



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2016 – 08:18 AM EDT

PDB ID : 5GIJ  
Title : Crystal structure of TDR-TDIF complex  
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Deposited on : 2016-06-23  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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-20027939

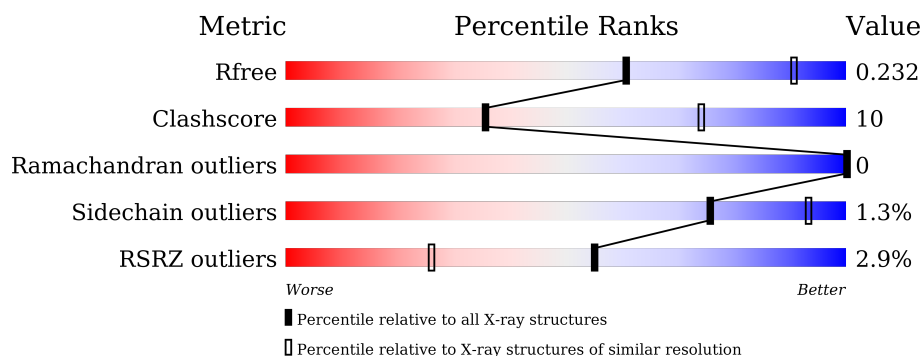
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	607	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>22%</div> <div>..</div> </div> </div>
2	D	12	<div> <div>67%</div> <div>33%</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
3	NAG	B	723	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5064 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 Leucine-rich repeat receptor-like protein kinase TDR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	603	Total	C	N	O	S	0	0	0
			4657	2990	771	885	11			

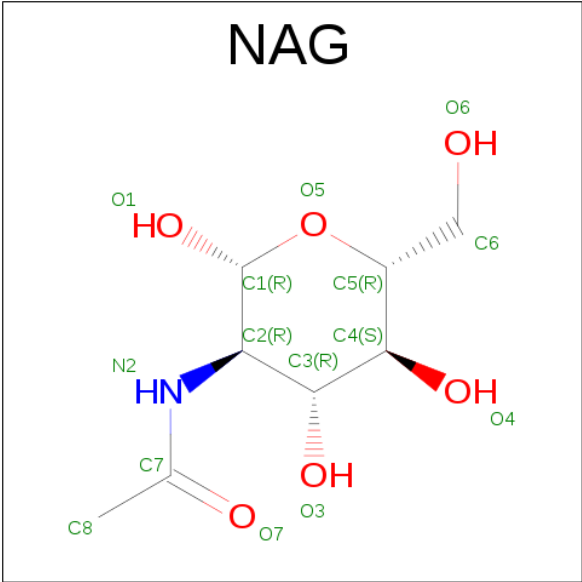
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	259	ALA	CYS	engineered mutation	UNP Q9FII5
B	540	SER	CYS	engineered mutation	UNP Q9FII5
B	632	SER	-	expression tag	UNP Q9FII5
B	633	GLY	-	expression tag	UNP Q9FII5
B	634	LEU	-	expression tag	UNP Q9FII5
B	635	GLU	-	expression tag	UNP Q9FII5
B	636	VAL	-	expression tag	UNP Q9FII5
B	637	LEU	-	expression tag	UNP Q9FII5

- Molecule 2 is a protein called Peptide from CLAVATA3/ESR (CLE)-related protein 41.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	0	0	0
			90	53	16	21			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



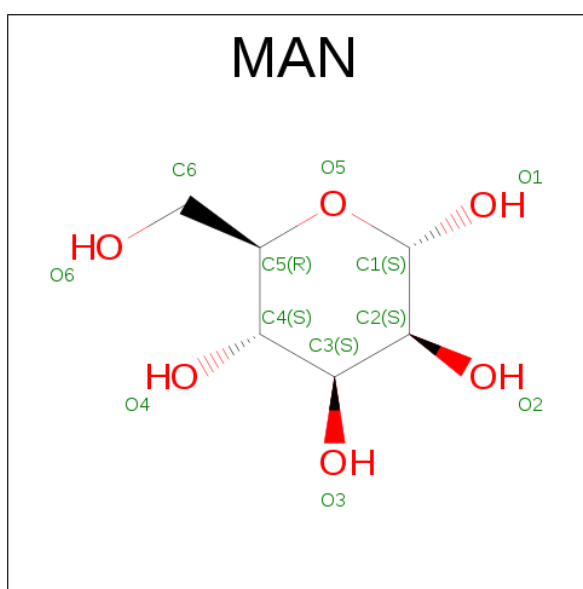
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1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

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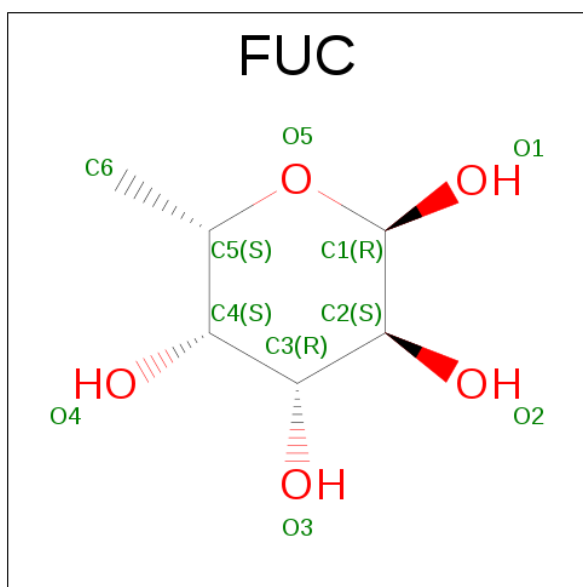
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	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		
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<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).

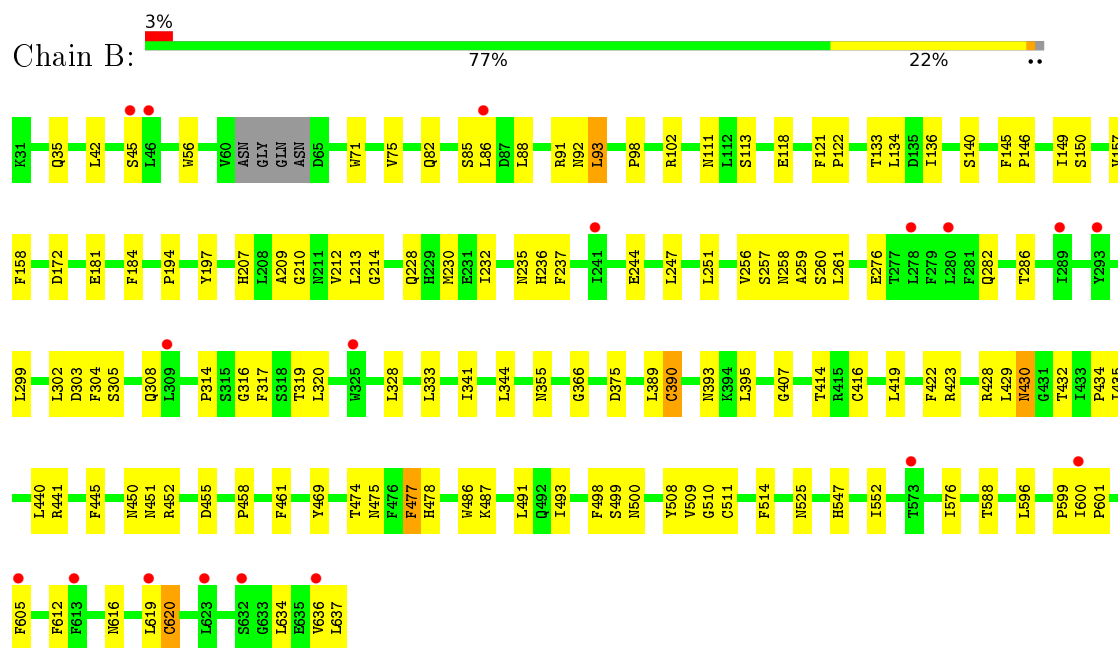


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		

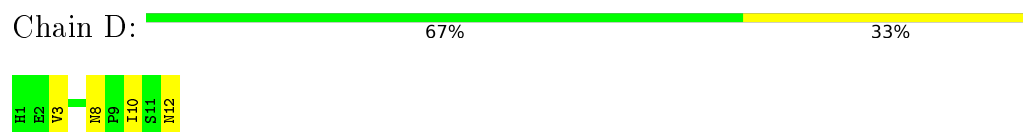
### 3 Residue-property plots

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: Leucine-rich repeat receptor-like protein kinase TDR



- Molecule 2: Peptide from CLAVATA3/ESR (CLE)-related protein 41





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.92Å 132.92Å 229.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	57.56 – 3.00 102.93 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (57.56-3.00) 94.9 (102.93-3.00)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.217 , 0.237 0.207 , 0.232	Depositor DCC
$R_{free}$ test set	2269 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.2	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5064	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: HYP, FUC, 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	B	0.54	2/4773 (0.0%)	0.77	3/6495 (0.0%)
2	D	0.66	0/73	0.84	0/94
All	All	0.54	2/4846 (0.0%)	0.77	3/6589 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	620	CYS	CB-SG	-5.41	1.73	1.81
1	B	390	CYS	CB-SG	-5.30	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	LEU	CA-CB-CG	8.81	135.55	115.30
1	B	435	ILE	C-N-CA	-6.67	108.28	122.30
1	B	42	LEU	CA-CB-CG	5.40	127.72	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	258	ASN	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	B	4657	0	4551	93	0
2	D	90	0	81	4	0
3	B	252	0	223	5	0
4	B	55	0	48	1	0
5	B	10	0	10	0	0
All	All	5064	0	4913	97	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 10.

All (97) 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:616:ASN:HB3	1:B:619:LEU:HD23	1.51	0.92
1:B:333:LEU:HB2	1:B:355:ASN:HD22	1.35	0.90
1:B:213:LEU:HB2	1:B:235:ASN:HD22	1.47	0.78
1:B:596:LEU:HB2	1:B:619:LEU:HD21	1.70	0.72
1:B:316:GLY:O	1:B:319:THR:HG22	1.92	0.69
1:B:149:ILE:HG23	1:B:172:ASP:HB2	1.75	0.68
1:B:596:LEU:HD12	1:B:616:ASN:OD1	1.95	0.67
1:B:35:GLN:NE2	1:B:82:GLN:OE1	2.28	0.67
1:B:333:LEU:HB2	1:B:355:ASN:ND2	2.10	0.66
1:B:118:GLU:HA	1:B:140:SER:O	1.96	0.66
1:B:299:LEU:HD21	1:B:302:LEU:HD12	1.78	0.66
1:B:601:PRO:HG2	1:B:605:PHE:CD2	2.34	0.62
1:B:474:THR:HA	1:B:498:PHE:O	2.01	0.61
1:B:525:ASN:HA	1:B:547:HIS:O	2.01	0.61
1:B:305:SER:HB2	2:D:8:ASN:HD22	1.66	0.60
1:B:303:ASP:OD1	1:B:305:SER:OG	2.16	0.59
1:B:432:THR:HG22	1:B:455:ASP:HB2	1.87	0.57
1:B:636:VAL:HG12	1:B:637:LEU:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:SER:HB2	1:B:98:PRO:HG3	1.88	0.56
1:B:207:HIS:CE1	1:B:209:ALA:HB3	2.42	0.55
1:B:75:VAL:HB	1:B:85:SER:HB3	1.89	0.54
2:D:8:ASN:HD21	2:D:10:ILE:HD11	1.73	0.54
1:B:194:PRO:HG2	1:B:197:TYR:CE1	2.43	0.52
1:B:158:PHE:HE2	1:B:184:PHE:CZ	2.28	0.51
1:B:487:LYS:HE2	1:B:509:VAL:HG21	1.90	0.51
1:B:121:PHE:CD1	1:B:122:PRO:HD2	2.46	0.51
1:B:207:HIS:HE1	1:B:209:ALA:HB3	1.75	0.51
1:B:213:LEU:CB	1:B:235:ASN:HD22	2.22	0.50
1:B:194:PRO:HG2	1:B:197:TYR:CZ	2.46	0.49
1:B:91:ARG:O	1:B:92:ASN:C	2.50	0.49
1:B:390:CYS:SG	1:B:395:LEU:HB3	2.52	0.49
1:B:429:LEU:HB2	1:B:451:ASN:ND2	2.27	0.48
1:B:375:ASP:OD2	2:D:12:ASN:HB2	2.13	0.48
1:B:445:PHE:CE2	1:B:469:TYR:CD2	3.02	0.48
1:B:230:MET:CE	1:B:232:ILE:HD11	2.44	0.48
1:B:212:VAL:O	1:B:212:VAL:HG12	2.14	0.48
1:B:423:ARG:HG2	1:B:445:PHE:CE1	2.49	0.47
1:B:486:TRP:CE2	1:B:508:TYR:CE1	3.02	0.47
1:B:428:ARG:HG2	1:B:452:ARG:NH1	2.29	0.47
1:B:86:LEU:HG	1:B:88:LEU:HD13	1.95	0.47
1:B:157:VAL:HG13	1:B:181:GLU:HB2	1.96	0.47
1:B:150:SER:HB3	1:B:172:ASP:HB3	1.96	0.47
1:B:341:ILE:HG23	1:B:344:LEU:HD12	1.97	0.47
1:B:228:GLN:HA	1:B:251:LEU:HA	1.97	0.46
3:B:711:NAG:H3	3:B:711:NAG:H83	1.96	0.46
1:B:317:PHE:HA	1:B:320:LEU:HD13	1.98	0.46
1:B:486:TRP:HD1	1:B:508:TYR:H	1.64	0.46
1:B:491:LEU:HD23	1:B:514:PHE:CZ	2.51	0.46
1:B:419:LEU:HD21	1:B:422:PHE:HB2	1.97	0.45
1:B:286:THR:HA	1:B:308:GLN:O	2.17	0.45
3:B:719:NAG:O3	4:B:720:MAN:H2	2.17	0.45
1:B:299:LEU:CD2	1:B:302:LEU:HD12	2.47	0.45
1:B:237:PHE:O	1:B:260:SER:OG	2.34	0.45
1:B:282:GLN:HE22	3:B:704:NAG:H82	1.83	0.45
1:B:455:ASP:O	1:B:477:PHE:HB2	2.16	0.44
1:B:478:HIS:HA	1:B:500:ASN:O	2.18	0.44
1:B:133:THR:HB	1:B:157:VAL:HB	2.00	0.44
1:B:111:ASN:OD1	1:B:113:SER:HB3	2.18	0.44
1:B:407:GLY:C	1:B:430:ASN:HB2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:ILE:HG13	1:B:619:LEU:HD12	1.99	0.44
1:B:445:PHE:CZ	1:B:469:TYR:CD2	3.06	0.44
1:B:469:TYR:HD1	1:B:493:ILE:HB	1.83	0.44
1:B:475:ASN:O	1:B:499:SER:HA	2.17	0.44
1:B:616:ASN:CB	1:B:619:LEU:HD23	2.34	0.43
1:B:56:TRP:CD1	1:B:71:TRP:HB3	2.52	0.43
1:B:407:GLY:O	1:B:430:ASN:HB2	2.18	0.43
1:B:441:ARG:HH21	3:B:713:NAG:HN2	1.67	0.43
1:B:407:GLY:O	1:B:430:ASN:N	2.52	0.43
1:B:276:GLU:HA	1:B:299:LEU:HA	2.01	0.42
1:B:235:ASN:O	1:B:259:ALA:HA	2.19	0.42
1:B:552:ILE:HG21	1:B:552:ILE:HD13	1.79	0.42
1:B:145:PHE:HA	1:B:146:PRO:HD3	1.91	0.42
1:B:414:THR:HG21	1:B:434:PRO:HB2	2.01	0.42
1:B:509:VAL:HG23	1:B:510:GLY:H	1.84	0.42
1:B:210:GLY:HA3	2:D:3:VAL:HG11	2.02	0.42
1:B:599:PRO:HA	1:B:620:CYS:HB3	2.02	0.42
1:B:458:PRO:HG2	1:B:461:PHE:CE2	2.55	0.41
1:B:366:GLY:HA3	1:B:389:LEU:HA	2.01	0.41
1:B:450:ASN:HA	1:B:474:THR:OG1	2.20	0.41
1:B:596:LEU:HB2	1:B:619:LEU:CD2	2.44	0.41
1:B:299:LEU:HA	1:B:299:LEU:HD12	1.83	0.41
1:B:257:SER:C	1:B:259:ALA:H	2.24	0.41
1:B:487:LYS:HG2	1:B:509:VAL:HG23	2.03	0.41
1:B:314:PRO:HD2	1:B:317:PHE:HE2	1.86	0.41
1:B:576:ILE:HG12	1:B:596:LEU:HD22	2.03	0.41
3:B:707:NAG:H4	3:B:708:NAG:H2	1.95	0.41
1:B:247:LEU:HD13	1:B:247:LEU:HA	1.91	0.41
1:B:416:CYS:O	1:B:440:LEU:HD22	2.21	0.41
1:B:302:LEU:HD21	1:B:304:PHE:CZ	2.56	0.41
1:B:134:LEU:HD23	1:B:158:PHE:CE1	2.56	0.41
1:B:244:GLU:OE1	1:B:244:GLU:N	2.49	0.41
1:B:588:THR:HG23	1:B:612:PHE:CZ	2.56	0.40
1:B:136:ILE:O	1:B:136:ILE:HG22	2.21	0.40
1:B:232:ILE:HD13	1:B:232:ILE:HG21	1.82	0.40
1:B:214:GLY:HA2	1:B:236:HIS:O	2.20	0.40
1:B:256:VAL:HG21	1:B:261:LEU:HD11	2.04	0.40
1:B:328:LEU:HA	1:B:328:LEU:HD23	1.81	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	B	599/607 (99%)	567 (95%)	32 (5%)	0	100	100
2	D	8/12 (67%)	6 (75%)	2 (25%)	0	100	100
All	All	607/619 (98%)	573 (94%)	34 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	B	530/540 (98%)	523 (99%)	7 (1%)	76	93
2	D	9/9 (100%)	9 (100%)	0	100	100
All	All	539/549 (98%)	532 (99%)	7 (1%)	76	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	93	LEU
1	B	102	ARG
1	B	393	ASN
1	B	430	ASN
1	B	477	PHE
1	B	511	CYS
1	B	634	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	35	GLN
1	B	235	ASN
1	B	355	ASN
2	D	1	HIS
2	D	8	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	HYP	D	4	2	6,8,9	1.14	0	5,10,12	1.71	0
2	HYP	D	7	2	6,8,9	0.65	0	5,10,12	2.15	1 (20%)

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	HYP	D	4	2	-	0/0/11/13	0/1/1/1
2	HYP	D	7	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	7	HYP	CB-CG-CD	4.41	108.49	103.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

24 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	NAG	B	701	1,3	14,14,15	0.31	0	15,19,21	0.47	0
3	NAG	B	702	3,4	14,14,15	0.59	0	15,19,21	1.26	3 (20%)
4	MAN	B	703	3	11,11,12	1.68	2 (18%)	15,15,17	1.33	2 (13%)
3	NAG	B	704	1	14,14,15	0.87	1 (7%)	15,19,21	0.81	1 (6%)
3	NAG	B	705	1	14,14,15	0.68	1 (7%)	15,19,21	1.09	1 (6%)
3	NAG	B	706	1	14,14,15	0.44	0	15,19,21	1.26	2 (13%)
3	NAG	B	707	1,3	14,14,15	0.30	0	15,19,21	0.85	1 (6%)
3	NAG	B	708	3	14,14,15	0.84	1 (7%)	15,19,21	0.86	1 (6%)
3	NAG	B	709	1,3	14,14,15	0.63	0	15,19,21	1.13	1 (6%)
3	NAG	B	710	3	14,14,15	0.58	0	15,19,21	0.28	0
3	NAG	B	711	1,3	14,14,15	1.68	1 (7%)	15,19,21	1.79	3 (20%)
3	NAG	B	712	3	14,14,15	2.06	2 (14%)	15,19,21	1.51	1 (6%)
3	NAG	B	713	1	14,14,15	0.51	0	15,19,21	0.48	0
3	NAG	B	714	1,3	14,14,15	0.38	0	15,19,21	0.80	1 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	715	3,4	14,14,15	0.31	0	15,19,21	0.87	0
4	MAN	B	716	3,4	11,11,12	1.28	1 (9%)	15,15,17	2.62	4 (26%)
4	MAN	B	717	4	11,11,12	1.90	4 (36%)	15,15,17	1.62	3 (20%)
3	NAG	B	718	1,3,5	14,14,15	0.36	0	15,19,21	0.71	0
3	NAG	B	719	3,4	14,14,15	0.81	2 (14%)	15,19,21	0.71	0
4	MAN	B	720	3,4	11,11,12	1.70	2 (18%)	15,15,17	2.53	8 (53%)
4	MAN	B	721	4	11,11,12	1.86	3 (27%)	15,15,17	1.89	5 (33%)
5	FUC	B	722	3	10,10,11	2.17	3 (30%)	13,14,16	1.67	2 (15%)
3	NAG	B	723	1,3	14,14,15	0.55	0	15,19,21	0.89	1 (6%)
3	NAG	B	724	3	14,14,15	0.68	1 (7%)	15,19,21	0.20	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	NAG	B	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	702	3,4	-	0/6/23/26	0/1/1/1
4	MAN	B	703	3	-	0/2/19/22	1/1/1/1
3	NAG	B	704	1	-	0/6/23/26	0/1/1/1
3	NAG	B	705	1	-	0/6/23/26	0/1/1/1
3	NAG	B	706	1	-	0/6/23/26	0/1/1/1
3	NAG	B	707	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	708	3	-	0/6/23/26	0/1/1/1
3	NAG	B	709	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	710	3	-	0/6/23/26	0/1/1/1
3	NAG	B	711	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	712	3	-	0/6/23/26	0/1/1/1
3	NAG	B	713	1	-	0/6/23/26	0/1/1/1
3	NAG	B	714	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	715	3,4	-	0/6/23/26	0/1/1/1
4	MAN	B	716	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	717	4	-	0/2/19/22	0/1/1/1
3	NAG	B	718	1,3,5	-	0/6/23/26	0/1/1/1
3	NAG	B	719	3,4	-	0/6/23/26	0/1/1/1
4	MAN	B	720	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	721	4	-	0/2/19/22	0/1/1/1
5	FUC	B	722	3	-	0/0/17/20	0/1/1/1
3	NAG	B	723	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	724	3	-	0/6/23/26	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	711	NAG	O5-C1	-5.91	1.34	1.43
4	B	721	MAN	O5-C1	-3.31	1.38	1.43
3	B	719	NAG	O5-C1	-2.08	1.40	1.43
3	B	719	NAG	C1-C2	2.09	1.55	1.52
3	B	705	NAG	O5-C1	2.12	1.47	1.43
3	B	724	NAG	C1-C2	2.12	1.55	1.52
3	B	712	NAG	C1-C2	2.22	1.55	1.52
4	B	716	MAN	C1-C2	2.23	1.57	1.52
4	B	717	MAN	C4-C5	2.28	1.58	1.53
5	B	722	FUC	C6-C5	2.36	1.57	1.51
4	B	717	MAN	C1-C2	2.54	1.58	1.52
4	B	720	MAN	O5-C5	2.54	1.49	1.43
4	B	717	MAN	C4-C3	2.57	1.59	1.52
3	B	708	NAG	C1-C2	2.80	1.56	1.52
4	B	703	MAN	C1-C2	2.84	1.59	1.52
3	B	704	NAG	O5-C1	3.12	1.48	1.43
4	B	721	MAN	C1-C2	3.26	1.60	1.52
4	B	721	MAN	C2-C3	3.42	1.57	1.52
4	B	703	MAN	O5-C5	3.45	1.51	1.43
4	B	720	MAN	C1-C2	3.74	1.61	1.52
5	B	722	FUC	C4-C5	3.93	1.60	1.53
4	B	717	MAN	C2-C3	4.05	1.58	1.52
5	B	722	FUC	C4-C3	4.57	1.64	1.52
3	B	712	NAG	O5-C1	7.35	1.55	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	720	MAN	C3-C4-C5	-4.91	101.47	110.23
4	B	720	MAN	C2-C3-C4	-4.78	102.70	111.05
3	B	706	NAG	C1-O5-C5	-3.17	107.47	112.14
4	B	721	MAN	C3-C4-C5	-2.79	105.26	110.23
4	B	720	MAN	O6-C6-C5	-2.46	103.08	111.30
3	B	714	NAG	O4-C4-C3	-2.43	104.88	110.36
4	B	721	MAN	O5-C5-C4	-2.21	106.48	110.13
3	B	708	NAG	C1-O5-C5	-2.02	109.16	112.14
3	B	707	NAG	O4-C4-C5	-2.00	103.95	109.23
3	B	702	NAG	C3-C4-C5	2.03	113.84	110.23
4	B	717	MAN	O5-C1-C2	2.12	114.28	110.89
3	B	711	NAG	C1-O5-C5	2.16	115.31	112.14
4	B	720	MAN	O5-C1-C2	2.17	114.37	110.89
4	B	703	MAN	C1-C2-C3	2.25	112.28	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	716	MAN	O3-C3-C2	2.45	114.49	110.01
4	B	721	MAN	O3-C3-C2	2.47	114.53	110.01
4	B	720	MAN	O3-C3-C4	2.52	116.05	110.36
3	B	723	NAG	C1-O5-C5	2.55	115.88	112.14
3	B	704	NAG	C1-O5-C5	2.55	115.89	112.14
4	B	716	MAN	O5-C5-C4	2.59	114.43	110.13
4	B	720	MAN	O4-C4-C3	2.69	116.43	110.36
4	B	717	MAN	C1-O5-C5	2.70	116.11	112.14
3	B	702	NAG	O5-C5-C4	2.72	114.64	110.13
4	B	720	MAN	C1-O5-C5	2.82	116.28	112.14
3	B	711	NAG	C3-C4-C5	2.86	115.32	110.23
3	B	702	NAG	C1-O5-C5	2.91	116.41	112.14
3	B	709	NAG	C1-O5-C5	2.91	116.42	112.14
5	B	722	FUC	C2-C3-C4	2.95	116.19	111.05
3	B	706	NAG	C2-N2-C7	2.98	126.98	123.11
4	B	720	MAN	O3-C3-C2	2.99	115.48	110.01
4	B	721	MAN	C1-O5-C5	3.01	116.57	112.14
4	B	703	MAN	C1-O5-C5	3.20	116.84	112.14
4	B	717	MAN	C1-C2-C3	3.37	113.63	109.55
4	B	721	MAN	C1-C2-C3	3.47	113.75	109.55
3	B	705	NAG	C1-O5-C5	3.51	117.30	112.14
5	B	722	FUC	C3-C4-C5	4.01	115.65	109.66
4	B	716	MAN	O5-C1-C2	4.28	117.73	110.89
3	B	711	NAG	C2-N2-C7	4.93	129.52	123.11
3	B	712	NAG	C1-O5-C5	5.38	120.06	112.14
4	B	716	MAN	C1-O5-C5	7.80	123.61	112.14

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	703	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	704	NAG	1	0
3	B	707	NAG	1	0
3	B	708	NAG	1	0
3	B	711	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	713	NAG	1	0
3	B	719	NAG	1	0
4	B	720	MAN	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	B	603/607 (99%)	0.78	18 (2%) 54 25	56, 71, 101, 138	0
2	D	10/12 (83%)	0.77	0 100 100	64, 71, 78, 82	0
All	All	613/619 (99%)	0.78	18 (2%) 55 26	56, 71, 101, 138	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	632	SER	3.0
1	B	86	LEU	2.9
1	B	623	LEU	2.9
1	B	636	VAL	2.9
1	B	619	LEU	2.9
1	B	309	LEU	2.8
1	B	605	PHE	2.6
1	B	45	SER	2.6
1	B	280	LEU	2.5
1	B	293	TYR	2.4
1	B	278	LEU	2.4
1	B	289	ILE	2.3
1	B	613	PHE	2.1
1	B	600	ILE	2.1
1	B	241	ILE	2.1
1	B	573	THR	2.1
1	B	46	LEU	2.1
1	B	325	TRP	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	HYP	D	7	8/9	0.95	0.30	-	61,67,68,69	0
2	HYP	D	4	8/9	0.97	0.31	-	62,65,70,76	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	B	723	14/15	0.86	0.38	2.09	101,111,127,134	0
3	NAG	B	718	14/15	0.96	0.23	-0.46	50,61,71,71	0
3	NAG	B	714	14/15	0.95	0.24	-0.59	64,69,78,79	0
4	MAN	B	721	11/12	0.94	0.24	-1.03	68,73,79,84	0
3	NAG	B	701	14/15	0.96	0.21	-1.11	69,83,92,97	0
3	NAG	B	709	14/15	0.89	0.20	-	89,101,123,126	0
3	NAG	B	710	14/15	0.87	0.21	-	133,141,146,148	0
4	MAN	B	717	11/12	0.81	0.17	-	138,145,151,153	0
3	NAG	B	713	14/15	0.92	0.34	-	97,100,106,107	0
3	NAG	B	724	14/15	0.80	0.28	-	122,143,152,153	0
3	NAG	B	712	14/15	0.85	0.21	-	128,137,141,144	0
4	MAN	B	703	11/12	0.79	0.31	-	131,137,143,145	0
3	NAG	B	702	14/15	0.89	0.23	-	100,114,131,136	0
3	NAG	B	715	14/15	0.91	0.21	-	84,95,108,122	0
3	NAG	B	719	14/15	0.97	0.21	-	71,75,84,84	0
3	NAG	B	711	14/15	0.87	0.19	-	108,115,125,129	0
3	NAG	B	708	14/15	0.84	0.25	-	136,143,148,148	0
3	NAG	B	706	14/15	0.91	0.18	-	75,83,104,107	0
4	MAN	B	720	11/12	0.92	0.19	-	81,83,89,95	0
5	FUC	B	722	10/11	0.93	0.19	-	68,71,85,94	0
3	NAG	B	707	14/15	0.90	0.18	-	107,117,128,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	705	14/15	0.75	0.22	-	114,127,132,134	0
3	NAG	B	704	14/15	0.86	0.28	-	101,108,123,124	0
4	MAN	B	716	11/12	0.80	0.12	-	125,133,142,143	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.