



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:42 PM GMT

PDB ID : 4WI4  
Title : Structural mapping of the human IgG1 binding site for FcRn: hu3S193 Fc mutation S254A  
Authors : Farrugia, W.; Burvenich, I.J.G.; Scott, A.M.; Ramsland, P.A.  
Deposited on : 2014-09-25  
Resolution : 2.80 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

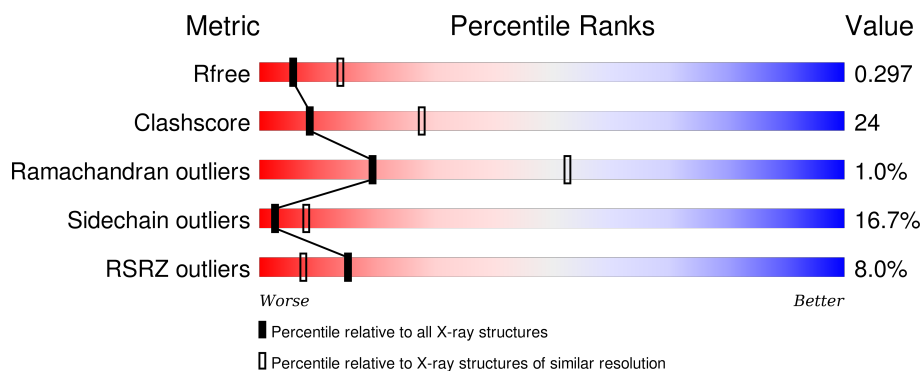
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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	207	<div> <div>6%</div> <div>54%</div> <div>35%</div> <div>8%</div> <div>..</div> </div>
1	B	207	<div> <div>10%</div> <div>50%</div> <div>39%</div> <div>9%</div> <div>.</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	A	507	-	-	-	X
2	NAG	B	501	X	-	-	-
6	EDO	A	509	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3548 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.

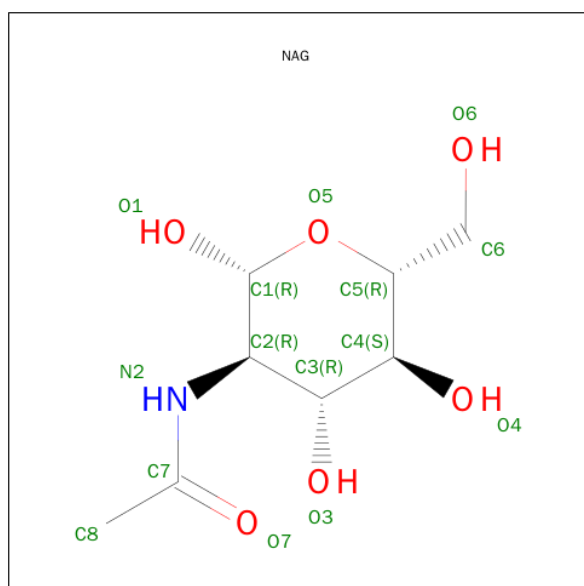
- Molecule 1 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1646	1049	277	314	6			
1	B	207	Total	C	N	O	S	0	0	0
			1659	1057	279	317	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	ALA	SER	engineered mutation	UNP P01857
B	254	ALA	SER	engineered mutation	UNP P01857

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



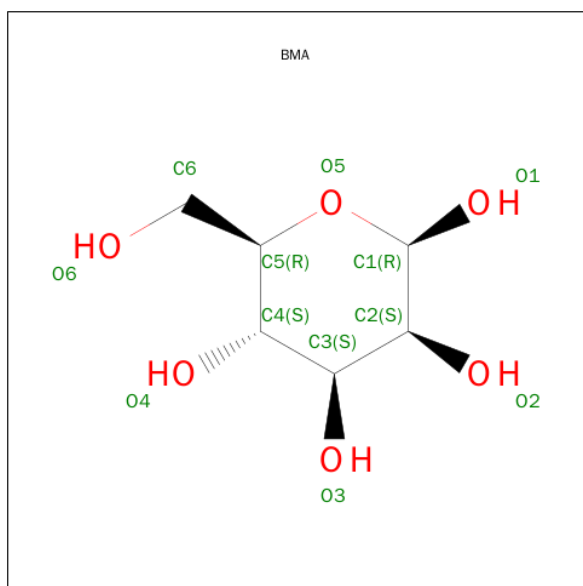
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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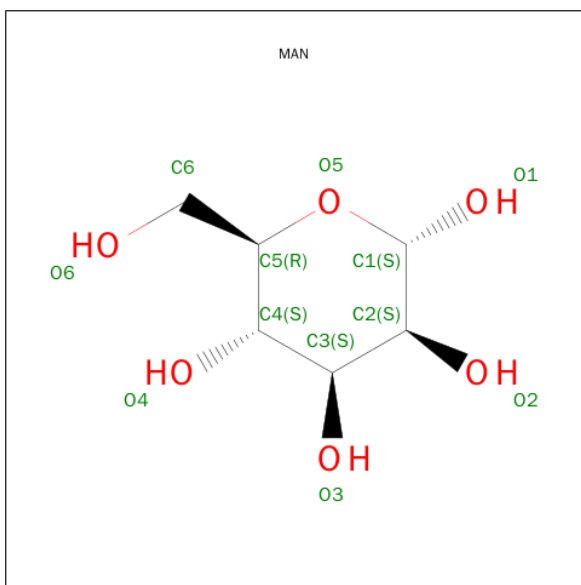
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



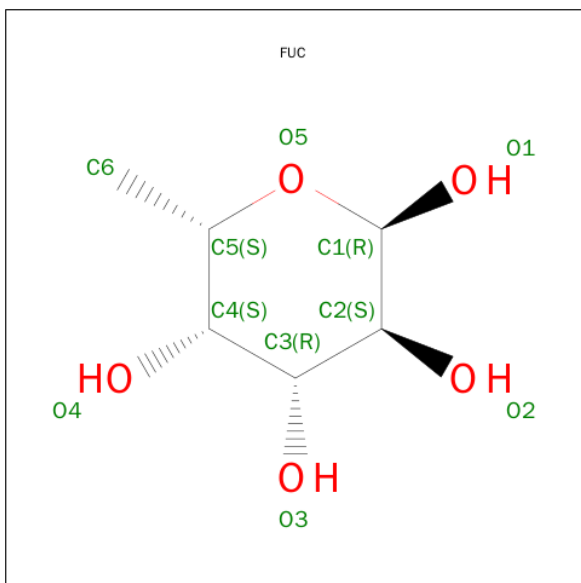
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



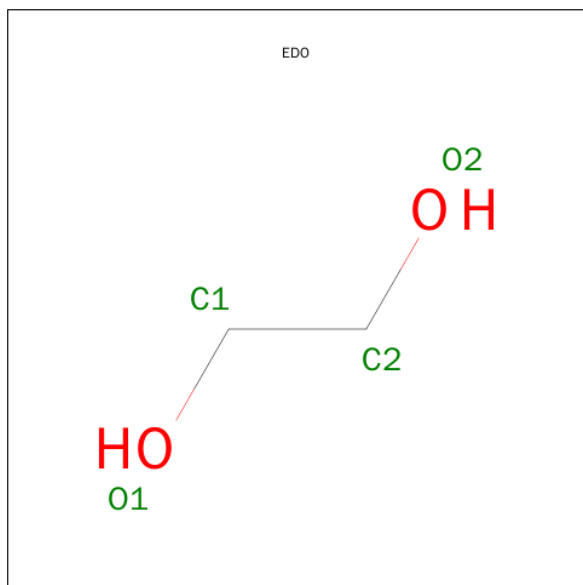
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

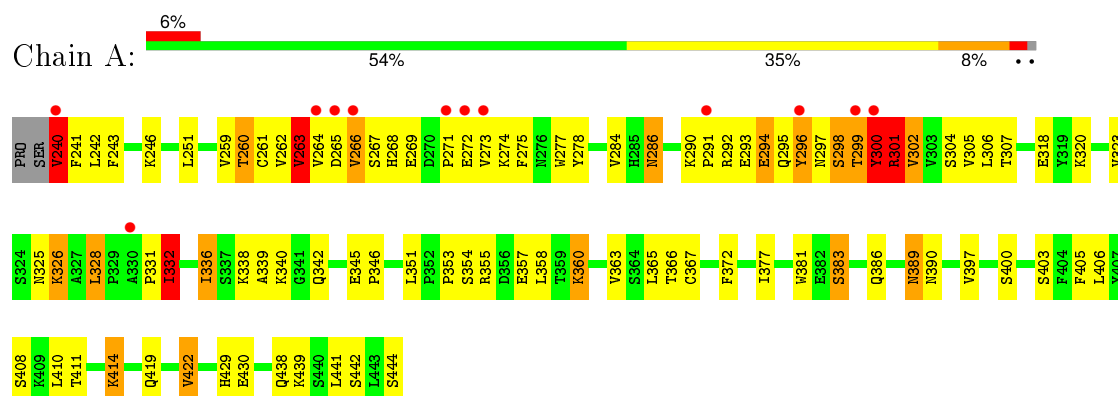
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	16	Total	O	0	0
			16	16		
7	B	17	Total	O	0	0
			17	17		

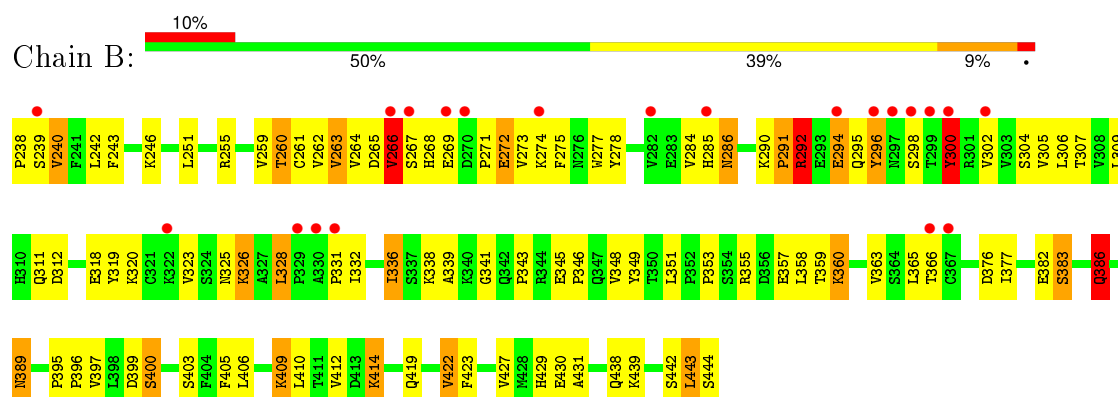
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.16 Å 79.11 Å 141.21 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.67 – 2.80 28.67 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (28.67-2.80) 96.8 (28.67-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.80 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.240 , 0.308 0.231 , 0.297	Depositor DCC
$R_{free}$ test set	1371 reflections (10.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.1	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 66.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 13712 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3548	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.24% 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, 0.375 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: FUC, MAN, BMA, NAG, EDO

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	0.82	6/1691 (0.4%)	0.94	7/2304 (0.3%)
1	B	0.84	6/1705 (0.4%)	0.97	9/2323 (0.4%)
All	All	0.83	12/3396 (0.4%)	0.96	16/4627 (0.3%)

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	B	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	TYR	CE1-CZ	-8.76	1.27	1.38
1	B	300	TYR	CD1-CE1	-8.74	1.26	1.39
1	A	386	GLN	CD-OE1	-7.73	1.06	1.24
1	B	266	VAL	CB-CG2	-7.14	1.37	1.52
1	B	386	GLN	CD-OE1	-6.92	1.08	1.24
1	A	419	GLN	CB-CG	-6.43	1.35	1.52
1	B	300	TYR	CG-CD2	6.23	1.47	1.39
1	B	266	VAL	C-O	6.21	1.35	1.23
1	B	419	GLN	CB-CG	-6.04	1.36	1.52
1	A	240	VAL	CB-CG2	-5.60	1.41	1.52
1	A	266	VAL	CB-CG1	-5.56	1.41	1.52
1	A	263	VAL	CB-CG2	-5.39	1.41	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ARG	NE-CZ-NH1	-9.85	115.37	120.30
1	B	291	PRO	CA-C-N	8.33	135.52	117.20
1	B	300	TYR	CZ-CE2-CD2	-8.00	112.60	119.80
1	A	263	VAL	CG1-CB-CG2	-7.42	99.03	110.90
1	A	266	VAL	CG1-CB-CG2	6.85	121.86	110.90
1	A	291	PRO	O-C-N	6.77	133.53	122.70
1	B	272	GLU	OE1-CD-OE2	6.67	131.31	123.30
1	A	332	ILE	CG1-CB-CG2	-6.29	97.56	111.40
1	B	266	VAL	CG1-CB-CG2	5.93	120.38	110.90
1	A	291	PRO	CA-C-N	-5.91	104.20	117.20
1	A	301	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	291	PRO	C-N-CA	5.30	134.95	121.70
1	B	409	LYS	CD-CE-NZ	5.29	123.88	111.70
1	B	266	VAL	N-CA-C	-5.14	97.12	111.00
1	B	291	PRO	C-N-CA	5.12	134.50	121.70
1	B	292	ARG	NE-CZ-NH2	5.07	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	291	PRO	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	A	1646	0	1615	88	0
1	B	1659	0	1628	79	1
2	A	56	0	49	6	0
2	B	56	0	49	0	0
3	A	11	0	8	1	0
3	B	11	0	8	0	0
4	A	22	0	18	0	0
4	B	22	0	18	1	0
5	A	10	0	10	0	0
5	B	10	0	10	0	0
6	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	8	0	12	1	0
7	A	16	0	0	7	0
7	B	17	0	0	1	0
All	All	3548	0	3431	165	1

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 24.

All (165) 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:B:240:VAL:HG23	1:B:263:VAL:HG13	1.41	1.02
1:A:240:VAL:HG23	1:A:263:VAL:HG12	1.44	0.98
1:B:263:VAL:HG23	1:B:302:VAL:O	1.69	0.91
1:A:294:GLU:HA	1:A:300:TYR:HB3	1.52	0.90
1:A:275:PHE:CD2	1:A:304:SER:HB2	2.10	0.87
1:B:275:PHE:CD2	1:B:304:SER:HB2	2.10	0.87
1:A:300:TYR:HD1	1:A:300:TYR:H	1.24	0.86
1:B:240:VAL:CG2	1:B:263:VAL:HG13	2.11	0.81
1:B:240:VAL:HG23	1:B:263:VAL:CG1	2.12	0.80
1:A:264:VAL:HG11	2:A:502:NAG:H2	1.62	0.79
1:A:325:ASN:H	1:A:328:LEU:HD11	1.47	0.79
1:B:383:SER:OG	1:B:422:VAL:O	2.02	0.77
1:A:240:VAL:HG23	1:A:263:VAL:CG1	2.14	0.77
1:A:293:GLU:O	1:A:295:GLN:NE2	2.17	0.77
1:B:267:SER:O	1:B:300:TYR:OH	2.03	0.76
1:B:325:ASN:H	1:B:328:LEU:HD11	1.48	0.76
1:A:383:SER:OG	1:A:422:VAL:O	2.04	0.74
1:B:295:GLN:HG3	1:B:296:TYR:H	1.51	0.74
1:B:403:SER:OG	7:B:615:HOH:O	2.06	0.73
1:B:325:ASN:OD1	1:B:326:LYS:N	2.18	0.72
1:B:275:PHE:HD2	1:B:304:SER:HB2	1.56	0.71
1:A:267:SER:O	1:A:300:TYR:OH	2.10	0.70
1:A:263:VAL:HG23	1:A:302:VAL:O	1.91	0.70
1:B:292:ARG:HH22	1:B:300:TYR:HB3	1.57	0.69
1:A:278:TYR:HB2	1:A:320:LYS:HB3	1.74	0.69
1:A:275:PHE:HD2	1:A:304:SER:HB2	1.55	0.69
1:B:300:TYR:HD1	1:B:300:TYR:H	1.37	0.69
1:B:292:ARG:NH1	1:B:300:TYR:HD2	1.91	0.68
1:B:278:TYR:HB2	1:B:320:LYS:HB3	1.75	0.67
1:B:292:ARG:HG2	1:B:302:VAL:HG23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:TYR:N	1:A:300:TYR:HD1	1.93	0.66
1:A:342:GLN:HG2	7:A:601:HOH:O	1.95	0.66
1:B:443:LEU:HG	1:B:444:SER:N	2.09	0.65
1:A:353:PRO:HD3	1:A:365:LEU:HD23	1.79	0.64
1:A:240:VAL:HG21	1:A:323:VAL:HG21	1.80	0.64
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.79	0.64
1:A:271:PRO:HA	1:A:300:TYR:OH	1.99	0.61
1:A:365:LEU:HD12	1:A:410:LEU:HD23	1.82	0.61
1:A:292:ARG:HA	1:A:302:VAL:HG23	1.83	0.60
1:B:240:VAL:HG21	1:B:323:VAL:HG21	1.83	0.59
1:B:377:ILE:HG13	1:B:429:HIS:HB2	1.83	0.59
1:B:277:TRP:HZ2	1:B:304:SER:HB3	1.67	0.59
1:A:295:GLN:H	1:A:300:TYR:HA	1.66	0.58
1:B:300:TYR:HD1	1:B:300:TYR:N	2.03	0.57
1:A:360:LYS:HB3	7:A:615:HOH:O	2.05	0.57
1:A:277:TRP:HZ2	1:A:304:SER:HB3	1.68	0.57
1:A:240:VAL:HG11	1:A:332:ILE:HG21	1.87	0.57
1:B:300:TYR:N	1:B:300:TYR:CD1	2.72	0.56
1:B:292:ARG:HH12	1:B:300:TYR:HD2	1.51	0.56
1:A:300:TYR:N	1:A:300:TYR:CD1	2.68	0.56
1:B:353:PRO:HD3	1:B:365:LEU:HD23	1.87	0.56
1:A:263:VAL:CG2	1:A:302:VAL:O	2.54	0.56
1:B:243:PHE:HE2	1:B:262:VAL:HB	1.71	0.56
1:B:271:PRO:HA	1:B:300:TYR:OH	2.06	0.55
1:A:377:ILE:HG13	1:A:429:HIS:HB2	1.89	0.55
1:A:306:LEU:HD12	1:A:307:THR:N	2.22	0.55
1:B:306:LEU:HD12	1:B:307:THR:N	2.21	0.55
1:B:389:ASN:OD1	1:B:389:ASN:N	2.38	0.54
1:A:243:PHE:HE2	1:A:262:VAL:HB	1.73	0.54
1:A:267:SER:C	1:A:300:TYR:HE1	2.10	0.54
1:A:338:LYS:HZ1	1:A:430:GLU:CD	2.10	0.53
1:B:341:GLY:O	1:B:343:PRO:HD3	2.08	0.53
1:A:389:ASN:N	1:A:389:ASN:OD1	2.41	0.53
1:A:397:VAL:HB	1:A:405:PHE:CE2	2.43	0.53
1:B:243:PHE:CE1	4:B:506:MAN:H2	2.44	0.53
1:B:338:LYS:NZ	1:B:430:GLU:OE1	2.43	0.52
1:B:348:VAL:HG21	1:B:427:VAL:HG21	1.91	0.52
1:A:242:LEU:HD23	1:A:336:ILE:HB	1.90	0.51
1:B:286:ASN:OD1	1:B:286:ASN:N	2.43	0.51
1:B:242:LEU:HD23	1:B:336:ILE:HB	1.93	0.51
1:A:354:SER:HB2	1:B:349:TYR:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:CYS:HB2	1:B:277:TRP:CH2	2.47	0.50
1:A:338:LYS:HG2	1:A:339:ALA:N	2.26	0.50
1:A:296:TYR:O	1:A:298:SER:N	2.36	0.50
1:B:422:VAL:HA	1:B:442:SER:HB3	1.93	0.50
1:A:275:PHE:CE1	1:A:323:VAL:HG13	2.47	0.50
1:A:296:TYR:C	1:A:298:SER:H	2.15	0.50
1:A:338:LYS:NZ	1:A:430:GLU:OE1	2.44	0.49
1:A:355:ARG:HA	1:A:358:LEU:HD23	1.95	0.49
1:B:275:PHE:CE1	1:B:323:VAL:HG13	2.47	0.49
1:A:241:PHE:CZ	3:A:503:BMA:H2	2.48	0.49
1:A:342:GLN:NE2	7:A:601:HOH:O	1.81	0.49
1:B:267:SER:C	1:B:300:TYR:HE1	2.16	0.49
1:B:271:PRO:HA	1:B:300:TYR:CZ	2.47	0.49
1:A:422:VAL:HA	1:A:442:SER:HB3	1.94	0.49
1:A:263:VAL:HG21	1:A:302:VAL:HG12	1.94	0.48
1:B:332:ILE:HD12	6:B:510:EDO:O2	2.12	0.48
1:B:264:VAL:HG23	1:B:265:ASP:OD1	2.13	0.48
1:B:397:VAL:HB	1:B:405:PHE:CE2	2.49	0.48
1:A:301:ARG:NH1	1:A:301:ARG:HG2	2.29	0.48
1:B:338:LYS:HZ1	1:B:430:GLU:CD	2.17	0.47
1:A:286:ASN:N	1:A:286:ASN:OD1	2.47	0.47
1:A:260:THR:HG23	1:A:305:VAL:HG22	1.97	0.47
1:B:348:VAL:CG2	1:B:427:VAL:HG21	2.45	0.46
1:B:238:PRO:HA	1:B:265:ASP:O	2.14	0.46
1:A:275:PHE:HE1	1:A:323:VAL:HG13	1.81	0.46
1:A:274:LYS:HE3	1:A:274:LYS:HB3	1.68	0.46
1:B:274:LYS:HB3	1:B:274:LYS:HE3	1.70	0.46
1:A:241:PHE:HE2	2:A:502:NAG:H4	1.81	0.46
1:B:338:LYS:HG2	1:B:339:ALA:N	2.30	0.46
1:B:355:ARG:HA	1:B:358:LEU:HD23	1.98	0.46
1:A:271:PRO:HA	1:A:300:TYR:CZ	2.51	0.46
1:B:292:ARG:HD2	1:B:292:ARG:HH11	1.51	0.45
1:A:340:LYS:N	7:A:609:HOH:O	2.39	0.45
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.52	0.45
1:B:444:SER:OG	1:B:444:SER:O	2.34	0.45
1:A:345:GLU:HA	1:A:346:PRO:HD2	1.75	0.45
1:A:295:GLN:HB2	1:A:299:THR:O	2.16	0.45
1:B:290:LYS:HE2	1:B:290:LYS:HB3	1.58	0.45
1:A:301:ARG:HH11	1:A:301:ARG:HG2	1.82	0.45
1:A:354:SER:CB	1:B:349:TYR:HB3	2.45	0.45
1:A:353:PRO:HG3	1:A:363:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:GLU:OE1	1:B:269:GLU:N	2.49	0.45
1:A:357:GLU:O	1:A:360:LYS:HG2	2.17	0.45
1:B:358:LEU:HD12	1:B:414:LYS:HE3	1.99	0.45
1:A:351:LEU:HB2	1:A:366:THR:HB	1.97	0.45
1:A:390:ASN:OD1	1:A:411:THR:HB	2.17	0.44
1:A:290:LYS:HE2	1:A:290:LYS:HB3	1.53	0.44
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.51	0.44
1:A:264:VAL:HG23	1:A:265:ASP:OD1	2.16	0.44
1:A:300:TYR:HB2	1:A:301:ARG:H	1.60	0.44
1:B:266:VAL:O	1:B:300:TYR:CD1	2.70	0.44
1:B:295:GLN:HG3	1:B:296:TYR:N	2.25	0.44
1:B:357:GLU:O	1:B:360:LYS:HG2	2.18	0.44
1:A:263:VAL:CG2	1:A:302:VAL:HG12	2.47	0.44
1:B:328:LEU:HD13	1:B:331:PRO:HA	1.98	0.44
1:A:325:ASN:CG	1:A:326:LYS:H	2.21	0.44
1:B:382:GLU:HB2	1:B:386:GLN:O	2.18	0.44
1:A:240:VAL:HG11	1:A:332:ILE:CG2	2.47	0.43
1:A:268:HIS:NE2	1:A:298:SER:HA	2.33	0.43
1:A:328:LEU:HD13	1:A:331:PRO:HA	2.01	0.43
1:A:439:LYS:HA	1:A:439:LYS:HD3	1.84	0.43
1:A:240:VAL:CG1	1:A:332:ILE:HG21	2.48	0.43
1:A:301:ARG:HD2	2:A:502:NAG:H82	2.01	0.43
1:A:444:SER:OG	1:A:444:SER:O	2.36	0.43
1:B:376:ASP:O	1:B:429:HIS:HD2	2.01	0.43
1:A:358:LEU:HD12	1:A:414:LYS:HE3	2.01	0.43
1:B:260:THR:HG23	1:B:305:VAL:HG22	2.01	0.42
1:A:441:LEU:HA	7:A:607:HOH:O	2.19	0.42
1:A:301:ARG:HD2	2:A:502:NAG:C8	2.49	0.42
1:A:430:GLU:N	7:A:606:HOH:O	2.27	0.42
1:B:275:PHE:HE1	1:B:323:VAL:HG13	1.83	0.42
1:A:265:ASP:OD1	2:A:501:NAG:H3	2.19	0.42
1:B:353:PRO:HG3	1:B:363:VAL:HG13	2.02	0.42
1:A:271:PRO:CA	1:A:300:TYR:OH	2.66	0.41
1:A:264:VAL:CG1	2:A:502:NAG:H2	2.40	0.41
1:A:342:GLN:CG	7:A:601:HOH:O	2.58	0.41
1:B:351:LEU:HB2	1:B:366:THR:HB	2.02	0.41
1:A:301:ARG:HH11	1:A:301:ARG:CG	2.33	0.41
1:B:345:GLU:HA	1:B:346:PRO:HD2	1.70	0.41
1:B:255:ARG:HE	1:B:255:ARG:HB3	1.63	0.41
1:B:292:ARG:HE	1:B:292:ARG:HB3	1.52	0.41
1:A:269:GLU:OE1	1:A:269:GLU:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:LYS:HA	1:B:439:LYS:HD3	1.83	0.41
1:A:397:VAL:HB	1:A:405:PHE:CZ	2.56	0.41
1:A:266:VAL:HG23	1:A:266:VAL:H	1.73	0.41
1:B:399:ASP:OD1	1:B:400:SER:N	2.48	0.41
1:B:275:PHE:CE2	1:B:304:SER:HB2	2.54	0.40
1:A:346:PRO:HB3	1:A:372:PHE:HB3	2.03	0.40
1:B:345:GLU:HG3	1:B:431:ALA:O	2.21	0.40
1:B:312:ASP:HB3	1:B:319:TYR:OH	2.22	0.40
1:B:395:PRO:HA	1:B:396:PRO:HD3	1.94	0.40
1:B:359:THR:OG1	1:B:360:LYS:HD3	2.21	0.40
1:B:412:VAL:HG11	1:B:423:PHE:CE2	2.57	0.40
1:B:309:LEU:HD23	1:B:309:LEU:HA	1.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:HIS:ND1	1:B:285:HIS:O[4_555]	1.99	0.21

## 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	203/207 (98%)	181 (89%)	20 (10%)	2 (1%)	19	52
1	B	205/207 (99%)	181 (88%)	22 (11%)	2 (1%)	19	52
All	All	408/414 (99%)	362 (89%)	42 (10%)	4 (1%)	19	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	GLU

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Mol	Chain	Res	Type
1	B	292	ARG
1	A	297	ASN
1	B	294	GLU

### 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	191/193 (99%)	160 (84%)	31 (16%)	3	8
1	B	193/193 (100%)	160 (83%)	33 (17%)	2	7
All	All	384/386 (100%)	320 (83%)	64 (17%)	3	8

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	VAL
1	A	246	LYS
1	A	251	LEU
1	A	259	VAL
1	A	260	THR
1	A	263	VAL
1	A	272	GLU
1	A	273	VAL
1	A	284	VAL
1	A	286	ASN
1	A	296	TYR
1	A	298	SER
1	A	299	THR
1	A	300	TYR
1	A	301	ARG
1	A	302	VAL
1	A	318	GLU
1	A	326	LYS
1	A	328	LEU
1	A	332	ILE

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Mol	Chain	Res	Type
1	A	336	ILE
1	A	360	LYS
1	A	383	SER
1	A	389	ASN
1	A	400	SER
1	A	403	SER
1	A	406	LEU
1	A	408	SER
1	A	414	LYS
1	A	422	VAL
1	A	438	GLN
1	B	239	SER
1	B	240	VAL
1	B	246	LYS
1	B	251	LEU
1	B	259	VAL
1	B	260	THR
1	B	263	VAL
1	B	266	VAL
1	B	272	GLU
1	B	273	VAL
1	B	284	VAL
1	B	286	ASN
1	B	292	ARG
1	B	294	GLU
1	B	296	TYR
1	B	298	SER
1	B	300	TYR
1	B	311	GLN
1	B	318	GLU
1	B	326	LYS
1	B	328	LEU
1	B	336	ILE
1	B	360	LYS
1	B	383	SER
1	B	386	GLN
1	B	389	ASN
1	B	400	SER
1	B	406	LEU
1	B	409	LYS
1	B	414	LYS
1	B	422	VAL

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Mol	Chain	Res	Type
1	B	438	GLN
1	B	443	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	311	GLN
1	B	429	HIS

### 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 carbohydrates in this entry.

## 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	$\# Z  > 2$
2	NAG	A	501	1,2,5	14,14,15	0.65	0	15,19,21	1.72	2 (13%)
2	NAG	A	502	3,2	14,14,15	0.66	0	15,19,21	1.63	2 (13%)
3	BMA	A	503	2,4	11,11,12	0.54	0	15,15,17	1.73	3 (20%)
4	MAN	A	504	3,2	11,11,12	0.59	0	15,15,17	1.16	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	505	4	14,14,15	0.52	0	15,19,21	0.58	0
4	MAN	A	506	3,2	11,11,12	0.62	0	15,15,17	1.44	3 (20%)
2	NAG	A	507	4	14,14,15	0.52	0	15,19,21	1.43	2 (13%)
5	FUC	A	508	2	10,10,11	0.70	0	13,14,16	1.54	2 (15%)
6	EDO	A	509	-	3,3,3	0.49	0	2,2,2	0.38	0
2	NAG	B	501	1,2,5	14,14,15	0.34	0	15,19,21	2.10	2 (13%)
2	NAG	B	502	3,2	14,14,15	0.41	0	15,19,21	0.86	1 (6%)
3	BMA	B	503	2,4	11,11,12	0.64	0	15,15,17	1.55	2 (13%)
4	MAN	B	504	3,2	11,11,12	0.53	0	15,15,17	1.30	2 (13%)
2	NAG	B	505	4	14,14,15	0.61	0	15,19,21	0.73	0
4	MAN	B	506	3,2	11,11,12	0.79	1 (9%)	15,15,17	1.54	3 (20%)
2	NAG	B	507	4	14,14,15	0.56	0	15,19,21	1.27	2 (13%)
5	FUC	B	508	2	10,10,11	0.58	0	13,14,16	0.94	0
6	EDO	B	509	-	3,3,3	0.46	0	2,2,2	0.58	0
6	EDO	B	510	-	3,3,3	0.48	0	2,2,2	0.28	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	501	1,2,5	-	0/6/23/26	0/1/1/1
2	NAG	A	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	503	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	504	3,2	-	0/2/19/22	0/1/1/1
2	NAG	A	505	4	-	2/6/23/26	0/1/1/1
4	MAN	A	506	3,2	-	0/2/19/22	0/1/1/1
2	NAG	A	507	4	-	0/6/23/26	0/1/1/1
5	FUC	A	508	2	-	0/0/17/20	0/1/1/1
6	EDO	A	509	-	-	0/1/1/1	0/0/0/0
2	NAG	B	501	1,2,5	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	503	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	504	3,2	-	0/2/19/22	0/1/1/1
2	NAG	B	505	4	-	0/6/23/26	0/1/1/1
4	MAN	B	506	3,2	-	0/2/19/22	0/1/1/1
2	NAG	B	507	4	-	0/6/23/26	0/1/1/1
5	FUC	B	508	2	-	0/0/17/20	0/1/1/1
6	EDO	B	509	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	510	-	-	0/1/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	506	MAN	O5-C1	-2.01	1.40	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	504	MAN	C2-C3-C4	-3.43	105.06	111.05
4	B	506	MAN	O5-C1-C2	-3.43	105.41	110.89
4	A	506	MAN	O5-C1-C2	-2.93	106.21	110.89
4	B	506	MAN	C1-C2-C3	-2.76	106.21	109.55
4	A	504	MAN	O5-C1-C2	-2.60	106.75	110.89
3	B	503	BMA	O5-C1-C2	-2.50	106.90	110.89
4	A	506	MAN	C1-C2-C3	-2.49	106.53	109.55
2	A	507	NAG	C2-N2-C7	-2.14	120.32	123.11
5	A	508	FUC	O5-C1-C2	-2.09	107.55	110.89
3	A	503	BMA	O5-C5-C6	2.02	111.66	107.34
4	B	506	MAN	C3-C4-C5	2.03	113.84	110.23
2	B	502	NAG	O5-C5-C6	2.17	111.98	107.34
3	A	503	BMA	C1-O5-C5	2.18	115.34	112.14
4	A	506	MAN	C3-C4-C5	2.21	114.17	110.23
2	A	502	NAG	O5-C5-C4	2.51	114.29	110.13
2	B	507	NAG	C3-C4-C5	2.52	114.73	110.23
4	B	504	MAN	C1-O5-C5	2.55	115.89	112.14
2	B	507	NAG	C4-C3-C2	2.75	115.61	111.34
3	B	503	BMA	C3-C4-C5	3.37	116.23	110.23
2	A	501	NAG	C4-C3-C2	3.38	116.59	111.34
5	A	508	FUC	C3-C4-C5	3.48	114.86	109.66
2	B	501	NAG	O5-C5-C4	3.70	116.26	110.13
2	A	501	NAG	C1-O5-C5	3.94	117.94	112.14
2	A	507	NAG	C4-C3-C2	3.99	117.53	111.34
2	A	502	NAG	C1-O5-C5	4.58	118.88	112.14
3	A	503	BMA	C1-C2-C3	5.38	116.07	109.55
2	B	501	NAG	C1-O5-C5	7.06	122.52	112.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	501	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	505	NAG	C8-C7-N2-C2
2	A	505	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	1	0
2	A	502	NAG	5	0
3	A	503	BMA	1	0
4	B	506	MAN	1	0
6	B	510	EDO	1	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, 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	A	205/207 (99%)	0.22	12 (5%) 26 16	39, 80, 185, 253	0
1	B	207/207 (100%)	0.33	21 (10%) 9 4	40, 82, 182, 250	0
All	All	412/414 (99%)	0.27	33 (8%) 15 7	39, 81, 183, 253	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	PRO	6.8
1	A	272	GLU	5.5
1	A	271	PRO	5.2
1	A	330	ALA	4.5
1	A	265	ASP	4.4
1	B	298	SER	4.4
1	B	330	ALA	4.2
1	B	300	TYR	4.0
1	B	296	TYR	3.9
1	A	300	TYR	3.8
1	A	273	VAL	3.5
1	A	299	THR	3.2
1	B	367	CYS	2.9
1	B	297	ASN	2.9
1	A	264	VAL	2.9
1	B	294	GLU	2.8
1	B	282	VAL	2.8
1	A	296	TYR	2.8
1	B	266	VAL	2.7
1	B	239	SER	2.7
1	B	274	LYS	2.6
1	B	299	THR	2.6
1	B	322	LYS	2.5
1	B	366	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	291	PRO	2.5
1	A	240	VAL	2.4
1	B	269	GLU	2.4
1	B	285	HIS	2.4
1	B	267	SER	2.3
1	B	331	PRO	2.3
1	B	270	ASP	2.3
1	A	266	VAL	2.1
1	B	302	VAL	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 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	EDO	A	509	4/4	0.92	0.47	4.11	71,113,113,120	0
2	NAG	A	507	14/15	0.80	0.27	3.61	72,110,150,180	0
6	EDO	B	509	4/4	0.90	0.23	1.49	52,67,72,96	0
2	NAG	B	507	14/15	0.81	0.18	-0.05	74,104,120,134	0
2	NAG	A	502	14/15	0.88	0.27	-0.56	107,127,137,145	0
2	NAG	A	501	14/15	0.74	0.32	-0.78	115,147,185,197	0
3	BMA	A	503	11/12	0.86	0.18	-	111,122,140,146	0
3	BMA	B	503	11/12	0.87	0.17	-	148,165,184,195	0
4	MAN	A	506	11/12	0.82	0.21	-	70,124,147,162	0
6	EDO	B	510	4/4	0.94	0.15	-	86,92,99,108	0
4	MAN	B	506	11/12	0.91	0.20	-	69,123,131,133	0
5	FUC	A	508	10/11	0.74	0.25	-	88,138,178,197	0

*Continued on next page...*



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	FUC	B	508	10/11	0.71	0.42	-	108,166,188,200	0
4	MAN	A	504	11/12	0.82	0.25	-	93,127,148,151	0
2	NAG	B	502	14/15	0.80	0.39	-	128,160,179,190	0
2	NAG	B	501	14/15	0.76	0.35	-	162,183,195,203	0
4	MAN	B	504	11/12	0.77	0.34	-	106,130,181,183	0
2	NAG	A	505	14/15	0.77	0.32	-	101,136,164,164	0
2	NAG	B	505	14/15	0.81	0.24	-	60,130,143,145	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.