



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:13 am GMT

PDB ID : 3V95
Title : Crystal structure of monoclonal human anti-rhesus D Fc and IgG1 t125(yb2/0) in the presence of EDTA
Authors : Menez, R.; A Stura, E.; Bourel, D.; Siberil, S.; Jorieux, S.; De Romeuf, C.; Ducancel, F.; Fridman, W.H.; Teillaud, J.L.
Deposited on : 2011-12-23
Resolution : 2.70 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

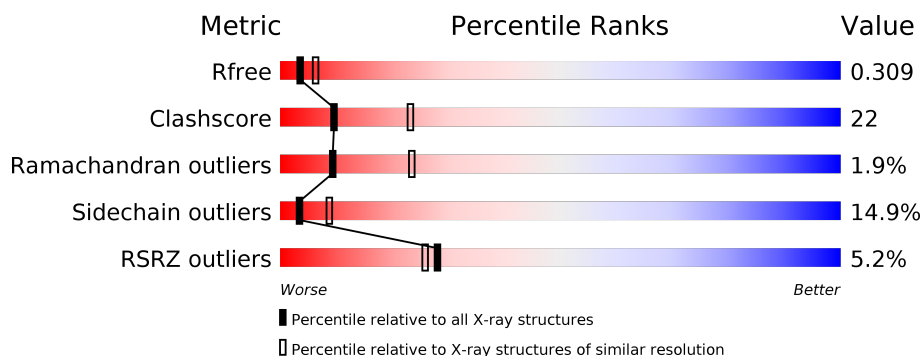
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	212	<div> <div></div> <div>62%</div> <div>28%</div> <div>10%</div> </div>
1	B	212	<div> <div>9%</div> <div>53%</div> <div>35%</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	GAL	A	506	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3676 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.

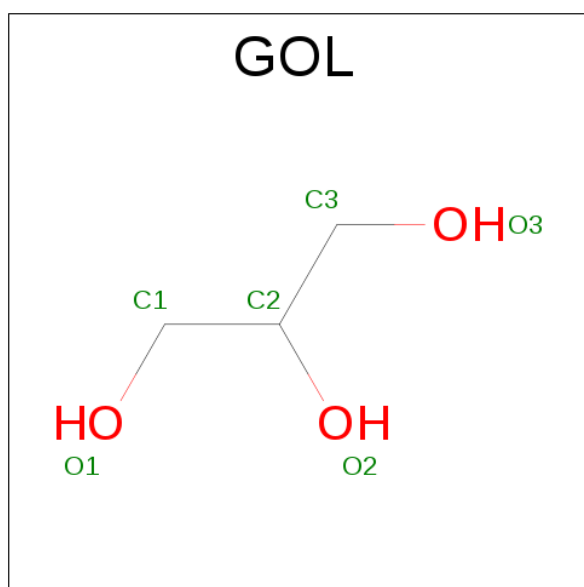
- Molecule 1 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1689	1074	285	324	6			
1	B	209	Total	C	N	O	S	0	0	0
			1667	1062	280	319	6			

- Molecule 2 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	8	Total	C	N	O	0	0
			100	56	4	40		
2	B	8	Total	C	N	O	0	0
			100	56	4	40		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

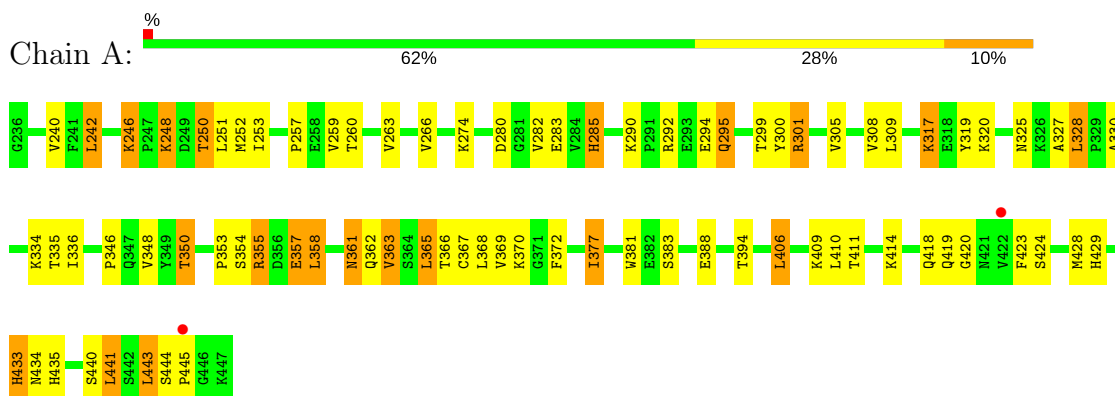
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		
4	B	51	Total	O	0	0
			51	51		

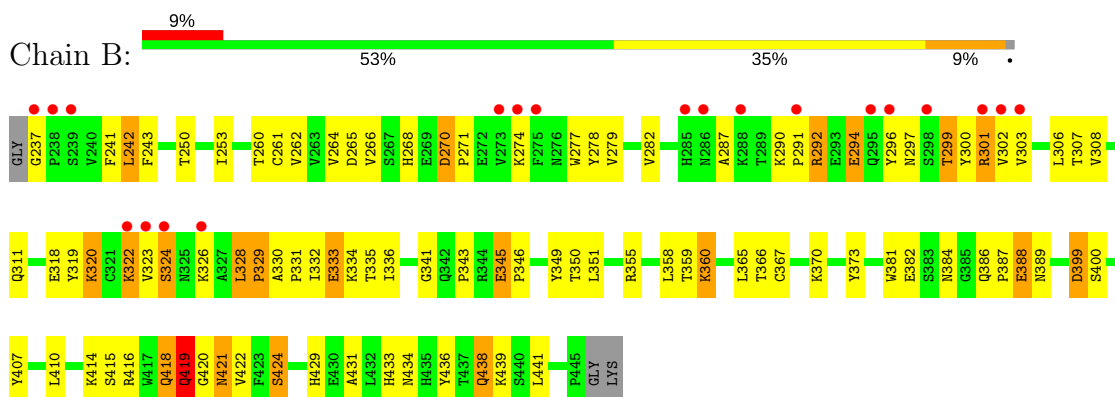
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 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	49.38Å 79.12Å 138.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.89 – 2.70 40.25 – 2.69	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.89-2.70) 99.4 (40.25-2.69)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.251 , 0.321 0.249 , 0.309	Depositor DCC
R_{free} test set	779 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3676	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.65	0/1736	0.74	0/2363
1	B	0.70	0/1714	0.74	0/2337
All	All	0.68	0/3450	0.74	0/4700

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1689	0	1656	64	0
1	B	1667	0	1631	92	0
2	A	100	0	85	7	0
2	B	100	0	85	7	0
3	A	12	0	16	1	0
4	A	57	0	0	4	0
4	B	51	0	0	2	0
All	All	3676	0	3473	152	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 22.

All (152) 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:330:ALA:HB1	1:B:331:PRO:HD2	1.33	1.09
1:A:428:MET:HB2	1:A:435:HIS:O	1.70	0.92
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.53	0.91
1:B:237:GLY:HA2	1:B:328:LEU:HD12	1.54	0.90
1:B:328:LEU:HB2	1:B:329:PRO:HD2	1.54	0.89
1:A:253:ILE:HD12	1:A:253:ILE:H	1.43	0.81
1:B:264:VAL:HG12	1:B:265:ASP:N	1.96	0.81
1:B:241:PHE:CE1	2:B:502:NAG:H62	2.17	0.80
1:A:443:LEU:H	1:A:443:LEU:HD12	1.46	0.79
1:A:350:THR:HB	1:A:441:LEU:HD13	1.64	0.78
1:B:264:VAL:HG12	1:B:265:ASP:H	1.48	0.75
1:B:419:GLN:HA	1:B:419:GLN:HE21	1.51	0.75
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.24	0.72
1:B:328:LEU:CB	1:B:329:PRO:HD2	2.18	0.72
1:A:409:LYS:HE2	4:A:646:HOH:O	1.89	0.72
1:A:295:GLN:HE21	2:A:501:NAG:H62	1.55	0.72
1:B:301:ARG:HG3	1:B:301:ARG:HH11	1.53	0.72
1:B:264:VAL:CG1	1:B:265:ASP:H	2.02	0.71
1:B:241:PHE:HE1	2:B:502:NAG:H62	1.53	0.71
1:B:237:GLY:CA	1:B:328:LEU:HD12	2.21	0.70
1:B:323:VAL:HG22	1:B:332:ILE:HB	1.74	0.70
1:A:285:HIS:ND1	4:A:655:HOH:O	2.24	0.70
1:A:420:GLY:HA2	1:A:443:LEU:HD11	1.74	0.69
1:B:330:ALA:HB1	1:B:331:PRO:CD	2.17	0.69
1:B:328:LEU:CB	1:B:329:PRO:CD	2.71	0.69
1:A:369:VAL:HB	1:A:406:LEU:HD22	1.75	0.69
1:B:243:PHE:HE2	1:B:262:VAL:CG1	2.06	0.68
1:B:333:GLU:O	1:B:334:LYS:HG2	1.92	0.68
1:B:414:LYS:O	1:B:418:GLN:HG2	1.94	0.67
1:A:420:GLY:HA2	1:A:443:LEU:CD1	2.24	0.67
1:A:361:ASN:HD22	1:A:361:ASN:N	1.92	0.67
1:B:265:ASP:OD2	2:B:501:NAG:H83	1.95	0.67
1:A:253:ILE:CD1	1:A:253:ILE:H	2.07	0.66
1:A:325:ASN:OD1	1:A:327:ALA:HB3	1.96	0.66
1:A:354:SER:HB2	1:B:349:TYR:HB3	1.78	0.66
1:A:357:GLU:HG3	1:B:349:TYR:CZ	2.32	0.65
1:B:350:THR:HB	1:B:441:LEU:HD22	1.79	0.64
1:B:268:HIS:O	1:B:271:PRO:HD3	1.98	0.64
1:B:311:GLN:HA	1:B:311:GLN:NE2	2.12	0.64
1:A:346:PRO:HG3	1:A:372:PHE:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:TYR:OH	1:B:438:GLN:NE2	2.33	0.62
1:B:419:GLN:CA	1:B:419:GLN:HE21	2.12	0.62
1:B:287:ALA:HB2	1:B:306:LEU:HD12	1.80	0.62
1:B:297:ASN:OD1	1:B:299:THR:HB	1.98	0.62
1:A:361:ASN:ND2	4:A:602:HOH:O	2.32	0.61
1:B:243:PHE:CE2	1:B:262:VAL:CG1	2.83	0.61
1:A:295:GLN:NE2	1:A:301:ARG:HG2	2.16	0.61
1:B:388:GLU:OE2	1:B:416:ARG:NH1	2.33	0.60
1:A:369:VAL:HB	1:A:406:LEU:CD2	2.33	0.58
1:A:253:ILE:HD12	1:A:253:ILE:N	2.16	0.58
1:B:382:GLU:HA	1:B:388:GLU:H	1.69	0.57
1:B:266:VAL:HG13	1:B:300:TYR:HB2	1.85	0.57
1:B:294:GLU:HA	1:B:300:TYR:HA	1.87	0.56
1:B:301:ARG:HG3	1:B:301:ARG:NH1	2.15	0.56
1:B:290:LYS:HD3	1:B:303:VAL:HB	1.88	0.56
1:A:283:GLU:HG2	4:A:655:HOH:O	2.05	0.55
1:B:270:ASP:N	1:B:271:PRO:HD3	2.23	0.54
1:B:274:LYS:HB3	1:B:324:SER:HB2	1.89	0.54
1:B:323:VAL:O	1:B:323:VAL:HG23	2.07	0.53
1:A:357:GLU:HG3	1:B:349:TYR:CE2	2.44	0.53
1:B:333:GLU:O	1:B:334:LYS:CG	2.56	0.53
1:A:250:THR:HG22	1:A:251:LEU:HG	1.91	0.53
1:A:355:ARG:O	1:A:358:LEU:HD22	2.08	0.53
1:B:241:PHE:CZ	2:B:502:NAG:H62	2.44	0.53
1:B:330:ALA:CB	1:B:331:PRO:HD2	2.22	0.52
1:B:433:HIS:O	1:B:434:ASN:HB2	2.10	0.52
2:A:508:NAG:H82	2:A:508:NAG:C1	2.40	0.52
1:B:264:VAL:CG1	1:B:265:ASP:N	2.59	0.51
1:A:246:LYS:HB2	2:A:506:GAL:H61	1.92	0.51
1:B:301:ARG:CG	1:B:301:ARG:HH11	2.23	0.51
1:B:242:LEU:HD23	1:B:260:THR:O	2.10	0.51
1:B:264:VAL:HG11	2:B:502:NAG:O5	2.11	0.51
1:B:311:GLN:HA	1:B:311:GLN:HE21	1.76	0.50
1:A:424:SER:HA	1:A:440:SER:HA	1.93	0.50
1:B:311:GLN:CA	1:B:311:GLN:HE21	2.24	0.50
1:B:262:VAL:HG21	1:B:301:ARG:NH1	2.27	0.49
1:A:246:LYS:HD2	2:A:506:GAL:H61	1.94	0.49
1:A:266:VAL:O	1:A:300:TYR:HB2	2.13	0.49
1:B:355:ARG:O	1:B:358:LEU:HB2	2.13	0.48
1:B:359:THR:O	1:B:360:LYS:HG2	2.14	0.48
1:A:414:LYS:O	1:A:418:GLN:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:SER:HB2	1:A:423:PHE:CD2	2.48	0.48
1:B:242:LEU:HD13	1:B:336:ILE:HB	1.95	0.48
1:A:320:LYS:HE3	3:A:510:GOL:H2	1.96	0.47
1:A:242:LEU:HD13	1:A:336:ILE:HB	1.95	0.47
1:A:406:LEU:C	1:A:406:LEU:HD23	2.34	0.47
1:B:268:HIS:O	1:B:271:PRO:CD	2.62	0.47
2:A:508:NAG:C8	2:A:508:NAG:C1	2.92	0.47
1:A:424:SER:HB3	1:A:440:SER:HB3	1.96	0.47
1:A:358:LEU:O	1:A:414:LYS:NZ	2.46	0.47
1:B:311:GLN:CA	1:B:311:GLN:NE2	2.77	0.47
1:A:361:ASN:ND2	1:A:361:ASN:N	2.62	0.47
1:B:290:LYS:HG2	1:B:291:PRO:O	2.16	0.46
1:B:320:LYS:HD2	1:B:320:LYS:N	2.30	0.46
1:B:306:LEU:HD23	1:B:308:VAL:HG22	1.98	0.46
1:A:363:VAL:HG22	1:A:414:LYS:HA	1.98	0.45
1:B:266:VAL:HG13	1:B:300:TYR:CB	2.46	0.45
1:B:278:TYR:HB2	1:B:320:LYS:HD3	1.98	0.45
1:B:429:HIS:CD2	1:B:431:ALA:H	2.34	0.45
1:A:444:SER:N	1:A:445:PRO:HD3	2.32	0.45
1:B:345:GLU:HA	1:B:346:PRO:HD3	1.88	0.45
1:B:359:THR:C	1:B:360:LYS:HG2	2.37	0.45
1:B:355:ARG:HA	1:B:358:LEU:HD12	1.98	0.45
1:B:420:GLY:O	1:B:421:ASN:C	2.55	0.45
1:A:366:THR:OG1	1:B:407:TYR:OH	2.23	0.44
1:B:301:ARG:HH22	2:B:502:NAG:H2	1.82	0.44
1:B:243:PHE:HE2	1:B:262:VAL:HG13	1.80	0.44
1:B:301:ARG:NH2	2:B:502:NAG:H2	2.33	0.44
1:A:246:LYS:HD2	2:A:506:GAL:C6	2.47	0.44
1:A:308:VAL:HG22	1:A:319:TYR:CE2	2.52	0.44
1:B:261:CYS:HB2	1:B:277:TRP:CZ2	2.53	0.44
1:B:381:TRP:HA	1:B:424:SER:O	2.18	0.44
1:A:257:PRO:HG2	1:A:308:VAL:O	2.18	0.44
1:A:388:GLU:OE2	1:A:388:GLU:HA	2.17	0.43
1:B:328:LEU:HB3	1:B:329:PRO:CD	2.46	0.43
1:A:274:LYS:HE3	1:A:274:LYS:HB3	1.76	0.43
1:A:259:VAL:HG23	1:A:308:VAL:HG21	1.99	0.43
1:A:248:LYS:O	1:A:252:MET:HG3	2.18	0.43
1:A:294:GLU:HB2	1:A:300:TYR:CE1	2.54	0.43
1:A:319:TYR:O	1:A:335:THR:HA	2.19	0.43
1:A:363:VAL:O	1:A:411:THR:HA	2.19	0.42
1:A:388:GLU:HB3	1:A:410:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LYS:NZ	1:B:399:ASP:OD1	2.50	0.42
1:B:418:GLN:O	1:B:419:GLN:C	2.57	0.42
1:A:377:ILE:HG13	1:A:429:HIS:HB2	2.02	0.42
1:A:368:LEU:HD12	1:A:369:VAL:N	2.35	0.42
1:B:241:PHE:HB2	1:B:262:VAL:HG13	2.01	0.42
1:A:260:THR:HG23	1:A:305:VAL:HG22	2.02	0.42
1:A:328:LEU:HD13	1:A:330:ALA:O	2.19	0.42
1:A:353:PRO:HD3	1:A:365:LEU:HD12	2.02	0.42
1:B:292:ARG:HB3	1:B:302:VAL:HG22	2.02	0.42
1:B:360:LYS:NZ	4:B:615:HOH:O	2.51	0.42
1:A:348:VAL:HG12	1:A:348:VAL:O	2.19	0.42
1:A:246:LYS:H	2:A:506:GAL:C6	2.33	0.41
1:B:341:GLY:O	1:B:343:PRO:HD3	2.20	0.41
1:B:351:LEU:HD12	1:B:366:THR:HG21	2.01	0.41
1:B:266:VAL:CG2	1:B:271:PRO:HB3	2.50	0.41
1:B:278:TYR:HA	1:B:282:VAL:O	2.19	0.41
1:A:280:ASP:OD1	1:A:317:LYS:HG3	2.20	0.41
1:B:308:VAL:HG13	1:B:319:TYR:OH	2.20	0.41
1:A:354:SER:CB	1:B:349:TYR:HB3	2.50	0.41
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.56	0.41
1:B:386:GLN:HA	1:B:387:PRO:HD3	1.90	0.41
1:A:433:HIS:O	1:A:434:ASN:HB2	2.21	0.41
1:B:278:TYR:O	1:B:320:LYS:HD2	2.21	0.41
1:B:343:PRO:HA	1:B:373:TYR:O	2.21	0.41
1:A:370:LYS:HE3	1:A:370:LYS:HB2	1.76	0.40
1:B:415:SER:O	1:B:419:GLN:HG2	2.21	0.40
1:A:240:VAL:HG22	1:A:263:VAL:HG13	2.02	0.40
1:B:360:LYS:O	1:B:414:LYS:HD3	2.21	0.40
1:B:320:LYS:H	1:B:320:LYS:HD2	1.87	0.40
1:B:322:LYS:NZ	4:B:642:HOH:O	2.54	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	210/212 (99%)	200 (95%)	7 (3%)	3 (1%)	13	33
1	B	207/212 (98%)	180 (87%)	22 (11%)	5 (2%)	7	17
All	All	417/424 (98%)	380 (91%)	29 (7%)	8 (2%)	9	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	324	SER
1	A	292	ARG
1	A	419	GLN
1	B	421	ASN
1	B	419	GLN
1	A	377	ILE
1	B	270	ASP
1	B	329	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/196 (100%)	169 (86%)	27 (14%)	4	10
1	B	194/196 (99%)	163 (84%)	31 (16%)	3	7
All	All	390/392 (100%)	332 (85%)	58 (15%)	3	9

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	LEU
1	A	246	LYS
1	A	248	LYS
1	A	250	THR
1	A	282	VAL

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Mol	Chain	Res	Type
1	A	285	HIS
1	A	290	LYS
1	A	295	GLN
1	A	299	THR
1	A	301	ARG
1	A	309	LEU
1	A	317	LYS
1	A	328	LEU
1	A	334	LYS
1	A	350	THR
1	A	355	ARG
1	A	357	GLU
1	A	358	LEU
1	A	361	ASN
1	A	362	GLN
1	A	363	VAL
1	A	365	LEU
1	A	394	THR
1	A	406	LEU
1	A	433	HIS
1	A	441	LEU
1	A	443	LEU
1	B	242	LEU
1	B	250	THR
1	B	253	ILE
1	B	279	VAL
1	B	292	ARG
1	B	294	GLU
1	B	296	TYR
1	B	299	THR
1	B	301	ARG
1	B	307	THR
1	B	318	GLU
1	B	320	LYS
1	B	322	LYS
1	B	326	LYS
1	B	328	LEU
1	B	333	GLU
1	B	335	THR
1	B	345	GLU
1	B	360	LYS
1	B	370	LYS

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Mol	Chain	Res	Type
1	B	384	ASN
1	B	388	GLU
1	B	389	ASN
1	B	399	ASP
1	B	400	SER
1	B	418	GLN
1	B	419	GLN
1	B	422	VAL
1	B	424	SER
1	B	438	GLN
1	B	439	LYS

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	421	ASN
1	B	285	HIS
1	B	311	GLN
1	B	362	GLN
1	B	390	ASN
1	B	419	GLN
1	B	429	HIS
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](#)

16 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	$\# Z > 2$
2	NAG	A	501	1,2	14,14,15	0.52	0	15,19,21	1.37	1 (6%)
2	NAG	A	502	2	14,14,15	0.74	0	15,19,21	1.91	6 (40%)
2	MAN	A	503	2	11,11,12	0.78	0	13,15,17	2.91	4 (30%)
2	MAN	A	504	2	11,11,12	0.70	0	13,15,17	1.07	1 (7%)
2	NAG	A	505	2	14,14,15	0.47	0	15,19,21	1.21	1 (6%)
2	GAL	A	506	2	11,11,12	0.49	0	13,15,17	2.79	6 (46%)
2	MAN	A	507	2	11,11,12	0.66	0	13,15,17	2.24	8 (61%)
2	NAG	A	508	2	14,14,15	0.48	0	15,19,21	2.40	5 (33%)
2	NAG	B	501	1,2	14,14,15	0.66	0	15,19,21	1.35	2 (13%)
2	NAG	B	502	2	14,14,15	0.78	0	15,19,21	1.64	3 (20%)
2	MAN	B	503	2	11,11,12	0.56	0	13,15,17	1.83	4 (30%)
2	MAN	B	504	2	11,11,12	0.58	0	13,15,17	2.93	2 (15%)
2	NAG	B	505	2	14,14,15	0.47	0	15,19,21	2.96	6 (40%)
2	GAL	B	506	2	11,11,12	0.68	0	13,15,17	1.33	2 (15%)
2	MAN	B	507	2	11,11,12	0.77	0	13,15,17	1.50	3 (23%)
2	NAG	B	508	2	14,14,15	0.71	0	15,19,21	1.29	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
2	NAG	A	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
2	MAN	A	503	2	-	0/2/19/22	0/1/1/1
2	MAN	A	504	2	-	0/2/19/22	0/1/1/1
2	NAG	A	505	2	-	0/6/23/26	0/1/1/1
2	GAL	A	506	2	-	0/2/19/22	0/1/1/1
2	MAN	A	507	2	-	0/2/19/22	0/1/1/1
2	NAG	A	508	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	502	2	-	0/6/23/26	0/1/1/1
2	MAN	B	503	2	-	0/2/19/22	0/1/1/1
2	MAN	B	504	2	-	0/2/19/22	0/1/1/1
2	NAG	B	505	2	-	0/6/23/26	0/1/1/1
2	GAL	B	506	2	-	0/2/19/22	0/1/1/1
2	MAN	B	507	2	-	0/2/19/22	0/1/1/1
2	NAG	B	508	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	506	GAL	C1-C2-C3	-3.96	104.64	109.65
2	A	506	GAL	O3-C3-C4	-3.82	102.04	110.36
2	B	505	NAG	C4-C3-C2	-3.46	105.94	111.02
2	A	507	MAN	C1-C2-C3	-3.34	105.41	109.65
2	A	507	MAN	O2-C2-C1	-2.74	103.61	109.18
2	A	507	MAN	C2-C3-C4	-2.61	106.33	110.88
2	A	502	NAG	C1-C2-N2	-2.48	106.25	110.49
2	B	505	NAG	O4-C4-C3	-2.48	104.97	110.36
2	B	502	NAG	O3-C3-C4	-2.45	105.02	110.36
2	B	508	NAG	C3-C4-C5	-2.43	105.94	110.22
2	A	506	GAL	O4-C4-C3	-2.42	105.09	110.36
2	A	502	NAG	C2-N2-C7	-2.42	119.42	122.94
2	A	502	NAG	O3-C3-C2	-2.39	104.28	109.39
2	A	508	NAG	C4-C3-C2	-2.33	107.60	111.02
2	B	503	MAN	C6-C5-C4	-2.32	107.57	113.00
2	A	506	GAL	C6-C5-C4	-2.24	107.76	113.00
2	A	502	NAG	C4-C3-C2	-2.23	107.75	111.02
2	A	507	MAN	C3-C4-C5	-2.13	106.47	110.22
2	A	503	MAN	C6-C5-C4	-2.09	108.11	113.00
2	B	503	MAN	O3-C3-C2	-2.04	106.31	110.02
2	A	502	NAG	C1-O5-C5	2.11	115.08	112.17
2	B	505	NAG	O3-C3-C2	2.13	113.96	109.39
2	A	507	MAN	O3-C3-C4	2.22	115.19	110.36
2	A	503	MAN	O5-C1-C2	2.26	114.34	110.79
2	A	507	MAN	O4-C4-C5	2.29	115.05	109.28
2	B	507	MAN	O2-C2-C1	2.30	113.84	109.18
2	A	505	NAG	C1-O5-C5	2.33	115.38	112.17
2	B	505	NAG	C1-C2-N2	2.44	114.65	110.49
2	A	507	MAN	C1-O5-C5	2.44	115.53	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	507	MAN	C1-C2-C3	2.48	112.79	109.65
2	A	508	NAG	C8-C7-N2	2.52	120.65	116.11
2	B	501	NAG	C1-O5-C5	2.52	115.64	112.17
2	A	506	GAL	O2-C2-C3	2.54	115.16	110.17
2	A	508	NAG	O5-C1-C2	2.61	115.10	111.47
2	B	506	GAL	C1-O5-C5	2.64	115.80	112.17
2	B	506	GAL	C1-C2-C3	2.77	113.16	109.65
2	B	501	NAG	C4-C3-C2	2.87	115.23	111.02
2	B	507	MAN	O2-C2-C3	2.94	115.95	110.17
2	A	504	MAN	C1-O5-C5	3.11	116.45	112.17
2	B	508	NAG	C1-O5-C5	3.18	116.56	112.17
2	A	507	MAN	O3-C3-C2	3.29	116.01	110.02
2	B	504	MAN	O5-C1-C2	3.33	116.00	110.79
2	B	502	NAG	O4-C4-C3	3.41	117.77	110.36
2	B	503	MAN	C1-C2-C3	3.71	114.35	109.65
2	A	501	NAG	C1-C2-N2	3.75	116.89	110.49
2	B	502	NAG	C4-C3-C2	3.96	116.82	111.02
2	B	503	MAN	C1-O5-C5	4.10	117.82	112.17
2	A	502	NAG	O4-C4-C3	4.56	120.29	110.36
2	B	505	NAG	C2-N2-C7	4.64	129.72	122.94
2	A	503	MAN	C1-C2-C3	4.76	115.68	109.65
2	A	508	NAG	C2-N2-C7	4.79	129.94	122.94
2	A	508	NAG	C1-O5-C5	6.23	120.76	112.17
2	A	506	GAL	C1-O5-C5	7.03	121.86	112.17
2	A	503	MAN	C1-O5-C5	8.21	123.48	112.17
2	B	505	NAG	C1-O5-C5	8.29	123.59	112.17
2	B	504	MAN	C1-O5-C5	9.30	124.99	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	1	0
2	A	506	GAL	4	0
2	A	508	NAG	2	0
2	B	501	NAG	1	0
2	B	502	NAG	6	0

5.6 Ligand geometry

2 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	$\# Z > 2$
3	GOL	A	509	-	5,5,5	0.38	0	5,5,5	0.26	0
3	GOL	A	510	-	5,5,5	0.44	0	5,5,5	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	509	-	-	0/4/4/4	0/0/0/0
3	GOL	A	510	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	510	GOL	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	212/212 (100%)	-0.03	2 (0%) 84 85	11, 31, 52, 78	1 (0%)
1	B	209/212 (98%)	0.40	20 (9%) 9 6	11, 43, 75, 86	1 (0%)
All	All	421/424 (99%)	0.18	22 (5%) 28 26	11, 34, 73, 86	2 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	GLY	4.7
1	B	239	SER	4.0
1	B	323	VAL	3.8
1	A	445	PRO	3.6
1	B	295	GLN	3.4
1	B	273	VAL	3.3
1	B	326	LYS	3.2
1	B	238	PRO	3.1
1	A	422	VAL	2.6
1	B	296	TYR	2.6
1	B	298	SER	2.6
1	B	324	SER	2.5
1	B	302	VAL	2.4
1	B	303	VAL	2.2
1	B	285	HIS	2.2
1	B	301	ARG	2.2
1	B	288	LYS	2.2
1	B	286	ASN	2.1
1	B	291	PRO	2.0
1	B	274	LYS	2.0
1	B	275	PHE	2.0
1	B	322	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

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(Å ²)	Q<0.9
2	GAL	A	506	11/12	0.76	0.29	4.88	34,36,37,37	11
2	GAL	B	506	11/12	0.90	0.29	1.83	42,45,46,46	11
2	NAG	B	505	14/15	0.91	0.20	0.01	47,51,55,56	0
2	NAG	B	501	14/15	0.64	0.24	-0.71	79,82,83,83	0
2	NAG	A	505	14/15	0.94	0.13	-0.96	34,37,44,44	0
2	MAN	B	507	11/12	0.83	0.21	-	73,73,74,75	0
2	MAN	B	504	11/12	0.91	0.17	-	52,54,55,56	0
2	NAG	A	508	14/15	0.85	0.18	-	58,61,63,64	0
2	NAG	B	508	14/15	0.81	0.23	-	75,76,78,78	0
2	MAN	A	504	11/12	0.94	0.14	-	33,35,36,36	0
2	NAG	B	502	14/15	0.67	0.30	-	78,82,82,82	0
2	NAG	A	502	14/15	0.93	0.18	-	29,31,34,34	0
2	MAN	A	503	11/12	0.94	0.14	-	34,35,41,42	0
2	MAN	A	507	11/12	0.87	0.16	-	43,44,47,53	0
2	MAN	B	503	11/12	0.83	0.23	-	60,71,73,74	0
2	NAG	A	501	14/15	0.94	0.12	-	23,27,29,29	0

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
3	GOL	A	510	6/6	0.80	0.19	-	48,49,50,50	0
3	GOL	A	509	6/6	0.66	0.23	-	89,90,90,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.