



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2017 – 03:02 PM EDT

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 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
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-20029077

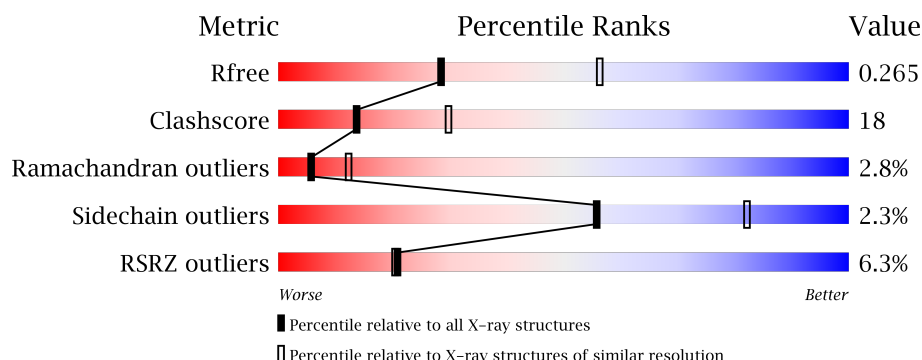
# 1 Overall quality at a glance

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))
$R_{free}$	100719	3342 (2.78-2.70)
Clashscore	112137	3731 (2.78-2.70)
Ramachandran outliers	110173	3670 (2.78-2.70)
Sidechain outliers	110143	3671 (2.78-2.70)
RSRZ outliers	101464	3362 (2.78-2.70)

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  $\geq 3$ , 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	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></div> <div>75%</div> <div>25%</div> </div> </div>
2	D	12	<div> <div></div> <div> <div></div> <div>92%</div> <div>8%</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.

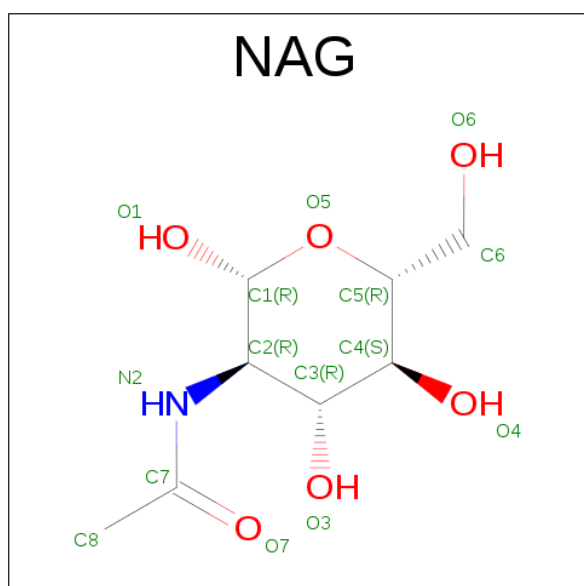
- Molecule 1 is a protein called Leucine-rich repeat receptor-like protein kinase TDR.

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 N-ACETYL-D-GLUCOSAMINE (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		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

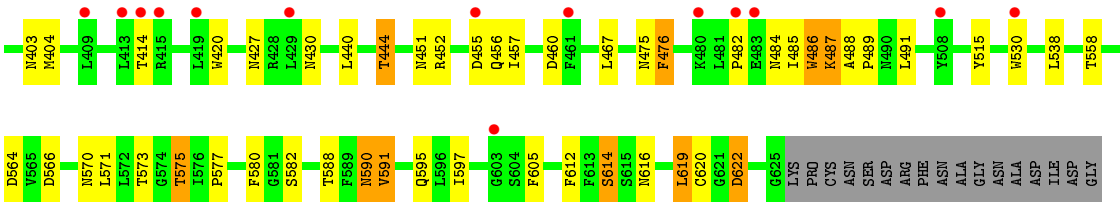
- Molecule 4 is water.

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		

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.

- Chain A:
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- [illegible]



• Molecule 2: CLE41



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.214 , 0.267 0.209 , 0.265	Depositor DCC
$R_{free}$ test set	1605 reflections (3.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<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, NAG

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

All (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
1	B	175	ARG	CD-NE	-5.51	1.37	1.46
1	B	69	CYS	CB-SG	-5.32	1.73	1.81
1	B	117	LEU	CG-CD2	-5.08	1.33	1.51

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	A	559	LEU	CB-CG-CD1	7.08	123.03	111.00
1	A	558	THR	C-N-CA	7.05	139.33	121.70
1	B	68	TRP	CB-CG-CD2	-6.90	117.63	126.60
1	B	172	ASP	CB-CG-OD1	6.82	124.44	118.30
1	B	175	ARG	CB-CG-CD	-6.79	93.94	111.60
1	B	619	LEU	CA-CB-CG	6.69	130.68	115.30
1	B	93	LEU	CA-CB-CG	5.94	128.96	115.30
1	A	96	ARG	CB-CA-C	-5.94	98.52	110.40
1	B	619	LEU	CB-CG-CD2	5.79	120.85	111.00
1	B	67	VAL	CG1-CB-CG2	-5.77	101.66	110.90
1	B	58	VAL	CG1-CB-CG2	-5.41	102.24	110.90
1	B	68	TRP	CA-CB-CG	-5.41	103.43	113.70
1	A	76	CYS	CA-CB-SG	-5.32	104.42	114.00
1	A	395	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	69	CYS	CA-CB-SG	5.19	123.34	114.00
1	B	399	ILE	CG1-CB-CG2	-5.07	100.25	111.40

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:B:68:TRP:HZ3	1:B:93:LEU:CB	1.41	1.31
1:B:484:ASN:ND2	1:B:487:LYS:HZ3	1.32	1.25
1:A:68:TRP:CE3	1:A:94:SER:O	1.92	1.22
1:A:68:TRP:CZ2	1:A:96:ARG:N	2.09	1.20
1:B:150:SER:HA	1:B:175:ARG:NH2	0.87	1.20
1:A:68:TRP:CH2	1:A:95:GLY:CA	2.26	1.19
1:A:68:TRP:NE1	1:A:96:ARG:O	1.78	1.15
1:B:68:TRP:CZ2	1:B:117:LEU:HD23	1.82	1.13
1:B:68:TRP:HZ2	1:B:117:LEU:CD2	1.60	1.13
1:B:68:TRP:CZ2	1:B:117:LEU:CD2	2.32	1.12
1:B:150:SER:N	1:B:175:ARG:NH2	1.97	1.12
1:A:68:TRP:CZ3	1:A:95:GLY:CA	2.33	1.10
1:B:68:TRP:CZ3	1:B:93:LEU:CB	2.22	1.08
1:A:68:TRP:CZ3	1:A:94:SER:O	2.07	1.08
1:B:68:TRP:HZ2	1:B:117:LEU:HD23	0.93	1.08
1:A:621:GLY:O	1:A:622:ASP:OD2	1.71	1.07
1:B:58:VAL:HG12	1:B:59:PRO:CD	1.89	1.02
1:B:58:VAL:HG12	1:B:59:PRO:HD3	1.02	1.02
1:A:559:LEU:HD12	1:A:562:ILE:HG21	1.44	0.99
1:B:190:GLU:OE2	4:B:801:HOH:O	1.80	0.98
1:A:559:LEU:HD12	1:A:562:ILE:CG2	1.94	0.97
1:B:484:ASN:ND2	1:B:487:LYS:NZ	2.11	0.97
1:A:64:ASN:O	1:A:66:ALA:N	1.98	0.96
1:A:72:SER:O	1:A:74:VAL:N	2.00	0.94
1:B:40:LEU:O	4:B:803:HOH:O	1.86	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ARG:C	1:B:175:ARG:HD2	1.87	0.94
3:B:704:NAG:O7	4:B:802:HOH:O	1.84	0.94
1:B:58:VAL:CG1	1:B:59:PRO:HD3	1.97	0.92
1:A:310:SER:OG	4:A:801:HOH:O	1.86	0.91
1:A:240:ASN:HD22	1:A:241:ILE:H	1.09	0.90
1:B:486:TRP:O	1:B:488:ALA:N	2.05	0.89
1:A:430:ASN:ND2	4:A:807:HOH:O	2.06	0.87
1:A:68:TRP:HE3	1:A:94:SER:O	1.57	0.86
1:B:150:SER:N	1:B:175:ARG:HH21	1.66	0.86
1:B:75:VAL:HG12	4:B:805:HOH:O	1.75	0.86
1:B:614:SER:O	4:B:804:HOH:O	1.93	0.84
1:B:68:TRP:CZ3	1:B:93:LEU:HB2	2.14	0.83
1:B:240:ASN:HD22	1:B:241:ILE:H	1.25	0.83
1:B:619:LEU:HD23	1:B:620:CYS:H	1.45	0.82
1:B:484:ASN:CG	1:B:487:LYS:HZ3	1.83	0.82
1:A:82:GLN:NE2	4:A:813:HOH:O	2.15	0.80
1:B:68:TRP:CZ2	1:B:117:LEU:HD21	2.16	0.79
1:A:62:GLY:HA2	1:A:71:TRP:HZ2	1.48	0.79
1:B:484:ASN:HD22	1:B:487:LYS:HZ3	1.25	0.78
1:A:240:ASN:ND2	1:A:241:ILE:H	1.81	0.78
1:B:75:VAL:O	4:B:805:HOH:O	2.00	0.78
1:B:68:TRP:HZ3	1:B:93:LEU:HB3	0.65	0.78
1:A:149:ILE:HG21	1:A:173:VAL:HG12	1.66	0.78
1:A:309:LEU:H	1:A:331:ASN:HD22	1.32	0.77
1:A:68:TRP:CD1	1:A:69:CYS:N	2.51	0.77
1:A:292:SER:O	1:A:295:ASN:ND2	2.17	0.77
1:A:71:TRP:O	4:A:804:HOH:O	2.02	0.77
1:A:62:GLY:HA2	1:A:71:TRP:CZ2	2.20	0.76
1:B:68:TRP:CH2	1:B:93:LEU:HB2	2.19	0.76
1:A:554:TRP:O	1:A:557:SER:OG	2.03	0.76
1:A:501:LEU:H	1:A:522:ASN:HD22	1.34	0.76
1:A:619:LEU:O	1:A:621:GLY:N	2.19	0.76
1:A:68:TRP:CE2	1:A:96:ARG:O	2.38	0.75
1:A:58:VAL:HB	1:A:59:PRO:HD3	1.67	0.75
1:A:43:LYS:O	4:A:806:HOH:O	2.05	0.74
1:A:456:GLN:O	4:A:805:HOH:O	2.03	0.74
1:A:333:LEU:H	1:A:355:ASN:HD22	1.35	0.74
1:B:484:ASN:CG	1:B:487:LYS:NZ	2.40	0.74
1:B:273:SER:O	1:B:275:LEU:N	2.17	0.73
1:B:63:GLN:CD	1:B:64:ASN:H	1.90	0.73
1:B:430:ASN:ND2	4:B:811:HOH:O	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:VAL:HG12	1:B:94:SER:OG	1.87	0.73
1:B:150:SER:CA	1:B:175:ARG:CZ	2.37	0.73
1:B:64:ASN:O	1:B:66:ALA:N	2.22	0.73
1:B:61:ASN:O	4:B:807:HOH:O	2.07	0.72
1:A:68:TRP:CH2	1:A:96:ARG:N	2.46	0.72
2:C:658:ASN:O	4:C:701:HOH:O	2.07	0.72
1:B:69:CYS:SG	4:B:849:HOH:O	2.48	0.71
1:A:59:PRO:O	4:A:809:HOH:O	2.08	0.71
1:B:150:SER:HA	1:B:175:ARG:HH21	1.38	0.70
3:B:703:NAG:O4	4:B:806:HOH:O	2.01	0.70
1:A:484:ASN:HB3	1:A:487:LYS:HG3	1.73	0.69
1:B:132:THR:HG23	1:B:133:THR:HG23	1.73	0.69
1:B:70:SER:O	4:B:808:HOH:O	2.10	0.69
1:A:240:ASN:HD22	1:A:241:ILE:N	1.87	0.69
1:B:240:ASN:ND2	1:B:241:ILE:H	1.91	0.69
1:A:42:LEU:HA	1:A:91:ARG:HH22	1.58	0.68
1:A:455:ASP:HA	1:A:479:ARG:HH11	1.59	0.68
1:B:619:LEU:CD2	1:B:620:CYS:H	2.05	0.68
3:A:704:NAG:O7	4:A:811:HOH:O	2.12	0.68
1:A:72:SER:OG	1:A:73:GLY:N	2.25	0.68
1:B:456:GLN:OE1	1:B:457:ILE:N	2.23	0.67
1:A:204:LYS:HA	1:A:227:LEU:HA	1.75	0.67
1:B:149:ILE:C	1:B:175:ARG:NH2	2.47	0.67
1:A:67:VAL:HG23	1:A:94:SER:O	1.95	0.67
1:B:484:ASN:HB3	1:B:487:LYS:HE2	1.75	0.67
1:B:614:SER:O	1:B:614:SER:OG	2.12	0.66
1:B:68:TRP:CD1	1:B:96:ARG:O	2.48	0.66
1:B:374:MET:CE	1:B:389:LEU:HD22	2.25	0.66
3:A:704:NAG:O4	4:A:812:HOH:O	2.14	0.66
1:B:68:TRP:CH2	1:B:93:LEU:CB	2.75	0.66
1:A:58:VAL:HB	1:A:59:PRO:CD	2.26	0.66
1:B:373:THR:HG23	1:B:397:LYS:HB3	1.78	0.66
1:A:602:SER:HB3	1:A:619:LEU:HD21	1.78	0.65
1:A:68:TRP:CG	1:A:69:CYS:N	2.60	0.65
1:A:559:LEU:HD21	1:A:583:SER:HB2	1.77	0.65
1:A:501:LEU:H	1:A:522:ASN:ND2	1.95	0.64
1:A:599:PRO:HA	1:A:618:GLY:HA2	1.79	0.64
1:A:455:ASP:HA	1:A:479:ARG:NH1	2.12	0.64
1:A:572:LEU:H	1:A:594:ASN:ND2	1.94	0.64
1:B:63:GLN:OE1	1:B:64:ASN:N	2.31	0.63
1:A:570:ASN:HB2	1:A:594:ASN:HD21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:TRP:O	1:A:70:SER:N	2.32	0.62
1:A:579:ASP:O	1:A:582:SER:OG	2.16	0.62
1:A:307:ASN:HB2	1:A:331:ASN:HD21	1.63	0.62
1:A:456:GLN:HG3	1:A:457:ILE:H	1.63	0.62
1:A:555:GLU:HB2	4:A:825:HOH:O	1.98	0.62
1:A:444:THR:HA	1:A:467:LEU:HA	1.82	0.61
1:A:132:THR:HG23	1:A:133:THR:HG23	1.81	0.61
1:A:456:GLN:HG3	1:A:457:ILE:N	2.16	0.61
1:B:71:TRP:O	1:B:75:VAL:HG23	2.01	0.60
1:A:68:TRP:HZ2	1:A:96:ARG:HB2	1.66	0.60
1:B:374:MET:HE1	1:B:389:LEU:HD22	1.83	0.60
1:A:614:SER:O	1:A:614:SER:OG	2.19	0.60
1:A:78:ASN:O	1:A:80:THR:HG23	2.02	0.59
1:A:318:SER:OG	1:A:340:GLY:HA3	2.03	0.59
1:A:150:SER:OG	1:A:172:ASP:OD1	2.18	0.59
1:A:616:ASN:O	1:A:617:GLU:O	2.21	0.59
1:A:159:ASN:ND2	1:A:161:PHE:H	1.99	0.59
1:A:460:ASP:OD2	1:A:460:ASP:N	2.30	0.59
1:B:162:SER:HG	2:D:651:HIS:N	2.01	0.59
1:A:69:CYS:O	1:A:73:GLY:N	2.36	0.58
1:A:255:ASP:O	1:A:256:VAL:HG12	2.04	0.58
1:A:68:TRP:CZ3	1:A:94:SER:C	2.76	0.58
1:B:71:TRP:CG	1:B:71:TRP:O	2.56	0.58
1:B:75:VAL:O	1:B:78:ASN:ND2	2.36	0.58
1:A:333:LEU:H	1:A:355:ASN:ND2	2.01	0.58
1:A:75:VAL:HG11	4:A:867:HOH:O	2.03	0.58
1:B:244:GLU:N	1:B:244:GLU:OE1	2.33	0.58
1:B:530:TRP:CD1	4:B:821:HOH:O	2.52	0.58
1:B:62:GLY:HA2	1:B:71:TRP:CZ2	2.39	0.58
1:A:590:ASN:HD22	1:A:591:VAL:N	2.02	0.57
1:A:69:CYS:N	1:A:72:SER:HB3	2.19	0.57
1:B:175:ARG:HD2	1:B:175:ARG:O	2.03	0.57
1:A:273:SER:O	1:A:274:ASN:HB2	2.03	0.57
1:A:62:GLY:CA	1:A:71:TRP:HZ2	2.16	0.57
1:B:179:LEU:HD21	1:B:182:LEU:HB2	1.88	0.56
1:A:572:LEU:H	1:A:594:ASN:HD22	1.52	0.56
1:A:162:SER:HG	2:C:651:HIS:N	2.02	0.56
1:B:166:GLU:HB2	4:B:801:HOH:O	2.06	0.56
1:B:577:PRO:HG2	1:B:580:PHE:HE1	1.71	0.56
1:B:43:LYS:CB	1:B:60:VAL:HA	2.36	0.56
1:A:558:THR:O	1:A:560:PRO:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ASN:HB2	1:A:355:ASN:HD21	1.71	0.56
1:A:72:SER:OG	4:A:802:HOH:O	1.91	0.56
1:B:403:ASN:HB2	1:B:427:ASN:HD21	1.70	0.55
1:B:486:TRP:C	1:B:488:ALA:H	2.07	0.55
1:B:91:ARG:HB2	1:B:93:LEU:HG	1.87	0.55
1:B:156:LYS:HA	1:B:179:LEU:HA	1.89	0.55
1:A:161:PHE:HB2	1:A:183:ASN:OD1	2.07	0.55
1:B:240:ASN:HD22	1:B:241:ILE:N	2.01	0.55
1:A:68:TRP:HE3	1:A:68:TRP:H	1.56	0.54
1:A:93:LEU:H	1:A:115:ASN:ND2	2.06	0.54
1:A:91:ARG:H	1:A:115:ASN:HD21	1.55	0.53
1:B:460:ASP:N	1:B:460:ASP:OD2	2.34	0.53
1:A:67:VAL:HG23	1:A:68:TRP:CE3	2.44	0.53
1:B:374:MET:HE1	1:B:389:LEU:CD2	2.39	0.53
1:B:530:TRP:NE1	4:B:821:HOH:O	2.43	0.52
1:B:177:ARG:NH1	1:B:202:ARG:HH21	2.05	0.52
1:A:483:GLU:CD	1:A:483:GLU:H	2.12	0.52
1:A:462:ALA:HB1	1:A:484:ASN:O	2.09	0.52
1:A:562:ILE:O	1:A:585:THR:HG23	2.10	0.52
1:A:436:GLY:N	1:A:460:ASP:OD1	2.41	0.52
1:A:515:TYR:HA	1:A:538:LEU:HA	1.92	0.52
1:A:564:ASP:OD2	1:A:588:THR:HB	2.10	0.52
1:B:68:TRP:HD1	1:B:96:ARG:O	1.90	0.52
1:A:368:ASN:H	1:A:368:ASN:ND2	2.08	0.52
1:A:62:GLY:HA3	1:A:91:ARG:NH1	2.24	0.52
1:A:63:GLN:CD	1:A:64:ASN:H	2.14	0.52
1:A:68:TRP:CH2	1:A:95:GLY:C	2.83	0.52
1:A:355:ASN:C	3:A:705:NAG:H81	2.30	0.51
1:B:187:SER:C	1:B:211:ASN:HD22	2.14	0.51
1:B:318:SER:OG	1:B:340:GLY:HA3	2.10	0.51
1:B:397:LYS:HG2	1:B:399:ILE:HD13	1.90	0.51
1:B:515:TYR:HA	1:B:538:LEU:HA	1.91	0.51
1:A:68:TRP:CZ2	1:A:96:ARG:CA	2.90	0.51
1:A:88:LEU:HB2	1:A:112:LEU:HD23	1.91	0.51
1:A:294:SER:HA	1:A:320:LEU:HD21	1.93	0.51
1:B:356:ASN:OD1	1:B:356:ASN:O	2.29	0.51
1:B:156:LYS:HE3	1:B:180:GLU:OE1	2.11	0.50
1:B:564:ASP:OD2	1:B:588:THR:HB	2.11	0.50
1:B:185:GLY:HA3	1:B:207:HIS:CD2	2.47	0.50
1:A:573:THR:HG22	1:A:595:GLN:HB2	1.92	0.50
3:B:701:NAG:O4	4:B:810:HOH:O	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:H	1:A:115:ASN:HD22	1.58	0.50
1:A:620:CYS:C	1:A:622:ASP:H	2.14	0.50
1:B:144:SER:HA	1:B:166:GLU:O	2.12	0.50
1:B:484:ASN:HB3	1:B:487:LYS:CE	2.41	0.50
1:B:78:ASN:O	1:B:79:VAL:HG12	2.12	0.50
1:A:557:SER:HA	1:A:559:LEU:HD22	1.93	0.50
1:A:600:ILE:HD12	1:A:618:GLY:HA3	1.94	0.49
1:B:69:CYS:SG	1:B:96:ARG:HB2	2.52	0.49
1:A:68:TRP:HZ3	1:A:94:SER:O	1.84	0.49
1:B:255:ASP:O	1:B:256:VAL:HG12	2.11	0.49
1:A:68:TRP:HZ2	1:A:96:ARG:H	1.32	0.49
1:B:102:ARG:HG3	1:B:103:TYR:CD2	2.48	0.49
1:B:45:SER:O	1:B:47:SER:N	2.39	0.49
1:A:78:ASN:C	1:A:80:THR:HG23	2.33	0.49
1:A:68:TRP:HZ2	1:A:96:ARG:CB	2.26	0.49
1:A:63:GLN:CG	1:A:64:ASN:H	2.26	0.48
1:A:355:ASN:O	3:A:705:NAG:H81	2.13	0.48
1:A:499:SER:H	1:A:522:ASN:HD21	1.62	0.48
1:A:155:LEU:HD21	1:A:158:PHE:HB2	1.96	0.48
1:A:121:PHE:HE1	1:A:136:ILE:CD1	2.27	0.48
1:A:273:SER:C	1:A:275:LEU:H	2.17	0.48
1:A:47:SER:CB	1:A:80:THR:HG21	2.44	0.48
1:A:559:LEU:CD2	1:A:583:SER:HB2	2.44	0.48
1:B:167:GLY:N	4:B:801:HOH:O	1.99	0.48
1:B:273:SER:C	1:B:275:LEU:H	2.11	0.48
1:A:159:ASN:HD22	1:A:160:ALA:N	2.12	0.47
1:B:257:SER:HB2	1:B:281:PHE:O	2.14	0.47
1:B:368:ASN:H	1:B:368:ASN:ND2	2.11	0.47
1:A:333:LEU:N	1:A:355:ASN:HD22	2.08	0.47
1:A:63:GLN:CD	1:A:64:ASN:N	2.68	0.47
1:A:99:ILE:O	1:A:102:ARG:HG2	2.15	0.47
1:A:256:VAL:O	1:A:256:VAL:HG13	2.15	0.47
1:B:227:LEU:HD21	1:B:230:MET:HB2	1.97	0.47
1:A:244:GLU:N	1:A:244:GLU:OE1	2.42	0.47
1:B:590:ASN:HD22	1:B:591:VAL:N	2.12	0.47
1:B:59:PRO:HA	4:B:854:HOH:O	2.15	0.47
1:A:290:PRO:HG2	1:A:293:TYR:CZ	2.50	0.46
1:B:41:SER:HA	4:B:803:HOH:O	2.15	0.46
1:B:444:THR:HA	1:B:467:LEU:HA	1.96	0.46
1:A:268:GLU:N	1:A:268:GLU:OE1	2.33	0.46
1:A:456:GLN:CG	1:A:457:ILE:H	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ASN:CB	1:A:487:LYS:HG3	2.45	0.46
1:B:256:VAL:O	1:B:256:VAL:HG13	2.15	0.46
1:A:309:LEU:H	1:A:331:ASN:ND2	2.08	0.46
1:A:600:ILE:O	1:A:619:LEU:HB2	2.15	0.46
1:A:77:ASP:O	1:A:79:VAL:N	2.48	0.46
1:A:413:LEU:HA	1:A:413:LEU:HD12	1.80	0.46
1:A:615:SER:O	1:A:616:ASN:OD1	2.34	0.45
1:B:558:THR:O	1:B:558:THR:HG22	2.17	0.45
1:B:88:LEU:HB2	1:B:112:LEU:HD23	1.98	0.45
1:B:575:THR:HA	1:B:597:ILE:O	2.16	0.45
1:A:590:ASN:ND2	1:A:592:SER:H	2.14	0.45
1:B:150:SER:CA	1:B:175:ARG:HH21	1.88	0.45
1:B:209:ALA:HA	1:B:233:GLY:O	2.17	0.45
1:B:228:GLN:O	1:B:251:LEU:HD12	2.17	0.45
1:B:355:ASN:C	3:B:705:NAG:H81	2.37	0.45
1:A:474:THR:HA	1:A:498:PHE:O	2.17	0.44
1:B:68:TRP:HH2	1:B:93:LEU:HB2	1.74	0.44
1:A:577:PRO:O	1:A:580:PHE:HD1	1.99	0.44
1:A:583:SER:OG	1:A:585:THR:HG22	2.18	0.44
1:B:149:ILE:O	1:B:175:ARG:NH2	2.51	0.44
1:A:322:ASN:ND2	4:A:822:HOH:O	2.41	0.44
1:B:161:PHE:HB2	1:B:183:ASN:OD1	2.18	0.44
1:B:475:ASN:O	1:B:476:PHE:HB2	2.18	0.44
1:A:100:GLN:O	1:A:103:TYR:HD1	2.01	0.44
3:A:704:NAG:H61	4:A:838:HOH:O	2.17	0.44
1:B:588:THR:HG23	1:B:612:PHE:CZ	2.53	0.44
1:A:57:LYS:O	1:A:58:VAL:HG13	2.18	0.44
1:B:170:PRO:O	1:B:173:VAL:HG23	2.18	0.44
1:B:577:PRO:O	1:B:580:PHE:HD1	2.01	0.44
1:B:68:TRP:CG	1:B:69:CYS:N	2.82	0.44
1:B:151:LYS:HG3	1:B:151:LYS:H	1.44	0.44
1:B:386:PRO:HG2	1:B:389:LEU:HD21	2.00	0.43
1:B:108:LEU:O	1:B:132:THR:HG22	2.17	0.43
1:A:76:CYS:SG	1:A:100:GLN:O	2.74	0.43
1:A:541:LEU:HD11	1:A:543:LEU:HD21	1.99	0.43
1:A:480:LYS:HB2	1:A:480:LYS:HE3	1.85	0.43
1:A:620:CYS:O	1:A:622:ASP:N	2.49	0.43
1:A:257:SER:HB2	1:A:281:PHE:O	2.19	0.43
1:B:136:ILE:HA	1:B:136:ILE:HD13	1.77	0.43
1:B:172:ASP:O	1:B:175:ARG:HG3	2.19	0.43
1:A:492:GLN:HB3	1:A:515:TYR:CE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:PRO:HG2	1:A:580:PHE:HE1	1.82	0.43
1:B:482:PRO:HG2	1:B:485:ILE:HB	2.00	0.43
1:B:79:VAL:O	1:B:79:VAL:HG13	2.19	0.43
1:A:107:LEU:HD12	1:A:128:LEU:HD13	2.01	0.43
1:B:573:THR:HG22	1:B:595:GLN:HB2	2.01	0.43
1:B:63:GLN:CG	1:B:64:ASN:H	2.31	0.43
1:A:314:PRO:HG2	1:A:317:PHE:CE1	2.54	0.43
1:A:159:ASN:ND2	1:A:183:ASN:HB3	2.34	0.42
1:A:315:SER:O	1:A:318:SER:HB2	2.19	0.42
1:A:368:ASN:H	1:A:368:ASN:HD22	1.66	0.42
1:A:559:LEU:HD12	1:A:562:ILE:HG22	1.92	0.42
1:B:67:VAL:CG1	1:B:94:SER:OG	2.64	0.42
1:A:360:VAL:HG22	1:A:383:GLY:HA3	2.00	0.42
1:A:88:LEU:HD12	1:A:112:LEU:CD2	2.50	0.42
1:A:201:GLN:O	1:A:202:ARG:CB	2.66	0.42
1:B:155:LEU:HD21	1:B:158:PHE:HB2	2.02	0.42
1:A:68:TRP:CZ3	1:A:95:GLY:N	2.86	0.42
1:B:107:LEU:HD23	1:B:107:LEU:HA	1.81	0.42
1:A:442:ASN:ND2	4:A:803:HOH:O	1.94	0.42
1:A:323:LEU:HD23	1:A:323:LEU:HA	1.82	0.42
1:B:403:ASN:HB3	1:B:404:MET:H	1.74	0.42
1:B:187:SER:H	1:B:211:ASN:ND2	2.18	0.42
1:A:395:LEU:HD11	1:A:398:LEU:HB2	2.01	0.41
1:B:118:GLU:HG2	1:B:119:GLY:H	1.85	0.41
1:B:570:ASN:HB3	1:B:571:LEU:H	1.71	0.41
1:B:242:PRO:HG2	1:B:245:PHE:CE1	2.56	0.41
1:A:69:CYS:HA	1:A:98:PRO:HG3	2.03	0.41
1:A:252:LYS:HA	1:A:275:LEU:HA	2.02	0.41
1:B:566:ASP:OD1	1:B:590:ASN:HB3	2.21	0.41
1:A:508:TYR:CE2	1:A:532:ILE:HD12	2.56	0.41
1:A:69:CYS:O	1:A:73:GLY:HA3	2.21	0.41
1:A:590:ASN:HD22	1:A:592:SER:H	1.69	0.41
1:B:420:TRP:CD1	1:B:444:THR:HG23	2.56	0.41
1:B:451:ASN:HB3	1:B:452:ARG:H	1.66	0.41
3:B:704:NAG:O3	3:B:704:NAG:H82	2.20	0.41
1:B:42:LEU:HA	1:B:91:ARG:HH22	1.84	0.41
2:C:658:ASN:HA	2:C:659:PRO:HD3	1.93	0.41
1:A:471:ASN:OD1	1:A:473:SER:HB3	2.20	0.41
1:A:443:LEU:HD21	1:A:446:VAL:HG21	2.02	0.41
1:A:438:GLY:HA3	1:A:460:ASP:O	2.21	0.41
1:B:580:PHE:HB3	1:B:605:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLY:HA3	1:A:91:ARG:HH12	1.86	0.40
1:B:150:SER:O	1:B:175:ARG:NH1	2.54	0.40
1:B:307:ASN:HB3	1:B:308:GLN:H	1.74	0.40
1:A:556:ILE:O	1:A:559:LEU:HD13	2.20	0.40
1:A:240:ASN:ND2	1:A:241:ILE:N	2.57	0.40
1:B:414:THR:O	1:B:440:LEU:HD21	2.22	0.40
1:B:64:ASN:O	1:B:65:ASP:C	2.59	0.40

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

### 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	573/613 (94%)	482 (84%)	71 (12%)	20 (4%)	4	8
1	B	573/613 (94%)	491 (86%)	69 (12%)	13 (2%)	7	17
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%)	6	12

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ASP
1	A	69	CYS
1	A	72	SER

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Mol	Chain	Res	Type
1	A	73	GLY
1	A	80	THR
1	A	491	LEU
1	A	559	LEU
1	A	614	SER
1	A	617	GLU
1	A	620	CYS
1	A	622	ASP
1	A	623	LEU
1	B	486	TRP
1	B	487	LYS
1	B	614	SER
1	A	68	TRP
1	A	621	GLY
1	B	65	ASP
1	B	78	ASN
1	B	616	ASN
1	A	455	ASP
1	A	489	PRO
1	B	455	ASP
1	B	476	PHE
1	A	78	ASN
1	B	489	PRO
1	B	622	ASP
1	A	58	VAL
1	B	70	SER
1	A	488	ALA
1	B	274	ASN
1	B	256	VAL
1	A	256	VAL

### 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	505/544 (93%)	494 (98%)	11 (2%)	57 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	505/544 (93%)	492 (97%)	13 (3%)	51	79
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%)	56	82

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

Mol	Chain	Res	Type
1	A	70	SER
1	A	82	GLN
1	A	159	ASN
1	A	175	ARG
1	A	202	ARG
1	A	240	ASN
1	A	318	SER
1	A	371	LEU
1	A	421	ARG
1	A	557	SER
1	A	590	ASN
1	B	64	ASN
1	B	70	SER
1	B	177	ARG
1	B	240	ASN
1	B	348	THR
1	B	371	LEU
1	B	444	THR
1	B	491	LEU
1	B	575	THR
1	B	582	SER
1	B	590	ASN
1	B	591	VAL
1	B	622	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	159	ASN
1	A	240	ASN
1	A	331	ASN

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Mol	Chain	Res	Type
1	A	355	ASN
1	A	522	ASN
1	A	546	ASN
1	A	590	ASN
1	A	594	ASN
1	B	64	ASN
1	B	207	HIS
1	B	211	ASN
1	B	228	GLN
1	B	240	ASN
1	B	267	GLN
1	B	368	ASN
1	B	393	ASN
1	B	427	ASN
1	B	468	GLN
1	B	484	ASN
1	B	492	GLN
1	B	545	GLN
1	B	590	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	C	654	2	7,8,9	1.00	0	5,10,12	2.08	2 (40%)
2	HYP	C	657	2	7,8,9	1.30	1 (14%)	5,10,12	1.70	2 (40%)
2	HYP	D	654	2	7,8,9	0.90	0	5,10,12	2.32	3 (60%)
2	HYP	D	657	2	7,8,9	1.36	1 (14%)	5,10,12	1.80	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	C	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	D	654	2	-	0/0/11/13	0/1/1/1
2	HYP	D	657	2	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	657	HYP	CA-C	3.11	1.54	1.50
2	C	657	HYP	CA-C	3.13	1.54	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	654	HYP	OD1-CG-CB	-2.05	105.02	110.14
2	D	657	HYP	CG-CB-CA	2.13	106.74	103.93
2	C	657	HYP	CG-CB-CA	2.19	106.82	103.93
2	C	654	HYP	CB-CG-CD	2.58	106.75	103.33
2	C	657	HYP	CB-CG-CD	2.73	106.94	103.33
2	D	654	HYP	CB-CG-CD	2.92	107.20	103.33
2	D	657	HYP	CB-CG-CD	2.94	107.22	103.33
2	D	654	HYP	CG-CB-CA	3.14	108.07	103.93
2	C	654	HYP	CG-CB-CA	3.15	108.08	103.93

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](#)

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	0.92	1 (7%)	15,19,21	0.84	0
3	NAG	A	702	1	14,14,15	0.47	0	15,19,21	1.27	2 (13%)
3	NAG	A	703	1	14,14,15	0.90	2 (14%)	15,19,21	0.87	1 (6%)
3	NAG	A	704	1	14,14,15	1.04	2 (14%)	15,19,21	0.90	1 (6%)
3	NAG	A	705	1	14,14,15	0.83	1 (7%)	15,19,21	1.07	1 (6%)
3	NAG	B	701	1	14,14,15	1.23	2 (14%)	15,19,21	0.76	0
3	NAG	B	702	1	14,14,15	1.02	1 (7%)	15,19,21	1.27	2 (13%)
3	NAG	B	703	1	14,14,15	0.85	1 (7%)	15,19,21	1.00	1 (6%)
3	NAG	B	704	1	14,14,15	1.34	2 (14%)	15,19,21	1.82	1 (6%)
3	NAG	B	705	1	14,14,15	0.70	1 (7%)	15,19,21	0.98	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	A	701	1	-	0/6/23/26	0/1/1/1
3	NAG	A	702	1	-	0/6/23/26	0/1/1/1
3	NAG	A	703	1	-	0/6/23/26	0/1/1/1
3	NAG	A	704	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	701	1	-	0/6/23/26	0/1/1/1
3	NAG	B	702	1	-	0/6/23/26	0/1/1/1
3	NAG	B	703	1	-	0/6/23/26	0/1/1/1
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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	NAG	C1-C2	-3.20	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	705	NAG	O5-C1	-2.69	1.39	1.43
3	B	705	NAG	O5-C1	-2.22	1.40	1.43
3	A	703	NAG	C1-C2	2.19	1.55	1.52
3	B	703	NAG	C1-C2	2.26	1.55	1.52
3	B	701	NAG	C1-C2	2.26	1.55	1.52
3	A	704	NAG	C1-C2	2.26	1.55	1.52
3	A	703	NAG	O5-C1	2.28	1.47	1.43
3	B	704	NAG	C1-C2	2.42	1.55	1.52
3	A	701	NAG	O5-C1	2.67	1.48	1.43
3	A	704	NAG	O5-C1	3.08	1.48	1.43
3	B	701	NAG	O5-C1	3.91	1.50	1.43
3	B	704	NAG	O5-C1	4.37	1.50	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	NAG	C1-O5-C5	2.02	114.94	112.17
3	B	702	NAG	C3-C4-C5	2.10	113.92	110.22
3	A	705	NAG	C1-C2-N2	2.16	114.18	110.49
3	A	704	NAG	C1-O5-C5	2.37	115.44	112.17
3	B	703	NAG	C1-O5-C5	2.48	115.59	112.17
3	A	702	NAG	C1-O5-C5	2.71	115.89	112.17
3	A	702	NAG	C3-C4-C5	3.29	116.01	110.22
3	B	702	NAG	C1-O5-C5	3.66	117.22	112.17
3	B	704	NAG	C1-O5-C5	6.66	121.34	112.17

There are no chirality outliers.

There are no torsion outliers.

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	701	NAG	1	0
3	B	703	NAG	1	0
3	B	704	NAG	2	0
3	B	705	NAG	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, 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	A	577/613 (94%)	0.60	35 (6%) 22 22	40, 61, 93, 135	0
1	B	577/613 (94%)	0.59	39 (6%) 18 17	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%) 21 20	37, 61, 93, 135	0

All (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
1	A	67	VAL	4.5
1	B	65	ASP	4.3
1	B	455	ASP	4.1
1	A	559	LEU	3.9
1	B	483	GLU	3.8
1	A	68	TRP	3.8
1	A	77	ASP	3.8
1	B	75	VAL	3.7
1	A	256	VAL	3.6
1	A	313	ILE	3.5
1	A	620	CYS	3.4
1	A	411	LYS	3.4
1	A	66	ALA	3.3
1	A	71	TRP	3.3
1	A	467	LEU	3.0
1	B	413	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	74	VAL	2.9
1	B	197	TYR	2.8
1	A	197	TYR	2.8
1	A	198	GLY	2.8
1	B	67	VAL	2.7
1	B	81	ALA	2.7
1	A	65	ASP	2.7
1	B	71	TRP	2.7
1	A	245	PHE	2.7
1	B	77	ASP	2.7
1	B	318	SER	2.6
1	B	60	VAL	2.6
1	B	508	TYR	2.6
1	A	623	LEU	2.6
1	B	79	VAL	2.5
1	A	413	LEU	2.5
1	A	222	GLY	2.5
1	B	419	LEU	2.5
1	A	221	LEU	2.5
1	A	374	MET	2.5
1	A	278	LEU	2.5
1	A	97	ILE	2.4
1	B	482	PRO	2.4
1	A	200	LEU	2.4
1	A	95	GLY	2.4
1	B	429	LEU	2.4
1	B	103	TYR	2.4
1	A	80	THR	2.3
1	B	172	ASP	2.3
1	A	75	VAL	2.3
1	A	603	GLY	2.3
1	B	156	LYS	2.3
1	B	603	GLY	2.3
1	B	241	ILE	2.3
1	B	530	TRP	2.3
1	B	180	GLU	2.2
1	B	461	PHE	2.2
1	B	415	ARG	2.2
1	B	158	PHE	2.2
1	A	605	PHE	2.2
1	A	247	LEU	2.1
1	B	173	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	204	LYS	2.1
1	B	95	GLY	2.1
1	B	409	LEU	2.1
1	B	74	VAL	2.1
1	B	414	THR	2.1
1	A	280	LEU	2.1
1	A	220	ARG	2.1
1	A	149	ILE	2.0
1	B	76	CYS	2.0
1	B	480	LYS	2.0
1	A	452	ARG	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	657	8/9	0.97	0.17	-	61,65,68,72	0
2	HYP	C	657	8/9	0.97	0.19	-	67,71,72,77	0
2	HYP	C	654	8/9	0.95	0.18	-	66,70,74,79	0
2	HYP	D	654	8/9	0.97	0.18	-	63,67,70,74	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( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	701	14/15	0.90	0.17	-0.71	50,59,68,69	0
3	NAG	B	701	14/15	0.89	0.16	-0.97	39,57,66,68	0
3	NAG	B	703	14/15	0.97	0.15	-1.60	25,37,50,55	0
3	NAG	A	703	14/15	0.95	0.15	-1.78	29,41,52,53	0
3	NAG	B	704	14/15	0.80	0.17	-	66,84,92,95	0
3	NAG	A	702	14/15	0.88	0.17	-	76,91,101,101	0
3	NAG	A	705	14/15	0.94	0.23	-	56,69,81,83	0
3	NAG	B	705	14/15	0.88	0.19	-	54,74,87,91	0
3	NAG	B	702	14/15	0.80	0.24	-	83,95,103,103	0
3	NAG	A	704	14/15	0.86	0.11	-	81,92,109,112	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.