



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:42 PM GMT

PDB ID : 4WI5
Title : Structural mapping of the human IgG1 binding site for FcRn: hu3S193 Fc mutation H310A
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
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 : 1.7.1 (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

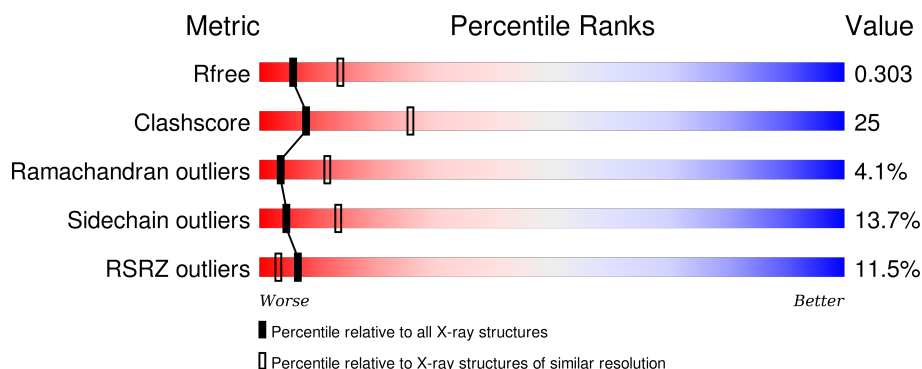
1 Overall quality at a glance

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 ≥ 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	208	<div> <div>12%</div> <div>50%</div> <div>41%</div> <div>8%</div> </div>
1	B	208	<div> <div>11%</div> <div>45%</div> <div>45%</div> <div>9%</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
6	EDO	A	509	-	-	-	X
6	EDO	B	509	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3536 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.

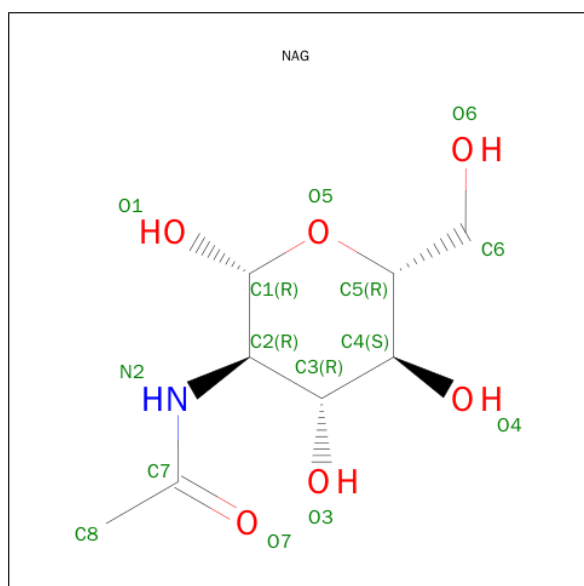
- Molecule 1 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1659	1056	278	319	6			
1	B	208	Total	C	N	O	S	0	0	0
			1659	1056	278	319	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	ALA	HIS	engineered mutation	UNP P01857
B	310	ALA	HIS	engineered mutation	UNP P01857

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



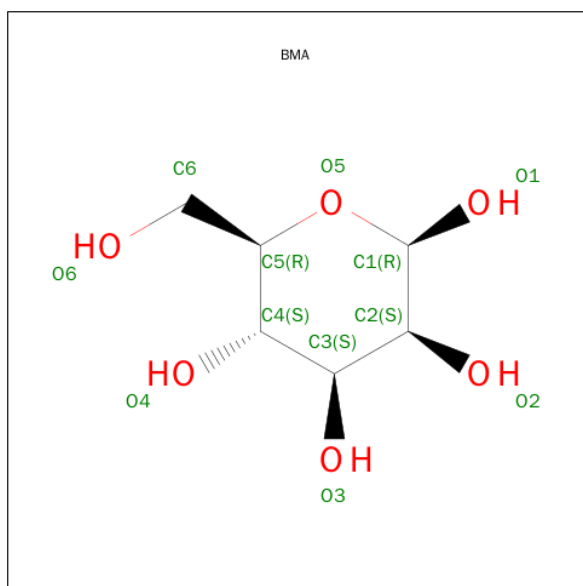
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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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: $C_6H_{12}O_6$).



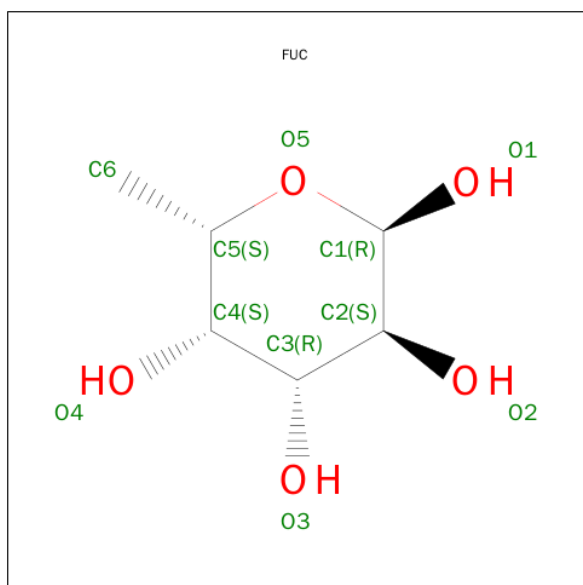
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



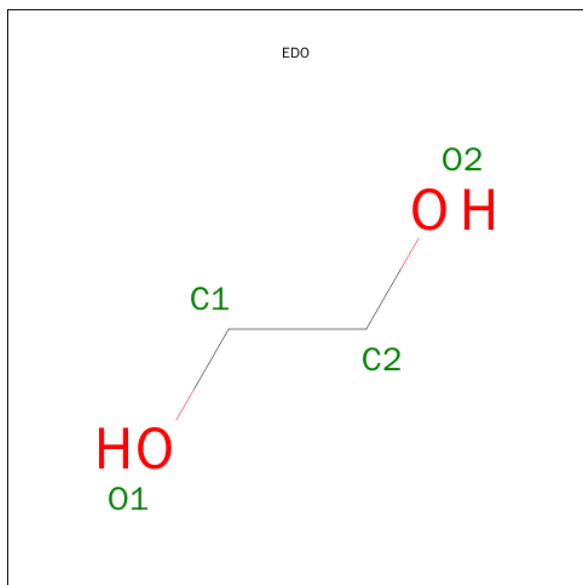
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- 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: C₂H₆O₂).



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		

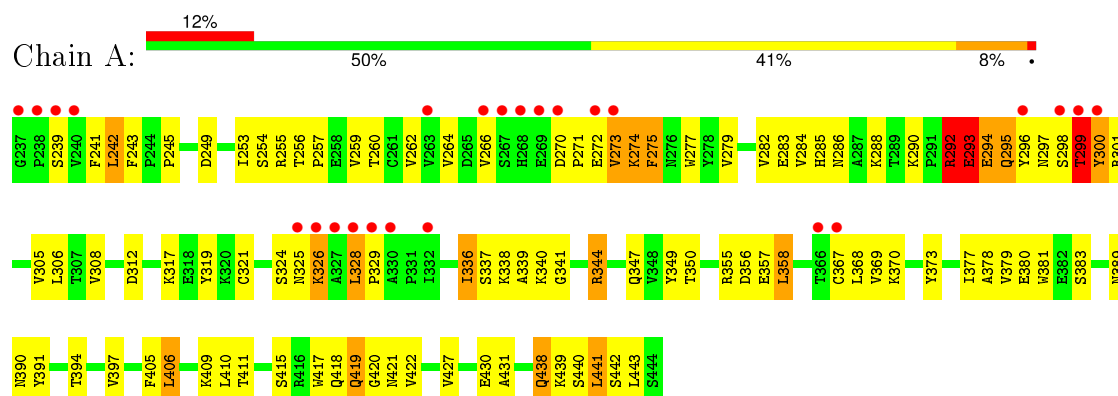
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	O	0	0
			4	4		
7	B	4	Total	O	0	0
			4	4		

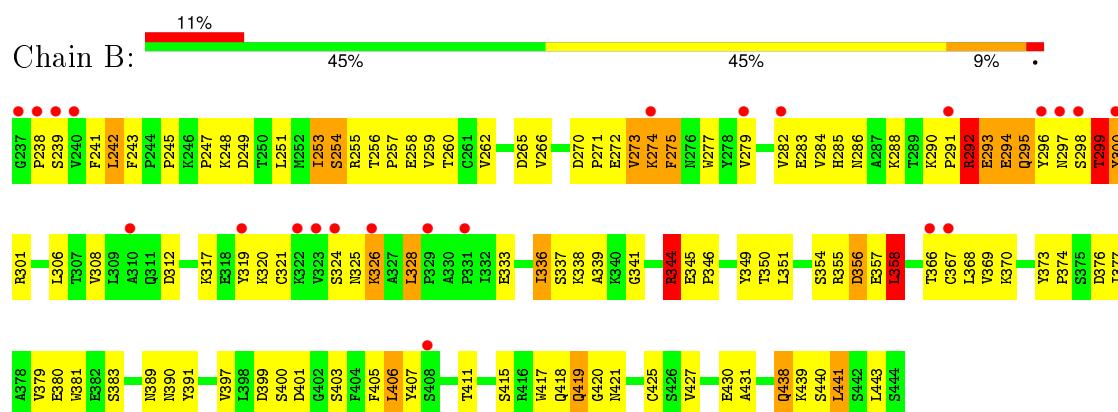
3 Residue-property plots

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 ($RSRZ > 2$). 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, α , β , γ	49.00 Å 77.48 Å 136.68 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 2.80 29.67 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.67-2.80) 97.0 (29.67-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.80 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.227 , 0.301 0.224 , 0.303	Depositor DCC
R_{free} test set	1300 reflections (10.02%)	DCC
Wilson B-factor (Å ²)	70.8	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 93.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 12993 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3536	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.06% 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: 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	0.78	6/1704 (0.4%)	1.01	12/2322 (0.5%)
1	B	0.73	4/1704 (0.2%)	0.98	11/2322 (0.5%)
All	All	0.75	10/3408 (0.3%)	0.99	23/4644 (0.5%)

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	2
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	TYR	CD2-CE2	-9.20	1.25	1.39
1	A	300	TYR	CB-CG	-8.91	1.38	1.51
1	B	300	TYR	CB-CG	-7.56	1.40	1.51
1	B	300	TYR	CD2-CE2	-7.48	1.28	1.39
1	A	300	TYR	CD1-CE1	-6.92	1.28	1.39
1	A	294	GLU	CB-CG	-6.29	1.40	1.52
1	A	274	LYS	CB-CG	-5.47	1.37	1.52
1	B	274	LYS	CB-CG	-5.44	1.37	1.52
1	B	300	TYR	CD1-CE1	-5.30	1.31	1.39
1	A	344	ARG	CG-CD	-5.15	1.39	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	A	344	ARG	NE-CZ-NH1	-11.45	114.58	120.30
1	B	344	ARG	NE-CZ-NH1	-10.09	115.26	120.30
1	B	300	TYR	CA-CB-CG	-9.28	95.76	113.40
1	A	358	LEU	CA-CB-CG	8.53	134.91	115.30
1	A	356	ASP	CB-CA-C	-8.30	93.81	110.40
1	A	300	TYR	CA-CB-CG	-8.25	97.73	113.40
1	A	356	ASP	CB-CG-OD2	-7.93	111.17	118.30
1	A	292	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	B	274	LYS	CB-CA-C	-7.04	96.32	110.40
1	B	292	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	B	358	LEU	CB-CG-CD2	6.59	122.21	111.00
1	B	358	LEU	CB-CG-CD1	-6.55	99.87	111.00
1	A	341	GLY	N-CA-C	-6.45	96.99	113.10
1	B	406	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	356	ASP	CB-CG-OD1	6.14	123.83	118.30
1	B	356	ASP	N-CA-CB	5.88	121.19	110.60
1	B	300	TYR	CB-CA-C	5.72	121.84	110.40
1	A	406	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	293	GLU	OE1-CD-OE2	5.50	129.90	123.30
1	B	341	GLY	N-CA-C	-5.50	99.36	113.10
1	A	358	LEU	N-CA-CB	-5.43	99.54	110.40
1	B	358	LEU	CA-CB-CG	5.43	127.78	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	299	THR	Peptide
1	B	291	PRO	Peptide
1	B	299	THR	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	1659	0	1628	85	0
1	B	1659	0	1627	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	56	0	49	10	0
2	B	56	0	49	6	0
3	A	11	0	8	0	0
3	B	11	0	8	1	0
4	A	22	0	18	2	0
4	B	22	0	18	1	0
5	A	10	0	10	2	0
5	B	10	0	10	0	0
6	A	4	0	6	0	0
6	B	8	0	12	1	0
7	A	4	0	0	2	0
7	B	4	0	0	2	0
All	All	3536	0	3443	173	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 25.

All (173) 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:292:ARG:HG2	1:A:292:ARG:HH11	1.10	1.14
1:B:266:VAL:HB	1:B:300:TYR:HB3	1.31	1.13
1:A:266:VAL:HB	1:A:300:TYR:HB3	1.30	1.05
1:B:292:ARG:HG2	1:B:292:ARG:HH11	1.29	0.96
1:A:292:ARG:HG3	1:A:300:TYR:CE2	2.04	0.92
1:A:292:ARG:HG3	1:A:300:TYR:HE2	1.36	0.91
1:A:241:PHE:HE2	2:A:502:NAG:H4	1.37	0.90
1:A:292:ARG:NH1	1:A:292:ARG:HG2	1.82	0.89
1:B:292:ARG:HG3	1:B:300:TYR:HE2	1.40	0.86
1:B:292:ARG:HG3	1:B:300:TYR:CE2	2.10	0.86
1:A:241:PHE:CE2	2:A:502:NAG:H4	2.17	0.79
1:B:295:GLN:HG3	1:B:296:TYR:H	1.48	0.78
1:A:292:ARG:CG	1:A:300:TYR:HE2	2.02	0.73
1:A:283:GLU:HG2	1:A:285:HIS:CE1	2.24	0.72
1:B:376:ASP:OD1	7:B:601:HOH:O	2.07	0.72
1:B:283:GLU:HG2	1:B:285:HIS:CE1	2.26	0.71
1:B:299:THR:OG1	1:B:300:TYR:N	2.16	0.71
1:B:292:ARG:CG	1:B:300:TYR:HE2	2.04	0.69
1:A:295:GLN:HG3	1:A:296:TYR:H	1.56	0.69
1:A:338:LYS:NZ	1:A:430:GLU:OE1	2.21	0.69
1:B:370:LYS:NZ	7:B:604:HOH:O	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLN:OE1	5:A:508:FUC:O2	2.01	0.68
1:A:242:LEU:HG	1:A:336:ILE:HG21	1.75	0.68
1:B:242:LEU:HG	1:B:336:ILE:HG21	1.75	0.68
1:A:242:LEU:HD12	1:A:243:PHE:H	1.59	0.67
1:B:295:GLN:HG3	1:B:296:TYR:N	2.09	0.66
1:A:273:VAL:HB	1:A:275:PHE:HE1	1.61	0.65
1:B:308:VAL:HG21	1:B:319:TYR:CE1	2.32	0.65
1:B:338:LYS:NZ	1:B:430:GLU:OE1	2.27	0.64
1:B:242:LEU:HD12	1:B:243:PHE:H	1.63	0.64
1:A:308:VAL:HG21	1:A:319:TYR:CE1	2.33	0.63
1:A:301:ARG:NH1	2:A:502:NAG:O7	2.25	0.63
1:B:273:VAL:HB	1:B:275:PHE:HE1	1.62	0.62
1:A:301:ARG:HH12	2:A:502:NAG:C7	2.10	0.62
1:B:379:VAL:O	1:B:380:GLU:HG3	1.99	0.62
1:B:350:THR:H	1:B:439:LYS:HZ3	1.47	0.62
1:A:299:THR:OG1	1:A:300:TYR:N	2.27	0.61
1:A:295:GLN:HG3	1:A:296:TYR:N	2.14	0.61
1:A:390:ASN:ND2	1:A:411:THR:HB	2.15	0.60
4:A:506:MAN:H61	2:A:507:NAG:H82	1.82	0.60
1:A:293:GLU:HG3	1:A:294:GLU:N	2.17	0.59
1:B:292:ARG:NH1	1:B:292:ARG:HG2	2.05	0.59
1:B:241:PHE:HE2	2:B:502:NAG:H4	1.69	0.58
1:B:273:VAL:HG12	1:B:274:LYS:H	1.69	0.58
1:B:338:LYS:HG2	1:B:339:ALA:N	2.19	0.57
1:A:292:ARG:NH1	1:A:292:ARG:CG	2.64	0.57
1:B:312:ASP:HB3	1:B:319:TYR:OH	2.05	0.56
1:B:295:GLN:CG	1:B:296:TYR:H	2.15	0.56
1:A:379:VAL:O	1:A:380:GLU:HG3	2.06	0.56
1:A:350:THR:H	1:A:439:LYS:HZ3	1.54	0.55
1:B:283:GLU:HG2	1:B:285:HIS:HE1	1.73	0.54
1:A:295:GLN:CG	1:A:296:TYR:H	2.19	0.54
1:A:336:ILE:HG12	1:A:337:SER:N	2.23	0.54
1:A:249:ASP:HA	1:A:255:ARG:HD3	1.89	0.54
1:A:338:LYS:HG2	1:A:339:ALA:N	2.23	0.53
1:B:241:PHE:CE2	2:B:502:NAG:H4	2.42	0.53
1:A:273:VAL:HG12	1:A:274:LYS:H	1.72	0.53
1:A:397:VAL:HB	1:A:405:PHE:CE2	2.43	0.53
1:B:277:TRP:O	1:B:283:GLU:HG3	2.08	0.53
1:A:357:GLU:HG3	1:B:349:TYR:CZ	2.44	0.53
1:A:312:ASP:HB3	1:A:319:TYR:OH	2.10	0.52
1:B:397:VAL:HB	1:B:405:PHE:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PHE:N	1:A:275:PHE:CD1	2.78	0.51
1:B:248:LYS:HD3	1:B:255:ARG:NH1	2.25	0.51
2:B:501:NAG:O6	2:B:502:NAG:N2	2.44	0.51
1:A:296:TYR:C	1:A:298:SER:H	2.14	0.51
1:B:249:ASP:HA	1:B:255:ARG:HD3	1.93	0.51
1:A:242:LEU:HD12	1:A:243:PHE:N	2.26	0.50
1:B:415:SER:O	1:B:419:GLN:HG3	2.10	0.50
1:B:390:ASN:ND2	1:B:411:THR:HB	2.26	0.50
1:B:275:PHE:N	1:B:275:PHE:CD1	2.79	0.50
1:B:368:LEU:HD12	1:B:369:VAL:H	1.76	0.50
2:A:502:NAG:O4	4:B:504:MAN:O4	2.27	0.50
1:A:275:PHE:N	1:A:275:PHE:HD1	2.10	0.50
1:B:257:PRO:HG2	1:B:308:VAL:O	2.12	0.49
1:A:377:ILE:HG12	1:A:378:ALA:N	2.26	0.49
1:B:296:TYR:C	1:B:298:SER:H	2.15	0.49
1:B:293:GLU:HG3	1:B:294:GLU:N	2.27	0.49
1:A:377:ILE:HD11	1:A:427:VAL:CG1	2.42	0.49
1:A:415:SER:O	1:A:419:GLN:HG3	2.12	0.49
1:A:390:ASN:HD22	1:A:411:THR:HB	1.78	0.49
1:A:283:GLU:HG2	1:A:285:HIS:HE1	1.74	0.49
1:B:279:VAL:HG23	1:B:284:VAL:HG21	1.95	0.49
1:B:275:PHE:N	1:B:275:PHE:HD1	2.11	0.49
1:A:368:LEU:HD12	1:A:369:VAL:H	1.78	0.48
1:B:274:LYS:HB2	1:B:324:SER:O	2.13	0.48
1:A:370:LYS:HB2	7:A:602:HOH:O	2.14	0.48
2:B:501:NAG:H61	2:B:502:NAG:H82	1.96	0.47
1:B:358:LEU:C	1:B:358:LEU:HD12	2.35	0.47
1:B:336:ILE:HG12	1:B:337:SER:N	2.28	0.47
1:B:286:ASN:HB3	1:B:306:LEU:HD12	1.97	0.47
1:A:262:VAL:HG11	1:A:301:ARG:NH2	2.30	0.47
2:A:501:NAG:H4	5:A:508:FUC:H5	1.95	0.47
1:A:308:VAL:HG21	1:A:319:TYR:CZ	2.49	0.47
1:B:301:ARG:NH2	2:B:502:NAG:O7	2.48	0.47
1:A:292:ARG:O	1:A:300:TYR:OH	2.32	0.47
1:B:438:GLN:O	1:B:438:GLN:HG2	2.15	0.47
1:B:245:PRO:HD3	1:B:259:VAL:HG12	1.96	0.47
1:B:381:TRP:HB2	1:B:391:TYR:CD1	2.50	0.47
1:B:262:VAL:HG11	1:B:301:ARG:NH2	2.30	0.46
1:A:264:VAL:CG2	2:A:501:NAG:H5	2.45	0.46
1:B:325:ASN:OD1	1:B:328:LEU:N	2.48	0.46
1:A:266:VAL:CG1	1:A:271:PRO:HA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:507:NAG:O6	2:B:507:NAG:O4	2.33	0.46
1:A:292:ARG:HG3	1:A:300:TYR:CZ	2.50	0.46
1:B:417:TRP:CZ2	1:B:443:LEU:HD13	2.52	0.45
1:B:294:GLU:HB3	1:B:300:TYR:HE1	1.81	0.45
1:A:325:ASN:OD1	1:A:328:LEU:N	2.49	0.45
1:A:350:THR:OG1	1:A:441:LEU:HB2	2.16	0.45
1:B:274:LYS:C	1:B:275:PHE:HD1	2.21	0.45
1:A:422:VAL:HG22	1:A:442:SER:HB3	1.99	0.45
1:A:245:PRO:HD3	1:A:259:VAL:HG12	1.99	0.45
1:A:391:TYR:HB3	1:A:410:LEU:HD12	1.99	0.45
1:B:338:LYS:HG2	1:B:339:ALA:H	1.83	0.44
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.52	0.44
1:A:277:TRP:O	1:A:283:GLU:HG3	2.16	0.44
1:A:270:ASP:OD1	1:A:326:LYS:HG2	2.18	0.44
1:B:351:LEU:HB2	1:B:366:THR:HB	2.00	0.44
1:A:340:LYS:HD3	1:A:340:LYS:HA	1.78	0.44
1:A:370:LYS:HE3	7:A:602:HOH:O	2.18	0.44
1:A:381:TRP:HB2	1:A:391:TYR:CD1	2.53	0.44
1:A:349:TYR:CZ	1:B:357:GLU:HG3	2.52	0.44
1:A:279:VAL:HG23	1:A:284:VAL:HG21	1.99	0.44
1:B:350:THR:OG1	1:B:441:LEU:HB2	2.18	0.44
1:B:345:GLU:HA	1:B:346:PRO:HD2	1.84	0.44
1:B:292:ARG:NH1	1:B:292:ARG:CG	2.78	0.44
1:A:249:ASP:HB3	1:A:257:PRO:HB3	2.00	0.44
1:B:401:ASP:OD1	1:B:403:SER:OG	2.27	0.44
1:B:317:LYS:HB2	1:B:319:TYR:CE2	2.53	0.43
1:A:274:LYS:HB3	1:A:324:SER:HB3	1.99	0.43
1:A:391:TYR:HB2	1:A:409:LYS:O	2.18	0.43
1:A:283:GLU:CG	1:A:285:HIS:HE1	2.32	0.43
1:A:274:LYS:HB3	1:A:324:SER:O	2.18	0.43
1:B:308:VAL:HG21	1:B:319:TYR:HE1	1.83	0.43
1:A:279:VAL:O	1:A:282:VAL:HB	2.19	0.43
2:A:502:NAG:O3	4:A:506:MAN:H3	2.18	0.43
1:A:257:PRO:HG2	1:A:308:VAL:O	2.18	0.43
1:B:443:LEU:HD12	1:B:443:LEU:HA	1.74	0.43
1:A:264:VAL:HG21	2:A:501:NAG:O4	2.18	0.43
1:A:349:TYR:HB3	1:B:354:SER:CB	2.47	0.43
1:B:270:ASP:OD1	1:B:326:LYS:HG2	2.18	0.43
1:A:438:GLN:O	1:A:438:GLN:HG2	2.19	0.43
1:B:266:VAL:CG1	1:B:271:PRO:HA	2.48	0.43
1:A:328:LEU:HA	1:A:329:PRO:HD3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:PRO:O	1:B:251:LEU:HG	2.19	0.43
1:B:344:ARG:HD2	1:B:344:ARG:HH11	1.41	0.42
1:A:443:LEU:HA	1:A:443:LEU:HD12	1.80	0.42
1:A:286:ASN:HB3	1:A:306:LEU:HD12	2.02	0.42
1:B:377:ILE:HD11	1:B:427:VAL:CG1	2.50	0.42
1:A:377:ILE:HG12	1:A:378:ALA:H	1.85	0.42
1:A:294:GLU:HA	1:A:300:TYR:CE1	2.54	0.42
1:A:296:TYR:O	1:A:298:SER:N	2.50	0.42
1:B:242:LEU:HD12	1:B:243:PHE:N	2.31	0.42
1:A:288:LYS:HB3	1:A:305:VAL:O	2.20	0.42
1:B:320:LYS:HD3	1:B:333:GLU:OE2	2.20	0.41
1:B:406:LEU:HD22	6:B:509:EDO:H12	2.02	0.41
1:B:238:PRO:HB3	1:B:265:ASP:O	2.20	0.41
1:B:425:CYS:O	1:B:438:GLN:HA	2.20	0.41
1:B:399:ASP:OD1	1:B:400:SER:N	2.51	0.41
1:A:338:LYS:HG2	1:A:339:ALA:H	1.86	0.41
1:B:308:VAL:HG21	1:B:319:TYR:CZ	2.55	0.41
1:A:394:THR:HA	1:B:397:VAL:HG21	2.03	0.41
1:B:253:ILE:HG13	1:B:254:SER:H	1.86	0.41
1:B:243:PHE:HE1	3:B:503:BMA:H62	1.86	0.41
1:B:373:TYR:CG	1:B:374:PRO:HA	2.55	0.41
1:B:367:CYS:O	1:B:407:TYR:HA	2.21	0.41
1:B:296:TYR:O	1:B:298:SER:N	2.51	0.41
1:A:312:ASP:O	1:A:317:LYS:HG2	2.21	0.40
1:A:417:TRP:CZ2	1:A:443:LEU:HD13	2.55	0.40
1:A:344:ARG:HB2	1:A:373:TYR:N	2.36	0.40
1:B:292:ARG:O	1:B:300:TYR:OH	2.39	0.40
1:B:373:TYR:CD2	1:B:374:PRO:HA	2.57	0.40
1:B:312:ASP:O	1:B:317:LYS:HG2	2.21	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	206/208 (99%)	170 (82%)	28 (14%)	8 (4%)	4	12
1	B	206/208 (99%)	171 (83%)	26 (13%)	9 (4%)	3	10
All	All	412/416 (99%)	341 (83%)	54 (13%)	17 (4%)	3	11

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	A	419	GLN
1	A	421	ASN
1	B	418	GLN
1	B	419	GLN
1	B	421	ASN
1	A	297	ASN
1	B	297	ASN
1	B	431	ALA
1	A	355	ARG
1	B	355	ARG
1	A	431	ALA
1	B	288	LYS
1	B	253	ILE
1	A	253	ILE
1	A	420	GLY
1	B	420	GLY

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	193/193 (100%)	168 (87%)	25 (13%)	5	15
1	B	193/193 (100%)	165 (86%)	28 (14%)	4	11
All	All	386/386 (100%)	333 (86%)	53 (14%)	4	13

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	SER
1	A	242	LEU
1	A	254	SER
1	A	256	THR
1	A	260	THR
1	A	272	GLU
1	A	273	VAL
1	A	275	PHE
1	A	290	LYS
1	A	292	ARG
1	A	293	GLU
1	A	295	GLN
1	A	299	THR
1	A	321	CYS
1	A	326	LYS
1	A	328	LEU
1	A	336	ILE
1	A	347	GLN
1	A	358	LEU
1	A	383	SER
1	A	389	ASN
1	A	406	LEU
1	A	438	GLN
1	A	440	SER
1	A	441	LEU
1	B	239	SER
1	B	242	LEU
1	B	254	SER
1	B	256	THR
1	B	258	GLU
1	B	260	THR
1	B	272	GLU
1	B	273	VAL
1	B	275	PHE
1	B	282	VAL
1	B	290	LYS
1	B	292	ARG
1	B	293	GLU
1	B	294	GLU
1	B	295	GLN
1	B	299	THR
1	B	321	CYS
1	B	326	LYS

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Mol	Chain	Res	Type
1	B	328	LEU
1	B	336	ILE
1	B	344	ARG
1	B	356	ASP
1	B	358	LEU
1	B	383	SER
1	B	389	ASN
1	B	438	GLN
1	B	440	SER
1	B	441	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	295	GLN

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	0.81	1 (7%)	15,19,21	2.14	6 (40%)
2	NAG	A	502	3,2	14,14,15	0.73	1 (7%)	15,19,21	1.51	3 (20%)
3	BMA	A	503	2,4	11,11,12	0.67	0	15,15,17	1.68	2 (13%)
4	MAN	A	504	3,2	11,11,12	0.55	0	15,15,17	1.19	2 (13%)
2	NAG	A	505	4	14,14,15	0.51	0	15,19,21	1.33	3 (20%)
4	MAN	A	506	3,2	11,11,12	0.69	0	15,15,17	1.77	4 (26%)
2	NAG	A	507	4	14,14,15	0.45	0	15,19,21	2.04	4 (26%)
5	FUC	A	508	2	10,10,11	0.82	0	13,14,16	1.13	1 (7%)
6	EDO	A	509	-	3,3,3	0.60	0	2,2,2	0.21	0
2	NAG	B	501	1,2,5	14,14,15	0.35	0	15,19,21	1.73	2 (13%)
2	NAG	B	502	3,2	14,14,15	0.67	0	15,19,21	1.75	4 (26%)
3	BMA	B	503	2,4	11,11,12	0.79	0	15,15,17	1.29	1 (6%)
4	MAN	B	504	3,2	11,11,12	0.57	0	15,15,17	1.15	1 (6%)
2	NAG	B	505	4	14,14,15	0.47	0	15,19,21	0.74	0
4	MAN	B	506	3,2	11,11,12	0.65	0	15,15,17	0.68	0
2	NAG	B	507	4	14,14,15	0.43	0	15,19,21	1.34	1 (6%)
5	FUC	B	508	2	10,10,11	0.67	0	13,14,16	1.32	3 (23%)
6	EDO	B	509	-	3,3,3	0.57	0	2,2,2	0.48	0
6	EDO	B	510	-	3,3,3	0.49	0	2,2,2	0.47	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	-	0/6/23/26	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	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	1/6/23/26	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
6	EDO	B	510	-	-	0/1/1/1	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	NAG	O5-C1	-2.00	1.40	1.43
2	A	501	NAG	C1-C2	2.30	1.55	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	507	NAG	C2-N2-C7	-4.63	117.09	123.11
2	B	502	NAG	C1-O5-C5	-4.21	105.95	112.14
2	A	507	NAG	C4-C3-C2	-4.00	105.12	111.34
2	A	502	NAG	C2-N2-C7	-3.96	117.96	123.11
3	A	503	BMA	O3-C3-C2	-3.13	104.28	110.01
2	B	502	NAG	C2-N2-C7	-2.85	119.39	123.11
4	A	506	MAN	C1-O5-C5	-2.22	108.88	112.14
4	A	506	MAN	O2-C2-C3	-2.17	105.81	110.19
4	A	504	MAN	C6-C5-C4	-2.12	107.67	112.99
2	A	501	NAG	O7-C7-C8	-2.10	118.20	122.07
4	A	506	MAN	O5-C5-C6	2.05	111.73	107.34
5	A	508	FUC	C1-C2-C3	2.11	112.10	109.55
2	A	502	NAG	C4-C3-C2	2.12	114.64	111.34
5	B	508	FUC	C3-C4-C5	2.20	112.94	109.66
4	A	504	MAN	C1-O5-C5	2.25	115.45	112.14
2	B	502	NAG	O4-C4-C5	2.29	115.25	109.23
2	A	502	NAG	C3-C4-C5	2.29	114.32	110.23
5	B	508	FUC	C1-C2-C3	2.43	112.50	109.55
5	B	508	FUC	O5-C5-C4	2.49	113.89	109.58
2	A	505	NAG	C1-O5-C5	2.57	115.92	112.14
2	A	505	NAG	O5-C5-C4	2.57	114.39	110.13
2	B	502	NAG	C6-C5-C4	2.60	119.50	112.99
3	B	503	BMA	C1-C2-C3	2.61	112.71	109.55
4	B	504	MAN	O2-C2-C1	2.71	114.65	109.23
2	A	505	NAG	C3-C4-C5	2.76	115.15	110.23
2	A	501	NAG	C3-C4-C5	2.77	115.17	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAG	O5-C5-C6	2.81	113.35	107.34
2	A	507	NAG	O5-C5-C4	2.81	114.79	110.13
2	A	507	NAG	C1-O5-C5	3.34	117.05	112.14
2	A	501	NAG	C4-C3-C2	3.43	116.67	111.34
2	A	501	NAG	C1-O5-C5	3.46	117.23	112.14
2	B	501	NAG	O5-C5-C4	3.56	116.03	110.13
2	A	501	NAG	O5-C5-C4	3.92	116.63	110.13
2	B	507	NAG	C1-O5-C5	4.12	118.20	112.14
3	A	503	BMA	C1-C2-C3	4.20	114.64	109.55
4	A	506	MAN	O2-C2-C1	4.51	118.26	109.23
2	B	501	NAG	C1-O5-C5	4.53	118.80	112.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	507	NAG	O7-C7-N2-C2

There are no ring outliers.

11 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	3	0
2	A	502	NAG	6	0
4	A	506	MAN	2	0
2	A	507	NAG	1	0
5	A	508	FUC	2	0
2	B	501	NAG	2	0
2	B	502	NAG	5	0
3	B	503	BMA	1	0
4	B	504	MAN	1	0
2	B	507	NAG	1	0
6	B	509	EDO	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

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	208/208 (100%)	0.44	25 (12%) 6 3	49, 107, 211, 295	0
1	B	208/208 (100%)	0.53	23 (11%) 7 3	47, 108, 213, 293	0
All	All	416/416 (100%)	0.49	48 (11%) 6 3	47, 107, 213, 295	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	SER	7.6
1	A	269	GLU	6.9
1	B	238	PRO	6.4
1	A	239	SER	6.3
1	A	330	ALA	6.1
1	A	329	PRO	5.5
1	A	263	VAL	5.4
1	A	332	ILE	5.2
1	A	325	ASN	4.1
1	A	266	VAL	3.8
1	B	326	LYS	3.8
1	B	300	TYR	3.8
1	B	237	GLY	3.7
1	B	298	SER	3.7
1	B	324	SER	3.6
1	A	240	VAL	3.6
1	B	367	CYS	3.6
1	B	329	PRO	3.5
1	A	328	LEU	3.5
1	A	296	TYR	3.5
1	A	327	ALA	3.4
1	A	237	GLY	3.4
1	A	268	HIS	3.3
1	A	273	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	272	GLU	3.1
1	A	300	TYR	3.0
1	B	366	THR	3.0
1	B	319	TYR	3.0
1	A	238	PRO	2.9
1	B	323	VAL	2.9
1	B	297	ASN	2.8
1	B	310	ALA	2.8
1	A	366	THR	2.7
1	A	298	SER	2.7
1	B	322	LYS	2.6
1	B	331	PRO	2.6
1	B	291	PRO	2.6
1	B	408	SER	2.5
1	B	279	VAL	2.4
1	B	282	VAL	2.4
1	A	270	ASP	2.4
1	A	326	LYS	2.3
1	B	274	LYS	2.3
1	A	299	THR	2.2
1	A	367	CYS	2.2
1	B	296	TYR	2.2
1	A	267	SER	2.2
1	B	240	VAL	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
6	EDO	A	509	4/4	0.83	0.88	10.25	97,102,116,121	0
6	EDO	B	509	4/4	0.87	0.27	2.30	53,66,78,96	0
2	NAG	B	507	14/15	0.88	0.23	0.94	98,153,170,173	0
2	NAG	B	502	14/15	0.72	0.29	-0.59	166,201,222,233	0
2	NAG	B	501	14/15	0.76	0.28	-0.94	192,205,229,254	0
2	NAG	A	501	14/15	0.84	0.25	-2.62	129,186,217,226	0
3	BMA	A	503	11/12	0.79	0.11	-	153,184,202,210	0
6	EDO	B	510	4/4	0.82	0.27	-	113,142,146,150	0
4	MAN	A	506	11/12	0.89	0.20	-	155,171,184,188	0
2	NAG	A	502	14/15	0.81	0.28	-	146,200,219,221	0
2	NAG	A	505	14/15	0.72	0.38	-	111,185,203,203	0
4	MAN	B	506	11/12	0.90	0.18	-	114,153,164,176	0
4	MAN	A	504	11/12	0.84	0.12	-	130,157,195,202	0
2	NAG	A	507	14/15	0.89	0.17	-	85,130,155,162	0
4	MAN	B	504	11/12	0.88	0.16	-	93,161,181,206	0
5	FUC	A	508	10/11	0.74	0.36	-	159,199,214,217	0
5	FUC	B	508	10/11	0.70	0.24	-	98,185,210,240	0
3	BMA	B	503	11/12	0.81	0.12	-	153,163,168,173	0
2	NAG	B	505	14/15	0.85	0.14	-	147,181,204,204	0

6.5 Other polymers [i](#)

There are no such residues in this entry.