



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 1, 2025 – 10:45 pm BST

PDB ID : 5T89 / pdb\_00005t89  
Title : Crystal structure of VEGF-A in complex with VEGFR-1 domains D1-6  
Authors : Markovic-Mueller, S.; Stuttfeld, E.; Asthana, M.; Weinert, T.; Bliven, S.; Goldie, K.N.; Kisko, K.; Capitani, G.; Ballmer-Hofer, K.  
Deposited on : 2016-09-07  
Resolution : 4.00 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

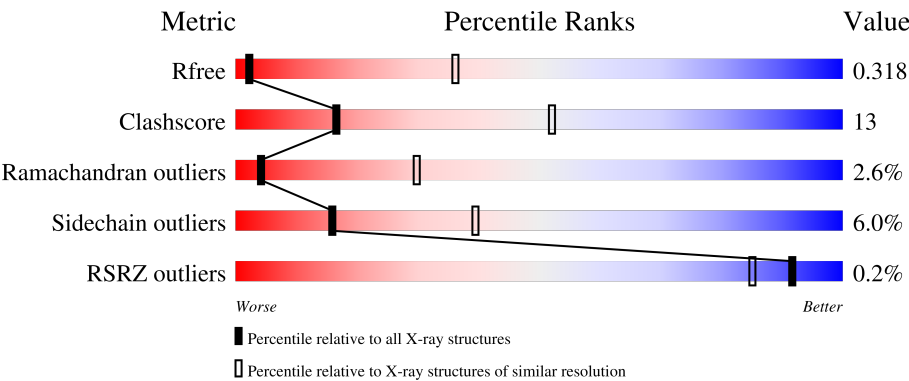
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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 <sub>free</sub>	164625	1028 (4.22-3.78)
Clashscore	180529	1055 (4.20-3.80)
Ramachandran outliers	177936	1004 (4.20-3.80)
Sidechain outliers	177891	1027 (4.22-3.78)
RSRZ outliers	164620	1029 (4.22-3.78)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	V	131	
1	W	131	
2	X	646	
2	Y	646	
3	A	2	

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Mol	Chain	Length	Quality of chain
3	B	2	 50%50%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11357 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 Vascular endothelial growth factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	V	96	Total	C	N	O	S	34	0	0
			779	489	131	146	13			
1	W	96	Total	C	N	O	S	0	0	0
			779	489	131	146	13			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-9	GLY	-	expression tag	UNP P15692
V	-8	SER	-	expression tag	UNP P15692
V	-7	HIS	-	expression tag	UNP P15692
V	-6	HIS	-	expression tag	UNP P15692
V	-5	HIS	-	expression tag	UNP P15692
V	-4	HIS	-	expression tag	UNP P15692
V	-3	HIS	-	expression tag	UNP P15692
V	-2	HIS	-	expression tag	UNP P15692
V	-1	GLY	-	expression tag	UNP P15692
V	0	SER	-	expression tag	UNP P15692
V	115	ASN	LYS	conflict	UNP P15692
W	-9	GLY	-	expression tag	UNP P15692
W	-8	SER	-	expression tag	UNP P15692
W	-7	HIS	-	expression tag	UNP P15692
W	-6	HIS	-	expression tag	UNP P15692
W	-5	HIS	-	expression tag	UNP P15692
W	-4	HIS	-	expression tag	UNP P15692
W	-3	HIS	-	expression tag	UNP P15692
W	-2	HIS	-	expression tag	UNP P15692
W	-1	GLY	-	expression tag	UNP P15692
W	0	SER	-	expression tag	UNP P15692
W	115	ASN	LYS	conflict	UNP P15692

- Molecule 2 is a protein called Vascular endothelial growth factor receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	596	Total 4734	C 3003	N 825	O 880	S 26	183	0	0
2	Y	597	Total 4743	C 3007	N 827	O 883	S 26	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

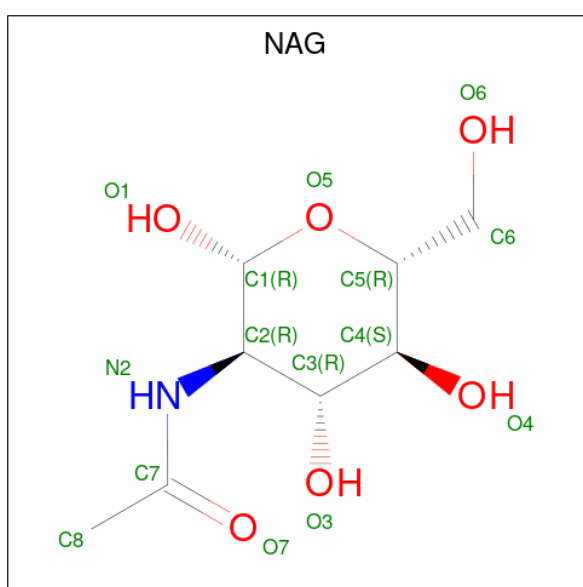
Chain	Residue	Modelled	Actual	Comment	Reference
X	657	ASP	-	expression tag	UNP P17948
X	658	GLN	-	expression tag	UNP P17948
X	659	GLU	-	expression tag	UNP P17948
X	660	ALA	-	expression tag	UNP P17948
X	661	ILE	-	expression tag	UNP P17948
X	662	GLU	-	expression tag	UNP P17948
X	663	GLY	-	expression tag	UNP P17948
X	664	ARG	-	expression tag	UNP P17948
X	665	HIS	-	expression tag	UNP P17948
X	666	HIS	-	expression tag	UNP P17948
X	667	HIS	-	expression tag	UNP P17948
X	668	HIS	-	expression tag	UNP P17948
X	669	HIS	-	expression tag	UNP P17948
X	670	HIS	-	expression tag	UNP P17948
X	671	HIS	-	expression tag	UNP P17948
X	672	HIS	-	expression tag	UNP P17948
Y	657	ASP	-	expression tag	UNP P17948
Y	658	GLN	-	expression tag	UNP P17948
Y	659	GLU	-	expression tag	UNP P17948
Y	660	ALA	-	expression tag	UNP P17948
Y	661	ILE	-	expression tag	UNP P17948
Y	662	GLU	-	expression tag	UNP P17948
Y	663	GLY	-	expression tag	UNP P17948
Y	664	ARG	-	expression tag	UNP P17948
Y	665	HIS	-	expression tag	UNP P17948
Y	666	HIS	-	expression tag	UNP P17948
Y	667	HIS	-	expression tag	UNP P17948
Y	668	HIS	-	expression tag	UNP P17948
Y	669	HIS	-	expression tag	UNP P17948
Y	670	HIS	-	expression tag	UNP P17948
Y	671	HIS	-	expression tag	UNP P17948
Y	672	HIS	-	expression tag	UNP P17948

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	V	1	Total	C	N	O	0	0
			14	8	1	5		
4	W	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		

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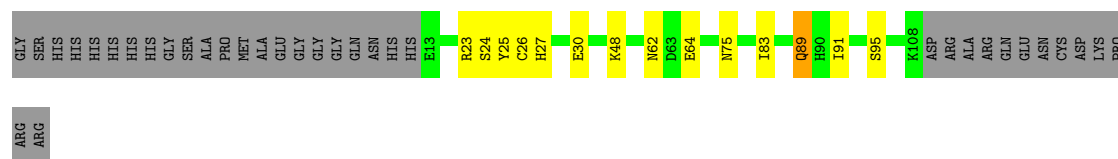
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		
4	Y	1	Total	C	N	O	0	0
			14	8	1	5		

### 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: Vascular endothelial growth factor A

Chain V: 



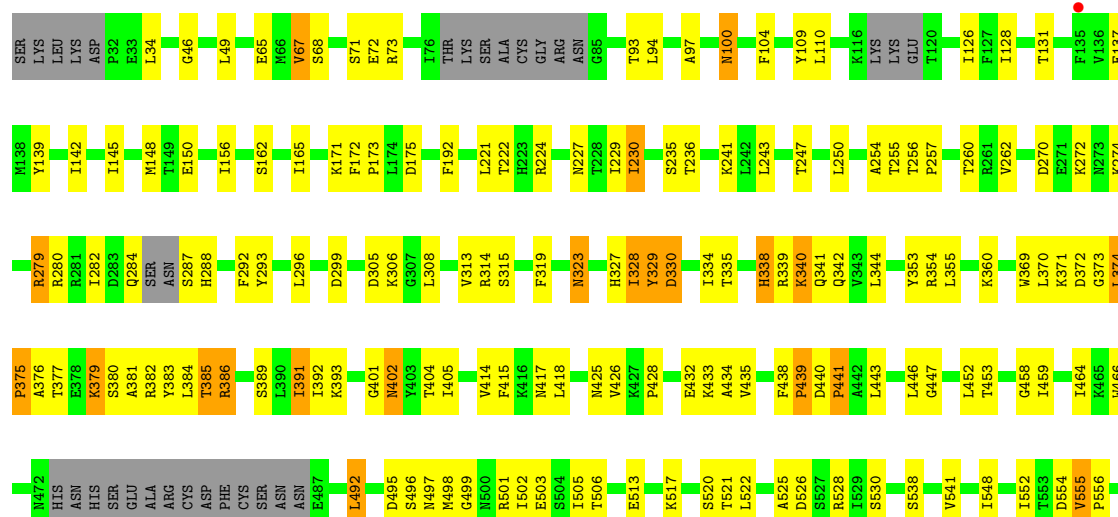
- Molecule 1: Vascular endothelial growth factor A

Chain W: 

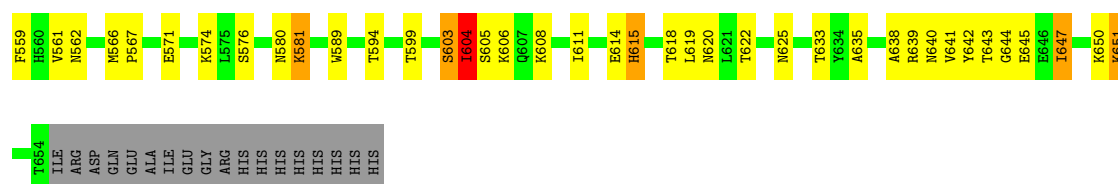


- Molecule 2: Vascular endothelial growth factor receptor 1

Chain X: 

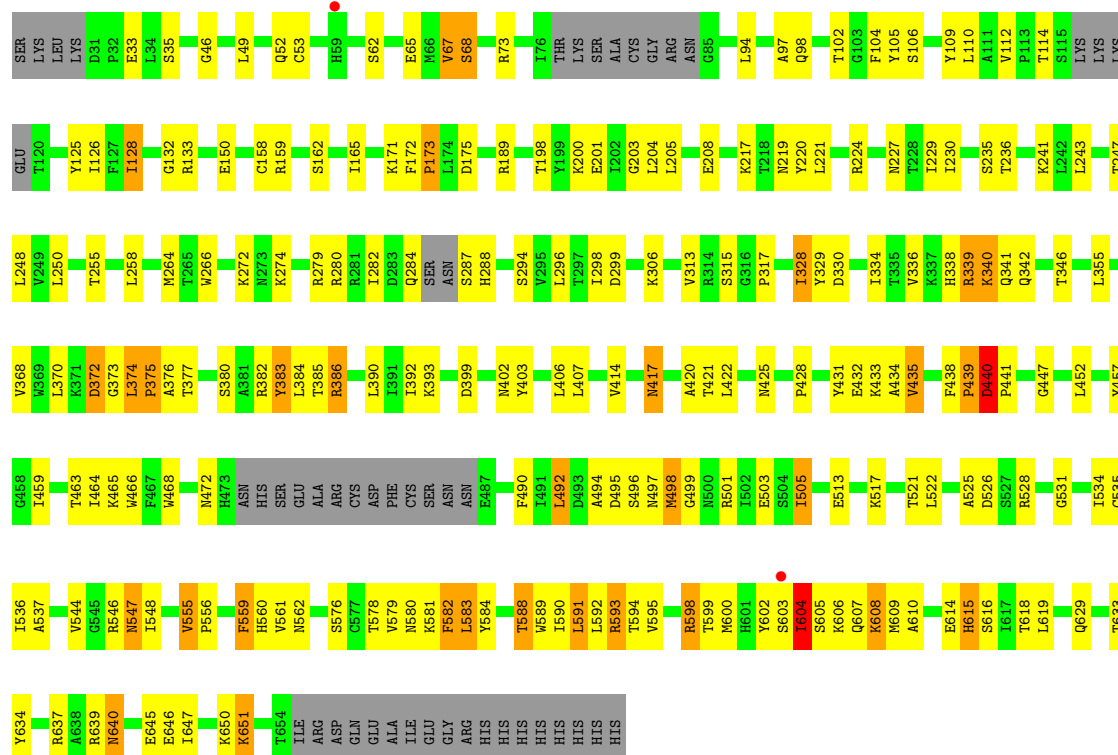






• Molecule 2: Vascular endothelial growth factor receptor 1

Chain Y: 59% 28% 5% 8%



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 100%



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.71Å 123.09Å 167.37Å 90.00° 109.56° 90.00°	Depositor
Resolution (Å)	19.99 – 4.00 19.99 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.99-4.00) 98.7 (19.99-4.00)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 4.00Å)	Xtriage
Refinement program	PHENIX dev_2420	Depositor
R, $R_{free}$	0.285 , 0.315 0.293 , 0.318	Depositor DCC
$R_{free}$ test set	803 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	138.9	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 148.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11357	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	219.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 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	V	0.27	0/797	0.43	0/1073
1	W	0.26	0/797	0.42	0/1073
2	X	0.27	0/4825	0.49	1/6531 (0.0%)
2	Y	0.27	0/4835	0.49	0/6547
All	All	0.27	0/11254	0.48	1/15224 (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
2	Y	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	X	603	SER	C-N-CA	5.55	135.57	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Y	372	ASP	Peptide
2	Y	440	ASP	Peptide

## 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	V	779	0	744	13	0
1	W	779	0	744	14	0
2	X	4734	0	4815	131	0
2	Y	4743	0	4811	143	0
3	A	28	0	25	0	0
3	B	28	0	25	1	0
4	V	14	0	13	0	0
4	W	14	0	13	3	0
4	X	112	0	104	3	0
4	Y	126	0	117	2	0
All	All	11357	0	11411	284	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 13.

All (284) 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)
2:Y:241:LYS:NZ	2:Y:330:ASP:OD2	2.08	0.86
2:Y:150:GLU:OE1	2:Y:224:ARG:NH1	2.12	0.81
2:Y:562:ASN:HB3	2:Y:576:SER:HB3	1.64	0.78
1:V:23:ARG:NH2	1:W:30:GLU:OE2	2.18	0.77
2:X:603:SER:HB3	2:X:604:ILE:O	1.87	0.75
2:Y:593:ARG:NH1	2:Y:629:GLN:O	2.21	0.74
2:Y:328:ILE:HG12	2:Y:329:TYR:H	1.53	0.73
1:V:24:SER:HB3	1:W:53:PRO:HD3	1.70	0.73
2:Y:603:SER:HB3	2:Y:604:ILE:O	1.88	0.72
2:X:375:PRO:HD2	2:X:376:ALA:HA	1.72	0.72
1:W:75:ASN:HD21	1:W:95:SER:HB3	1.54	0.71
2:X:381:ALA:O	2:Y:393:LYS:NZ	2.23	0.70
2:X:640:ASN:ND2	2:X:643:THR:OG1	2.23	0.70
2:Y:341:GLN:HG2	2:Y:342:GLN:HB3	1.73	0.70
2:Y:589:TRP:HE1	2:Y:619:LEU:HD22	1.58	0.69
2:X:241:LYS:NZ	2:X:330:ASP:OD2	2.27	0.68
2:Y:162:SER:HB3	2:Y:165:ILE:HG13	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:417:ASN:N	2:Y:417:ASN:OD1	2.28	0.67
2:X:384:LEU:HD21	2:X:386:ARG:HH12	1.58	0.66
2:Y:589:TRP:HB2	2:Y:604:ILE:HD13	1.78	0.66
2:X:517:LYS:NZ	2:Y:434:ALA:O	2.27	0.65
1:V:91:ILE:HG13	2:X:142:ILE:HD13	1.79	0.64
2:X:328:ILE:HG12	2:X:329:TYR:H	1.62	0.64
2:X:503:GLU:HB2	2:X:525:ALA:HB2	1.80	0.64
2:X:282:ILE:HG22	2:X:284:GLN:H	1.64	0.63
2:Y:375:PRO:HD2	2:Y:376:ALA:HA	1.80	0.63
2:X:589:TRP:HE1	2:X:619:LEU:HD22	1.64	0.63
2:X:492:LEU:H	2:X:495:ASP:HB2	1.64	0.63
2:Y:264:MET:HG2	2:Y:313:VAL:HG22	1.80	0.63
2:X:555:VAL:HG22	2:X:556:PRO:HD2	1.81	0.62
1:W:75:ASN:ND2	1:W:95:SER:HB3	2.15	0.62
2:X:562:ASN:HB3	2:X:576:SER:HB3	1.82	0.62
2:Y:67:VAL:HG13	2:Y:68:SER:H	1.64	0.62
2:Y:272:LYS:NZ	2:Y:272:LYS:HB3	2.15	0.62
2:Y:383:TYR:OH	2:Y:399:ASP:OD1	2.16	0.61
2:Y:425:ASN:HD22	2:Y:459:ILE:HG22	1.63	0.61
2:X:374:LEU:HB3	2:X:375:PRO:HD3	1.82	0.60
2:Y:503:GLU:HB2	2:Y:525:ALA:HB2	1.83	0.60
2:Y:339:ARG:HB2	2:Y:340:LYS:HD3	1.82	0.60
2:Y:452:LEU:HD12	2:Y:522:LEU:HD12	1.84	0.60
2:Y:590:ILE:HD11	2:Y:637:ARG:HD2	1.84	0.60
2:Y:591:LEU:HG	2:Y:602:TYR:HB2	1.84	0.60
1:W:96:PHE:HA	4:W:201:NAG:H82	1.83	0.60
1:V:83:ILE:HA	1:V:89:GLN:HB3	1.83	0.60
2:X:241:LYS:NZ	2:X:327:HIS:HD2	2.00	0.60
2:Y:102:THR:O	2:Y:159:ARG:NH1	2.24	0.60
2:Y:342:GLN:HB2	2:Y:421:THR:H	1.66	0.59
2:Y:579:VAL:HG13	2:Y:584:TYR:HD2	1.67	0.59
2:X:443:LEU:HD22	2:X:580:ASN:HD22	1.68	0.59
2:X:497:ASN:N	2:X:498:MET:HA	2.18	0.59
2:Y:62:SER:HB3	2:Y:106:SER:HB3	1.85	0.59
2:Y:640:ASN:OD1	2:Y:640:ASN:N	2.36	0.58
2:Y:374:LEU:HB3	2:Y:375:PRO:HD3	1.85	0.58
2:X:502:ILE:HD12	2:X:522:LEU:HD21	1.85	0.58
2:Y:497:ASN:N	2:Y:498:MET:HA	2.19	0.58
2:Y:588:THR:HG23	2:Y:637:ARG:HB3	1.84	0.58
2:Y:560:HIS:HB3	2:Y:578:THR:HB	1.86	0.58
2:Y:492:LEU:H	2:Y:495:ASP:HB2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:48:LYS:NZ	1:W:62:ASN:O	2.37	0.57
2:X:426:VAL:HG23	2:X:459:ILE:HB	1.86	0.57
2:Y:547:ASN:OD1	2:Y:547:ASN:N	2.35	0.57
2:X:162:SER:HB3	2:X:165:ILE:HG13	1.87	0.56
2:X:375:PRO:CD	2:X:376:ALA:HA	2.36	0.56
2:Y:607:GLN:HB3	2:Y:608:LYS:HA	1.88	0.56
2:Y:198:THR:N	2:Y:201:GLU:OE1	2.39	0.55
2:Y:370:LEU:HB3	2:Y:373:GLY:O	2.06	0.55
2:Y:229:ILE:HD13	2:Y:313:VAL:HG12	1.88	0.55
2:X:272:LYS:HB3	2:X:272:LYS:NZ	2.21	0.55
2:X:338:HIS:CD2	2:X:418:LEU:HD21	2.42	0.55
2:X:339:ARG:HB2	2:X:340:LYS:HD3	1.88	0.55
2:Y:589:TRP:H	2:Y:604:ILE:HG12	1.72	0.55
2:Y:402:ASN:HA	2:Y:421:THR:HA	1.88	0.55
2:X:434:ALA:HA	2:Y:513:GLU:HG3	1.88	0.55
2:Y:280:ARG:HH22	2:Y:282:ILE:HD11	1.72	0.55
2:X:625:ASN:OD1	4:X:709:NAG:N2	2.40	0.54
1:V:30:GLU:OE2	1:W:23:ARG:NH2	2.40	0.54
4:X:705:NAG:H83	4:X:705:NAG:H3	1.89	0.54
2:Y:49:LEU:H	2:Y:94:LEU:HB3	1.72	0.54
2:Y:346:THR:HG22	2:Y:422:LEU:HD11	1.89	0.54
2:X:279:ARG:HG2	2:X:293:TYR:HB2	1.89	0.53
2:Y:432:GLU:HB3	2:Y:546:ARG:NH1	2.23	0.53
2:X:71:SER:OG	2:X:93:THR:O	2.24	0.53
1:V:75:ASN:OD1	1:V:95:SER:OG	2.24	0.53
2:X:446:LEU:HB2	2:X:554:ASP:HA	1.91	0.53
2:Y:555:VAL:HG22	2:Y:556:PRO:HD2	1.90	0.53
2:Y:594:THR:HB	2:Y:599:THR:HG23	1.91	0.53
2:X:229:ILE:HD13	2:X:313:VAL:HG12	1.91	0.52
2:Y:534:ILE:HG12	2:Y:547:ASN:HB3	1.90	0.52
2:Y:609:MET:HG3	2:Y:610:ALA:H	1.74	0.52
1:V:25:TYR:O	1:V:27:HIS:ND1	2.37	0.52
2:X:67:VAL:HG22	2:X:68:SER:H	1.75	0.52
2:X:530:SER:HB2	2:X:552:ILE:HG22	1.91	0.52
2:Y:595:VAL:H	2:Y:598:ARG:HH11	1.56	0.52
2:Y:380:SER:O	2:Y:382:ARG:N	2.42	0.52
1:W:75:ASN:OD1	1:W:76:ILE:N	2.43	0.51
2:Y:227:ASN:ND2	2:Y:315:SER:O	2.33	0.51
2:Y:637:ARG:HH12	2:Y:639:ARG:HD3	1.75	0.51
2:X:566:MET:HB2	2:X:571:GLU:HB2	1.93	0.51
2:Y:580:ASN:OD1	2:Y:583:LEU:HD21	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:280:ARG:NH1	2:Y:282:ILE:HG12	2.26	0.50
2:X:353:TYR:HB3	2:X:392:ILE:HB	1.93	0.50
2:X:306:LYS:HB2	2:X:328:ILE:HG22	1.93	0.50
2:X:643:THR:HB	2:X:644:GLY:HA3	1.92	0.50
2:Y:98:GLN:HB3	4:Y:701:NAG:H2	1.94	0.50
2:X:241:LYS:HZ3	2:X:327:HIS:HD2	1.58	0.50
2:Y:375:PRO:CD	2:Y:376:ALA:HA	2.41	0.50
2:X:171:LYS:HB3	2:X:175:ASP:HB2	1.93	0.50
2:X:405:ILE:HG23	2:X:418:LEU:HB3	1.93	0.50
2:Y:505:ILE:HG12	2:Y:522:LEU:HD23	1.94	0.50
2:X:371:LYS:H	2:X:376:ALA:HB2	1.76	0.50
2:X:270:ASP:OD2	2:X:305:ASP:HA	2.11	0.50
2:Y:204:LEU:HD11	2:Y:219:ASN:HB3	1.94	0.50
2:Y:438:PHE:O	2:Y:440:ASP:HA	2.12	0.50
2:X:308:LEU:HD11	2:X:323:ASN:HB2	1.93	0.49
2:Y:593:ARG:HH12	2:Y:629:GLN:C	2.15	0.49
2:Y:306:LYS:HB2	2:Y:328:ILE:HG22	1.93	0.49
2:X:156:ILE:HB	2:X:192:PHE:HB2	1.93	0.49
2:Y:495:ASP:HB3	2:Y:496:SER:HB3	1.95	0.49
2:X:330:ASP:OD1	2:X:330:ASP:N	2.46	0.49
2:X:640:ASN:OD1	2:X:641:VAL:N	2.46	0.49
2:X:370:LEU:HB3	2:X:373:GLY:O	2.13	0.49
2:Y:158:CYS:HB3	2:Y:220:TYR:CE1	2.48	0.48
2:X:432:GLU:OE2	2:Y:435:VAL:HG23	2.12	0.48
2:Y:171:LYS:HE3	2:Y:203:GLY:HA3	1.96	0.48
2:Y:421:THR:OG1	4:Y:707:NAG:H62	2.14	0.48
2:X:230:ILE:HD12	2:X:255:THR:HG22	1.96	0.48
2:Y:132:GLY:HA2	2:Y:133:ARG:HA	1.54	0.48
2:X:100:ASN:OD1	2:X:100:ASN:N	2.38	0.48
2:Y:341:GLN:HA	2:Y:342:GLN:HA	1.59	0.48
2:X:452:LEU:HD13	2:X:548:ILE:HG21	1.96	0.48
2:Y:463:THR:O	2:Y:537:ALA:HA	2.13	0.48
2:X:440:ASP:O	2:X:441:PRO:C	2.52	0.47
2:X:372:ASP:OD1	2:X:401:GLY:HA3	2.14	0.47
2:Y:580:ASN:ND2	2:Y:616:SER:OG	2.46	0.47
2:X:272:LYS:HB3	2:X:272:LYS:HZ3	1.79	0.47
2:X:502:ILE:HG21	2:X:505:ILE:HD11	1.96	0.47
2:Y:336:VAL:HG21	2:Y:407:LEU:HD13	1.97	0.47
1:V:62:ASN:HB3	1:W:48:LYS:HZ2	1.80	0.47
2:X:235:SER:HA	2:X:236:THR:HA	1.59	0.47
2:X:521:THR:HG21	2:Y:438:PHE:CD2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:605:SER:O	2:Y:607:GLN:N	2.47	0.47
2:Y:227:ASN:ND2	2:Y:317:PRO:HD2	2.30	0.47
2:X:280:ARG:HH22	2:X:282:ILE:HD11	1.80	0.47
2:X:354:ARG:HA	2:X:391:ILE:HA	1.97	0.47
2:Y:227:ASN:OD1	2:Y:315:SER:OG	2.31	0.47
2:X:466:TRP:HZ3	2:X:548:ILE:HD12	1.78	0.46
2:Y:97:ALA:HB1	2:Y:128:ILE:HD13	1.96	0.46
2:Y:447:GLY:HA2	2:Y:526:ASP:OD1	2.15	0.46
2:X:323:ASN:OD1	2:X:323:ASN:N	2.48	0.46
2:X:594:THR:HG22	2:X:599:THR:HA	1.97	0.46
2:X:432:GLU:N	2:X:432:GLU:OE1	2.48	0.46
2:Y:287:SER:OG	2:Y:288:HIS:N	2.46	0.46
2:Y:46:GLY:N	2:Y:97:ALA:HB3	2.30	0.46
2:Y:272:LYS:HB3	2:Y:272:LYS:HZ2	1.80	0.46
2:X:501:ARG:O	2:X:525:ALA:N	2.45	0.46
2:Y:334:ILE:HD12	2:Y:414:VAL:HG12	1.98	0.46
2:X:241:LYS:NZ	2:X:327:HIS:CD2	2.84	0.46
2:Y:208:GLU:HG2	2:Y:217:LYS:HB3	1.98	0.46
2:X:341:GLN:HA	2:X:342:GLN:HA	1.64	0.46
2:X:438:PHE:N	2:X:439:PRO:HD2	2.31	0.46
2:X:247:THR:HG23	2:X:299:ASP:HA	1.99	0.46
2:X:334:ILE:HD12	2:X:414:VAL:HG12	1.98	0.46
2:X:633:THR:OG1	2:X:651:LYS:HG2	2.16	0.46
2:Y:607:GLN:CB	2:Y:608:LYS:HA	2.44	0.46
2:Y:464:ILE:HA	2:Y:536:ILE:O	2.17	0.45
2:Y:433:LYS:HD2	2:Y:546:ARG:HB2	1.97	0.45
2:X:513:GLU:HG3	2:Y:434:ALA:HA	1.98	0.45
2:Y:368:VAL:HG13	2:Y:406:LEU:HB3	1.97	0.45
2:X:314:ARG:HD3	2:X:319:PHE:CD1	2.52	0.45
2:X:580:ASN:OD1	2:X:581:LYS:N	2.49	0.45
2:Y:355:LEU:HB2	2:Y:390:LEU:HB3	1.98	0.45
2:Y:125:TYR:CE2	2:Y:189:ARG:HB3	2.52	0.45
2:X:150:GLU:OE1	2:X:224:ARG:NH1	2.50	0.45
2:X:274:LYS:HG3	2:X:299:ASP:H	1.82	0.45
2:X:383:TYR:CE1	2:X:392:ILE:HG23	2.51	0.45
2:Y:280:ARG:HH12	2:Y:282:ILE:CD1	2.30	0.45
1:W:48:LYS:HD3	2:Y:221:LEU:HD21	1.97	0.45
2:X:280:ARG:HH12	2:X:282:ILE:HD11	1.82	0.45
2:Y:235:SER:HA	2:Y:236:THR:HA	1.59	0.45
2:X:376:ALA:N	2:X:377:THR:HA	2.32	0.45
2:Y:328:ILE:O	2:Y:329:TYR:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:604:ILE:HD12	2:Y:604:ILE:HA	1.71	0.45
2:X:227:ASN:ND2	2:X:315:SER:O	2.45	0.45
2:Y:384:LEU:HD21	2:Y:386:ARG:HH12	1.82	0.45
2:Y:603:SER:HA	2:Y:604:ILE:HB	1.98	0.45
2:Y:35:SER:HB3	2:Y:52:GLN:HB2	1.99	0.44
2:Y:604:ILE:HG23	2:Y:605:SER:HB2	1.99	0.44
2:Y:633:THR:HA	2:Y:651:LYS:HA	1.99	0.44
2:Y:588:THR:OG1	2:Y:589:TRP:N	2.50	0.44
2:X:464:ILE:HG12	2:X:520:SER:HB2	1.99	0.44
2:X:495:ASP:HA	2:X:496:SER:HA	1.79	0.44
1:V:48:LYS:HD3	2:X:221:LEU:HD21	2.00	0.44
2:Y:465:LYS:HG2	2:Y:490:PHE:HD2	1.81	0.44
2:X:635:ALA:HB1	2:X:647:ILE:HD11	1.99	0.44
2:X:172:PHE:HA	2:X:173:PRO:HA	1.74	0.44
2:X:446:LEU:HD21	2:X:528:ARG:NH1	2.33	0.44
2:Y:599:THR:HB	2:Y:600:MET:H	1.56	0.44
1:W:39:TYR:CZ	4:W:201:NAG:H83	2.52	0.44
2:X:49:LEU:HB2	2:X:94:LEU:HB3	1.99	0.44
2:X:576:SER:HA	2:X:620:ASN:HA	1.99	0.44
2:Y:274:LYS:HB2	2:Y:298:ILE:HA	1.99	0.44
2:X:344:LEU:HD12	2:X:353:TYR:OH	2.18	0.44
2:X:574:LYS:HA	2:X:622:THR:HG22	1.99	0.44
2:X:603:SER:HA	2:X:604:ILE:HG23	1.99	0.44
2:Y:266:TRP:NE1	2:Y:294:SER:OG	2.48	0.44
1:V:89:GLN:OE1	2:X:145:ILE:HD12	2.17	0.43
2:X:287:SER:OG	2:X:288:HIS:N	2.50	0.43
2:X:380:SER:C	2:X:382:ARG:H	2.21	0.43
2:X:376:ALA:H	2:X:377:THR:HA	1.83	0.43
2:X:428:PRO:HG3	2:X:538:SER:HA	2.00	0.43
2:X:614:GLU:HA	2:X:615:HIS:HA	1.61	0.43
2:Y:248:LEU:HD11	2:Y:250:LEU:HD21	2.00	0.43
2:Y:614:GLU:HA	2:Y:615:HIS:HA	1.66	0.43
2:Y:172:PHE:CG	2:Y:173:PRO:HA	2.53	0.43
2:X:97:ALA:HB1	2:X:128:ILE:HD13	2.00	0.43
2:Y:497:ASN:HA	2:Y:498:MET:HG2	2.01	0.43
2:Y:439:PRO:HA	2:Y:440:ASP:CG	2.39	0.43
2:X:250:LEU:HD12	2:X:296:LEU:HD23	2.00	0.43
2:Y:370:LEU:HA	2:Y:376:ALA:HB2	2.01	0.43
2:Y:595:VAL:HG23	2:Y:598:ARG:NH1	2.34	0.43
2:X:433:LYS:NZ	2:X:433:LYS:HB3	2.34	0.43
2:X:254:ALA:HB3	2:X:292:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:338:HIS:HB2	2:X:339:ARG:H	1.66	0.43
2:X:447:GLY:HA2	2:X:526:ASP:OD1	2.19	0.43
2:X:453:THR:HB	2:X:521:THR:HG22	2.00	0.43
1:W:75:ASN:HB2	4:W:201:NAG:O5	2.19	0.42
2:X:369:TRP:HD1	2:X:385:THR:HG23	1.83	0.42
2:X:384:LEU:HD21	2:X:386:ARG:NH1	2.31	0.42
2:X:384:LEU:HB3	2:X:391:ILE:HG23	2.01	0.42
2:X:559:PHE:HE2	2:X:638:ALA:HB3	1.84	0.42
2:Y:247:THR:HG23	2:Y:299:ASP:HA	2.01	0.42
2:Y:428:PRO:HG2	2:Y:544:VAL:HG12	2.01	0.42
3:B:1:NAG:H4	3:B:2:NAG:H2	1.78	0.42
1:V:64:GLU:HB3	2:Y:258:LEU:HD22	2.00	0.42
2:X:34:LEU:H	2:X:34:LEU:HD23	1.84	0.42
2:Y:582:PHE:HD1	2:Y:582:PHE:HA	1.65	0.42
1:W:107:LYS:HZ2	2:X:284:GLN:CG	2.32	0.42
2:X:438:PHE:CD2	2:Y:521:THR:HG21	2.54	0.42
2:Y:431:TYR:CE1	2:Y:517:LYS:HD3	2.54	0.42
2:Y:583:LEU:O	2:Y:640:ASN:HB3	2.19	0.42
2:X:148:MET:HG2	2:X:222:THR:HB	2.02	0.42
2:X:229:ILE:HA	2:X:256:THR:HG22	2.02	0.42
2:Y:383:TYR:CE1	2:Y:392:ILE:HG23	2.55	0.42
2:Y:651:LYS:HB3	2:Y:651:LYS:HE3	1.85	0.42
2:Y:466:TRP:HA	2:Y:534:ILE:O	2.20	0.42
2:X:402:ASN:OD1	2:X:402:ASN:N	2.34	0.42
2:Y:376:ALA:N	2:Y:377:THR:HA	2.35	0.42
2:X:46:GLY:H	2:X:97:ALA:HB3	1.85	0.42
2:X:604:ILE:HD12	2:X:605:SER:HB2	2.01	0.42
2:Y:112:VAL:HG12	2:Y:114:THR:H	1.85	0.42
2:X:355:LEU:O	2:X:389:SER:OG	2.29	0.41
2:X:262:VAL:HB	2:X:313:VAL:HG13	2.01	0.41
2:X:589:TRP:NE1	2:X:619:LEU:HD22	2.33	0.41
2:Y:591:LEU:HB3	2:Y:634:TYR:CE1	2.54	0.41
2:X:71:SER:OG	2:X:72:GLU:N	2.53	0.41
2:X:376:ALA:HB1	2:X:379:LYS:HG2	2.01	0.41
2:Y:466:TRP:CZ3	2:Y:535:CYS:HB3	2.54	0.41
2:Y:559:PHE:HD1	2:Y:559:PHE:HA	1.70	0.41
1:V:62:ASN:HB3	1:W:48:LYS:NZ	2.35	0.41
2:X:374:LEU:CB	2:X:375:PRO:HD3	2.48	0.41
2:Y:376:ALA:H	2:Y:377:THR:HA	1.86	0.41
2:X:384:LEU:HD12	2:X:384:LEU:HA	1.88	0.41
2:Y:382:ARG:HG3	2:Y:383:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:452:LEU:O	2:Y:521:THR:HA	2.21	0.41
2:Y:457:TYR:HB2	2:Y:517:LYS:HG2	2.02	0.41
2:Y:466:TRP:HZ3	2:Y:548:ILE:HD12	1.86	0.41
2:Y:526:ASP:OD1	2:Y:528:ARG:HD3	2.20	0.41
2:Y:205:LEU:N	2:Y:220:TYR:O	2.46	0.41
2:Y:403:TYR:N	2:Y:420:ALA:O	2.53	0.41
2:Y:468:TRP:CH2	2:Y:531:GLY:HA3	2.56	0.41
2:X:137:GLU:HB3	2:X:139:TYR:CE2	2.55	0.41
2:X:415:PHE:HB2	4:X:707:NAG:H61	2.03	0.40
2:X:335:THR:N	2:X:360:LYS:O	2.52	0.40
2:X:425:ASN:HB3	2:X:541:VAL:HG21	2.02	0.40
2:X:426:VAL:HB	2:X:458:GLY:HA2	2.03	0.40
2:X:603:SER:HA	2:X:604:ILE:CG1	2.52	0.40
2:Y:105:TYR:HB2	2:Y:126:ILE:HD13	2.03	0.40
2:Y:390:LEU:HD21	2:Y:403:TYR:CD2	2.55	0.40
2:X:49:LEU:HD11	2:X:126:ILE:HG21	2.02	0.40
2:X:611:ILE:HG13	2:X:618:THR:O	2.21	0.40
2:Y:33:GLU:O	2:Y:53:CYS:HA	2.21	0.40
2:Y:230:ILE:HD12	2:Y:255:THR:HG22	2.03	0.40
2:Y:250:LEU:HD12	2:Y:296:LEU:HD23	2.02	0.40
2:Y:171:LYS:NZ	2:Y:200:LYS:O	2.52	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	Percentiles	
1	V	94/131 (72%)	90 (96%)	3 (3%)	1 (1%)	12	45
1	W	94/131 (72%)	90 (96%)	4 (4%)	0	100	100
2	X	586/646 (91%)	474 (81%)	96 (16%)	16 (3%)	4	29
2	Y	587/646 (91%)	483 (82%)	85 (14%)	19 (3%)	3	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1361/1554 (88%)	1137 (84%)	188 (14%)	36 (3%)	4	30

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	X	67	VAL
2	X	581	LYS
2	X	604	ILE
2	Y	68	SER
2	Y	604	ILE
2	X	375	PRO
2	X	441	PRO
2	Y	67	VAL
2	Y	173	PRO
2	Y	328	ILE
2	Y	375	PRO
2	Y	581	LYS
2	Y	593	ARG
2	Y	606	LYS
2	X	374	LEU
2	X	386	ARG
2	X	639	ARG
2	X	642	TYR
2	Y	374	LEU
2	Y	494	ALA
2	Y	499	GLY
2	X	257	PRO
2	X	393	LYS
2	X	439	PRO
2	X	499	GLY
2	Y	440	ASP
2	Y	472	ASN
2	Y	383	TYR
2	Y	441	PRO
2	Y	501	ARG
1	V	26	CYS
2	Y	386	ARG
2	X	230	ILE
2	X	567	PRO
2	X	328	ILE
2	Y	439	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	V	91/118 (77%)	90 (99%)	1 (1%)	70	80
1	W	91/118 (77%)	91 (100%)	0	100	100
2	X	537/582 (92%)	503 (94%)	34 (6%)	15	38
2	Y	538/582 (92%)	497 (92%)	41 (8%)	11	33
All	All	1257/1400 (90%)	1181 (94%)	76 (6%)	16	39

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	89	GLN
2	X	65	GLU
2	X	73	ARG
2	X	100	ASN
2	X	104	PHE
2	X	109	TYR
2	X	110	LEU
2	X	131	THR
2	X	243	LEU
2	X	260	THR
2	X	279	ARG
2	X	323	ASN
2	X	329	TYR
2	X	330	ASP
2	X	338	HIS
2	X	340	LYS
2	X	379	LYS
2	X	385	THR
2	X	391	ILE
2	X	402	ASN
2	X	404	THR
2	X	417	ASN
2	X	435	VAL
2	X	492	LEU

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Mol	Chain	Res	Type
2	X	506	THR
2	X	555	VAL
2	X	561	VAL
2	X	604	ILE
2	X	606	LYS
2	X	608	LYS
2	X	615	HIS
2	X	645	GLU
2	X	647	ILE
2	X	650	LYS
2	X	651	LYS
2	Y	65	GLU
2	Y	73	ARG
2	Y	104	PHE
2	Y	109	TYR
2	Y	110	LEU
2	Y	128	ILE
2	Y	175	ASP
2	Y	243	LEU
2	Y	279	ARG
2	Y	284	GLN
2	Y	338	HIS
2	Y	339	ARG
2	Y	340	LYS
2	Y	372	ASP
2	Y	385	THR
2	Y	417	ASN
2	Y	435	VAL
2	Y	440	ASP
2	Y	492	LEU
2	Y	498	MET
2	Y	505	ILE
2	Y	547	ASN
2	Y	555	VAL
2	Y	559	PHE
2	Y	561	VAL
2	Y	582	PHE
2	Y	583	LEU
2	Y	588	THR
2	Y	591	LEU
2	Y	592	LEU
2	Y	598	ARG

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Mol	Chain	Res	Type
2	Y	604	ILE
2	Y	608	LYS
2	Y	615	HIS
2	Y	618	THR
2	Y	640	ASN
2	Y	645	GLU
2	Y	646	GLU
2	Y	647	ILE
2	Y	650	LYS
2	Y	651	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	X	101	HIS
2	X	147	HIS
2	X	284	GLN
2	X	425	ASN
2	Y	284	GLN
2	Y	338	HIS
2	Y	425	ASN
2	Y	580	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](#)

4 monosaccharides 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	$\# Z  > 2$
3	NAG	A	1	3,2	14,14,15	0.55	0	17,19,21	0.49	0
3	NAG	A	2	3	14,14,15	0.28	0	17,19,21	0.56	0
3	NAG	B	1	3,2	14,14,15	0.77	1 (7%)	17,19,21	1.20	1 (5%)
3	NAG	B	2	3	14,14,15	0.50	0	17,19,21	0.48	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
3	NAG	A	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	A	2	3	-	3/6/23/26	0/1/1/1
3	NAG	B	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	NAG	O5-C1	2.72	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	C1-O5-C5	4.77	118.65	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	NAG	C4-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
3	A	2	NAG	O5-C5-C6-O6
3	A	1	NAG	O5-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6
3	B	2	NAG	O5-C5-C6-O6
3	A	1	NAG	C4-C5-C6-O6

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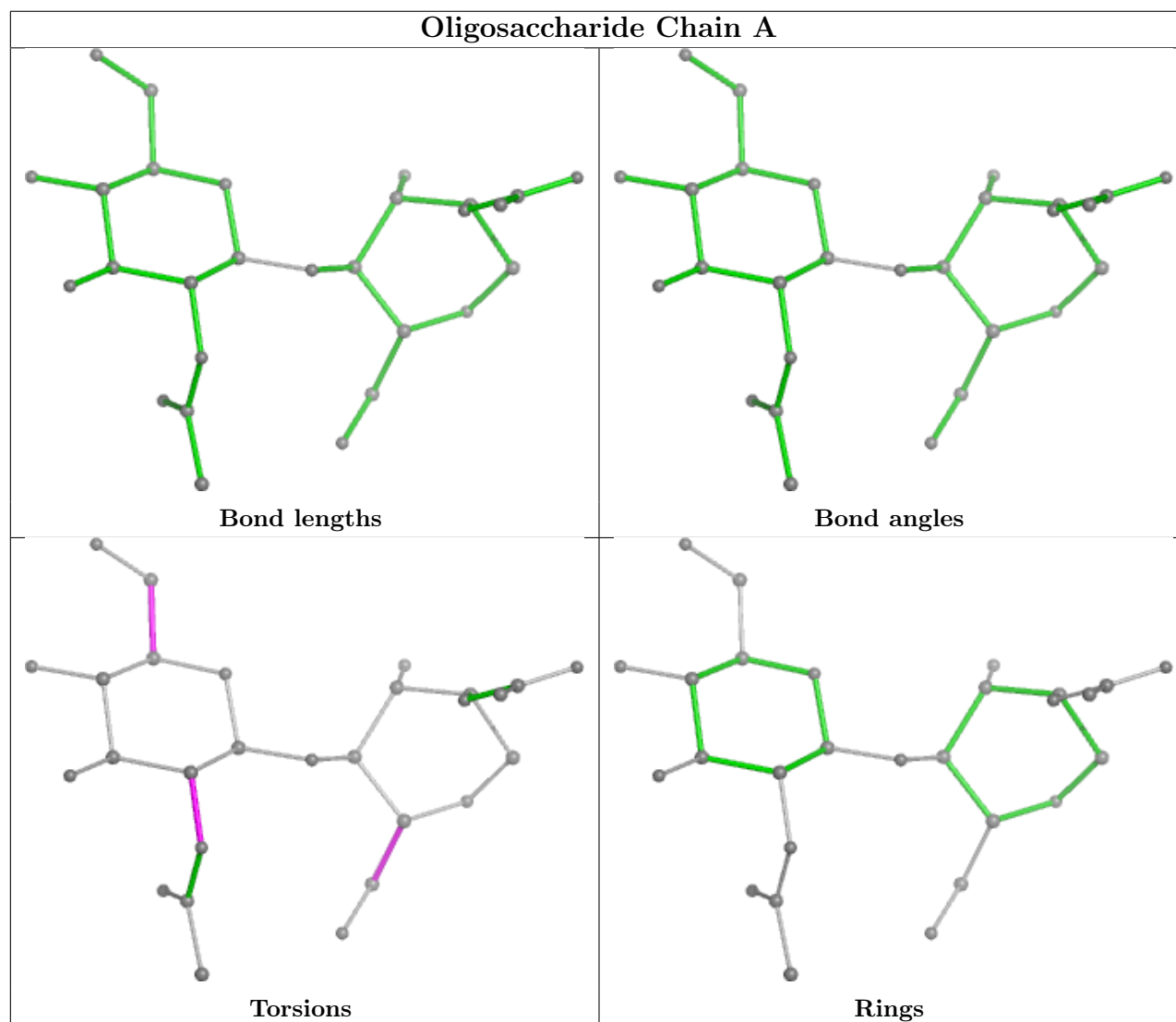
Mol	Chain	Res	Type	Atoms
3	B	2	NAG	C4-C5-C6-O6
3	A	2	NAG	C3-C2-N2-C7

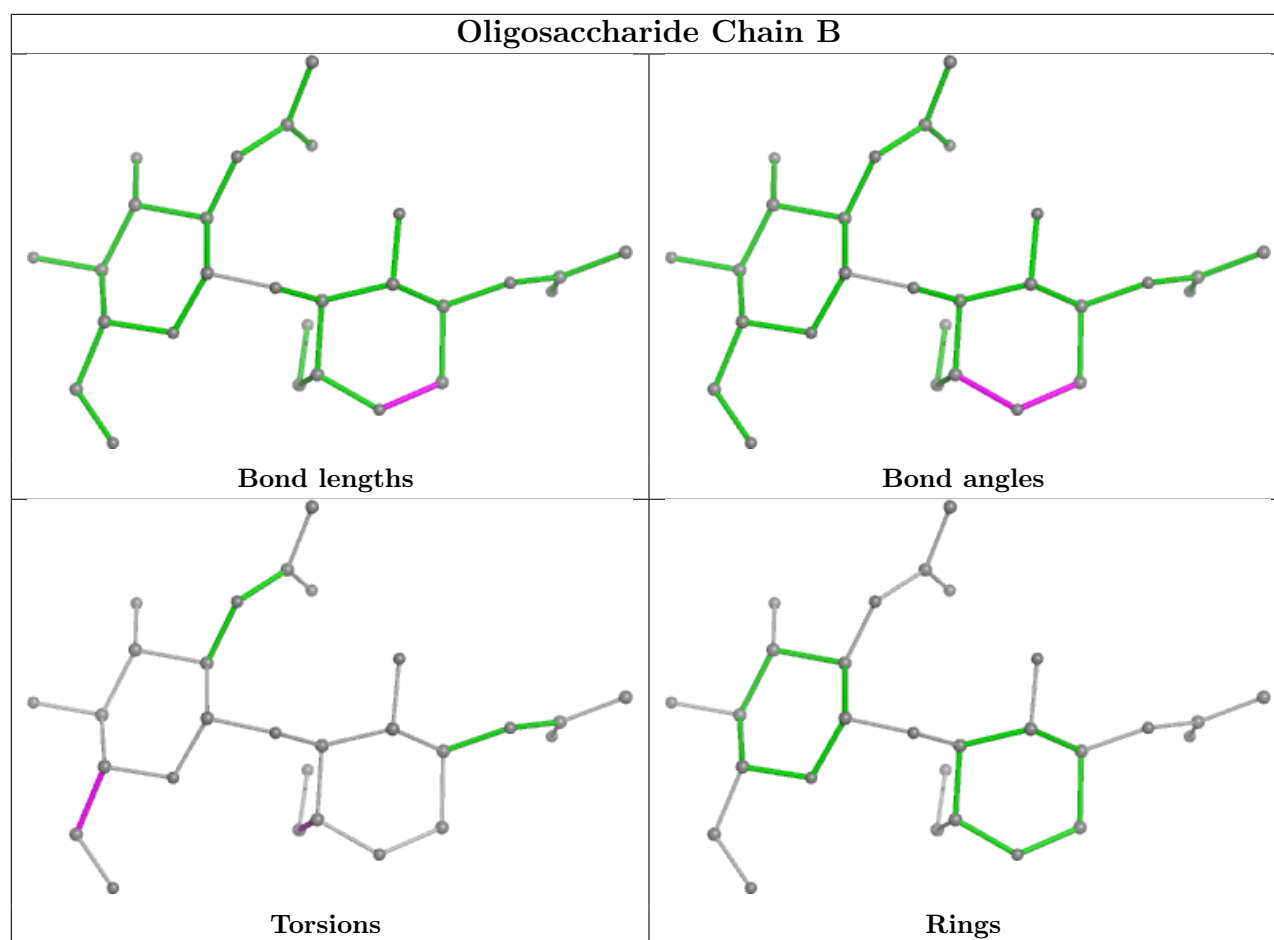
There are no ring outliers.

2 monomers are involved in 1 short contact:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





## 5.6 Ligand geometry [i](#)

19 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	$\# Z  > 2$
4	NAG	Y	705	2	14,14,15	0.22	0	17,19,21	0.47	0
4	NAG	Y	707	2	14,14,15	0.34	0	17,19,21	0.32	0
4	NAG	X	709	2	14,14,15	0.46	0	17,19,21	0.62	0
4	NAG	Y	710	2	14,14,15	0.26	0	17,19,21	0.44	0
4	NAG	Y	701	2	14,14,15	0.86	1 (7%)	17,19,21	1.32	1 (5%)
4	NAG	X	707	2	14,14,15	0.43	0	17,19,21	0.41	0
4	NAG	W	201	1	14,14,15	0.26	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	X	710	-	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	X	706	2	14,14,15	1.37	2 (14%)	17,19,21	1.74	4 (23%)
4	NAG	X	704	2	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	X	703	2	14,14,15	0.94	1 (7%)	17,19,21	1.25	1 (5%)
4	NAG	Y	711	-	14,14,15	0.25	0	17,19,21	0.39	0
4	NAG	X	708	2	14,14,15	0.19	0	17,19,21	0.46	0
4	NAG	Y	706	2	14,14,15	0.23	0	17,19,21	0.55	0
4	NAG	Y	702	2	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	Y	708	2	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	X	705	2	14,14,15	0.35	0	17,19,21	1.26	2 (11%)
4	NAG	V	201	1	14,14,15	0.48	0	17,19,21	0.66	0
4	NAG	Y	709	2	14,14,15	0.20	0	17,19,21	0.32	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
4	NAG	Y	705	2	-	0/6/23/26	0/1/1/1
4	NAG	Y	707	2	-	2/6/23/26	0/1/1/1
4	NAG	X	709	2	-	3/6/23/26	0/1/1/1
4	NAG	Y	710	2	-	2/6/23/26	0/1/1/1
4	NAG	Y	701	2	-	2/6/23/26	0/1/1/1
4	NAG	X	707	2	-	2/6/23/26	0/1/1/1
4	NAG	W	201	1	-	2/6/23/26	0/1/1/1
4	NAG	X	710	-	-	2/6/23/26	0/1/1/1
4	NAG	X	706	2	-	4/6/23/26	0/1/1/1
4	NAG	X	704	2	-	2/6/23/26	0/1/1/1
4	NAG	X	703	2	-	1/6/23/26	0/1/1/1
4	NAG	Y	711	-	-	4/6/23/26	0/1/1/1
4	NAG	X	708	2	-	2/6/23/26	0/1/1/1
4	NAG	Y	706	2	-	3/6/23/26	0/1/1/1
4	NAG	Y	702	2	-	2/6/23/26	0/1/1/1
4	NAG	Y	708	2	-	2/6/23/26	0/1/1/1
4	NAG	X	705	2	-	5/6/23/26	0/1/1/1
4	NAG	V	201	1	-	2/6/23/26	0/1/1/1
4	NAG	Y	709	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	706	NAG	O5-C1	-3.80	1.37	1.43
4	X	703	NAG	O5-C1	3.40	1.49	1.43
4	Y	701	NAG	O5-C1	3.08	1.48	1.43
4	X	706	NAG	C1-C2	2.72	1.56	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	703	NAG	C1-O5-C5	4.90	118.83	112.19
4	Y	701	NAG	C1-O5-C5	4.88	118.81	112.19
4	X	706	NAG	C2-N2-C7	4.44	129.22	122.90
4	X	705	NAG	C2-N2-C7	4.35	129.09	122.90
4	X	706	NAG	C4-C3-C2	3.89	116.72	111.02
4	X	706	NAG	C1-C2-N2	2.69	115.08	110.49
4	X	706	NAG	C3-C4-C5	2.26	114.28	110.24
4	X	705	NAG	C1-C2-N2	2.04	113.97	110.49

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Y	707	NAG	C4-C5-C6-O6
4	X	704	NAG	C4-C5-C6-O6
4	X	708	NAG	C4-C5-C6-O6
4	X	709	NAG	C4-C5-C6-O6
4	X	710	NAG	O5-C5-C6-O6
4	V	201	NAG	O5-C5-C6-O6
4	Y	709	NAG	O5-C5-C6-O6
4	X	707	NAG	O5-C5-C6-O6
4	Y	707	NAG	O5-C5-C6-O6
4	Y	708	NAG	O5-C5-C6-O6
4	Y	702	NAG	C4-C5-C6-O6
4	Y	702	NAG	O5-C5-C6-O6
4	X	704	NAG	O5-C5-C6-O6
4	Y	711	NAG	O5-C5-C6-O6
4	X	708	NAG	O5-C5-C6-O6
4	X	709	NAG	O5-C5-C6-O6
4	Y	710	NAG	C4-C5-C6-O6
4	Y	708	NAG	C4-C5-C6-O6
4	Y	711	NAG	C4-C5-C6-O6
4	X	705	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	X	705	NAG	O7-C7-N2-C2
4	X	706	NAG	C8-C7-N2-C2
4	X	706	NAG	O7-C7-N2-C2
4	Y	711	NAG	C8-C7-N2-C2
4	Y	711	NAG	O7-C7-N2-C2
4	X	705	NAG	O5-C5-C6-O6
4	Y	709	NAG	C4-C5-C6-O6
4	X	710	NAG	C4-C5-C6-O6
4	Y	706	NAG	C4-C5-C6-O6
4	V	201	NAG	C4-C5-C6-O6
4	X	707	NAG	C4-C5-C6-O6
4	Y	701	NAG	O5-C5-C6-O6
4	Y	710	NAG	O5-C5-C6-O6
4	X	706	NAG	O5-C5-C6-O6
4	Y	706	NAG	O5-C5-C6-O6
4	X	703	NAG	O5-C5-C6-O6
4	W	201	NAG	C1-C2-N2-C7
4	X	706	NAG	C3-C2-N2-C7
4	X	709	NAG	C3-C2-N2-C7
4	Y	701	NAG	C3-C2-N2-C7
4	Y	706	NAG	C3-C2-N2-C7
4	X	705	NAG	C4-C5-C6-O6
4	W	201	NAG	C3-C2-N2-C7
4	X	705	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	707	NAG	1	0
4	X	709	NAG	1	0
4	Y	701	NAG	1	0
4	X	707	NAG	1	0
4	W	201	NAG	3	0
4	X	705	NAG	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	V	92/131 (70%)	-0.34	0 100 100	168, 217, 251, 273	0
1	W	96/131 (73%)	-0.29	0 100 100	152, 226, 254, 268	0
2	X	571/646 (88%)	-0.12	1 (0%) 92 85	139, 233, 290, 338	0
2	Y	597/646 (92%)	-0.12	2 (0%) 90 82	122, 211, 273, 352	0
All	All	1356/1554 (87%)	-0.15	3 (0%) 92 85	122, 221, 281, 352	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	603	SER	2.6
2	Y	59	HIS	2.3
2	X	135	PHE	2.2

### 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](#)

SUGAR-RSR INFOmissingINFO

### 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	NAG	Y	707	14/15	0.31	0.13	241,241,241,241	0
4	NAG	X	703	14/15	0.32	0.12	322,322,322,322	0
4	NAG	X	706	14/15	0.35	0.12	284,284,284,284	0
4	NAG	V	201	14/15	0.36	0.11	262,262,262,262	0
4	NAG	Y	708	14/15	0.41	0.14	280,280,280,280	0
4	NAG	Y	702	14/15	0.43	0.10	296,296,296,296	0
4	NAG	X	707	14/15	0.46	0.11	297,297,297,297	0
4	NAG	Y	710	14/15	0.51	0.12	289,289,289,289	0
4	NAG	X	704	14/15	0.53	0.13	283,283,283,283	0
4	NAG	X	705	14/15	0.57	0.10	293,293,293,293	0
4	NAG	X	709	14/15	0.60	0.09	280,280,280,280	0
4	NAG	Y	706	14/15	0.63	0.11	243,243,243,243	0
4	NAG	Y	705	14/15	0.64	0.12	255,255,255,255	0
4	NAG	X	710	14/15	0.67	0.11	273,273,273,273	0
4	NAG	Y	711	14/15	0.67	0.13	247,247,247,247	0
4	NAG	Y	709	14/15	0.74	0.11	273,273,273,273	0
4	NAG	Y	701	14/15	0.75	0.15	240,240,240,240	0
4	NAG	W	201	14/15	0.76	0.13	248,248,248,248	0
4	NAG	X	708	14/15	0.82	0.11	265,265,265,265	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.