



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2017 – 02:21 AM EST

PDB ID : 5Y56
Title : Fc mutant (K392D/K409D/D399K)
Authors : Ye, S.; Xu, T.; Yu, J.; Wang, X.; Xu, T.; Jin, Q.; Duan, J.; Wu, J.; Wu, H.
Deposited on : unknown
Resolution : 2.65 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 : rb-20030345
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) : rb-20030345

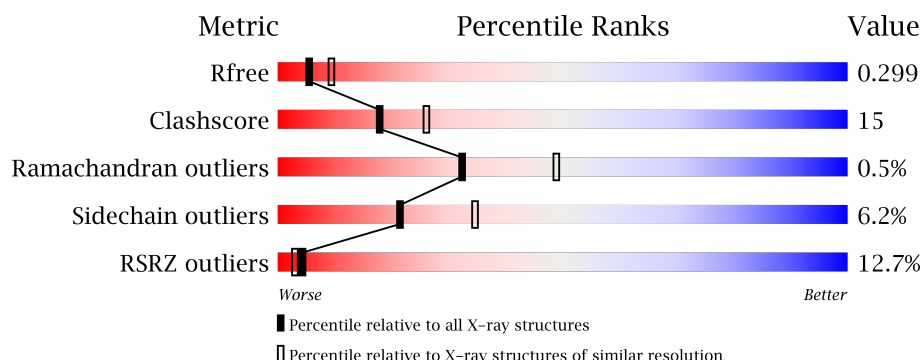
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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>3%</div> <div>73%</div> <div>25%</div> <div>.</div> </div>
1	B	208	<div> <div>23%</div> <div>69%</div> <div>25%</div> <div>6%</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
7	GAL	B	506	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 3613 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.

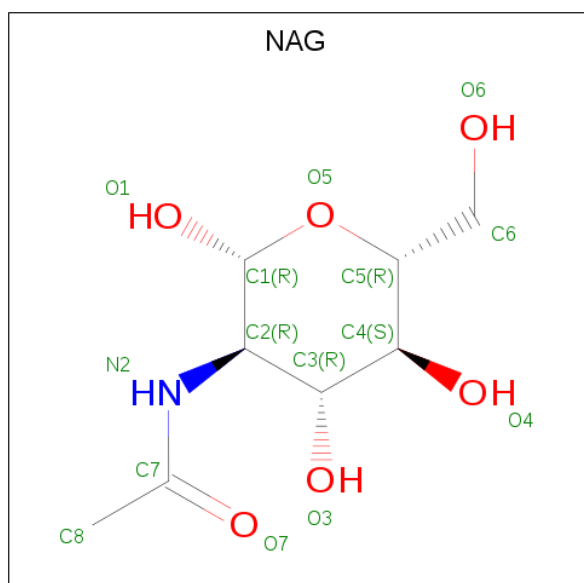
- Molecule 1 is a protein called Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1661	1056	279	320	6			
1	B	208	Total	C	N	O	S	0	0	0
			1661	1056	279	320	6			

There are 6 discrepancies between the modelled and reference sequences:

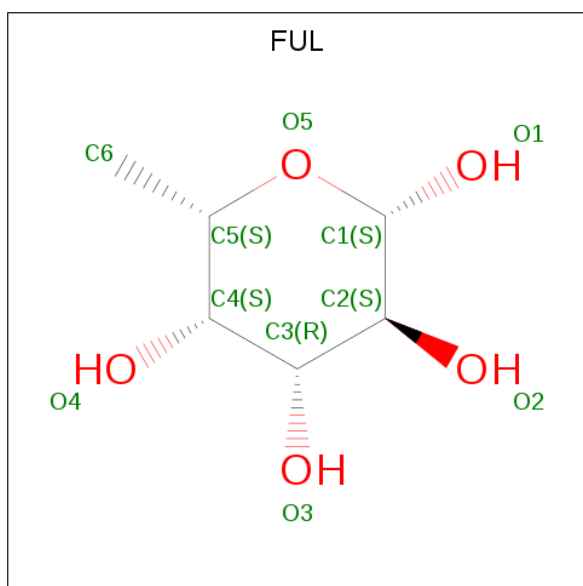
Chain	Residue	Modelled	Actual	Comment	Reference
A	392	ASP	LYS	engineered mutation	UNP P0DOX5
A	399	LYS	ASP	engineered mutation	UNP P0DOX5
A	409	ASP	LYS	engineered mutation	UNP P0DOX5
B	392	ASP	LYS	engineered mutation	UNP P0DOX5
B	399	LYS	ASP	engineered mutation	UNP P0DOX5
B	409	ASP	LYS	engineered mutation	UNP P0DOX5

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



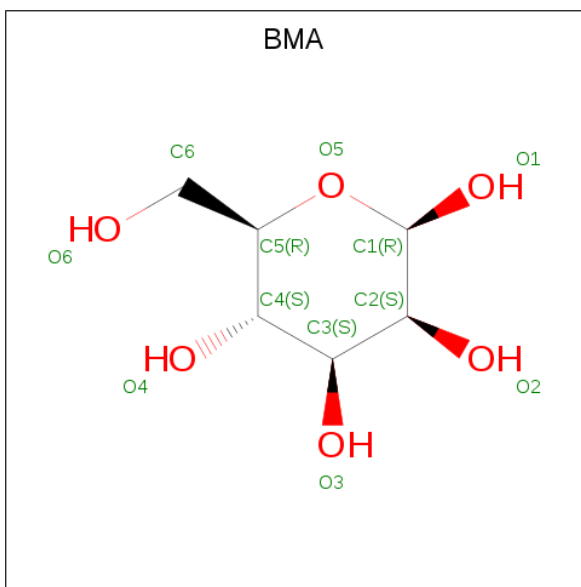
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-L-FUCOSE (three-letter code: FUL) (formula: $C_6H_{12}O_5$).



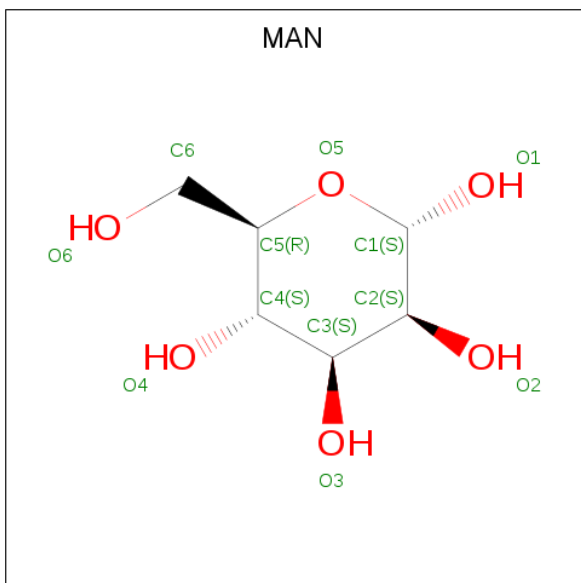
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

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



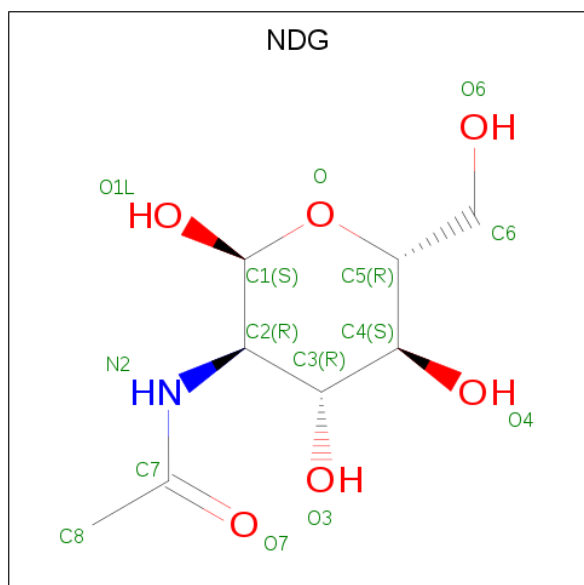
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



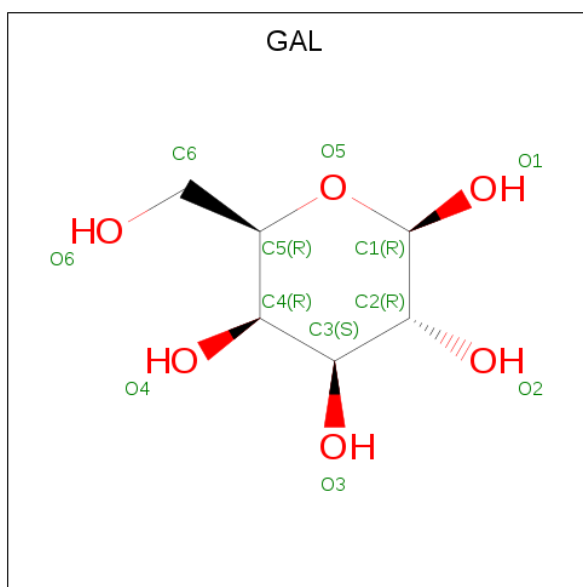
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is 2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



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

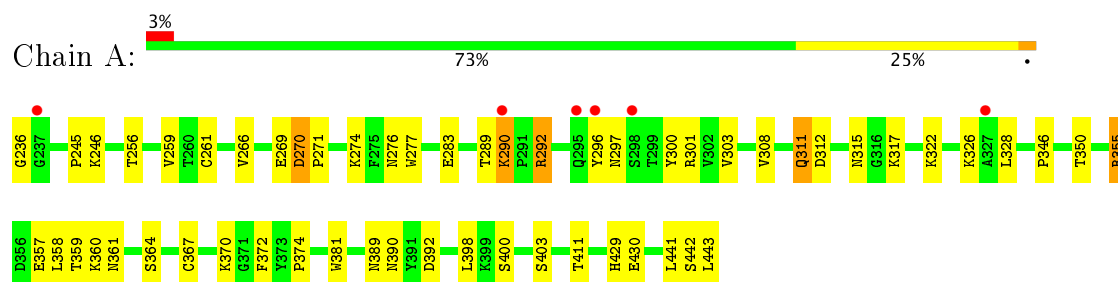
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	59	Total	O	0	0
			59	59		
8	B	36	Total	O	0	0
			36	36		

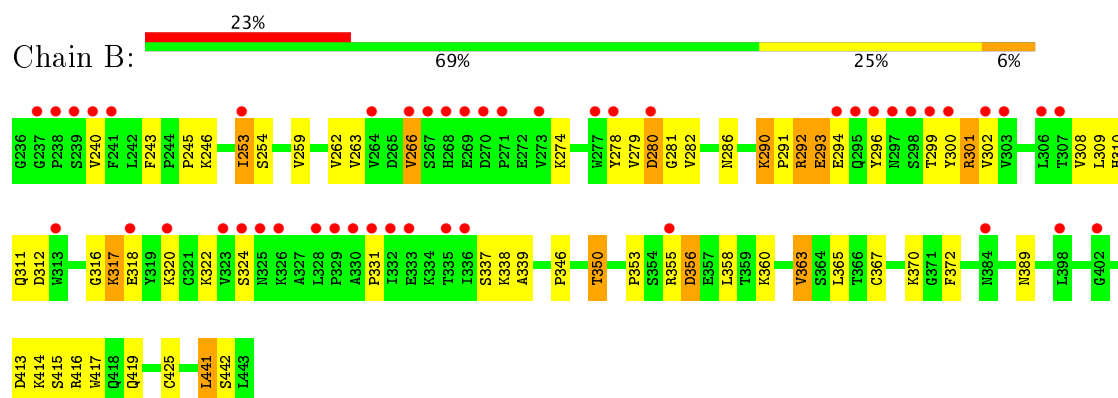
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Immunoglobulin gamma-1 heavy chain



- Molecule 1: Immunoglobulin gamma-1 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	65.13Å 65.13Å 477.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.45 – 2.65 36.45 – 2.65	Depositor EDS
% Data completeness (in resolution range)	96.1 (36.45-2.65) 96.1 (36.45-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.260 , 0.298 0.259 , 0.299	Depositor DCC
R_{free} test set	1803 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	85.2	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3613	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, NDG, GAL, FUL, 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	0.45	0/1707	0.62	1/2327 (0.0%)
1	B	0.39	0/1707	0.57	0/2327
All	All	0.42	0/3414	0.59	1/4654 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	LEU	CA-CB-CG	5.12	127.07	115.30

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	1661	0	1619	47	1
1	B	1661	0	1619	54	2
2	A	42	0	36	0	0
2	B	28	0	24	1	1
3	A	10	0	10	3	0
4	A	22	0	17	0	0
4	B	22	0	18	1	0
5	A	11	0	9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	11	0	9	1	0
6	A	14	0	12	1	0
6	B	14	0	12	1	0
7	A	11	0	10	4	0
7	B	11	0	10	4	0
8	A	59	0	0	18	1
8	B	36	0	0	16	0
All	All	3613	0	3405	105	3

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 15.

All (105) 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:370:LYS:NZ	8:A:601:HOH:O	1.91	1.02
1:B:367:CYS:SG	8:B:634:HOH:O	2.20	0.99
1:A:271:PRO:O	8:A:602:HOH:O	1.91	0.88
1:B:274:LYS:NZ	8:B:602:HOH:O	1.97	0.84
1:A:276:ASN:OD1	8:A:603:HOH:O	1.99	0.80
1:B:360:LYS:O	1:B:414:LYS:NZ	2.16	0.77
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.67	0.75
1:A:283:GLU:OE1	8:A:604:HOH:O	2.05	0.74
4:B:507:BMA:O2	8:B:603:HOH:O	2.06	0.72
1:B:322:LYS:HZ3	1:B:331:PRO:HB3	1.55	0.71
1:B:311:GLN:OE1	8:B:604:HOH:O	2.07	0.71
1:B:240:VAL:HG22	1:B:263:VAL:HG22	1.72	0.71
1:B:292:ARG:HG3	1:B:302:VAL:HG22	1.73	0.71
1:A:236:GLY:O	8:A:605:HOH:O	2.09	0.70
1:B:350:THR:HB	1:B:441:LEU:CD2	2.22	0.70
1:B:290:LYS:HG3	1:B:291:PRO:HD2	1.74	0.69
1:A:256:THR:OG1	8:A:606:HOH:O	2.10	0.69
1:B:310:HIS:NE2	8:B:607:HOH:O	2.26	0.69
1:B:416:ARG:NH1	1:B:419:GLN:OE1	2.24	0.69
1:A:297:ASN:O	8:A:607:HOH:O	2.11	0.69
1:A:361:ASN:ND2	8:A:614:HOH:O	2.26	0.69
1:A:290:LYS:HD2	1:A:303:VAL:H	1.60	0.67
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.77	0.66
1:B:243:PHE:HE1	5:B:504:MAN:H2	1.60	0.66
1:A:266:VAL:HG23	1:A:300:TYR:HB2	1.76	0.66
1:A:245:PRO:HA	7:A:507:GAL:H61	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:505:NDG:H4	7:B:506:GAL:O2	1.95	0.66
1:B:278:TYR:HB2	1:B:320:LYS:HB3	1.78	0.66
1:B:286:ASN:HA	8:B:616:HOH:O	1.97	0.65
1:A:296:TYR:HA	8:A:621:HOH:O	1.98	0.64
1:B:312:ASP:O	8:B:605:HOH:O	2.14	0.64
1:B:322:LYS:NZ	8:B:610:HOH:O	2.32	0.63
1:B:350:THR:HB	1:B:441:LEU:HG	1.82	0.61
1:A:276:ASN:ND2	8:A:604:HOH:O	2.25	0.61
3:A:502:FUL:O2	8:A:608:HOH:O	2.16	0.61
1:A:355:ARG:NH1	8:A:619:HOH:O	2.33	0.60
6:A:506:NDG:H4	7:A:507:GAL:O2	2.00	0.60
1:B:299:THR:HB	8:B:612:HOH:O	2.02	0.59
1:A:292:ARG:HG3	1:A:300:TYR:CE2	2.38	0.59
1:B:316:GLY:N	8:B:605:HOH:O	2.36	0.58
1:B:293:GLU:HG3	1:B:301:ARG:HB3	1.85	0.58
1:A:290:LYS:NZ	1:A:301:ARG:O	2.37	0.57
1:B:338:LYS:NZ	1:B:339:ALA:O	2.35	0.57
1:A:350:THR:HB	1:A:441:LEU:HD22	1.86	0.56
1:A:359:THR:OG1	8:A:610:HOH:O	2.18	0.56
1:B:246:LYS:HE3	7:B:506:GAL:H3	1.87	0.56
1:B:356:ASP:O	1:B:360:LYS:NZ	2.38	0.55
1:A:357:GLU:OE1	8:A:609:HOH:O	2.17	0.54
1:A:364:SER:O	8:A:611:HOH:O	2.18	0.54
1:A:246:LYS:HG2	7:A:507:GAL:H5	1.90	0.54
1:B:254:SER:N	8:B:601:HOH:O	1.90	0.54
1:B:350:THR:HB	1:B:441:LEU:HD23	1.90	0.53
1:B:350:THR:HB	1:B:441:LEU:CG	2.38	0.53
1:B:353:PRO:HB3	1:B:363:VAL:HG22	1.91	0.53
1:A:357:GLU:C	1:A:359:THR:H	2.12	0.53
1:A:311:GLN:O	1:A:315:ASN:ND2	2.43	0.50
1:A:270:ASP:OD1	1:A:270:ASP:N	2.45	0.50
1:A:322:LYS:NZ	8:A:623:HOH:O	2.37	0.49
1:A:296:TYR:HB2	3:A:502:FUL:H61	1.95	0.49
1:A:346:PRO:CB	1:A:372:PHE:HB3	2.41	0.49
1:B:389:ASN:OD1	1:B:389:ASN:N	2.45	0.49
1:B:417:TRP:CH2	1:B:442:SER:HA	2.48	0.49
1:A:389:ASN:HA	8:A:635:HOH:O	2.13	0.49
1:B:280:ASP:CB	1:B:317:LYS:HE3	2.43	0.49
1:B:280:ASP:HB3	1:B:317:LYS:HE3	1.95	0.48
1:A:312:ASP:HB3	1:A:317:LYS:HD2	1.95	0.48
1:B:294:GLU:HA	1:B:300:TYR:HA	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:PRO:O	1:A:429:HIS:HE1	1.97	0.47
1:B:425:CYS:SG	8:B:634:HOH:O	2.61	0.47
1:B:253:ILE:HG13	1:B:253:ILE:H	1.49	0.47
1:B:246:LYS:HG2	7:B:506:GAL:H5	1.96	0.47
1:B:279:VAL:O	1:B:281:GLY:N	2.47	0.47
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.50	0.47
1:B:360:LYS:HD2	1:B:360:LYS:H	1.81	0.46
1:B:425:CYS:HB2	8:B:634:HOH:O	2.16	0.45
1:A:346:PRO:HD3	1:A:429:HIS:CD2	2.52	0.45
1:B:266:VAL:HG22	1:B:300:TYR:HB2	1.99	0.45
1:A:290:LYS:C	1:A:290:LYS:HD3	2.37	0.45
1:B:355:ARG:HA	1:B:358:LEU:HD12	1.99	0.45
1:B:245:PRO:HA	7:B:506:GAL:H61	2.00	0.44
1:A:259:VAL:HG23	1:A:308:VAL:HG11	2.00	0.44
1:B:259:VAL:HG23	1:B:308:VAL:HG11	2.00	0.44
1:A:360:LYS:HD2	1:A:361:ASN:H	1.83	0.44
1:B:253:ILE:HD12	8:B:601:HOH:O	2.18	0.44
1:B:318:GLU:HG2	1:B:337:SER:HB2	2.00	0.43
1:A:398:LEU:HD12	1:A:403:SER:O	2.19	0.43
1:B:417:TRP:CZ3	1:B:442:SER:HA	2.54	0.43
1:A:296:TYR:HB2	3:A:502:FUL:C6	2.49	0.43
1:B:266:VAL:N	8:B:612:HOH:O	2.33	0.42
1:B:353:PRO:HB3	1:B:363:VAL:CG2	2.49	0.42
1:B:266:VAL:CG2	1:B:300:TYR:HB2	2.48	0.42
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.55	0.42
1:B:365:LEU:HD21	1:B:417:TRP:CZ3	2.55	0.42
1:A:274:LYS:HE2	1:A:274:LYS:HB3	1.73	0.42
1:A:442:SER:O	1:A:443:LEU:HB2	2.19	0.42
1:A:269:GLU:O	1:A:271:PRO:HD3	2.20	0.42
1:B:370:LYS:HE3	1:B:370:LYS:HB2	1.75	0.41
1:B:262:VAL:HG11	2:B:502:NAG:H81	2.01	0.41
1:A:290:LYS:HE3	1:A:303:VAL:HB	2.02	0.41
1:A:370:LYS:HE3	1:A:370:LYS:HB2	1.90	0.41
1:B:322:LYS:NZ	1:B:324:SER:OG	2.53	0.41
1:A:245:PRO:HA	7:A:507:GAL:C6	2.47	0.40
1:A:297:ASN:HB2	8:A:612:HOH:O	2.20	0.40
1:A:390:ASN:OD1	1:A:411:THR:OG1	2.39	0.40
1:B:254:SER:CB	8:B:601:HOH:O	2.69	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:SER:O	1:B:292:ARG:NH1[8_555]	2.06	0.14
1:B:296:TYR:OH	2:B:501:NAG:O6[8_555]	2.13	0.07
8:A:614:HOH:O	8:A:655:HOH:O[12_444]	2.17	0.03

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	206/208 (99%)	197 (96%)	8 (4%)	1 (0%)	32	49
1	B	206/208 (99%)	196 (95%)	9 (4%)	1 (0%)	32	49
All	All	412/416 (99%)	393 (95%)	17 (4%)	2 (0%)	32	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	280	ASP
1	A	358	LEU

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	193/193 (100%)	184 (95%)	9 (5%)	30	48
1	B	193/193 (100%)	178 (92%)	15 (8%)	15	24
All	All	386/386 (100%)	362 (94%)	24 (6%)	21	34

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	ASP
1	A	289	THR
1	A	290	LYS
1	A	292	ARG
1	A	311	GLN
1	A	326	LYS
1	A	355	ARG
1	A	392	ASP
1	A	430	GLU
1	B	253	ILE
1	B	266	VAL
1	B	282	VAL
1	B	290	LYS
1	B	292	ARG
1	B	293	GLU
1	B	301	ARG
1	B	309	LEU
1	B	317	LYS
1	B	350	THR
1	B	356	ASP
1	B	363	VAL
1	B	413	ASP
1	B	415	SER
1	B	441	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	429	HIS
1	B	347	GLN
1	B	438	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

16 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	1,3,2	14,14,15	1.05	1 (7%)	15,19,21	1.05	1 (6%)
3	FUL	A	502	2	9,10,11	2.08	2 (22%)	13,14,16	1.85	3 (23%)
2	NAG	A	503	2,4	14,14,15	0.50	0	15,19,21	0.47	0
4	BMA	A	504	2,5,4	11,11,12	1.13	1 (9%)	13,15,17	1.95	3 (23%)
5	MAN	A	505	4,6	11,11,12	1.05	1 (9%)	13,15,17	2.21	4 (30%)
6	NDG	A	506	5,7	14,14,15	1.03	1 (7%)	15,19,21	1.35	1 (6%)
7	GAL	A	507	6	11,11,12	1.60	3 (27%)	13,15,17	2.17	3 (23%)
4	BMA	A	508	2,4	11,11,12	1.16	1 (9%)	13,15,17	1.80	3 (23%)
2	NAG	A	509	4	14,14,15	1.23	1 (7%)	15,19,21	1.30	1 (6%)
2	NAG	B	501	1,2	14,14,15	0.36	0	15,19,21	0.44	0
2	NAG	B	502	2,4	14,14,15	0.17	0	15,19,21	0.53	0
4	BMA	B	503	2,5,4	11,11,12	1.31	2 (18%)	13,15,17	1.91	3 (23%)
5	MAN	B	504	4,6	11,11,12	1.00	0	13,15,17	1.50	1 (7%)
6	NDG	B	505	5,7	14,14,15	1.02	1 (7%)	15,19,21	1.41	2 (13%)
7	GAL	B	506	6	11,11,12	1.30	1 (9%)	13,15,17	1.89	3 (23%)
4	BMA	B	507	4	11,11,12	1.12	1 (9%)	13,15,17	0.96	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	1,3,2	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUL	A	502	2	-	0/0/17/20	0/1/1/1
2	NAG	A	503	2,4	-	0/6/23/26	0/1/1/1
4	BMA	A	504	2,5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	505	4,6	-	0/2/19/22	0/1/1/1
6	NDG	A	506	5,7	-	0/6/23/26	0/1/1/1
7	GAL	A	507	6	-	0/2/19/22	0/1/1/1
4	BMA	A	508	2,4	-	0/2/19/22	0/1/1/1
2	NAG	A	509	4	-	0/6/23/26	0/1/1/1
2	NAG	B	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	502	2,4	-	0/6/23/26	0/1/1/1
4	BMA	B	503	2,5,4	-	0/2/19/22	0/1/1/1
5	MAN	B	504	4,6	-	0/2/19/22	1/1/1/1
6	NDG	B	505	5,7	-	0/6/23/26	0/1/1/1
7	GAL	B	506	6	-	0/2/19/22	0/1/1/1
4	BMA	B	507	4	-	0/2/19/22	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	507	GAL	C2-C3	-3.60	1.47	1.52
3	A	502	FUL	C2-C3	-2.51	1.49	1.52
4	B	503	BMA	C1-C2	2.05	1.57	1.52
4	A	504	BMA	O3-C3	2.18	1.48	1.43
7	A	507	GAL	C1-C2	2.35	1.57	1.52
7	A	507	GAL	O5-C5	2.39	1.48	1.43
4	B	507	BMA	C4-C5	2.50	1.58	1.53
4	A	508	BMA	C4-C5	2.74	1.58	1.53
5	A	505	MAN	O5-C5	2.78	1.49	1.43
4	B	503	BMA	C2-C3	3.11	1.56	1.52
7	B	506	GAL	C1-C2	3.19	1.59	1.52
6	A	506	NDG	C1-C2	3.37	1.57	1.52
6	B	505	NDG	C1-C2	3.39	1.57	1.52
2	A	501	NAG	O5-C1	3.80	1.49	1.43
2	A	509	NAG	O5-C1	4.18	1.50	1.43
3	A	502	FUL	O5-C1	5.48	1.52	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	FUL	C1-C2-C3	-5.08	103.20	109.65
4	A	508	BMA	C1-C2-C3	-4.66	103.75	109.65
7	A	507	GAL	O5-C1-C2	-3.92	104.65	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	507	GAL	O2-C2-C3	-3.79	102.74	110.17
7	B	506	GAL	O2-C2-C3	-3.30	103.69	110.17
7	B	506	GAL	O5-C1-C2	-3.13	105.88	110.79
4	B	503	BMA	C1-C2-C3	-3.07	105.76	109.65
5	A	505	MAN	O2-C2-C3	-2.79	104.70	110.17
5	A	505	MAN	C1-C2-C3	-2.67	106.27	109.65
3	A	502	FUL	O5-C1-C2	-2.63	106.67	110.79
4	A	508	BMA	O5-C1-C2	-2.36	107.10	110.79
5	A	505	MAN	C2-C3-C4	-2.30	106.87	110.88
4	A	504	BMA	C1-C2-C3	-2.24	106.81	109.65
3	A	502	FUL	C1-O5-C5	-2.24	107.44	112.39
4	B	503	BMA	C3-C4-C5	-2.02	106.66	110.22
4	A	504	BMA	C1-O5-C5	2.24	115.26	112.17
6	B	505	NDG	C1-C2-N2	2.28	114.39	110.49
4	A	508	BMA	O3-C3-C2	2.62	114.79	110.02
6	B	505	NDG	C1-O-C5	2.68	115.86	112.17
6	A	506	NDG	C1-O-C5	2.99	116.29	112.17
2	A	501	NAG	C1-O5-C5	3.04	116.36	112.17
5	B	504	MAN	C1-O5-C5	4.17	117.91	112.17
7	B	506	GAL	O2-C2-C1	4.59	118.51	109.18
2	A	509	NAG	C1-O5-C5	4.74	118.70	112.17
7	A	507	GAL	O2-C2-C1	4.79	118.92	109.18
4	B	503	BMA	O3-C3-C2	5.32	119.70	110.02
4	A	504	BMA	O3-C3-C2	5.59	120.20	110.02
5	A	505	MAN	C1-O5-C5	5.87	120.25	112.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	504	MAN	C1-C2-C3-C4-C5-O5

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	FUL	3	0
6	A	506	NDG	1	0
7	A	507	GAL	4	0
2	B	501	NAG	0	1
2	B	502	NAG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	504	MAN	1	0
6	B	505	NDG	1	0
7	B	506	GAL	4	0
4	B	507	BMA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.36	6 (2%)	52	50	54, 88, 133, 159	4 (1%)
1	B	208/208 (100%)	1.35	47 (22%)	1	1	65, 119, 199, 257	3 (1%)
All	All	416/416 (100%)	0.85	53 (12%)	4	3	54, 101, 183, 257	7 (1%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	238	PRO	9.0
1	B	237	GLY	7.9
1	B	299	THR	7.7
1	B	295	GLN	7.3
1	B	271	PRO	7.2
1	B	300	TYR	7.2
1	B	269	GLU	6.8
1	B	267	SER	5.3
1	B	297	ASN	5.1
1	B	266	VAL	5.1
1	B	323	VAL	5.0
1	B	294	GLU	4.9
1	B	298	SER	4.8
1	A	237	GLY	4.7
1	A	296	TYR	4.6
1	B	240	VAL	4.6
1	B	273	VAL	4.6
1	B	302	VAL	4.6
1	B	296	TYR	4.1
1	B	268	HIS	4.0
1	B	333	GLU	4.0
1	B	320	LYS	3.7
1	B	270	ASP	3.7
1	B	239	SER	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	328	LEU	3.6
1	B	335	THR	3.5
1	B	402	GLY	3.5
1	B	331	PRO	3.3
1	B	384	ASN	3.3
1	B	313	TRP	3.2
1	B	241	PHE	3.2
1	A	298	SER	3.1
1	B	326	LYS	3.1
1	B	253	ILE	3.1
1	B	264	VAL	3.0
1	B	330	ALA	2.9
1	B	332	ILE	2.8
1	B	278	TYR	2.6
1	B	277	TRP	2.5
1	B	336	ILE	2.4
1	B	355	ARG	2.4
1	A	290	LYS	2.3
1	A	295	GLN	2.3
1	B	324	SER	2.2
1	B	398	LEU	2.2
1	B	306	LEU	2.1
1	B	307	THR	2.1
1	B	318	GLU	2.1
1	B	303	VAL	2.1
1	B	325	ASN	2.1
1	B	280	ASP	2.1
1	A	327	ALA	2.0
1	B	329	PRO	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 ⓘ

There are no carbohydrates in this entry.

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
7	GAL	B	506	11/12	0.85	0.35	3.00	141,158,168,181	0
7	GAL	A	507	11/12	0.88	0.22	1.48	81,107,124,142	0
6	NDG	B	505	14/15	0.89	0.26	1.01	112,130,143,144	0
6	NDG	A	506	14/15	0.92	0.12	-1.96	88,111,126,127	0
2	NAG	B	501	14/15	0.88	0.20	-1.97	112,149,162,173	0
4	BMA	A	504	11/12	0.95	0.16	-	91,100,113,117	0
4	BMA	B	507	11/12	0.88	0.27	-	135,158,168,175	0
3	FUL	A	502	10/11	0.80	0.50	-	101,136,154,159	0
4	BMA	B	503	11/12	0.80	0.14	-	155,163,175,177	0
5	MAN	B	504	11/12	0.79	0.24	-	155,161,180,184	0
2	NAG	A	501	14/15	0.88	0.18	-	96,107,146,150	0
5	MAN	A	505	11/12	0.91	0.13	-	95,103,117,126	0
2	NAG	A	509	14/15	0.83	0.21	-	124,154,162,162	0
2	NAG	B	502	14/15	0.82	0.22	-	133,180,188,195	0
4	BMA	A	508	11/12	0.90	0.14	-	116,137,144,145	0
2	NAG	A	503	14/15	0.94	0.17	-	95,110,130,133	0

6.5 Other polymers ⓘ

There are no such residues in this entry.