



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5JFI
Title : Crystal structure of a TDIF-TDR complex
Authors : Xu, G.; Li, Z.
Deposited on : 2016-04-19
Resolution : 2.75 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

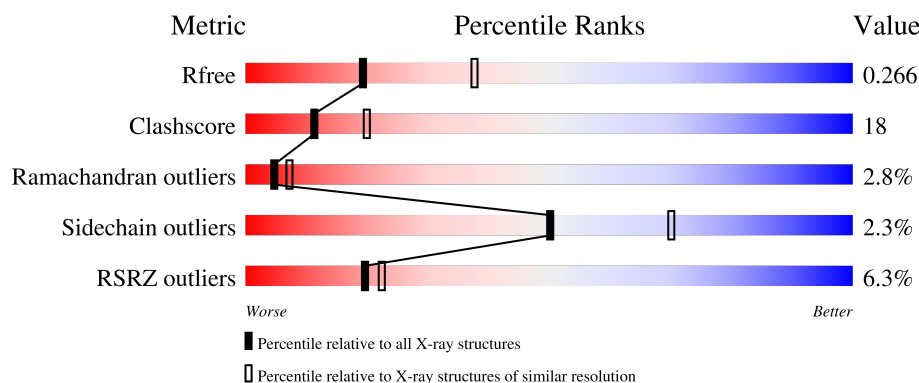
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	613	<div> <div>6%</div> <div> <div></div> <div>66%</div> <div>23%</div> <div>• 6%</div> </div> </div>
1	B	613	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>20%</div> <div>• 6%</div> </div> </div>
2	C	12	<div> <div></div> <div> <div>58%</div> <div>42%</div> </div> </div>
2	D	12	<div> <div></div> <div> <div>75%</div> <div>25%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9400 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	A	577	Total	C	N	O	S	0	0	0
			4463	2859	745	847	12			
1	B	577	Total	C	N	O	S	0	0	0
			4463	2859	745	847	12			

- Molecule 2 is a protein called CLE41.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	0	0	0
			89	53	16	20			
2	D	12	Total	C	N	O	0	0	0
			89	53	16	20			

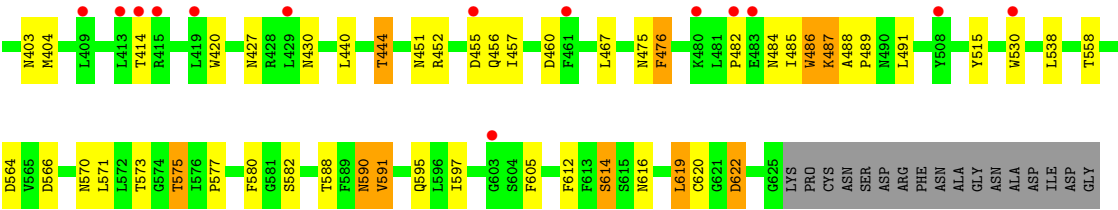
- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



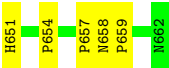
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	77	Total	O	0	0
			77	77		
4	C	2	Total	O	0	0
			2	2		
4	B	76	Total	O	0	0
			76	76		
4	D	1	Total	O	0	0
			1	1		



● Molecule 2: CLE41



● Molecule 2: CLE41



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	92.44Å 92.44Å 252.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.22 – 2.75 46.22 – 2.75	Depositor EDS
% Data completeness (in resolution range)	94.8 (46.22-2.75) 94.7 (46.22-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.214 , 0.267 0.214 , 0.266	Depositor DCC
R_{free} test set	1679 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9400	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: NAG, HYP

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	0.56	2/4571 (0.0%)	0.80	9/6214 (0.1%)
1	B	0.60	6/4571 (0.1%)	0.81	11/6214 (0.2%)
2	C	0.45	0/72	0.60	0/94
2	D	0.48	0/72	0.62	0/94
All	All	0.58	8/9286 (0.1%)	0.80	20/12616 (0.2%)

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

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	CYS	CB-SG	-12.21	1.61	1.82
1	B	68	TRP	CE3-CZ3	-10.91	1.20	1.38
1	A	67	VAL	CB-CG2	-9.13	1.33	1.52
1	B	175	ARG	CZ-NH1	-6.20	1.25	1.33
1	B	71	TRP	CB-CG	-6.04	1.39	1.50

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	559	LEU	CA-CB-CG	16.89	154.14	115.30
1	A	69	CYS	CB-CA-C	-7.73	94.94	110.40
1	A	559	LEU	CB-CA-C	-7.32	96.29	110.20
1	B	176	LEU	CB-CG-CD2	-7.13	98.88	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	559	LEU	CB-CG-CD1	7.08	123.03	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	68	TRP	Peptide

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	4463	0	4360	171	0
1	B	4463	0	4358	144	1
2	C	89	0	78	3	0
2	D	89	0	78	1	0
3	A	70	0	65	5	0
3	B	70	0	65	5	0
4	A	77	0	0	15	0
4	B	76	0	0	18	0
4	C	2	0	0	1	0
4	D	1	0	0	0	0
All	All	9400	0	9004	324	1

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 18.

The worst 5 of 324 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:68:TRP:CH2	1:A:95:GLY:HA3	1.41	1.55
1:B:150:SER:CA	1:B:175:ARG:NH2	1.68	1.55
1:A:68:TRP:CZ3	1:A:95:GLY:HA3	1.40	1.54
1:B:150:SER:HA	1:B:175:ARG:CZ	1.43	1.45
1:B:68:TRP:CZ3	1:B:93:LEU:HB3	1.54	1.39

All (1) 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:B:70:SER:OG	1:B:575:THR:N[3_645]	1.99	0.21

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	573/613 (94%)	482 (84%)	71 (12%)	20 (4%)	3	5
1	B	573/613 (94%)	491 (86%)	69 (12%)	13 (2%)	6	10
2	C	8/12 (67%)	7 (88%)	1 (12%)	0	100	100
2	D	8/12 (67%)	8 (100%)	0	0	100	100
All	All	1162/1250 (93%)	988 (85%)	141 (12%)	33 (3%)	5	7

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ASP
1	A	69	CYS
1	A	72	SER
1	A	73	GLY
1	A	80	THR

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	505/544 (93%)	494 (98%)	11 (2%)	52	71
1	B	505/544 (93%)	492 (97%)	13 (3%)	46	66
2	C	9/9 (100%)	9 (100%)	0	100	100
2	D	9/9 (100%)	9 (100%)	0	100	100
All	All	1028/1106 (93%)	1004 (98%)	24 (2%)	50	70

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	240	ASN
1	B	444	THR
1	B	371	LEU
1	B	491	LEU
1	A	318	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	267	GLN
1	B	427	ASN
1	B	393	ASN
1	B	468	GLN
1	A	546	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	654	2	6,8,9	0.73	0	5,10,12	2.37	3 (60%)
2	HYP	C	657	2	6,8,9	0.61	0	5,10,12	1.77	2 (40%)
2	HYP	C	654	2	6,8,9	0.80	0	5,10,12	2.13	2 (40%)
2	HYP	D	657	2	6,8,9	0.75	0	5,10,12	1.86	2 (40%)

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	654	2	-	0/0/11/13	0/1/1/1
2	HYP	C	657	2	-	0/0/11/13	0/1/1/1
2	HYP	C	654	2	-	0/0/11/13	0/1/1/1
2	HYP	D	657	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	654	HYP	CG-CB-CA	3.26	108.08	103.96
2	D	654	HYP	CG-CB-CA	3.25	108.07	103.96
2	D	657	HYP	CB-CG-CD	3.23	107.22	103.27
2	D	654	HYP	CB-CG-CD	3.21	107.20	103.27
2	C	657	HYP	CB-CG-CD	3.00	106.94	103.27

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	A	701	1	14,14,15	0.93	1 (7%)	17,19,21	0.83	0
3	NAG	A	704	1	14,14,15	1.04	2 (14%)	17,19,21	0.83	1 (5%)
3	NAG	B	702	1	14,14,15	0.96	1 (7%)	17,19,21	1.19	2 (11%)
3	NAG	A	705	1	14,14,15	0.84	1 (7%)	17,19,21	1.04	1 (5%)
3	NAG	B	703	1	14,14,15	0.83	1 (7%)	17,19,21	1.00	1 (5%)
3	NAG	B	701	1	14,14,15	1.24	2 (14%)	17,19,21	0.75	0
3	NAG	B	705	1	14,14,15	0.72	1 (7%)	17,19,21	0.94	0
3	NAG	A	702	1	14,14,15	0.46	0	17,19,21	1.20	2 (11%)
3	NAG	B	704	1	14,14,15	1.35	2 (14%)	17,19,21	1.74	1 (5%)
3	NAG	A	703	1	14,14,15	0.89	2 (14%)	17,19,21	0.89	1 (5%)

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	A	701	1	-	1/6/23/26	0/1/1/1
3	NAG	A	704	1	-	3/6/23/26	0/1/1/1
3	NAG	B	702	1	-	0/6/23/26	0/1/1/1
3	NAG	A	705	1	-	0/6/23/26	0/1/1/1
3	NAG	B	703	1	-	2/6/23/26	0/1/1/1
3	NAG	B	701	1	-	1/6/23/26	0/1/1/1
3	NAG	B	705	1	-	0/6/23/26	0/1/1/1
3	NAG	A	702	1	-	1/6/23/26	0/1/1/1
3	NAG	B	704	1	-	2/6/23/26	0/1/1/1
3	NAG	A	703	1	-	2/6/23/26	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	704	NAG	O5-C1	4.47	1.50	1.43
3	B	701	NAG	O5-C1	4.01	1.50	1.43
3	A	704	NAG	O5-C1	3.15	1.48	1.43
3	B	702	NAG	C1-C2	-2.90	1.48	1.52
3	A	705	NAG	O5-C1	-2.76	1.39	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	704	NAG	C1-O5-C5	6.75	121.34	112.19
3	B	702	NAG	C1-O5-C5	3.71	117.22	112.19
3	A	702	NAG	C3-C4-C5	3.24	116.01	110.24
3	A	702	NAG	C1-O5-C5	2.73	115.89	112.19
3	B	703	NAG	C1-O5-C5	2.51	115.59	112.19

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	703	NAG	O5-C5-C6-O6
3	A	703	NAG	O5-C5-C6-O6
3	A	703	NAG	C4-C5-C6-O6
3	B	703	NAG	C4-C5-C6-O6
3	A	704	NAG	C8-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	704	NAG	3	0
3	A	705	NAG	2	0
3	B	703	NAG	1	0
3	B	701	NAG	1	0
3	B	705	NAG	1	0
3	B	704	NAG	2	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 [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(Å ²)	Q<0.9
1	A	577/613 (94%)	0.61	35 (6%) 21 24	40, 61, 93, 135	0
1	B	577/613 (94%)	0.59	39 (6%) 17 19	37, 61, 93, 120	0
2	C	10/12 (83%)	0.60	0 100 100	44, 53, 69, 71	0
2	D	10/12 (83%)	0.44	0 100 100	45, 54, 63, 70	0
All	All	1174/1250 (93%)	0.60	74 (6%) 20 22	37, 61, 93, 135	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	619	LEU	8.8
1	B	68	TRP	8.1
1	B	62	GLY	6.6
1	B	80	THR	5.5
1	B	69	CYS	4.6

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. 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	B-factors(Å ²)	Q<0.9
2	HYP	C	654	8/9	0.95	0.18	66,70,74,79	0
2	HYP	C	657	8/9	0.97	0.19	67,71,72,77	0
2	HYP	D	654	8/9	0.97	0.18	63,67,70,74	0
2	HYP	D	657	8/9	0.97	0.17	61,65,68,72	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors(\AA^2)	Q<0.9
3	NAG	B	702	14/15	0.80	0.24	83,95,103,103	0
3	NAG	B	704	14/15	0.80	0.17	66,84,92,95	0
3	NAG	A	704	14/15	0.86	0.11	81,92,109,112	0
3	NAG	A	702	14/15	0.88	0.17	76,91,101,101	0
3	NAG	B	705	14/15	0.88	0.19	54,74,87,91	0
3	NAG	B	701	14/15	0.89	0.16	39,57,66,68	0
3	NAG	A	701	14/15	0.90	0.17	50,59,68,69	0
3	NAG	A	705	14/15	0.94	0.23	56,69,81,83	0
3	NAG	A	703	14/15	0.95	0.15	29,41,52,53	0
3	NAG	B	703	14/15	0.97	0.15	25,37,50,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.