Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:50 PM GMT

PDB ID : 3V8C

Title : Crystal structure of monoclonal human anti-rhesus D Fc IgG1 t125(yb2/0) double mutant (H310 and H435 in K)

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Deposited on : 2011-12-22

Resolution : 2.77 Å(reported)

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

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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.77 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	Percentile Ranks	Value
Rfree		0.309
Clashscore		30
Ramachandran outliers		3.6%
Sidechain outliers		19.2%
RSRZ outliers		12.4%

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
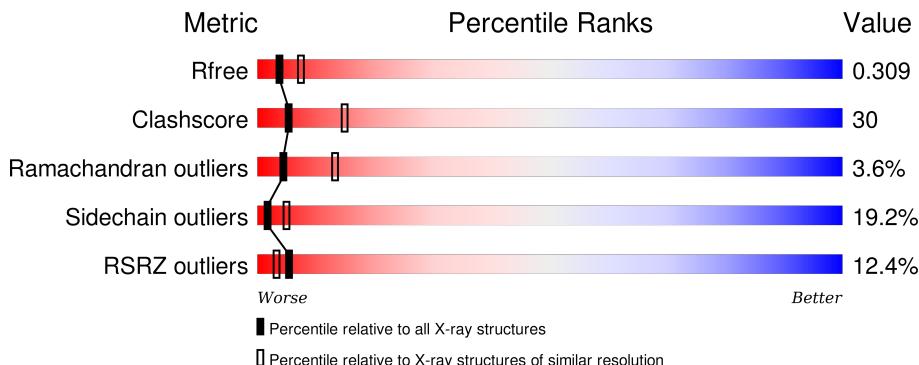
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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 <=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	212	6% / 52% 36% 12%
1	B	212	19% / 42% 42% 15% •
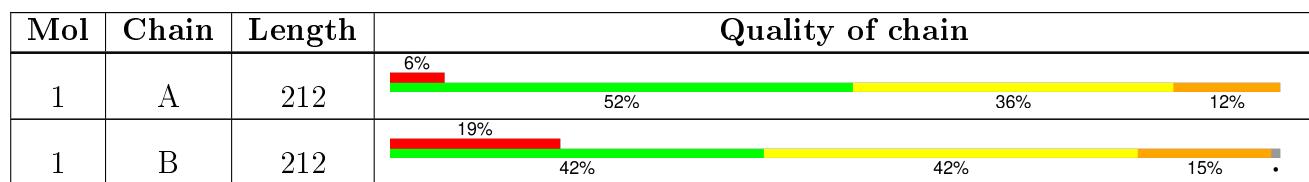
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	502	-	-	X	-
4	MAN	A	503	-	-	X	-
4	MAN	A	507	-	-	X	-
5	NAG	A	505	-	-	X	-
5	GAL	A	506	-	-	X	X
6	GAL	B	506	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3668 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	212	Total 1687	C 1074	N 283	O 324	S 6	0	0	0
1	B	209	Total 1665	C 1062	N 278	O 319	S 6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	LYS	HIS	ENGINEERED MUTATION	UNP P01857
A	435	LYS	HIS	ENGINEERED MUTATION	UNP P01857
B	310	LYS	HIS	ENGINEERED MUTATION	UNP P01857
B	435	LYS	HIS	ENGINEERED MUTATION	UNP P01857

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
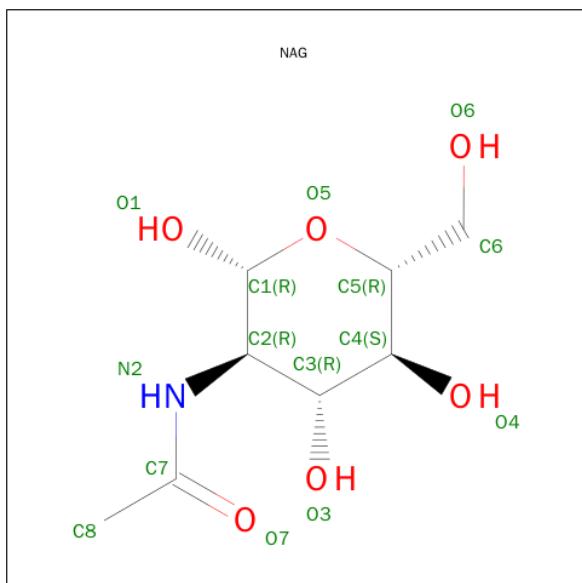
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
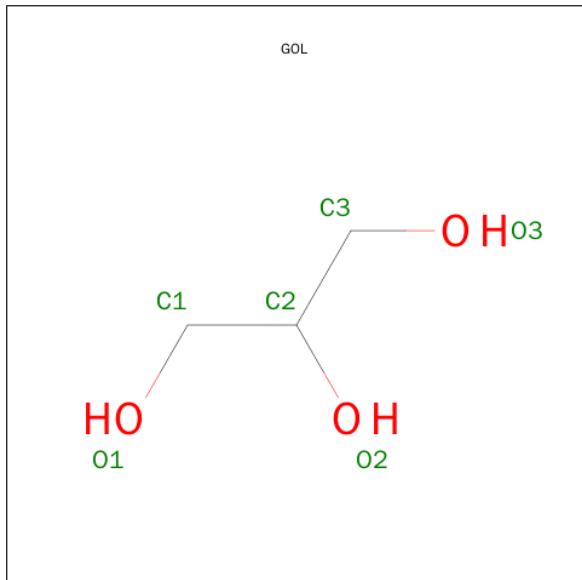
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0

- Molecule 4 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).
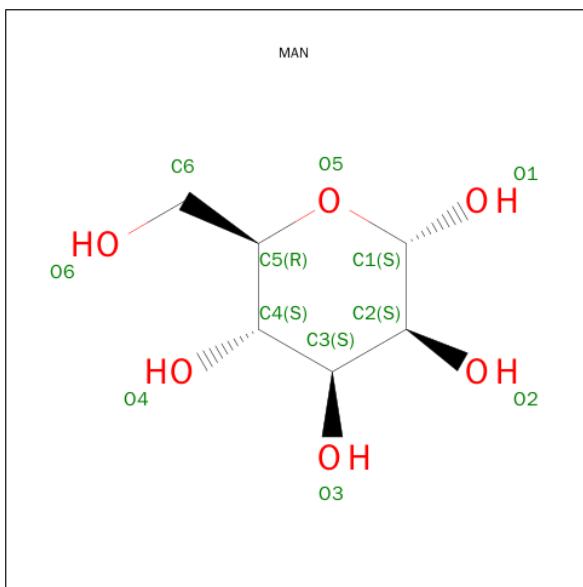
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 11	C 6	O 5	0	0
4	A	1	Total 11	C 6	O 5	0	0
4	A	1	Total 11	C 6	O 5	0	0
4	B	1	Total 11	C 6	O 5	0	0
4	B	1	Total 11	C 6	O 5	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total 25	C 14	N 1	O 10	0	0

- Molecule 6 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula: $C_6H_{12}O_6$).
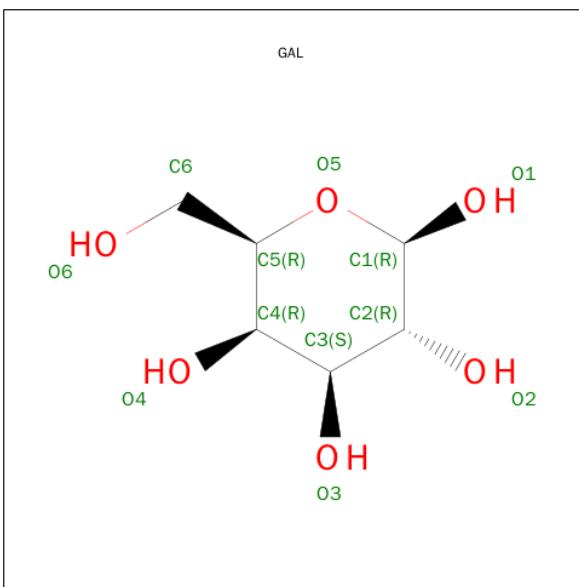
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 11	C 6	O 5	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	2	Total 25	C 14	N 1	O 10	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	50	Total 50	O 50	0	0
8	B	48	Total 48	O 48	0	0

3 Residue-property plots (i)

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
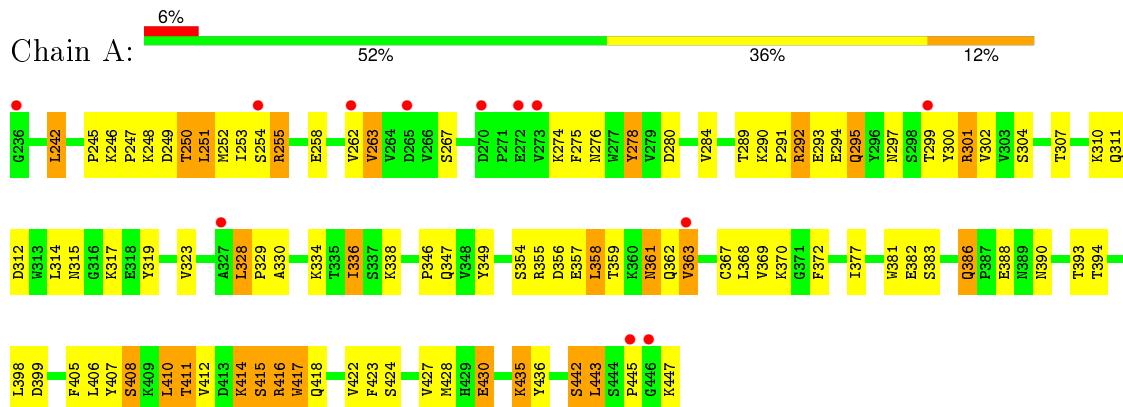
- Molecule 1: Ig gamma-1 chain C region
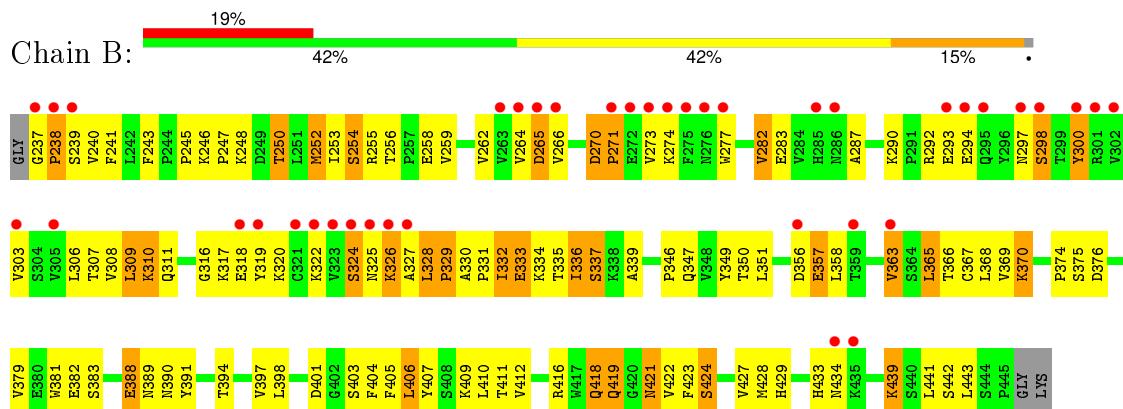
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.54Å 79.40Å 139.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.03 – 2.77 40.40 – 2.77	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.03-2.77) 99.3 (40.40-2.77)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$<I/\sigma(I)>$ [1]	2.80 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.254 , 0.316 0.251 , 0.309	Depositor DCC
R_{free} test set	723 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	61.6	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning [2]	$<|L|> = 0.47$, $<L^2> = 0.30$	Xtriage
Outliers	1 of 14465 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3668	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, GAL, NAG, MAN

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	0.70	0/1732	0.83	1/2355 (0.0%)
1	B	0.67	0/1710	0.72	0/2329
All	All	0.68	0/3442	0.78	1/4684 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	442	SER	N-CA-C	-5.18	97.02	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1687	0	1669	79	0
1	B	1665	0	1644	108	0
2	A	42	0	39	16	0
2	B	42	0	39	6	0
3	A	12	0	16	0	0
3	B	6	0	8	1	0
4	A	33	0	30	19	0
4	B	22	0	20	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	25	0	21	12	0
6	B	11	0	10	5	0
7	B	25	0	22	2	0
8	A	50	0	0	1	0
8	B	48	0	0	3	0
All	All	3668	0	3518	214	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 30.

All (214) 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)
5:A:505:NAG:O4	5:A:506:GAL:C2	1.64	1.43
2:A:502:NAG:O4	4:A:503:MAN:C1	1.72	1.36
1:B:328:LEU:CB	1:B:329:PRO:HD3	1.86	1.05
1:A:247:PRO:O	1:A:251:LEU:HD12	1.54	1.03
5:A:505:NAG:O4	5:A:506:GAL:C1	2.07	1.02
1:B:328:LEU:HB2	1:B:329:PRO:HD3	1.02	1.01
1:A:242:LEU:HD13	1:A:336:ILE:HB	1.42	1.01
1:B:328:LEU:HB2	1:B:329:PRO:CD	1.91	0.99
1:B:347:GLN:NE2	1:B:349:TYR:OH	1.98	0.97
1:B:266:VAL:HG13	1:B:300:TYR:HB3	1.49	0.95
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.30	0.95
1:A:361:ASN:H	1:A:361:ASN:HD22	1.11	0.95
2:A:502:NAG:O4	4:A:503:MAN:C2	2.17	0.92
1:B:418:GLN:HA	1:B:418:GLN:HE21	1.36	0.90
4:A:507:MAN:O2	2:A:508:NAG:H2	1.71	0.89
1:B:282:VAL:HG12	1:B:283:GLU:H	1.42	0.84
1:B:330:ALA:HB1	1:B:331:PRO:HD2	1.58	0.83
1:A:297:ASN:HD21	2:A:501:NAG:C1	1.92	0.83
1:B:391:TYR:HB3	1:B:410:LEU:HD12	1.60	0.83
1:A:361:ASN:H	1:A:361:ASN:ND2	1.77	0.81
1:A:255:ARG:CG	1:A:255:ARG:HH11	1.94	0.79
1:A:357:GLU:HG3	1:B:349:TYR:CZ	2.19	0.77
1:B:406:LEU:HD12	1:B:406:LEU:O	1.84	0.76
1:A:398:LEU:HD13	1:A:399:ASP:O	1.86	0.76
1:A:255:ARG:HG2	1:A:255:ARG:NH1	2.01	0.76
1:B:418:GLN:CA	1:B:418:GLN:HE21	1.98	0.76
2:A:502:NAG:C4	4:A:503:MAN:C1	2.65	0.75
4:A:504:MAN:O2	5:A:505:NAG:C1	2.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:VAL:HG11	1:A:323:VAL:HG11	1.69	0.75
1:B:248:LYS:HE2	1:B:255:ARG:NH1	2.02	0.75
1:B:306:LEU:HD23	1:B:308:VAL:HG22	1.70	0.73
2:A:502:NAG:O4	4:A:503:MAN:H2	1.88	0.72
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.69	0.72
1:B:336:ILE:HD12	1:B:337:SER:H	1.53	0.72
1:A:361:ASN:N	1:A:361:ASN:HD22	1.83	0.72
1:B:297:ASN:O	1:B:298:SER:HB3	1.87	0.72
4:A:507:MAN:O2	2:A:508:NAG:C2	2.38	0.71
1:A:393:THR:OG1	1:A:408:SER:HB2	1.90	0.71
1:B:406:LEU:C	1:B:406:LEU:HD12	2.11	0.70
1:A:338:LYS:NZ	1:A:430:GLU:OE2	2.25	0.70
1:A:255:ARG:O	1:A:310:LYS:NZ	2.25	0.69
4:B:503:MAN:O3	7:B:507:MAN:H3	1.91	0.69
1:A:311:GLN:O	1:A:315:ASN:HB2	1.93	0.68
1:A:415:SER:O	1:A:418:GLN:N	2.27	0.67
1:B:332:ILE:CG2	1:B:333:GLU:N	2.58	0.67
4:A:503:MAN:O3	4:A:507:MAN:H2	1.95	0.66
1:A:247:PRO:O	1:A:251:LEU:CD1	2.38	0.66
1:A:328:LEU:HD11	1:A:330:ALA:O	1.96	0.66
1:A:246:LYS:NZ	5:A:505:NAG:O3	2.24	0.65
1:B:293:GLU:HG2	1:B:294:GLU:HG3	1.77	0.65
1:B:317:LYS:HB2	1:B:319:TYR:HE1	1.61	0.65
1:B:347:GLN:CD	1:B:349:TYR:OH	2.35	0.64
1:A:297:ASN:ND2	2:A:501:NAG:C1	2.60	0.64
1:B:410:LEU:HG	1:B:411:THR:N	2.12	0.64
1:A:346:PRO:HG3	1:A:372:PHE:HB3	1.79	0.64
1:B:287:ALA:HB2	1:B:306:LEU:HD12	1.80	0.64
1:A:293:GLU:HG2	1:A:301:ARG:HG3	1.80	0.64
1:A:293:GLU:HG3	1:A:295:GLN:HE22	1.62	0.63
1:B:332:ILE:HG23	1:B:333:GLU:H	1.64	0.63
4:A:507:MAN:HO2	2:A:508:NAG:H2	1.64	0.62
1:A:377:ILE:HD11	1:A:427:VAL:CG1	2.29	0.62
4:B:504:MAN:O2	2:B:505:NAG:C1	2.48	0.62
4:B:503:MAN:H4	7:B:507:MAN:C1	2.30	0.62
5:A:505:NAG:C4	5:A:506:GAL:C2	2.76	0.62
2:A:502:NAG:C3	4:A:503:MAN:C1	2.77	0.62
1:B:350:THR:HB	1:B:441:LEU:HD22	1.82	0.62
1:B:365:LEU:CD1	1:B:410:LEU:HD23	2.29	0.61
1:B:433:HIS:O	1:B:434:ASN:HB2	2.00	0.61
1:A:275:PHE:CE2	1:A:304:SER:HB2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:503:MAN:O6	4:A:504:MAN:H3	2.02	0.60
1:B:246:LYS:HG2	6:B:506:GAL:O4	2.01	0.59
1:A:280:ASP:OD1	1:A:317:LYS:HG3	2.02	0.59
1:B:351:LEU:HB2	1:B:366:THR:HB	1.83	0.59
1:B:357:GLU:HG2	1:B:357:GLU:O	2.02	0.59
1:B:254:SER:HA	1:B:310:LYS:HZ1	1.68	0.59
1:A:394:THR:HG23	1:A:407:TYR:O	2.02	0.59
1:B:397:VAL:HB	1:B:405:PHE:CE2	2.38	0.58
1:B:243:PHE:HE2	1:B:262:VAL:HG22	1.67	0.58
1:B:336:ILE:HD12	1:B:337:SER:N	2.18	0.58
1:B:394:THR:HG23	1:B:407:TYR:O	2.02	0.58
1:A:312:ASP:HB3	1:A:319:TYR:OH	2.04	0.58
1:A:328:LEU:CD1	1:A:330:ALA:O	2.51	0.58
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.38	0.58
1:A:361:ASN:ND2	1:A:361:ASN:N	2.47	0.57
1:B:246:LYS:HE3	6:B:506:GAL:H61	1.86	0.57
1:B:241:PHE:CE2	2:B:502:NAG:H62	2.39	0.57
1:B:318:GLU:C	1:B:319:TYR:HD1	2.08	0.57
2:B:505:NAG:O4	6:B:506:GAL:C1	2.53	0.57
1:A:245:PRO:HA	5:A:506:GAL:H4	1.86	0.57
1:B:397:VAL:O	1:B:404:PHE:HA	2.04	0.57
1:B:406:LEU:C	1:B:406:LEU:CD1	2.74	0.56
1:B:308:VAL:HG11	1:B:319:TYR:CE2	2.40	0.56
1:B:332:ILE:CG2	1:B:333:GLU:H	2.15	0.56
1:B:388:GLU:OE2	1:B:416:ARG:NH1	2.33	0.56
1:B:381:TRP:HA	1:B:424:SER:O	2.05	0.56
1:A:347:GLN:NE2	1:A:349:TYR:OH	2.36	0.56
1:A:297:ASN:OD1	2:A:501:NAG:C1	2.53	0.56
1:B:274:LYS:HB3	1:B:324:SER:HB3	1.88	0.56
4:A:503:MAN:O3	4:A:507:MAN:C2	2.54	0.56
1:B:245:PRO:HA	6:B:506:GAL:O3	2.06	0.56
4:A:503:MAN:O3	4:A:507:MAN:C1	2.55	0.55
1:A:443:LEU:O	1:A:445:PRO:HD3	2.06	0.55
1:A:383:SER:HB2	1:A:423:PHE:CD2	2.41	0.55
4:B:504:MAN:O2	2:B:505:NAG:O5	2.24	0.55
1:B:309:LEU:HD23	1:B:311:GLN:H	1.71	0.54
1:B:308:VAL:HG11	1:B:319:TYR:HE2	1.71	0.54
1:B:401:ASP:OD1	1:B:403:SER:OG	2.25	0.54
2:A:501:NAG:O4	2:A:502:NAG:C1	2.56	0.54
3:B:509:GOL:H12	8:B:629:HOH:O	2.07	0.54
1:B:270:ASP:N	1:B:271:PRO:HD3	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:HG22	1:B:333:GLU:N	2.23	0.53
1:B:306:LEU:CD2	1:B:308:VAL:HG22	2.38	0.53
1:A:393:THR:HA	1:A:408:SER:HA	1.90	0.53
1:A:407:TYR:OH	1:B:409:LYS:HG3	2.08	0.53
1:B:388:GLU:OE2	1:B:423:PHE:HE2	1.93	0.52
1:B:318:GLU:C	1:B:319:TYR:CD1	2.83	0.52
1:B:418:GLN:NE2	1:B:418:GLN:CA	2.71	0.52
1:A:377:ILE:HD11	1:A:427:VAL:HG13	1.90	0.52
1:B:421:ASN:OD1	1:B:421:ASN:N	2.43	0.51
1:B:237:GLY:HA2	1:B:329:PRO:HD2	1.92	0.51
1:B:308:VAL:CG1	1:B:319:TYR:HE2	2.24	0.51
1:A:289:THR:HG22	1:A:290:LYS:N	2.24	0.51
1:B:243:PHE:O	1:B:259:VAL:HG23	2.11	0.51
1:B:390:ASN:OD1	1:B:411:THR:HG23	2.11	0.51
1:B:317:LYS:HB2	1:B:319:TYR:CE1	2.43	0.50
1:A:390:ASN:ND2	1:A:411:THR:O	2.37	0.50
1:A:278:TYR:CD2	1:A:278:TYR:N	2.80	0.50
1:A:358:LEU:O	1:A:414:LYS:HE3	2.12	0.49
1:A:382:GLU:HB2	1:A:386:GLN:O	2.11	0.49
1:A:290:LYS:HB3	1:A:291:PRO:CD	2.43	0.49
1:B:356:ASP:C	1:B:358:LEU:H	2.16	0.49
1:B:365:LEU:HD12	1:B:410:LEU:CD2	2.41	0.49
1:B:350:THR:HG23	1:B:439:LYS:HB3	1.96	0.48
1:A:292:ARG:HD3	1:A:300:TYR:CD1	2.47	0.48
1:B:252:MET:HG3	1:B:428:MET:HE1	1.96	0.48
1:B:282:VAL:HG12	1:B:283:GLU:N	2.20	0.48
1:A:377:ILE:HD11	1:A:427:VAL:HG11	1.95	0.48
1:B:356:ASP:O	1:B:358:LEU:N	2.47	0.48
1:A:354:SER:HB2	1:B:349:TYR:HB3	1.96	0.48
1:B:368:LEU:HD13	1:B:407:TYR:CZ	2.49	0.48
1:A:245:PRO:HA	5:A:506:GAL:C4	2.44	0.47
1:A:294:GLU:C	1:A:295:GLN:HE21	2.18	0.47
1:A:249:ASP:OD2	5:A:506:GAL:H62	2.14	0.47
1:B:379:VAL:HG22	1:B:427:VAL:HG22	1.97	0.47
1:B:290:LYS:HZ1	1:B:293:GLU:HG3	1.80	0.47
1:B:390:ASN:O	1:B:411:THR:HG22	2.13	0.47
1:A:414:LYS:O	1:A:415:SER:C	2.53	0.47
2:A:502:NAG:O3	4:A:503:MAN:C1	2.63	0.47
1:B:346:PRO:HD3	1:B:429:HIS:CD2	2.50	0.47
1:A:368:LEU:HD12	1:A:369:VAL:N	2.31	0.47
1:B:388:GLU:OE1	1:B:388:GLU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:GLN:NE2	1:B:418:GLN:HA	2.17	0.46
1:B:243:PHE:HE2	1:B:262:VAL:CG2	2.28	0.46
2:A:502:NAG:HO4	4:A:503:MAN:C1	2.13	0.46
1:A:263:VAL:CG1	1:A:323:VAL:HG11	2.43	0.46
1:B:258:GLU:O	6:B:506:GAL:O3	2.25	0.46
1:B:347:GLN:CD	1:B:349:TYR:HH	2.20	0.45
1:B:241:PHE:CE2	2:B:502:NAG:C6	3.00	0.45
1:B:252:MET:HG3	1:B:428:MET:CE	2.47	0.45
1:B:255:ARG:H	1:B:310:LYS:NZ	2.15	0.45
1:B:266:VAL:O	1:B:300:TYR:HB2	2.17	0.45
1:A:295:GLN:N	1:A:295:GLN:HE21	2.15	0.44
1:A:289:THR:CG2	1:A:290:LYS:N	2.79	0.44
1:B:247:PRO:O	1:B:250:THR:HG22	2.16	0.44
1:B:264:VAL:O	1:B:265:ASP:HB2	2.17	0.44
1:A:388:GLU:OE1	1:A:416:ARG:NH2	2.50	0.44
1:B:273:VAL:HG13	1:B:325:ASN:HB2	1.99	0.44
1:A:246:LYS:O	1:A:249:ASP:HB2	2.16	0.44
1:B:241:PHE:HE2	2:B:502:NAG:C6	2.31	0.44
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.53	0.44
1:B:290:LYS:HD2	1:B:303:VAL:HB	2.00	0.43
1:A:428:MET:HB2	1:A:435:LYS:O	2.18	0.43
1:A:295:GLN:OE1	1:A:301:ARG:HG2	2.17	0.43
1:B:328:LEU:CB	1:B:329:PRO:CD	2.68	0.43
1:A:422:VAL:HG22	1:A:442:SER:HB3	2.01	0.43
1:B:347:GLN:HB2	1:B:370:LYS:O	2.18	0.43
1:B:363:VAL:HG23	1:B:412:VAL:CG2	2.49	0.43
1:A:295:GLN:CA	1:A:295:GLN:HE21	2.32	0.43
1:A:388:GLU:HB3	1:A:410:LEU:CD1	2.49	0.42
1:A:436:TYR:C	1:A:436:TYR:CD2	2.91	0.42
4:A:507:MAN:O2	2:A:508:NAG:N2	2.52	0.42
1:A:247:PRO:O	1:A:250:THR:HB	2.19	0.42
1:B:316:GLY:O	1:B:317:LYS:C	2.57	0.42
1:B:238:PRO:HB2	1:B:239:SER:H	1.69	0.42
1:B:336:ILE:CD1	1:B:337:SER:H	2.29	0.42
1:B:241:PHE:HB2	1:B:262:VAL:CG2	2.49	0.42
1:A:276:ASN:HB3	1:A:278:TYR:HE2	1.85	0.42
1:B:256:THR:HG23	1:B:307:THR:HG23	2.01	0.42
1:A:258:GLU:O	5:A:506:GAL:H4	2.19	0.42
1:A:398:LEU:HD13	1:A:398:LEU:C	2.40	0.42
1:B:410:LEU:HG	1:B:411:THR:H	1.83	0.41
1:B:240:VAL:HG12	1:B:334:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LYS:HE2	1:A:370:LYS:HB2	1.46	0.41
1:A:415:SER:O	1:A:417:TRP:N	2.53	0.41
1:B:334:LYS:NZ	8:B:647:HOH:O	2.53	0.41
1:A:363:VAL:HG23	1:A:412:VAL:HG23	2.02	0.41
4:A:504:MAN:C2	5:A:505:NAG:C1	2.99	0.41
4:A:503:MAN:C3	4:A:507:MAN:C1	2.98	0.41
1:B:241:PHE:HB2	1:B:262:VAL:HG22	2.02	0.41
1:A:369:VAL:O	1:A:405:PHE:HA	2.20	0.41
1:B:419:GLN:HB2	1:B:421:ASN:OD1	2.21	0.41
1:A:246:LYS:NZ	5:A:505:NAG:C3	2.84	0.41
1:A:249:ASP:OD2	5:A:506:GAL:C6	2.69	0.40
1:A:275:PHE:CD2	1:A:304:SER:HB2	2.55	0.40
1:A:284:VAL:HG12	8:A:601:HOH:O	2.20	0.40
1:B:369:VAL:O	1:B:405:PHE:HA	2.21	0.40
1:A:242:LEU:HA	1:A:242:LEU:HD23	1.93	0.40
1:B:339:ALA:HB3	1:B:374:PRO:HB3	2.04	0.40
1:B:422:VAL:HG12	1:B:442:SER:HB3	2.02	0.40
2:A:501:NAG:C4	2:A:502:NAG:C1	2.99	0.40
4:A:503:MAN:O6	4:A:504:MAN:C3	2.69	0.40
1:B:319:TYR:N	1:B:319:TYR:CD1	2.90	0.40
1:A:394:THR:H	1:A:394:THR:HG23	1.65	0.40
1:B:382:GLU:CB	8:B:626:HOH:O	2.69	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	A	210/212 (99%)	183 (87%)	23 (11%)	4 (2%)	10	30
1	B	207/212 (98%)	173 (84%)	23 (11%)	11 (5%)	2	6
All	All	417/424 (98%)	356 (85%)	46 (11%)	15 (4%)	4	13

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ARG
1	B	271	PRO
1	B	328	LEU
1	B	329	PRO
1	B	238	PRO
1	B	326	LYS
1	B	327	ALA
1	B	298	SER
1	B	357	GLU
1	B	265	ASP
1	A	267	SER
1	B	270	ASP
1	B	282	VAL
1	A	253	ILE
1	A	329	PRO

5.3.2 Protein sidechains (i)

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	196/196 (100%)	155 (79%)	41 (21%)	1	3
1	B	194/196 (99%)	160 (82%)	34 (18%)	2	6
All	All	390/392 (100%)	315 (81%)	75 (19%)	2	5

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	LEU
1	A	248	LYS
1	A	250	THR
1	A	251	LEU
1	A	252	MET
1	A	254	SER
1	A	255	ARG
1	A	262	VAL

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Mol	Chain	Res	Type
1	A	263	VAL
1	A	274	LYS
1	A	278	TYR
1	A	295	GLN
1	A	299	THR
1	A	301	ARG
1	A	302	VAL
1	A	307	THR
1	A	314	LEU
1	A	328	LEU
1	A	334	LYS
1	A	336	ILE
1	A	355	ARG
1	A	356	ASP
1	A	358	LEU
1	A	359	THR
1	A	361	ASN
1	A	362	GLN
1	A	363	VAL
1	A	386	GLN
1	A	406	LEU
1	A	408	SER
1	A	410	LEU
1	A	411	THR
1	A	414	LYS
1	A	415	SER
1	A	416	ARG
1	A	417	TRP
1	A	424	SER
1	A	430	GLU
1	A	435	LYS
1	A	443	LEU
1	A	447	LYS
1	B	250	THR
1	B	252	MET
1	B	253	ILE
1	B	254	SER
1	B	277	TRP
1	B	292	ARG
1	B	300	TYR
1	B	309	LEU
1	B	310	LYS

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Mol	Chain	Res	Type
1	B	320	LYS
1	B	322	LYS
1	B	324	SER
1	B	326	LYS
1	B	332	ILE
1	B	333	GLU
1	B	335	THR
1	B	336	ILE
1	B	337	SER
1	B	363	VAL
1	B	365	LEU
1	B	370	LYS
1	B	375	SER
1	B	376	ASP
1	B	383	SER
1	B	388	GLU
1	B	389	ASN
1	B	398	LEU
1	B	406	LEU
1	B	418	GLN
1	B	419	GLN
1	B	421	ASN
1	B	424	SER
1	B	439	LYS
1	B	443	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	GLN
1	A	347	GLN
1	A	361	ASN
1	A	362	GLN
1	A	390	ASN
1	B	276	ASN
1	B	315	ASN
1	B	347	GLN
1	B	362	GLN
1	B	384	ASN
1	B	418	GLN
1	B	438	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)

4 carbohydrates 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	$\#|Z| > 2$
5	NAG	A	505	-	14,14,15	0.80	0	15,19,21	1.52	3 (20%)
5	GAL	A	506	-	11,11,12	0.73	0	14,15,17	2.54	6 (42%)
7	MAN	B	507	7	11,11,12	0.67	0	14,15,17	0.99	0
7	NAG	B	508	7	14,14,15	0.63	0	15,19,21	1.39	2 (13%)

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
5	NAG	A	505	-	-	0/6/23/26	0/1/1/1
5	GAL	A	506	-	-	0/2/19/22	0/1/1/1
7	MAN	B	507	7	-	0/2/19/22	0/1/1/1
7	NAG	B	508	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	505	NAG	O4-C4-C3	-3.13	103.28	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	506	GAL	C3-C4-C5	-2.98	105.01	110.20
5	A	505	NAG	C2-N2-C7	-2.18	120.23	123.04
5	A	506	GAL	C6-C5-C4	-2.03	108.00	113.02
7	B	508	NAG	C4-C3-C2	2.53	115.16	111.23
5	A	506	GAL	O5-C1-C2	2.60	115.08	110.86
5	A	506	GAL	O5-C5-C6	3.13	114.13	107.35
5	A	506	GAL	C1-O5-C5	3.48	116.67	112.25
5	A	505	NAG	C3-C4-C5	3.50	116.30	110.20
7	B	508	NAG	C3-C4-C5	4.19	117.50	110.20
5	A	506	GAL	C1-C2-C3	6.66	117.42	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	NAG	7	0
5	A	506	GAL	8	0
7	B	507	MAN	2	0

5.6 Ligand geometry (i)

15 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	-	14,14,15	0.63	0	15,19,21	1.61	2 (13%)
2	NAG	A	502	-	14,14,15	0.88	1 (7%)	15,19,21	1.60	2 (13%)
4	MAN	A	503	-	11,11,12	0.65	0	14,15,17	1.45	2 (14%)
4	MAN	A	504	-	11,11,12	0.82	0	14,15,17	1.93	3 (21%)
4	MAN	A	507	-	11,11,12	0.99	1 (9%)	14,15,17	1.78	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	NAG	A	508	-	14,14,15	0.66	0	15,19,21	2.95	7 (46%)
3	GOL	A	509	-	5,5,5	0.25	0	5,5,5	0.48	0
3	GOL	A	510	-	5,5,5	0.35	0	5,5,5	0.30	0
2	NAG	B	501	-	14,14,15	0.49	0	15,19,21	0.92	1 (6%)
2	NAG	B	502	-	14,14,15	0.70	1 (7%)	15,19,21	1.21	2 (13%)
4	MAN	B	503	-	11,11,12	0.77	0	14,15,17	1.53	3 (21%)
4	MAN	B	504	-	11,11,12	0.53	0	14,15,17	2.21	5 (35%)
2	NAG	B	505	-	14,14,15	0.50	0	15,19,21	2.35	5 (33%)
6	GAL	B	506	-	11,11,12	0.75	0	14,15,17	1.24	2 (14%)
3	GOL	B	509	-	5,5,5	0.34	0	5,5,5	0.43	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	-	-	0/6/23/26	0/1/1/1
2	NAG	A	502	-	-	0/6/23/26	0/1/1/1
4	MAN	A	503	-	-	0/2/19/22	1/1/1/1
4	MAN	A	504	-	-	0/2/19/22	0/1/1/1
4	MAN	A	507	-	-	0/2/19/22	0/1/1/1
2	NAG	A	508	-	-	0/6/23/26	0/1/1/1
3	GOL	A	509	-	-	0/4/4/4	0/0/0/0
3	GOL	A	510	-	-	0/4/4/4	0/0/0/0
2	NAG	B	501	-	-	0/6/23/26	0/1/1/1
2	NAG	B	502	-	-	0/6/23/26	0/1/1/1
4	MAN	B	503	-	-	0/2/19/22	0/1/1/1
4	MAN	B	504	-	-	0/2/19/22	0/1/1/1
2	NAG	B	505	-	-	0/6/23/26	0/1/1/1
6	GAL	B	506	-	-	0/2/19/22	0/1/1/1
3	GOL	B	509	-	-	0/4/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	NAG	O5-C1	-2.44	1.39	1.43
2	B	502	NAG	C1-C2	2.05	1.55	1.52
4	A	507	MAN	C2-C3	2.22	1.55	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	508	NAG	C4-C3-C2	-4.00	105.02	111.23
2	A	502	NAG	C1-O5-C5	-3.83	107.38	112.25
2	B	505	NAG	C4-C3-C2	-3.61	105.61	111.23
2	A	502	NAG	C2-N2-C7	-3.56	118.46	123.04
6	B	506	GAL	O5-C1-C2	-3.11	105.81	110.86
4	B	504	MAN	O3-C3-C2	-2.90	104.77	110.00
4	B	504	MAN	O2-C2-C3	-2.74	104.62	110.12
4	A	504	MAN	O2-C2-C1	-2.33	104.54	109.21
2	A	508	NAG	O7-C7-C8	-2.12	118.17	122.06
6	B	506	GAL	C1-C2-C3	-2.03	107.14	109.54
2	B	501	NAG	C3-C4-C5	2.06	113.78	110.20
4	A	507	MAN	O2-C2-C3	2.23	114.61	110.12
2	A	501	NAG	C2-N2-C7	2.24	125.92	123.04
4	A	503	MAN	O5-C5-C6	2.28	112.28	107.35
2	B	502	NAG	C4-C3-C2	2.28	114.78	111.23
2	B	505	NAG	O3-C3-C2	2.30	113.67	109.11
4	B	503	MAN	C3-C4-C5	2.35	114.29	110.20
2	B	505	NAG	C3-C2-N2	2.35	116.19	110.56
4	A	504	MAN	C2-C3-C4	2.37	115.06	111.04
4	A	507	MAN	C2-C3-C4	2.41	115.13	111.04
2	A	508	NAG	C3-C2-N2	2.44	116.41	110.56
2	A	508	NAG	C3-C4-C5	2.48	114.53	110.20
2	B	502	NAG	C2-N2-C7	2.79	126.62	123.04
2	A	508	NAG	C1-O5-C5	2.99	116.05	112.25
2	A	508	NAG	C8-C7-N2	3.06	121.96	116.11
4	B	503	MAN	C1-C2-C3	3.10	113.21	109.54
4	B	503	MAN	C2-C3-C4	3.20	116.48	111.04
4	B	504	MAN	C2-C3-C4	3.35	116.72	111.04
4	B	504	MAN	C1-C2-C3	3.44	113.61	109.54
2	B	505	NAG	C2-N2-C7	3.59	127.65	123.04
4	A	503	MAN	C1-O5-C5	3.94	117.24	112.25
4	B	504	MAN	C3-C4-C5	4.04	117.24	110.20
2	A	501	NAG	C3-C4-C5	4.11	117.36	110.20
4	A	507	MAN	C1-C2-C3	4.70	115.10	109.54
4	A	504	MAN	C1-C2-C3	5.31	115.82	109.54
2	B	505	NAG	C1-O5-C5	6.05	119.92	112.25
2	A	508	NAG	C2-N2-C7	8.68	134.19	123.04

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	MAN	C1-C2-C3-C4-C5-O5

12 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	5	0
2	A	502	NAG	9	0
4	A	503	MAN	13	0
4	A	504	MAN	4	0
4	A	507	MAN	8	0
2	A	508	NAG	4	0
2	B	502	NAG	3	0
4	B	503	MAN	2	0
4	B	504	MAN	2	0
2	B	505	NAG	3	0
6	B	506	GAL	5	0
3	B	509	GOL	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 (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, 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(Å²)	Q<0.9
1	A	212/212 (100%)	0.47	12 (5%)	27	20	19, 49, 74, 89	1 (0%)
1	B	209/212 (98%)	1.02	40 (19%)	2	1	22, 60, 102, 105	1 (0%)
All	All	421/424 (99%)	0.75	52 (12%)	5	3	19, 54, 99, 105	2 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	VAL	6.5
1	A	327	ALA	6.1
1	B	276	ASN	5.8
1	B	300	TYR	5.6
1	B	274	LYS	5.5
1	B	323	VAL	5.5
1	B	293	GLU	5.4
1	B	266	VAL	5.3
1	B	264	VAL	5.2
1	B	294	GLU	5.2
1	B	324	SER	4.8
1	B	325	ASN	4.7
1	B	302	VAL	4.7
1	A	236	GLY	4.6
1	B	265	ASP	4.3
1	B	285	HIS	4.2
1	B	301	ARG	4.1
1	B	239	SER	4.0
1	B	275	PHE	3.9
1	A	363	VAL	3.8
1	B	363	VAL	3.8
1	B	286	ASN	3.6
1	B	327	ALA	3.5
1	B	273	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	272	GLU	3.4
1	B	326	LYS	3.4
1	B	359	THR	3.3
1	B	298	SER	3.3
1	B	238	PRO	3.2
1	A	445	PRO	3.0
1	B	277	TRP	3.0
1	B	321	CYS	2.9
1	A	446	GLY	2.9
1	A	270	ASP	2.8
1	B	271	PRO	2.8
1	B	305	VAL	2.7
1	B	322	LYS	2.7
1	A	262	VAL	2.7
1	A	265	ASP	2.7
1	B	295	GLN	2.4
1	A	299	THR	2.3
1	A	272	GLU	2.3
1	A	254	SER	2.2
1	B	356	ASP	2.2
1	B	263	VAL	2.2
1	B	318	GLU	2.2
1	A	273	VAL	2.2
1	B	319	TYR	2.1
1	B	297	ASN	2.1
1	B	237	GLY	2.1
1	B	435	LYS	2.1
1	B	434	ASN	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)

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(Å²)	Q<0.9
5	GAL	A	506	11/12	0.83	0.37	6.64	48,51,53,53	11
5	NAG	A	505	14/15	0.94	0.20	-0.04	59,62,67,68	0
7	NAG	B	508	14/15	0.82	0.20	-	78,83,84,85	0
7	MAN	B	507	11/12	0.93	0.14	-	79,79,79,80	0

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(Å²)	Q<0.9
6	GAL	B	506	11/12	0.67	0.44	4.07	54,56,57,57	11
2	NAG	B	505	14/15	0.89	0.19	-0.57	60,64,66,66	0
2	NAG	A	501	14/15	0.90	0.14	-	59,60,62,62	0
2	NAG	B	501	14/15	0.51	0.43	-	144,146,147,147	0
4	MAN	B	504	11/12	0.84	0.18	-	68,70,72,73	0
2	NAG	A	502	14/15	0.89	0.21	-	59,62,68,68	0
3	GOL	A	509	6/6	0.81	0.17	-	59,62,63,64	0
2	NAG	B	502	14/15	0.40	0.46	-	147,149,149,150	0
4	MAN	A	503	11/12	0.87	0.26	-	59,60,62,63	0
2	NAG	A	508	14/15	0.75	0.19	-	84,86,87,88	0
4	MAN	A	507	11/12	0.84	0.23	-	73,74,75,76	0
3	GOL	B	509	6/6	0.83	0.18	-	66,67,68,69	0
3	GOL	A	510	6/6	0.80	0.29	-	79,80,80,80	0
4	MAN	A	504	11/12	0.90	0.15	-	67,68,70,71	0
4	MAN	B	503	11/12	0.58	0.32	-	128,129,129,129	0

6.5 Other polymers (i)

There are no such residues in this entry.