.46
1:B:125:TRP:CE3	1:B:135:ARG:HD2	2.51	0.46
1:A:431:PHE:CE1	1:A:437:PRO:HD3	2.51	0.46
1:B:362:ALA:HA	1:B:421:ALA:HB2	1.97	0.46
1:B:482:VAL:HG13	1:B:482:VAL:O	2.15	0.46
1:B:251:ALA:HB2	1:B:490:ARG:HD3	1.98	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:B:381:VAL:O	1:B:398:ILE:HA	2.16	0.46
1:B:108:ASP:O	1:B:115:ARG:HD2	2.15	0.46
1:A:503:ASP:OD2	1:A:565:ARG:NH1	2.45	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:420:ILE:HD13	1:B:566:LEU:HD22	1.98	0.45
1:B:93:TYR:CD1	1:B:94:PRO:HA	2.52	0.45
1:B:334:TRP:O	1:B:336:VAL:HG23	2.16	0.45
1:B:532:LYS:HE2	1:B:537:ASN:OD1	2.16	0.45
1:B:424:LYS:HE3	1:B:577:PHE:CE2	2.52	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:B:76:HIS:HD2	2:B:703:NAG:C8	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:THR:C	1:A:471:ASN:N	2.70	0.44
1:B:529:PHE:CD1	1:B:542:MET:HB2	2.52	0.44
1:B:119:SER:O	1:B:120:SER:O	2.35	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:B:366:LEU:HA	1:B:372:LYS:O	2.18	0.43
1:B:326:ASP:OD1	1:B:479:VAL:HG21	2.18	0.43
1:A:415:ASN:O	1:A:416:LEU:HB2	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:415:ASN:ND2	1:B:500:ARG:H	2.13	0.42
1:B:357:TRP:CZ3	1:B:424:LYS:HB2	2.54	0.42
1:B:92:ARG:HD3	1:B:96:LYS:HG3	2.01	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:CA	1:A:468:TRP:CE3	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: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:213:GLN:H	1:A:213:GLN:HG2	1.74	0.41
1:A:471:ASN:O	1:A:473:GLY:N	2.51	0.41
1:B:469:THR:C	1:B:471:ASN:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:TRP:HA	1:B:352:LEU:HB3	2.02	0.41
1:B:520:ALA:O	1:B:521:CYS:CB	2.68	0.41
1:B:194:TRP:HZ3	1:B:232:TYR:CD2	2.36	0.41
1:B:333:PRO:HD2	1:B:334:TRP:CE3	2.56	0.41
1:B:315:SER:O	1:B:316:TYR:C	2.59	0.41
1:A:333:PRO:HD2	1:A:334:TRP:CZ3	2.56	0.41
1:B:342:SER:HA	1:B:343:PRO:HA	1.85	0.41
1:B:99:ILE:HG23	1:B:104:HIS:HB2	2.02	0.41
1:B:179:GLN:HB2	1:B:179:GLN:HE21	1.66	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: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:186:THR:HG21	1:B:409:ARG:NE	2.36	0.40
1:B:221:ASN:HB2	1:B:229:VAL:HG12	2.04	0.40
1:B:130:ASP:HA	1:B:131:PRO:HD3	1.92	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 ⓘ

5.3.1 Protein backbone ⓘ

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	Percentiles	
1	A	388/533 (73%)	325 (84%)	51 (13%)	12 (3%)	5	32
1	B	462/533 (87%)	358 (78%)	72 (16%)	32 (7%)	1	11
All	All	850/1066 (80%)	683 (80%)	123 (14%)	44 (5%)	2	18

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	TRP

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

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Mol	Chain	Res	Type
1	B	237	PRO

5.3.2 Protein sidechains ⓘ

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	Percentiles	
1	A	335/456 (74%)	314 (94%)	21 (6%)	22	60
1	B	404/456 (89%)	365 (90%)	39 (10%)	10	38
All	All	739/912 (81%)	679 (92%)	60 (8%)	15	48

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

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

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

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

Mol	Chain	Res	Type
1	A	282	ASN
1	A	386	HIS
1	A	536	ASN
1	A	541	GLN
1	B	76	HIS
1	B	112	ASN
1	B	136	GLN
1	B	177	GLN
1	B	179	GLN
1	B	415	ASN
1	B	536	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	701	1	14,14,15	0.53	0	15,19,21	1.39	1 (6%)
2	NAG	B	701	1	14,14,15	0.45	0	15,19,21	1.01	1 (6%)
2	NAG	B	702	1	14,14,15	0.50	0	15,19,21	0.99	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	703	1	14,14,15	0.57	0	15,19,21	0.87	0

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	A	701	1	-	0/6/23/26	0/1/1/1
2	NAG	B	701	1	-	0/6/23/26	0/1/1/1
2	NAG	B	702	1	-	0/6/23/26	0/1/1/1
2	NAG	B	703	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	NAG	C1-O5-C5	2.52	115.44	112.25
2	B	701	NAG	C1-O5-C5	3.17	116.27	112.25
2	A	701	NAG	C1-O5-C5	4.74	118.27	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	702	NAG	1	0
2	B	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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	A	392/533 (73%)	-0.05	5 (1%) 79 74	20, 38, 70, 82	0
1	B	468/533 (87%)	0.45	25 (5%) 30 24	48, 66, 105, 112	0
All	All	860/1066 (80%)	0.22	30 (3%) 48 40	20, 59, 101, 112	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	ALA	7.5
1	B	552	ASP	4.4
1	B	274	THR	4.2
1	B	579	GLU	3.9
1	B	181	ARG	3.5
1	B	205	HIS	3.4
1	B	473	GLY	3.4
1	B	275	SER	3.3
1	B	197	ALA	3.1
1	A	318	ASP	3.0
1	B	555	GLY	3.0
1	A	201	ALA	2.9
1	B	578	GLY	2.8
1	B	276	GLU	2.8
1	B	517	ARG	2.8
1	B	526	GLY	2.7
1	B	196	SER	2.6
1	B	206	GLN	2.5
1	B	194	TRP	2.4
1	B	512	PRO	2.4
1	B	83	GLY	2.4
1	B	170	CYS	2.3
1	A	515	GLY	2.2
1	B	514	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	277	TYR	2.2
1	B	554	ASP	2.2
1	B	198	GLN	2.2
1	B	122	THR	2.2
1	A	173	ASP	2.0
1	A	319	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	B	703	14/15	0.62	0.43	2.45	69,70,71,71	0
2	NAG	B	702	14/15	0.82	0.24	-0.05	61,61,62,62	0
2	NAG	B	701	14/15	0.78	0.21	-	54,56,56,56	0
2	NAG	A	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.