



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:37 am GMT

PDB ID : 2V5S  
Title : STRUCTURAL BASIS FOR DSCAM ISOFORM SPECIFICITY  
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Deposited on : 2007-07-09  
Resolution : 2.30 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 : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

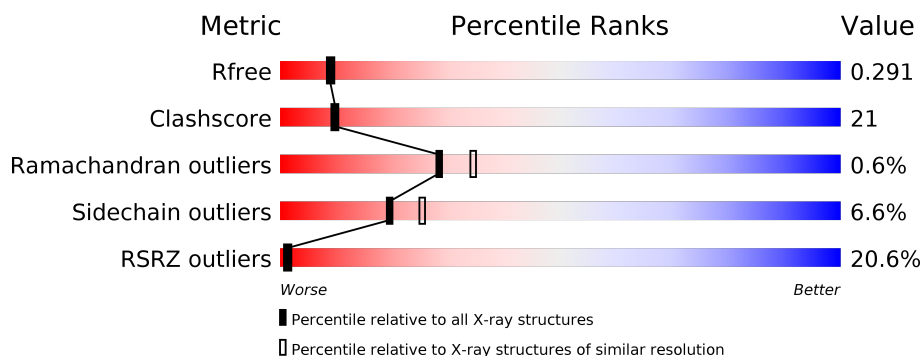
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	394	
1	B	394	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1391	X	-	X	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6627 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 DSCAM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	19	0
			3110	1962	538	597	13			
1	B	394	Total	C	N	O	S	0	21	0
			3159	1994	545	607	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	EXPRESSION TAG	UNP Q9NBA1
A	-4	TYR	-	EXPRESSION TAG	UNP Q9NBA1
A	-3	PHE	-	EXPRESSION TAG	UNP Q9NBA1
A	-2	GLN	-	EXPRESSION TAG	UNP Q9NBA1
A	-1	GLY	-	EXPRESSION TAG	UNP Q9NBA1
A	0	ASP	-	EXPRESSION TAG	UNP Q9NBA1
A	207	ILE	VAL	VARIANT SEE REMARK 99	UNP Q9NBA1
A	211	ALA	PRO	VARIANT SEE REMARK 99	UNP Q9NBA1
A	213	ARG	LYS	VARIANT SEE REMARK 99	UNP Q9NBA1
A	214	THR	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
A	215	PRO	ASN	VARIANT SEE REMARK 99	UNP Q9NBA1
A	216	ALA	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
A	218	VAL	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
A	219	GLN	TYR	VARIANT SEE REMARK 99	UNP Q9NBA1
A	222	LEU	ASN	VARIANT SEE REMARK 99	UNP Q9NBA1
A	223	GLU	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
A	224	LEU	VAL	VARIANT SEE REMARK 99	UNP Q9NBA1
A	225	MET	GLU	VARIANT SEE REMARK 99	UNP Q9NBA1
A	226	VAL	SER	VARIANT SEE REMARK 99	UNP Q9NBA1
A	227	ALA	MET	VARIANT SEE REMARK 99	UNP Q9NBA1
A	228	HIS	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
A	229	THR	SER	VARIANT SEE REMARK 99	UNP Q9NBA1
A	230	ILE	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
A	231	SER	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
A	232	LEU	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	239	PHE	TYR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	-5	ALA	-	EXPRESSION TAG	UNP Q9NBA1
B	-4	TYR	-	EXPRESSION TAG	UNP Q9NBA1
B	-3	PHE	-	EXPRESSION TAG	UNP Q9NBA1
B	-2	GLN	-	EXPRESSION TAG	UNP Q9NBA1
B	-1	GLY	-	EXPRESSION TAG	UNP Q9NBA1
B	0	ASP	-	EXPRESSION TAG	UNP Q9NBA1
B	207	ILE	VAL	VARIANT SEE REMARK 99	UNP Q9NBA1
B	211	ALA	PRO	VARIANT SEE REMARK 99	UNP Q9NBA1
B	213	ARG	LYS	VARIANT SEE REMARK 99	UNP Q9NBA1
B	214	THR	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
B	215	PRO	ASN	VARIANT SEE REMARK 99	UNP Q9NBA1
B	216	ALA	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	218	VAL	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	219	GLN	TYR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	222	LEU	ASN	VARIANT SEE REMARK 99	UNP Q9NBA1
B	223	GLU	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
B	224	LEU	VAL	VARIANT SEE REMARK 99	UNP Q9NBA1
B	225	MET	GLU	VARIANT SEE REMARK 99	UNP Q9NBA1
B	226	VAL	SER	VARIANT SEE REMARK 99	UNP Q9NBA1
B	227	ALA	MET	VARIANT SEE REMARK 99	UNP Q9NBA1
B	228	HIS	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
B	229	THR	SER	VARIANT SEE REMARK 99	UNP Q9NBA1
B	230	ILE	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	231	SER	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
B	232	LEU	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
B	239	PHE	TYR	VARIANT SEE REMARK 99	UNP Q9NBA1

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

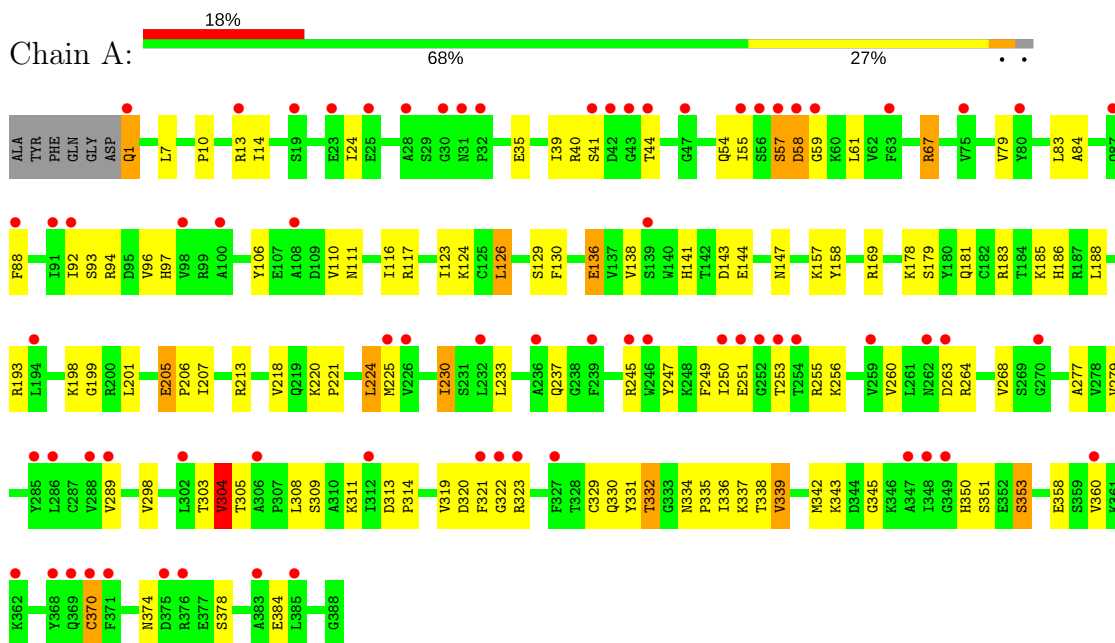
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total 119	O 119	0	0
3	B	127	Total 127	O 127	0	0

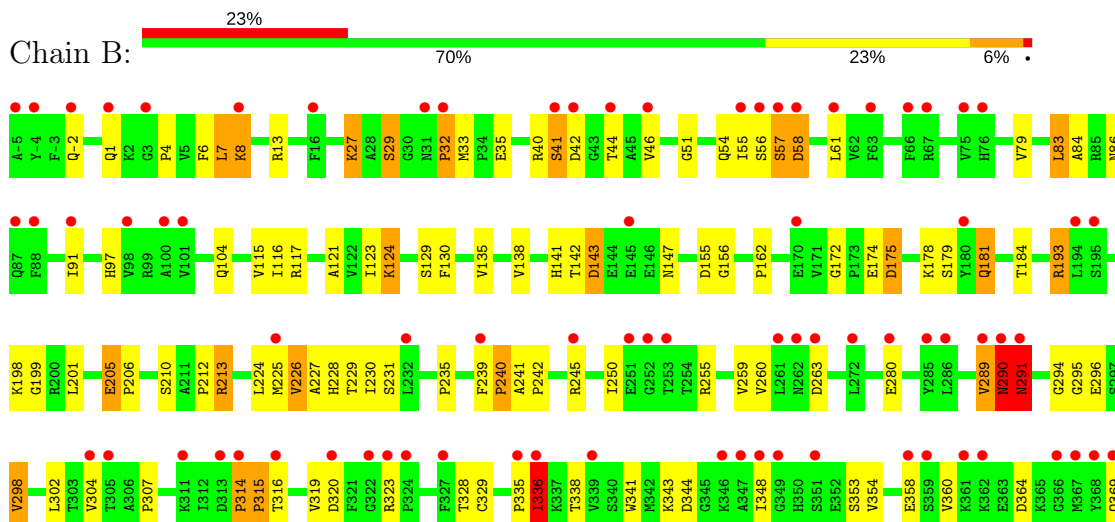
### 3 Residue-property plots

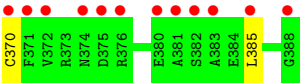
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: DSCAM



#### • Molecule 1: DSCAM







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.77Å 166.84Å 125.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.30 19.90 – 2.29	Depositor EDS
% Data completeness (in resolution range)	95.6 (19.99-2.30) 94.7 (19.90-2.29)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 2.28Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.227 , 0.287 0.235 , 0.291	Depositor DCC
$R_{free}$ test set	2254 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 67.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6627	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.25 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.8332e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 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	0.46	0/3243	1.17	12/4394 (0.3%)
1	B	0.48	1/3299 (0.0%)	1.18	8/4470 (0.2%)
All	All	0.47	1/6542 (0.0%)	1.18	20/8864 (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	A	0	4
1	B	0	7
2	B	1	0
All	All	1	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	-2	GLN	CD-OE1	6.29	1.37	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	MET	N-CA-C	-9.04	86.58	111.00
1	A	183	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	B	143[A]	ASP	CB-CG-OD1	7.54	125.09	118.30
1	B	143[B]	ASP	CB-CG-OD1	7.54	125.09	118.30
1	B	213	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	233	LEU	CB-CG-CD2	-6.96	99.17	111.00
1	A	158	TYR	CB-CG-CD2	-6.13	117.32	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	ARG	CB-CA-C	-5.97	98.46	110.40
1	A	353	SER	N-CA-CB	-5.90	101.64	110.50
1	B	175	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	126	LEU	CB-CG-CD1	5.68	120.66	111.00
1	A	322	GLY	N-CA-C	-5.65	98.97	113.10
1	A	264	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	304	VAL	N-CA-C	5.60	126.12	111.00
1	A	370	CYS	CA-CB-SG	-5.40	104.28	114.00
1	A	67	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	290	ASN	N-CA-C	5.33	125.39	111.00
1	B	336	ILE	N-CA-C	5.25	125.16	111.00
1	A	264	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	339	VAL	CB-CA-C	-5.01	101.88	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1391	NAG	C1

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	THR	Peptide
1	A	321	PHE	Peptide
1	A	41	SER	Peptide
1	A	59	GLY	Peptide
1	B	155	ASP	Peptide
1	B	240	PRO	Peptide
1	B	290	ASN	Mainchain
1	B	314	PRO	Peptide
1	B	32	PRO	Peptide
1	B	335	PRO	Peptide
1	B	41	SER	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	3110	0	3088	119	2
1	B	3159	0	3123	146	2
2	A	56	0	50	2	0
2	B	56	0	50	33	0
3	A	119	0	0	27	1
3	B	127	0	0	19	0
All	All	6627	0	6311	269	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 21.

All (269) 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:291[B]:ASN:ND2	1:B:294:GLY:O	1.75	1.20
1:B:294:GLY:O	2:B:1391:NAG:C1	1.91	1.19
1:B:291[A]:ASN:ND2	1:B:294:GLY:O	1.76	1.17
1:A:106:TYR:O	3:A:2019:HOH:O	1.62	1.16
2:B:1391:NAG:H82	3:B:2110:HOH:O	1.48	1.13
1:A:224:LEU:HD22	1:A:230[A]:ILE:HD11	1.23	1.12
1:A:298:VAL:HG23	3:A:2092:HOH:O	1.48	1.11
1:A:117:ARG:HD2	1:A:205[B]:GLU:OE1	1.53	1.07
1:B:295:GLY:HA3	2:B:1391:NAG:C5	1.88	1.03
1:A:224:LEU:HD22	1:A:230[A]:ILE:CD1	1.92	1.00
1:B:295:GLY:HA3	2:B:1391:NAG:C6	1.93	0.97
1:B:143[A]:ASP:OD2	1:B:179:SER:HB3	1.65	0.95
1:A:44:THR:HG22	3:A:2005:HOH:O	1.66	0.94
1:B:295:GLY:HA3	2:B:1391:NAG:O5	1.67	0.92
1:B:295:GLY:CA	2:B:1391:NAG:C6	2.48	0.92
1:B:295:GLY:HA3	2:B:1391:NAG:H61	1.54	0.90
1:B:295:GLY:CA	2:B:1391:NAG:H61	2.02	0.90
1:B:224:LEU:HD22	1:B:230[A]:ILE:CG1	2.03	0.89
1:B:298:VAL:HG12	3:B:2114:HOH:O	1.71	0.88
1:B:206:PRO:CB	3:B:2074:HOH:O	2.21	0.88
1:B:224:LEU:HD22	1:B:230[B]:ILE:CG1	2.04	0.88
1:A:61:LEU:HD12	3:A:2010:HOH:O	1.76	0.86
1:A:350:HIS:ND1	3:A:2103:HOH:O	2.08	0.86
1:A:54:GLN:O	3:A:2010:HOH:O	1.94	0.85
1:A:224:LEU:HD13	1:A:230[B]:ILE:HG12	1.56	0.85
1:B:295:GLY:C	2:B:1391:NAG:H61	1.96	0.85
1:A:116:ILE:HG23	1:A:206:PRO:HG3	1.57	0.84
1:B:294:GLY:O	2:B:1391:NAG:O5	1.95	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:PHE:HA	3:B:2037:HOH:O	1.78	0.83
2:B:1391:NAG:O6	2:B:1392:NAG:N2	2.12	0.83
1:A:343:LYS:HG2	3:A:2108:HOH:O	1.79	0.82
1:B:4:PRO:HA	1:B:29:SER:O	1.80	0.80
1:A:250:ILE:HD12	1:A:255:ARG:HB2	1.64	0.80
1:B:295:GLY:CA	2:B:1391:NAG:O5	2.29	0.80
1:A:141:HIS:HD2	1:A:147:ASN:HD22	1.29	0.79
1:B:290:ASN:HA	1:B:291[A]:ASN:ND2	1.99	0.78
1:A:141:HIS:CD2	1:A:147:ASN:HD22	2.02	0.78
2:B:1392:NAG:O7	2:B:1392:NAG:O3	2.01	0.78
1:B:225[B]:MET:HE3	1:B:307:PRO:HD3	1.65	0.77
1:A:67:ARG:HA	2:A:1389:NAG:H83	1.65	0.76
1:B:40:ARG:HB2	3:B:2015:HOH:O	1.84	0.76
1:A:323:ARG:O	1:A:360:VAL:HG22	1.86	0.75
1:A:44:THR:CG2	3:A:2005:HOH:O	2.27	0.75
1:B:290:ASN:HA	1:B:291[B]:ASN:ND2	2.00	0.75
1:B:116:ILE:HG23	1:B:206:PRO:HG3	1.70	0.73
1:B:7:LEU:HD21	1:B:29:SER:CB	2.18	0.73
1:A:250:ILE:O	1:A:253:THR:OG1	2.06	0.73
1:B:206:PRO:CA	3:B:2074:HOH:O	2.36	0.72
1:A:129:SER:O	1:B:213:ARG:HD3	1.89	0.72
1:A:116:ILE:H	1:A:237:GLN:NE2	1.88	0.72
1:B:7:LEU:HD21	1:B:29:SER:HB2	1.70	0.72
2:A:1389:NAG:H81	3:A:2116:HOH:O	1.90	0.71
1:A:224:LEU:HD13	1:A:230[A]:ILE:HD13	1.72	0.71
1:B:323:ARG:O	1:B:360:VAL:HG22	1.91	0.70
1:B:290:ASN:HA	2:B:1391:NAG:C1	2.22	0.69
1:B:225[B]:MET:CE	1:B:307:PRO:HD3	2.22	0.69
1:A:224:LEU:HD13	1:A:230[A]:ILE:CG1	2.23	0.69
1:A:143[A]:ASP:OD2	1:A:179:SER:HB3	1.93	0.68
1:A:224:LEU:CD2	1:A:230[A]:ILE:HD11	2.14	0.68
1:B:224:LEU:HD22	1:B:230[A]:ILE:HD11	1.75	0.68
1:B:40:ARG:HG3	1:B:46:VAL:HG12	1.73	0.68
1:B:123:ILE:HD11	1:B:201:LEU:HD21	1.75	0.68
1:B:290:ASN:CG	2:B:1391:NAG:H5	2.13	0.68
1:B:13[A]:ARG:HD2	3:B:2008:HOH:O	1.94	0.68
1:B:343:LYS:NZ	1:B:344:ASP:OD2	2.28	0.67
1:B:294:GLY:C	2:B:1391:NAG:O5	2.32	0.66
1:B:295:GLY:CA	2:B:1391:NAG:C5	2.69	0.66
1:B:290:ASN:OD1	2:B:1391:NAG:H5	1.94	0.66
1:B:224:LEU:HD22	1:B:230[A]:ILE:CD1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245[A]:ARG:HD2	3:B:2092:HOH:O	1.94	0.66
1:A:124[A]:LYS:HD2	1:A:126:LEU:HD23	1.76	0.66
1:A:116:ILE:HG23	1:A:206:PRO:CG	2.25	0.65
1:A:250:ILE:HB	1:A:253:THR:OG1	1.97	0.65
1:A:224:LEU:HD13	1:A:230[A]:ILE:CD1	2.26	0.65
1:B:226:VAL:O	1:B:227:ALA:HB3	1.97	0.65
1:A:308:LEU:HA	1:A:332:THR:O	1.98	0.63
2:B:1392:NAG:C7	2:B:1392:NAG:O3	2.44	0.63
1:A:79:VAL:HG22	1:A:97:HIS:ND1	2.14	0.63
1:B:130:PHE:CA	3:B:2037:HOH:O	2.38	0.63
1:A:224:LEU:CD2	1:A:230[A]:ILE:CD1	2.75	0.62
1:B:329:CYS:HG	1:B:370:CYS:HG	1.44	0.62
1:A:342:MET:CE	1:A:345:GLY:O	2.47	0.62
1:A:250:ILE:HD12	1:A:255:ARG:CB	2.29	0.62
1:B:212:PRO:HD3	1:B:291[A]:ASN:CG	2.20	0.62
1:B:212:PRO:HD3	1:B:291[B]:ASN:CG	2.20	0.62
1:B:224:LEU:HD22	1:B:230[B]:ILE:HG12	1.82	0.62
1:A:92:ILE:HG22	1:A:93:SER:O	2.00	0.62
1:B:83:LEU:HD23	1:B:84:ALA:N	2.15	0.61
1:A:129:SER:O	1:B:213:ARG:CD	2.48	0.61
1:A:141:HIS:HD2	1:A:147:ASN:ND2	1.95	0.61
1:B:328:THR:HG23	1:B:354:VAL:HG22	1.82	0.61
1:A:144[A]:GLU:OE1	1:A:178[A]:LYS:HE2	2.00	0.61
1:B:245[A]:ARG:CD	3:B:2092:HOH:O	2.48	0.61
1:A:343:LYS:CG	3:A:2108:HOH:O	2.43	0.61
1:A:342:MET:HE1	1:A:345:GLY:O	2.01	0.60
1:A:225[B]:MET:HG3	3:A:2080:HOH:O	2.00	0.60
1:A:111:ASN:ND2	1:A:126:LEU:HD12	2.17	0.60
1:A:329:CYS:HG	1:A:370:CYS:HG	1.47	0.60
1:B:116:ILE:HG23	1:B:206:PRO:CG	2.31	0.60
1:A:320:ASP:O	1:A:360:VAL:HG23	2.03	0.59
1:A:245[B]:ARG:HG2	1:A:247:TYR:CZ	2.38	0.58
1:B:341:TRP:CB	1:B:348:ILE:HD11	2.33	0.58
1:B:294:GLY:C	2:B:1391:NAG:C1	2.70	0.58
1:B:341:TRP:HB2	1:B:348:ILE:HD11	1.85	0.58
1:B:291[A]:ASN:CG	1:B:294:GLY:O	2.39	0.58
1:A:186:HIS:CE1	1:A:188:LEU:HB2	2.39	0.58
1:A:224:LEU:HD13	1:A:230[A]:ILE:HG12	1.86	0.57
1:B:193:ARG:HD2	3:B:2024:HOH:O	2.04	0.57
1:B:295:GLY:N	2:B:1391:NAG:O5	2.38	0.57
1:B:32:PRO:O	1:B:86:ASN:ND2	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:VAL:HG11	1:B:121:ALA:HB2	1.85	0.57
1:A:1:GLN:NE2	1:A:88:PHE:HB2	2.20	0.57
1:B:239:PHE:HA	1:B:240:PRO:C	2.24	0.57
1:A:13[A]:ARG:HD2	1:A:97:HIS:HB2	1.87	0.57
1:B:295:GLY:C	2:B:1391:NAG:C6	2.71	0.56
1:A:305:THR:HG22	1:A:335:PRO:HD3	1.88	0.56
1:B:296:GLU:N	2:B:1391:NAG:H61	2.21	0.56
1:A:207:ILE:N	1:A:207:ILE:HD13	2.20	0.56
1:B:206:PRO:HB3	3:B:2074:HOH:O	1.96	0.56
1:B:329:CYS:CB	1:B:370:CYS:HG	2.19	0.56
1:B:224:LEU:HD22	1:B:230[B]:ILE:HG13	1.85	0.56
1:A:88:PHE:CE2	1:A:384:GLU:HG3	2.41	0.55
1:B:51:GLY:H	1:B:54:GLN:HE21	1.54	0.55
1:B:224:LEU:HD22	1:B:230[A]:ILE:HG12	1.83	0.55
1:A:110:VAL:HG12	1:A:199:GLY:HA3	1.89	0.55
1:A:10:PRO:HB2	1:A:96:VAL:HG21	1.89	0.55
1:A:213:ARG:CD	1:B:129:SER:O	2.55	0.55
1:A:335:PRO:O	1:A:374:ASN:HB3	2.07	0.55
1:A:218:VAL:HG12	3:A:2075:HOH:O	2.05	0.55
1:B:245[B]:ARG:NH1	1:B:259:VAL:O	2.39	0.55
1:B:224:LEU:HD22	1:B:230[B]:ILE:HD11	1.88	0.55
1:B:319:VAL:HG12	1:B:360:VAL:HG21	1.89	0.55
1:B:7:LEU:HD21	1:B:29:SER:HB3	1.88	0.54
1:A:124[B]:LYS:NZ	1:A:124[B]:LYS:HB2	2.22	0.54
1:B:141:HIS:ND1	1:B:147:ASN:ND2	2.54	0.54
1:B:55:ILE:CD1	1:B:61:LEU:CD1	2.86	0.54
1:B:290:ASN:CG	2:B:1391:NAG:C5	2.76	0.54
1:B:7:LEU:CD2	1:B:29:SER:CB	2.85	0.54
1:A:250:ILE:HD13	1:A:255:ARG:NH1	2.23	0.53
1:B:178[A]:LYS:HD2	3:B:2059:HOH:O	2.08	0.53
1:B:224:LEU:HD22	1:B:230[B]:ILE:CD1	2.35	0.53
1:B:142:THR:HG21	1:B:178[B]:LYS:HE2	1.91	0.53
1:A:55:ILE:HD13	3:A:2007:HOH:O	2.09	0.53
1:A:10:PRO:HB2	1:A:96:VAL:CG2	2.38	0.53
1:B:55:ILE:HD11	1:B:61:LEU:CD1	2.39	0.53
1:A:224:LEU:CD1	1:A:230[A]:ILE:HG12	2.39	0.52
1:B:320:ASP:O	1:B:360:VAL:CG2	2.57	0.52
1:B:6:PHE:CD2	1:B:91:ILE:HD12	2.43	0.52
1:B:83:LEU:C	1:B:83:LEU:HD23	2.30	0.52
1:B:35:GLU:O	1:B:84:ALA:HA	2.09	0.52
1:B:290:ASN:CA	2:B:1391:NAG:C1	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LYS:HG2	1:A:338:THR:HG23	1.92	0.52
1:B:174:GLU:N	1:B:174:GLU:OE1	2.39	0.52
1:B:83:LEU:CD2	1:B:83:LEU:C	2.78	0.52
1:A:54:GLN:C	3:A:2010:HOH:O	2.42	0.52
1:A:224:LEU:HD22	1:A:230[A]:ILE:CG1	2.38	0.51
1:A:245[B]:ARG:CZ	3:A:2085:HOH:O	2.58	0.51
1:A:224:LEU:O	1:A:304:VAL:HA	2.11	0.51
1:A:186:HIS:HE1	1:A:188:LEU:HB2	1.76	0.51
1:B:242:PRO:HA	1:B:290:ASN:O	2.10	0.51
1:B:44:THR:HB	3:B:2015:HOH:O	2.11	0.51
1:A:14:ILE:HG12	1:A:24:ILE:HD11	1.93	0.51
1:A:213:ARG:HD2	1:B:129:SER:O	2.10	0.50
1:A:279:VAL:HG13	1:A:334:ASN:ND2	2.26	0.50
1:B:225[B]:MET:HE1	1:B:307:PRO:HG3	1.94	0.50
1:B:123:ILE:HD11	1:B:201:LEU:CD2	2.41	0.50
1:B:8:LYS:HB2	1:B:27:LYS:HB2	1.94	0.50
1:A:117:ARG:HD2	1:A:205[B]:GLU:CD	2.27	0.50
1:B:7:LEU:CD2	1:B:29:SER:HB3	2.42	0.50
1:A:230[B]:ILE:HD11	1:A:277:ALA:HB2	1.93	0.50
1:A:358[B]:GLU:CD	1:A:358[B]:GLU:H	2.13	0.50
1:B:206:PRO:HA	3:B:2074:HOH:O	2.07	0.50
1:A:39:ILE:HD12	1:A:40:ARG:O	2.12	0.49
1:A:224:LEU:CD1	1:A:230[B]:ILE:HG12	2.36	0.49
1:A:193:ARG:CD	3:A:2019:HOH:O	2.61	0.49
1:A:224:LEU:HD22	1:A:230[B]:ILE:CG1	2.43	0.49
1:B:280:GLU:HA	3:B:2107:HOH:O	2.12	0.49
1:A:342:MET:HE2	1:A:345:GLY:O	2.13	0.48
1:B:295:GLY:CA	2:B:1391:NAG:H62	2.41	0.48
2:B:1392:NAG:C7	2:B:1392:NAG:HO3	2.21	0.48
2:B:1389:NAG:H82	2:B:1389:NAG:O3	2.13	0.48
1:B:124[B]:LYS:HE3	1:B:124[B]:LYS:HB2	1.43	0.48
1:B:212:PRO:HD3	1:B:291[B]:ASN:OD1	2.13	0.47
1:B:291[A]:ASN:OD1	1:B:294:GLY:N	2.35	0.47
1:B:79:VAL:HG22	1:B:97:HIS:ND1	2.30	0.47
1:A:14:ILE:HG23	1:A:14:ILE:O	2.15	0.47
1:B:117:ARG:HD2	1:B:205[B]:GLU:OE1	2.15	0.47
1:B:341:TRP:HA	1:B:369:GLN:O	2.14	0.47
1:A:220:LYS:HB2	1:A:221:PRO:CD	2.45	0.47
1:A:245[B]:ARG:NH2	3:A:2085:HOH:O	2.48	0.47
1:A:116:ILE:H	1:A:237:GLN:HE22	1.58	0.47
1:A:206:PRO:CA	3:A:2068:HOH:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HD22	1:A:230[B]:ILE:HG12	1.95	0.47
1:A:178[A]:LYS:NZ	3:A:2057:HOH:O	2.48	0.47
1:A:329:CYS:SG	1:A:370:CYS:CB	3.03	0.47
1:A:106:TYR:C	3:A:2019:HOH:O	2.30	0.47
1:A:304:VAL:O	1:A:334:ASN:ND2	2.37	0.47
1:B:40:ARG:HD2	3:B:2015:HOH:O	2.14	0.47
1:B:358[B]:GLU:CD	1:B:358[B]:GLU:H	2.17	0.46
1:A:178[A]:LYS:NZ	3:A:2056:HOH:O	2.37	0.46
1:B:290:ASN:CA	1:B:291[A]:ASN:ND2	2.74	0.46
1:B:212:PRO:HD2	1:B:295:GLY:HA2	1.97	0.46
1:A:309:SER:O	1:A:331:TYR:HA	2.16	0.46
1:A:94:ARG:HB2	1:A:378:SER:OG	2.16	0.46
1:B:224:LEU:HD21	1:B:228:HIS:HB2	1.97	0.46
1:A:249:PHE:HA	1:A:256:LYS:HA	1.97	0.46
1:B:179:SER:HA	1:B:199:GLY:O	2.15	0.46
1:B:336:ILE:HD13	1:B:336:ILE:N	2.31	0.46
1:A:206:PRO:HA	3:A:2068:HOH:O	2.16	0.46
1:A:178[B]:LYS:HE3	3:A:2057:HOH:O	2.16	0.46
1:B:235:PRO:HA	3:B:2087:HOH:O	2.16	0.46
1:B:57:SER:HA	1:B:58:ASP:HA	1.58	0.45
1:A:136[A]:GLU:HB2	3:A:2034:HOH:O	2.16	0.45
1:A:319:VAL:HG12	1:A:360:VAL:HG21	1.98	0.45
1:A:169[B]:ARG:HH21	1:A:268:VAL:HG13	1.81	0.45
1:A:339:VAL:HG13	1:A:370:CYS:SG	2.57	0.45
1:B:290:ASN:CA	1:B:291[B]:ASN:ND2	2.76	0.45
1:B:162:PRO:HG2	1:B:231:SER:HB3	1.99	0.45
1:B:212:PRO:HD3	1:B:291[A]:ASN:OD1	2.15	0.45
1:A:224:LEU:CD1	1:A:230[A]:ILE:HD13	2.44	0.45
1:A:260:VAL:HG12	3:A:2088:HOH:O	2.16	0.44
1:B:242:PRO:CA	1:B:290:ASN:O	2.65	0.44
1:B:290:ASN:OD1	2:B:1391:NAG:C5	2.64	0.44
1:B:172:GLY:O	1:B:175:ASP:HB2	2.18	0.44
1:A:329:CYS:HG	1:A:370:CYS:CB	2.31	0.43
1:B:135:VAL:CG1	1:B:184:THR:HB	2.48	0.43
1:B:230[B]:ILE:HD13	1:B:302:LEU:HD21	2.00	0.43
1:A:123:ILE:HD11	1:A:201:LEU:HD21	2.01	0.43
1:A:313:ASP:HB2	1:A:330:GLN:HE22	1.83	0.43
1:B:224:LEU:HD22	1:B:230[A]:ILE:HG13	1.87	0.43
1:B:250:ILE:HD12	1:B:255:ARG:NH1	2.33	0.43
1:B:290:ASN:CG	2:B:1391:NAG:H83	2.38	0.43
1:A:313:ASP:HA	1:A:314:PRO:HA	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:ARG:HD2	1:B:323:ARG:HA	1.90	0.43
1:A:313:ASP:CB	1:A:330:GLN:HE22	2.31	0.43
1:A:138:VAL:HG21	1:A:185:LYS:HB2	2.01	0.43
1:A:224:LEU:CB	1:A:230[A]:ILE:HD13	2.48	0.43
1:A:336:ILE:HD12	1:A:336:ILE:HG23	1.69	0.43
1:B:205[A]:GLU:HG2	3:B:2073:HOH:O	2.19	0.43
1:B:226:VAL:O	1:B:227:ALA:CB	2.63	0.42
1:B:55:ILE:N	1:B:55:ILE:HD12	2.34	0.42
1:B:364:ASP:O	1:B:385:LEU:HD23	2.20	0.42
1:B:40:ARG:CG	1:B:46:VAL:HG12	2.48	0.42
1:B:230[A]:ILE:HD13	1:B:302:LEU:HD21	2.01	0.42
1:A:136[A]:GLU:CB	3:A:2034:HOH:O	2.68	0.41
1:B:295:GLY:N	2:B:1391:NAG:H62	2.35	0.41
1:B:224:LEU:O	1:B:304:VAL:HA	2.19	0.41
1:A:57:SER:HA	1:A:58:ASP:HA	1.74	0.41
1:A:35:GLU:O	1:A:84:ALA:HA	2.20	0.41
1:B:242:PRO:HB2	1:B:289[A]:VAL:HG23	2.02	0.41
1:B:314:PRO:HA	1:B:315:PRO:HD2	1.68	0.41
1:A:245[B]:ARG:HG2	1:A:247:TYR:CE2	2.56	0.41
1:A:351:SER:HB3	3:A:2101:HOH:O	2.20	0.41
1:B:115:VAL:HG11	1:B:121:ALA:CB	2.49	0.41
1:A:279:VAL:HA	1:A:304:VAL:HB	2.04	0.40
1:B:295:GLY:N	2:B:1391:NAG:C6	2.84	0.40
1:A:10:PRO:CB	1:A:96:VAL:HG21	2.50	0.40
1:B:13[A]:ARG:CD	1:B:97:HIS:HB2	2.51	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:198:LYS:NZ	1:B:181:GLN:OE1[3_655]	1.98	0.22
3:A:2064:HOH:O	3:A:2064:HOH:O[3_655]	1.99	0.21
1:A:181:GLN:NE2	1:B:198:LYS:NZ[3_655]	2.15	0.05

## 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	404/394 (102%)	382 (95%)	21 (5%)	1 (0%)	51	63
1	B	411/394 (104%)	386 (94%)	20 (5%)	5 (1%)	15	16
All	All	815/788 (103%)	768 (94%)	41 (5%)	6 (1%)	28	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	VAL
1	B	315	PRO
1	B	156	GLY
1	B	241	ALA
1	B	291[A]	ASN
1	B	291[B]	ASN

### 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	350/336 (104%)	329 (94%)	21 (6%)	22	30
1	B	355/336 (106%)	324 (91%)	31 (9%)	12	14
All	All	705/672 (105%)	653 (93%)	52 (7%)	19	20

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	7	LEU
1	A	57	SER
1	A	58	ASP
1	A	83	LEU
1	A	130	PHE

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Mol	Chain	Res	Type
1	A	136[A]	GLU
1	A	136[B]	GLU
1	A	205[A]	GLU
1	A	205[B]	GLU
1	A	224	LEU
1	A	230[A]	ILE
1	A	230[B]	ILE
1	A	251	GLU
1	A	263[A]	ASP
1	A	263[B]	ASP
1	A	289[A]	VAL
1	A	304	VAL
1	A	311	LYS
1	A	332	THR
1	A	353	SER
1	B	1	GLN
1	B	7	LEU
1	B	8	LYS
1	B	27	LYS
1	B	29	SER
1	B	41	SER
1	B	42	ASP
1	B	56	SER
1	B	57	SER
1	B	58	ASP
1	B	83	LEU
1	B	124[A]	LYS
1	B	124[B]	LYS
1	B	138	VAL
1	B	181	GLN
1	B	205[A]	GLU
1	B	205[B]	GLU
1	B	210	SER
1	B	226	VAL
1	B	260	VAL
1	B	263[A]	ASP
1	B	263[B]	ASP
1	B	289[A]	VAL
1	B	290	ASN
1	B	291[A]	ASN
1	B	291[B]	ASN
1	B	298	VAL

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Mol	Chain	Res	Type
1	B	316	THR
1	B	336	ILE
1	B	338	THR
1	B	353	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	31	ASN
1	A	54	GLN
1	A	87	GLN
1	A	111	ASN
1	A	141	HIS
1	A	147	ASN
1	A	181	GLN
1	A	237	GLN
1	A	330	GLN
1	B	31	ASN
1	B	54	GLN
1	B	73	GLN
1	B	147	ASN

### 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 ⓘ

8 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	1389	1,2	14,14,15	0.53	0	15,19,21	1.91	4 (26%)
2	NAG	A	1390	2	14,14,15	0.60	0	15,19,21	1.30	2 (13%)
2	NAG	A	1391	1,2	14,14,15	0.48	0	15,19,21	1.99	3 (20%)
2	NAG	A	1392	2	14,14,15	0.52	0	15,19,21	1.55	2 (13%)
2	NAG	B	1389	1,2	14,14,15	0.51	0	15,19,21	1.68	2 (13%)
2	NAG	B	1390	2	14,14,15	0.50	0	15,19,21	1.30	2 (13%)
2	NAG	B	1391	1,2	14,14,15	1.05	1 (7%)	15,19,21	5.75	11 (73%)
2	NAG	B	1392	2	14,14,15	0.64	0	15,19,21	2.91	5 (33%)

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	1389	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1390	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1391	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1392	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1389	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1390	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1391	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	1392	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1391	NAG	C1-C2	3.17	1.56	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1391	NAG	O5-C1-C2	-7.74	100.71	111.47
2	B	1391	NAG	C6-C5-C4	-6.38	98.07	113.00
2	B	1392	NAG	O5-C1-C2	-5.89	103.27	111.47
2	B	1389	NAG	O5-C1-C2	-4.93	104.61	111.47
2	B	1391	NAG	O7-C7-C8	-3.90	114.95	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1389	NAG	O5-C1-C2	-3.88	106.07	111.47
2	A	1391	NAG	O3-C3-C4	-3.60	102.52	110.36
2	A	1389	NAG	C3-C4-C5	-3.44	104.16	110.22
2	B	1392	NAG	O7-C7-C8	-3.23	116.17	122.06
2	A	1392	NAG	C4-C3-C2	-2.60	107.20	111.02
2	B	1391	NAG	O3-C3-C4	-2.50	104.92	110.36
2	B	1390	NAG	C1-C2-N2	2.04	113.97	110.49
2	B	1389	NAG	C8-C7-N2	2.06	119.82	116.11
2	B	1390	NAG	O4-C4-C5	2.09	114.56	109.28
2	A	1390	NAG	C1-C2-N2	2.11	114.08	110.49
2	B	1391	NAG	O6-C6-C5	2.11	118.44	111.34
2	B	1391	NAG	C8-C7-N2	2.37	120.39	116.11
2	A	1390	NAG	C1-O5-C5	2.49	115.60	112.17
2	A	1389	NAG	C2-N2-C7	2.74	126.94	122.94
2	B	1392	NAG	C1-O5-C5	2.84	116.08	112.17
2	A	1392	NAG	C1-C2-N2	2.86	115.38	110.49
2	B	1392	NAG	O3-C3-C2	3.03	115.88	109.39
2	A	1391	NAG	C3-C4-C5	3.29	116.01	110.22
2	B	1391	NAG	C1-C2-N2	3.65	116.73	110.49
2	A	1389	NAG	C1-O5-C5	3.72	117.29	112.17
2	A	1391	NAG	C1-O5-C5	4.10	117.81	112.17
2	B	1391	NAG	C2-N2-C7	4.44	129.43	122.94
2	B	1392	NAG	C1-C2-N2	7.06	122.55	110.49
2	B	1391	NAG	O4-C4-C3	7.27	126.19	110.36
2	B	1391	NAG	C4-C3-C2	8.41	123.35	111.02
2	B	1391	NAG	C1-O5-C5	14.27	131.83	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1391	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1389	NAG	2	0
2	B	1389	NAG	1	0
2	B	1391	NAG	29	0
2	B	1392	NAG	4	0

## 5.6 Ligand geometry

There are no ligands in this entry.

## 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	388/394 (98%)	1.13	71 (18%)	<b>1</b> <b>2</b>	56, 65, 72, 81	7 (1%)
1	B	394/394 (100%)	1.30	90 (22%)	<b>1</b> <b>1</b>	52, 65, 73, 82	5 (1%)
All	All	782/788 (99%)	1.22	161 (20%)	<b>1</b> <b>1</b>	52, 65, 72, 82	12 (1%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	347	ALA	8.4
1	A	55	ILE	8.1
1	B	58	ASP	7.6
1	A	385	LEU	6.3
1	B	358[A]	GLU	6.1
1	A	88	PHE	6.1
1	B	252	GLY	5.9
1	A	41	SER	5.3
1	A	31	ASN	5.3
1	A	289[A]	VAL	5.1
1	A	87	GLN	5.0
1	A	253	THR	5.0
1	B	32	PRO	4.9
1	A	98	VAL	4.6
1	A	347	ALA	4.6
1	A	58	ASP	4.5
1	A	323	ARG	4.5
1	A	57	SER	4.4
1	B	289[A]	VAL	4.4
1	B	381	ALA	4.3
1	B	382	SER	4.3
1	B	348	ILE	4.3
1	B	253	THR	4.2
1	B	339	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	-2	GLN	4.1
1	B	375	ASP	4.0
1	A	250	ILE	4.0
1	B	44	THR	4.0
1	B	385	LEU	4.0
1	B	361	LYS	4.0
1	A	368	TYR	3.9
1	A	1	GLN	3.9
1	A	306	ALA	3.9
1	B	194	LEU	3.9
1	A	375	ASP	3.9
1	B	263[A]	ASP	3.8
1	A	322	GLY	3.7
1	B	291[A]	ASN	3.7
1	B	-5	ALA	3.7
1	B	75	VAL	3.7
1	B	322	GLY	3.7
1	A	348	ILE	3.7
1	B	100	ALA	3.6
1	A	75	VAL	3.5
1	B	1	GLN	3.5
1	B	56	SER	3.5
1	B	351	SER	3.5
1	B	368	TYR	3.5
1	B	98	VAL	3.4
1	B	359	SER	3.4
1	A	139	SER	3.4
1	A	42	ASP	3.4
1	B	87	GLN	3.4
1	A	28	ALA	3.4
1	A	262	ASN	3.4
1	B	388	GLY	3.3
1	B	-4	TYR	3.3
1	B	145[A]	GLU	3.3
1	B	31	ASN	3.3
1	B	367	MET	3.3
1	A	63	PHE	3.2
1	B	280	GLU	3.2
1	B	8	LYS	3.2
1	A	59	GLY	3.1
1	B	262	ASN	3.1
1	B	63	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	252	GLY	3.0
1	A	32	PRO	3.0
1	B	57	SER	3.0
1	B	327	PHE	3.0
1	A	232	LEU	2.9
1	A	43	GLY	2.9
1	B	349	GLY	2.9
1	B	286	LEU	2.9
1	B	180	TYR	2.9
1	B	371	PHE	2.9
1	A	236	ALA	2.9
1	B	320	ASP	2.9
1	A	312	ILE	2.8
1	A	44	THR	2.8
1	B	251	GLU	2.8
1	B	366	GLY	2.8
1	A	47	GLY	2.8
1	B	323	ARG	2.8
1	A	376	ARG	2.8
1	B	225[A]	MET	2.8
1	B	314	PRO	2.7
1	B	376	ARG	2.8
1	B	101	VAL	2.7
1	B	316	THR	2.7
1	A	251	GLU	2.7
1	A	239	PHE	2.7
1	B	170[A]	GLU	2.7
1	B	41	SER	2.7
1	B	383	ALA	2.7
1	B	374	ASN	2.7
1	B	272	LEU	2.7
1	A	194	LEU	2.6
1	A	56	SER	2.6
1	B	311	LYS	2.6
1	B	55	ILE	2.6
1	B	369	GLN	2.6
1	A	246	TRP	2.6
1	A	302	LEU	2.6
1	B	66	PHE	2.5
1	B	285	TYR	2.5
1	A	80	TYR	2.5
1	A	91	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	369	GLN	2.5
1	B	372	VAL	2.5
1	A	371	PHE	2.5
1	B	46	VAL	2.5
1	A	225[A]	MET	2.5
1	A	30	GLY	2.4
1	B	16	PHE	2.4
1	B	76	HIS	2.4
1	B	336	ILE	2.4
1	A	286	LEU	2.4
1	B	370	CYS	2.4
1	B	245[A]	ARG	2.4
1	A	285	TYR	2.4
1	A	349	GLY	2.4
1	B	61	LEU	2.4
1	A	259	VAL	2.4
1	A	362	LYS	2.3
1	A	92	ILE	2.3
1	B	239	PHE	2.3
1	A	288	VAL	2.3
1	A	360	VAL	2.3
1	B	305	THR	2.3
1	A	23[A]	GLU	2.3
1	A	108	ALA	2.3
1	B	195	SER	2.3
1	B	232	LEU	2.3
1	B	346	LYS	2.3
1	B	290	ASN	2.2
1	A	226	VAL	2.2
1	A	327	PHE	2.2
1	B	335	PRO	2.2
1	B	42	ASP	2.2
1	B	313	ASP	2.2
1	A	254	THR	2.2
1	A	263[A]	ASP	2.2
1	B	380	GLU	2.2
1	A	19	SER	2.2
1	A	321	PHE	2.2
1	B	362	LYS	2.2
1	A	25	GLU	2.2
1	A	383	ALA	2.1
1	B	261	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	67	ARG	2.1
1	A	245[A]	ARG	2.1
1	B	304	VAL	2.1
1	A	13[A]	ARG	2.1
1	A	270	GLY	2.1
1	B	324	PRO	2.1
1	B	91	ILE	2.0
1	A	100	ALA	2.0
1	A	370	CYS	2.0
1	B	88	PHE	2.0
1	B	3	GLY	2.0

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

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

## 6.3 Carbohydrates [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	NAG	B	1391	14/15	-0.03	1.02	7.78	96,107,112,114	0
2	NAG	A	1391	14/15	0.68	0.36	1.51	77,82,85,89	0
2	NAG	A	1389	14/15	0.79	0.18	0.01	56,63,70,78	0
2	NAG	B	1389	14/15	0.83	0.20	-0.01	52,62,67,74	0
2	NAG	A	1390	14/15	0.54	0.46	-	88,94,96,97	0
2	NAG	B	1390	14/15	0.68	0.34	-	71,81,85,86	0
2	NAG	A	1392	14/15	0.52	0.47	-	93,96,97,98	0
2	NAG	B	1392	14/15	0.18	0.57	-	119,122,129,129	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.