



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:16 PM GMT

PDB ID : 2V5R  
Title : STRUCTURAL BASIS FOR DSCAM ISOFORM SPECIFICITY  
Authors : Meijers, R.; Puettmann-Holgado, R.; Skiniotis, G.; Liu, J.-H.; Walz, T.;  
Schmucker, D.; Wang, J.-H.  
Deposited on : 2007-07-09  
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

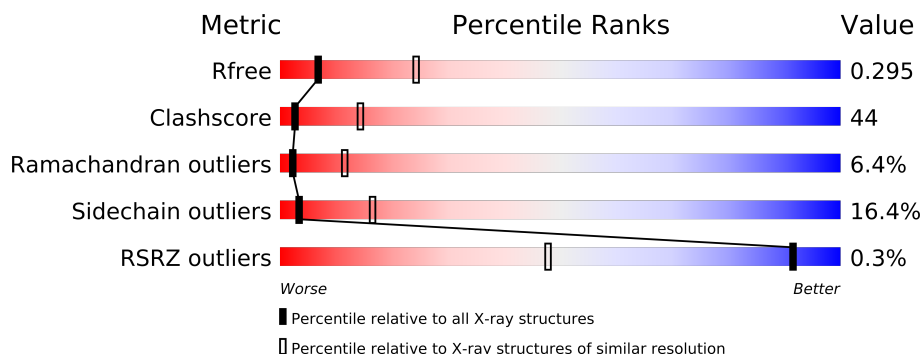
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	391	
1	B	391	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	B	1397	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6232 atoms, of which 0 are hydrogen and 0 are deuterium.

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	391	Total	C	N	O	S	0	0	0
			3054	1920	530	591	13			
1	B	391	Total	C	N	O	S	0	0	0
			3054	1920	530	591	13			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ILE	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
A	105	SER	TYR	VARIANT SEE REMARK 99	UNP Q9NBA1
A	108	SER	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
A	109	GLU	ASP	VARIANT SEE REMARK 99	UNP Q9NBA1
A	110	ALA	VAL	VARIANT SEE REMARK 99	UNP Q9NBA1
A	111	ASP	ASN	VARIANT SEE REMARK 99	UNP Q9NBA1
A	112	ASN	LYS	VARIANT SEE REMARK 99	UNP Q9NBA1
A	114	TYR	HIS	VARIANT SEE REMARK 99	UNP Q9NBA1
A	121	VAL	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
A	123	MET	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
A	126	GLU	LEU	VARIANT SEE REMARK 99	UNP Q9NBA1
A	130	TYR	PHE	VARIANT SEE REMARK 99	UNP Q9NBA1
A	136	PHE	GLU	VARIANT SEE REMARK 99	UNP Q9NBA1
A	138	ASP	VAL	VARIANT SEE REMARK 99	UNP Q9NBA1
A	139	LEU	SER	VARIANT SEE REMARK 99	UNP Q9NBA1
A	141	LEU	HIS	VARIANT SEE REMARK 99	UNP Q9NBA1
A	142	ASP	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
A	143	SER	ASP	VARIANT SEE REMARK 99	UNP Q9NBA1
A	145	GLY	GLU	VARIANT SEE REMARK 99	UNP Q9NBA1
A	146	ARG	GLU	VARIANT SEE REMARK 99	UNP Q9NBA1
A	149	TYR	PHE	VARIANT SEE REMARK 99	UNP Q9NBA1
A	153	ALA	GLY	VARIANT SEE REMARK 99	UNP Q9NBA1
A	156	THR	TYR	VARIANT SEE REMARK 99	UNP Q9NBA1
A	210	GLY	SER	VARIANT SEE REMARK 99	UNP Q9NBA1
A	212	VAL	SER	VARIANT SEE REMARK 99	UNP Q9NBA1

*Continued on next page...*

*Continued from previous page...*

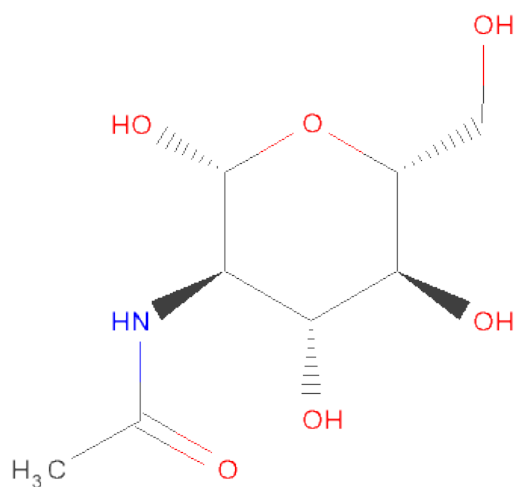
Chain	Residue	Modelled	Actual	Comment	Reference
A	213	ARG	PRO	VARIANT SEE REMARK 99	UNP Q9NBA1
A	216	VAL	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
A	218	PRO	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
A	219	GLN	LEU	VARIANT SEE REMARK 99	UNP Q9NBA1
A	220	ASP	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
A	221	LYS	TYR	VARIANT SEE REMARK 99	UNP Q9NBA1
A	222	HIS	LYS	VARIANT SEE REMARK 99	UNP Q9NBA1
A	223	GLN	PRO	VARIANT SEE REMARK 99	UNP Q9NBA1
A	224	PHE	ASN	VARIANT SEE REMARK 99	UNP Q9NBA1
A	229	LEU	SER	VARIANT SEE REMARK 99	UNP Q9NBA1
A	230	ALA	MET	VARIANT SEE REMARK 99	UNP Q9NBA1
A	231	SER	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
A	233	TYR	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
A	234	SER	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
A	235	LEU	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
A	238	MET	PRO	VARIANT SEE REMARK 99	UNP Q9NBA1
A	241	SER	GLY	VARIANT SEE REMARK 99	UNP Q9NBA1
A	244	THR	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
B	103	ILE	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
B	105	SER	TYR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	108	SER	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
B	109	GLU	ASP	VARIANT SEE REMARK 99	UNP Q9NBA1
B	110	ALA	VAL	VARIANT SEE REMARK 99	UNP Q9NBA1
B	111	ASP	ASN	VARIANT SEE REMARK 99	UNP Q9NBA1
B	112	ASN	LYS	VARIANT SEE REMARK 99	UNP Q9NBA1
B	114	TYR	HIS	VARIANT SEE REMARK 99	UNP Q9NBA1
B	121	VAL	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
B	123	MET	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
B	126	GLU	LEU	VARIANT SEE REMARK 99	UNP Q9NBA1
B	130	TYR	PHE	VARIANT SEE REMARK 99	UNP Q9NBA1
B	136	PHE	GLU	VARIANT SEE REMARK 99	UNP Q9NBA1
B	138	ASP	VAL	VARIANT SEE REMARK 99	UNP Q9NBA1
B	139	LEU	SER	VARIANT SEE REMARK 99	UNP Q9NBA1
B	141	LEU	HIS	VARIANT SEE REMARK 99	UNP Q9NBA1
B	142	ASP	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	143	SER	ASP	VARIANT SEE REMARK 99	UNP Q9NBA1
B	145	GLY	GLU	VARIANT SEE REMARK 99	UNP Q9NBA1
B	146	ARG	GLU	VARIANT SEE REMARK 99	UNP Q9NBA1
B	149	TYR	PHE	VARIANT SEE REMARK 99	UNP Q9NBA1
B	153	ALA	GLY	VARIANT SEE REMARK 99	UNP Q9NBA1
B	156	THR	TYR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	210	GLY	SER	VARIANT SEE REMARK 99	UNP Q9NBA1

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	212	VAL	SER	VARIANT SEE REMARK 99	UNP Q9NBA1
B	213	ARG	PRO	VARIANT SEE REMARK 99	UNP Q9NBA1
B	216	VAL	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
B	218	PRO	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	219	GLN	LEU	VARIANT SEE REMARK 99	UNP Q9NBA1
B	220	ASP	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	221	LYS	TYR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	222	HIS	LYS	VARIANT SEE REMARK 99	UNP Q9NBA1
B	223	GLN	PRO	VARIANT SEE REMARK 99	UNP Q9NBA1
B	224	PHE	ASN	VARIANT SEE REMARK 99	UNP Q9NBA1
B	229	LEU	SER	VARIANT SEE REMARK 99	UNP Q9NBA1
B	230	ALA	MET	VARIANT SEE REMARK 99	UNP Q9NBA1
B	231	SER	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
B	233	TYR	THR	VARIANT SEE REMARK 99	UNP Q9NBA1
B	234	SER	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1
B	235	LEU	ILE	VARIANT SEE REMARK 99	UNP Q9NBA1
B	238	MET	PRO	VARIANT SEE REMARK 99	UNP Q9NBA1
B	241	SER	GLY	VARIANT SEE REMARK 99	UNP Q9NBA1
B	244	THR	ALA	VARIANT SEE REMARK 99	UNP Q9NBA1

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



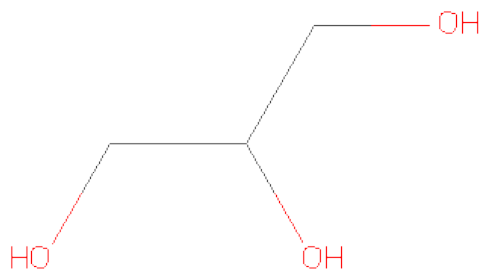
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

*Continued from previous page...*

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



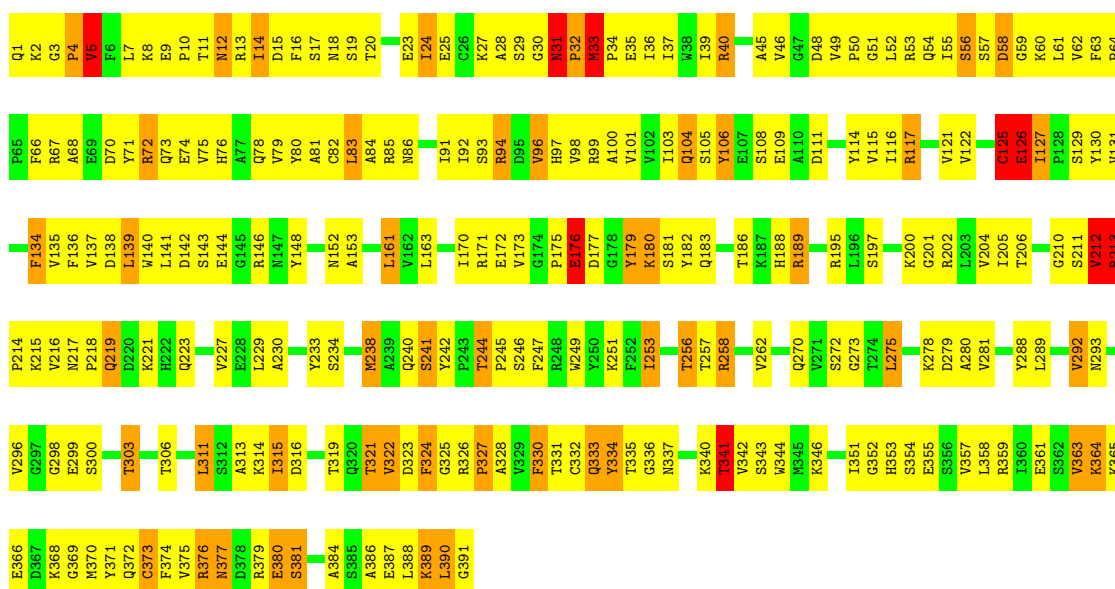
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

### 3 Residue-property plots

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

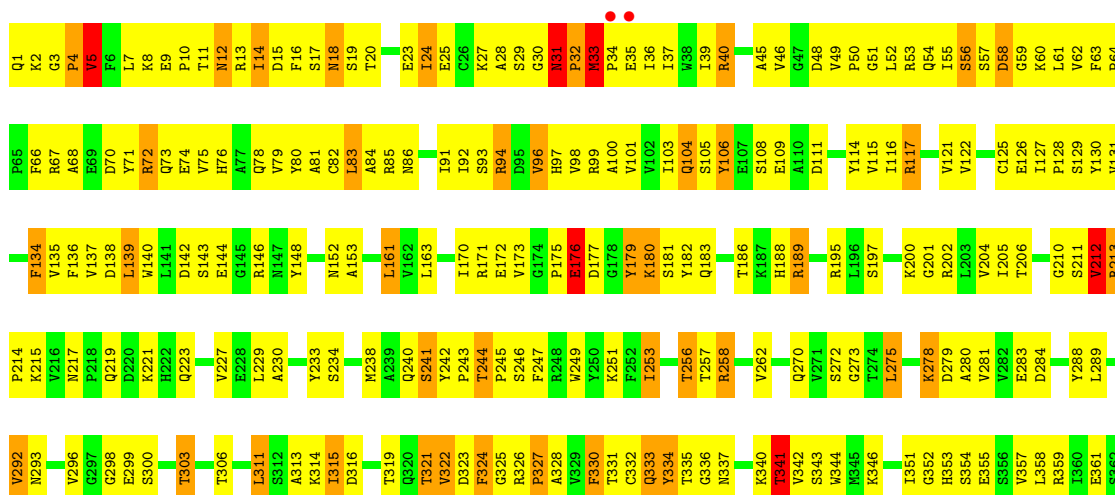
#### • Molecule 1: DSCAM

Chain A:



#### • Molecule 1: DSCAM

Chain B:



V363	K364	K365	E366	D367	K368	G369	M370	Y371	Q372	C373	F374	V375	R376	N377	D378	R379	E380	S381	A384	S385	A386	F387	I388	K389	L390	G391
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	277.78Å 70.55Å 72.77Å 90.00° 105.13° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.93 – 3.01	Depositor EDS
% Data completeness (in resolution range)	86.0 (20.00-3.00) 85.7 (19.93-3.01)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.71 (at 2.98Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.271 , 0.303 0.268 , 0.295	Depositor DCC
$R_{free}$ test set	1160 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.6	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 32.8	EDS
Estimated twinning fraction	0.030 for -h+k-l,-l,-k 0.022 for -h-k-l,l,k 0.448 for -h-2*l,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 23412 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	6232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	1.19	4/3117 (0.1%)	1.22	9/4226 (0.2%)
1	B	0.64	2/3117 (0.1%)	0.84	3/4226 (0.1%)
All	All	0.96	6/6234 (0.1%)	1.05	12/8452 (0.1%)

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	6
1	B	0	3
All	All	0	9

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	CYS	C-N	-45.17	0.30	1.34
1	A	126	GLU	C-N	-31.19	0.62	1.34
1	A	213	ARG	C-N	-24.45	0.87	1.34
1	B	213	ARG	C-N	-20.25	0.95	1.34
1	B	212	VAL	C-N	-16.25	0.96	1.34
1	A	212	VAL	C-N	-14.53	1.00	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	GLU	O-C-N	-44.21	51.96	122.70
1	B	212	VAL	O-C-N	-31.24	72.71	122.70
1	A	212	VAL	O-C-N	-29.62	75.31	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	GLU	CA-C-N	23.48	168.86	117.20
1	A	125	CYS	O-C-N	-22.97	85.95	122.70
1	A	126	GLU	C-N-CA	15.67	160.87	121.70
1	A	212	VAL	CA-C-N	9.74	138.64	117.20
1	B	212	VAL	CA-C-N	9.64	138.42	117.20
1	A	213	ARG	O-C-N	-8.87	104.25	121.10
1	A	213	ARG	CA-C-N	6.06	134.06	117.10
1	A	125	CYS	C-N-CA	-5.75	107.31	121.70
1	B	213	ARG	O-C-N	-5.43	110.78	121.10

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	CYS	Mainchain
1	A	126	GLU	Mainchain
1	A	212	VAL	Mainchain,Peptide
1	A	213	ARG	Mainchain
1	A	31	ASN	Peptide
1	B	212	VAL	Mainchain,Peptide
1	B	31	ASN	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3054	0	3014	271	0
1	B	3054	0	3016	270	0
2	A	56	0	52	12	0
2	B	56	0	52	11	0
3	B	12	0	16	4	0
All	All	6232	0	6150	546	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 44.

All (546) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:293:ASN:HD21	2:B:1396:NAG:C1	1.62	1.12
1:A:10:PRO:HB2	1:A:96:VAL:HG11	1.32	1.11
1:A:68:ALA:HB2	2:A:1392:NAG:H61	1.33	1.10
1:A:293:ASN:HD21	2:A:1395:NAG:C1	1.65	1.08
1:B:10:PRO:HB2	1:B:96:VAL:HG11	1.33	1.05
1:A:359:ARG:HH21	1:A:361:GLU:HG2	1.17	1.04
1:B:359:ARG:HH21	1:B:361:GLU:HG2	1.17	1.03
1:B:68:ALA:HB2	2:B:1393:NAG:H61	1.34	1.03
1:B:52:LEU:O	1:B:64:PRO:HD2	1.65	0.96
1:A:52:LEU:O	1:A:64:PRO:HD2	1.67	0.93
1:B:212:VAL:HG13	1:B:242:TYR:H	1.35	0.91
1:A:72:ARG:HG3	1:A:72:ARG:HH11	1.36	0.90
1:A:219:GLN:NE2	1:A:219:GLN:H	1.70	0.90
1:B:311:LEU:HA	1:B:336:GLY:HA3	1.54	0.90
1:B:364:LYS:HG3	1:B:365:LYS:H	1.38	0.89
1:A:380:GLU:HG2	1:A:381:SER:H	1.38	0.88
1:B:106:TYR:CE1	1:B:188:HIS:HD2	1.91	0.88
1:A:364:LYS:HG3	1:A:365:LYS:H	1.37	0.88
1:A:311:LEU:HA	1:A:336:GLY:HA3	1.54	0.88
1:B:72:ARG:HH11	1:B:72:ARG:HG3	1.39	0.87
1:A:212:VAL:HG13	1:A:242:TYR:H	1.37	0.87
1:B:359:ARG:NH2	1:B:361:GLU:HG2	1.90	0.87
1:A:106:TYR:CE1	1:A:188:HIS:HD2	1.92	0.86
1:A:105:SER:HB2	2:A:1394:NAG:H81	1.58	0.86
1:B:106:TYR:HE1	1:B:188:HIS:HD2	1.23	0.86
1:B:72:ARG:H	1:B:76:HIS:HD2	1.24	0.86
1:B:380:GLU:HG2	1:B:381:SER:H	1.39	0.85
1:A:72:ARG:H	1:A:76:HIS:HD2	1.24	0.85
1:A:72:ARG:CG	1:A:72:ARG:HH11	1.88	0.85
1:A:359:ARG:NH2	1:A:361:GLU:HG2	1.91	0.84
1:B:105:SER:HB2	2:B:1395:NAG:H81	1.58	0.84
1:A:223:GLN:HB2	1:A:303:THR:HG23	1.60	0.84
1:A:72:ARG:NH1	1:A:72:ARG:HB2	1.92	0.84
1:A:343:SER:HB2	1:A:374:PHE:HB2	1.60	0.83
1:B:72:ARG:HH11	1:B:72:ARG:CG	1.90	0.83
1:B:37:ILE:HD12	1:B:83:LEU:HD13	1.58	0.83
1:A:37:ILE:HD12	1:A:83:LEU:HD13	1.58	0.83
1:B:72:ARG:NH1	1:B:72:ARG:HB2	1.93	0.83
1:A:364:LYS:HG3	1:A:365:LYS:N	1.93	0.83
1:B:249:TRP:CD1	1:B:275:LEU:HD13	2.14	0.83
1:A:106:TYR:HE1	1:A:188:HIS:HD2	1.24	0.83
1:B:343:SER:HB2	1:B:374:PHE:HB2	1.61	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:249:TRP:CD1	1:A:275:LEU:HD13	2.15	0.82
1:B:293:ASN:ND2	2:B:1396:NAG:C1	2.42	0.81
1:B:364:LYS:HG3	1:B:365:LYS:N	1.93	0.81
1:A:39:ILE:HA	1:A:45:ALA:HA	1.62	0.81
1:B:39:ILE:HA	1:B:45:ALA:HA	1.63	0.81
1:B:223:GLN:HB2	1:B:303:THR:HG23	1.61	0.81
1:A:76:HIS:HB3	1:A:100:ALA:HB3	1.62	0.80
1:B:76:HIS:HB3	1:B:100:ALA:HB3	1.64	0.80
1:A:293:ASN:ND2	2:A:1395:NAG:C1	2.45	0.80
1:A:1:GLN:HB2	1:A:31:ASN:OD1	1.83	0.79
1:B:1:GLN:HB2	1:B:31:ASN:OD1	1.83	0.79
1:B:321:THR:HB	1:B:389:LYS:HG3	1.65	0.78
1:A:321:THR:HB	1:A:389:LYS:HG3	1.66	0.78
1:A:215:LYS:HE2	1:A:299:GLU:OE1	1.85	0.76
1:B:4:PRO:HD2	1:B:370:MET:SD	2.24	0.76
1:A:4:PRO:HD2	1:A:370:MET:SD	2.25	0.75
1:B:106:TYR:HE1	1:B:188:HIS:CD2	2.05	0.74
1:A:52:LEU:HD21	1:A:70:ASP:HB3	1.69	0.74
1:B:215:LYS:HE2	1:B:299:GLU:OE1	1.87	0.74
1:A:106:TYR:HE1	1:A:188:HIS:CD2	2.05	0.74
1:A:68:ALA:CB	2:A:1392:NAG:H61	2.15	0.73
1:A:10:PRO:HB2	1:A:96:VAL:CG1	2.16	0.73
1:B:179:TYR:O	1:B:180:LYS:HB2	1.85	0.73
1:A:72:ARG:HH22	1:A:75:VAL:HG21	1.54	0.73
1:A:18:ASN:HB2	2:A:1392:NAG:C1	2.19	0.73
1:B:52:LEU:HD21	1:B:70:ASP:HB3	1.69	0.73
1:B:114:TYR:CE1	1:B:204:VAL:HG21	2.23	0.73
1:B:18:ASN:HB2	2:B:1393:NAG:C1	2.18	0.72
1:A:114:TYR:CE1	1:A:204:VAL:HG21	2.23	0.72
1:B:10:PRO:HB2	1:B:96:VAL:CG1	2.17	0.72
1:B:72:ARG:HH22	1:B:75:VAL:HG21	1.55	0.72
1:A:179:TYR:O	1:A:180:LYS:HB2	1.87	0.72
1:B:143:SER:HB3	1:B:181:SER:OG	1.90	0.72
1:A:328:ALA:HB3	1:A:359:ARG:HA	1.71	0.71
1:B:328:ALA:HB3	1:B:359:ARG:HA	1.71	0.71
1:A:143:SER:HB3	1:A:181:SER:OG	1.91	0.69
1:B:319:THR:HG22	1:B:387:GLU:HG2	1.76	0.68
1:B:212:VAL:HG22	1:B:213:ARG:N	2.07	0.68
1:A:212:VAL:HG22	1:A:213:ARG:N	2.07	0.68
1:B:127:ILE:HD13	1:B:135:VAL:O	1.94	0.68
1:A:12:ASN:OD1	1:A:97:HIS:HD2	1.77	0.68
1:A:127:ILE:HD13	1:A:135:VAL:O	1.94	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:319:THR:HG22	1:A:387:GLU:HG2	1.76	0.67
1:A:72:ARG:NH1	1:A:72:ARG:CB	2.58	0.67
1:B:68:ALA:CB	2:B:1393:NAG:H61	2.17	0.67
1:A:39:ILE:HG12	1:A:81:ALA:O	1.95	0.67
1:B:39:ILE:HG12	1:B:81:ALA:O	1.96	0.66
1:B:12:ASN:OD1	1:B:97:HIS:HD2	1.78	0.66
1:A:326:ARG:HB3	1:A:327:PRO:HD2	1.78	0.65
1:A:80:TYR:HE2	1:A:98:VAL:HG11	1.61	0.65
1:B:80:TYR:HE2	1:B:98:VAL:HG11	1.60	0.65
1:B:66:PHE:HD2	1:B:67:ARG:O	1.79	0.65
1:B:72:ARG:NH1	1:B:72:ARG:CB	2.59	0.65
1:A:247:PHE:CG	1:A:273:GLY:HA3	2.32	0.65
1:B:23:GLU:HB3	1:B:62:VAL:HG13	1.79	0.64
1:A:134:PHE:HA	1:A:189:ARG:HD2	1.78	0.64
1:B:326:ARG:HB3	1:B:327:PRO:HD2	1.79	0.64
1:A:66:PHE:HD2	1:A:67:ARG:O	1.81	0.64
1:B:134:PHE:HA	1:B:189:ARG:HD2	1.77	0.64
1:B:247:PHE:CG	1:B:273:GLY:HA3	2.33	0.64
1:A:23:GLU:HB3	1:A:62:VAL:HG13	1.79	0.63
1:B:321:THR:CB	1:B:389:LYS:HG3	2.28	0.63
1:B:13:ARG:HH12	1:B:99:ARG:NH2	1.96	0.63
1:A:17:SER:HB2	1:A:101:VAL:O	1.98	0.63
1:A:24:ILE:O	1:A:60:LYS:HA	1.99	0.63
1:A:140:TRP:HB2	1:A:148:TYR:HB2	1.79	0.63
1:B:359:ARG:HH21	1:B:361:GLU:CG	2.02	0.62
1:A:213:ARG:HH22	1:A:215:LYS:HE3	1.64	0.62
1:A:180:LYS:H	1:A:202:ARG:NH2	1.98	0.62
1:B:72:ARG:HH11	1:B:72:ARG:CB	2.13	0.62
1:B:180:LYS:H	1:B:202:ARG:NH2	1.96	0.62
1:B:326:ARG:H	1:B:363:VAL:HG23	1.64	0.62
1:A:80:TYR:CE2	1:A:98:VAL:HG11	2.35	0.62
1:B:24:ILE:O	1:B:60:LYS:HA	1.99	0.62
1:B:140:TRP:HB2	1:B:148:TYR:HB2	1.81	0.62
1:B:17:SER:HB2	1:B:101:VAL:O	1.99	0.62
1:A:359:ARG:HH21	1:A:361:GLU:CG	2.02	0.62
1:A:321:THR:CB	1:A:389:LYS:HG3	2.29	0.62
1:A:326:ARG:H	1:A:363:VAL:HG23	1.64	0.62
1:B:80:TYR:CE2	1:B:98:VAL:HG11	2.34	0.61
1:A:380:GLU:CG	1:A:381:SER:H	2.12	0.61
1:A:247:PHE:CD1	1:A:273:GLY:HA3	2.36	0.61
1:B:139:LEU:HD22	1:B:140:TRP:H	1.66	0.61
1:A:121:VAL:HG12	1:A:170:ILE:HB	1.83	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:247:PHE:CD1	1:B:273:GLY:HA3	2.36	0.61
1:A:72:ARG:CG	1:A:72:ARG:NH1	2.56	0.61
1:A:13:ARG:HH12	1:A:99:ARG:NH2	1.98	0.60
1:A:72:ARG:CB	1:A:72:ARG:HH11	2.12	0.60
1:B:323:ASP:HB2	1:B:326:ARG:HG3	1.82	0.60
1:A:219:GLN:NE2	1:A:219:GLN:N	2.48	0.60
1:A:340:LYS:O	1:A:341:THR:HG23	2.01	0.60
1:A:24:ILE:HG12	1:A:61:LEU:HB3	1.84	0.60
1:B:253:ILE:HD11	1:B:258:ARG:HB2	1.84	0.60
1:A:253:ILE:HD11	1:A:258:ARG:HB2	1.84	0.59
1:B:39:ILE:HG21	1:B:83:LEU:HD12	1.84	0.59
1:A:37:ILE:HB	1:A:83:LEU:HB3	1.83	0.59
1:B:340:LYS:O	1:B:341:THR:HG23	2.02	0.59
1:B:24:ILE:HG12	1:B:61:LEU:HB3	1.84	0.59
1:B:28:ALA:H	1:B:36:ILE:HD11	1.67	0.59
1:A:39:ILE:HG21	1:A:83:LEU:HD12	1.84	0.59
1:A:9:GLU:HG2	1:A:10:PRO:CD	2.33	0.59
1:B:18:ASN:ND2	2:B:1393:NAG:O5	2.35	0.59
1:A:321:THR:HA	1:A:389:LYS:O	2.03	0.59
1:A:323:ASP:HB2	1:A:326:ARG:HG3	1.83	0.59
1:A:28:ALA:H	1:A:36:ILE:HD11	1.67	0.59
1:B:9:GLU:HG2	1:B:10:PRO:CD	2.33	0.58
1:B:4:PRO:O	1:B:5:VAL:HB	2.02	0.58
1:A:106:TYR:CE1	1:A:188:HIS:CD2	2.82	0.58
1:A:4:PRO:O	1:A:5:VAL:HB	2.03	0.58
1:A:78:GLN:O	1:A:98:VAL:HG12	2.03	0.58
1:B:121:VAL:HG12	1:B:170:ILE:HB	1.86	0.58
1:B:72:ARG:H	1:B:76:HIS:CD2	2.13	0.58
1:B:37:ILE:HB	1:B:83:LEU:HB3	1.83	0.58
1:B:78:GLN:O	1:B:98:VAL:HG12	2.03	0.58
1:A:23:GLU:OE2	1:A:60:LYS:HD2	2.03	0.58
1:A:139:LEU:HD22	1:A:140:TRP:H	1.68	0.58
1:A:72:ARG:H	1:A:76:HIS:CD2	2.13	0.58
1:A:72:ARG:CZ	1:A:72:ARG:HB2	2.34	0.58
2:A:1392:NAG:H4	2:A:1393:NAG:C1	2.34	0.57
1:A:115:VAL:O	1:A:206:THR:HG22	2.04	0.57
1:B:23:GLU:OE2	1:B:60:LYS:HD2	2.04	0.57
1:A:214:PRO:HA	1:A:240:GLN:O	2.05	0.57
1:B:72:ARG:CZ	1:B:72:ARG:HB2	2.34	0.57
1:B:206:THR:HG23	1:B:206:THR:O	2.05	0.57
1:B:130:TYR:CD2	1:B:131:VAL:HG13	2.40	0.57
1:A:380:GLU:HG2	1:A:381:SER:N	2.15	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:53:ARG:O	1:B:54:GLN:HG3	2.05	0.56
1:B:380:GLU:CG	1:B:381:SER:H	2.13	0.56
1:A:183:GLN:HB3	1:A:200:LYS:HB3	1.87	0.56
1:B:115:VAL:O	1:B:206:THR:HG22	2.05	0.56
1:B:321:THR:HA	1:B:389:LYS:O	2.05	0.56
1:B:234:SER:HB2	1:B:275:LEU:O	2.06	0.56
1:B:183:GLN:HB3	1:B:200:LYS:HB3	1.86	0.56
1:A:229:LEU:HD23	1:A:230:ALA:HB2	1.88	0.56
1:A:18:ASN:ND2	2:A:1392:NAG:O5	2.37	0.56
1:A:279:ASP:O	1:A:281:VAL:N	2.38	0.56
1:A:130:TYR:CD2	1:A:131:VAL:HG13	2.41	0.56
1:A:253:ILE:HG13	1:A:256:THR:OG1	2.05	0.56
1:B:229:LEU:HD23	1:B:230:ALA:HB2	1.87	0.56
1:B:72:ARG:NH1	1:B:72:ARG:CG	2.58	0.55
1:A:206:THR:O	1:A:206:THR:HG23	2.05	0.55
2:B:1393:NAG:H4	2:B:1394:NAG:C1	2.36	0.55
1:A:234:SER:HB2	1:A:275:LEU:O	2.06	0.55
1:B:344:TRP:HB2	1:B:353:HIS:O	2.07	0.55
1:B:49:VAL:HG23	1:B:53:ARG:NH2	2.21	0.55
1:A:175:PRO:HA	1:A:205:ILE:HG12	1.89	0.55
1:A:330:PHE:HB2	1:A:358:LEU:O	2.07	0.55
1:A:315:ILE:HD13	1:A:344:TRP:CH2	2.42	0.55
1:B:315:ILE:HD13	1:B:344:TRP:CH2	2.42	0.55
1:A:53:ARG:O	1:A:54:GLN:HG3	2.07	0.55
1:A:344:TRP:HB2	1:A:353:HIS:O	2.07	0.55
1:B:48:ASP:OD1	1:B:54:GLN:HA	2.07	0.55
1:B:330:PHE:HB2	1:B:358:LEU:O	2.07	0.55
1:A:49:VAL:HG23	1:A:53:ARG:NH2	2.21	0.54
1:B:114:TYR:CD1	1:B:204:VAL:HB	2.42	0.54
1:B:214:PRO:HA	1:B:240:GLN:O	2.07	0.54
1:A:326:ARG:CB	1:A:327:PRO:HD2	2.37	0.54
1:A:92:ILE:H	1:A:372:GLN:HE22	1.55	0.54
1:B:253:ILE:HG13	1:B:256:THR:OG1	2.07	0.54
1:B:36:ILE:HG23	1:B:82:CYS:SG	2.47	0.54
1:B:92:ILE:H	1:B:372:GLN:HE22	1.55	0.54
1:B:334:TYR:HD2	1:B:334:TYR:O	1.90	0.54
1:A:114:TYR:CD1	1:A:204:VAL:HB	2.42	0.54
1:B:326:ARG:CB	1:B:327:PRO:HD2	2.38	0.54
1:B:279:ASP:O	1:B:281:VAL:N	2.41	0.54
1:B:212:VAL:CG2	1:B:213:ARG:N	2.71	0.54
1:B:380:GLU:HG2	1:B:381:SER:N	2.16	0.54
1:B:370:MET:SD	1:B:387:GLU:HB3	2.48	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:211:SER:HB3	1:B:296:VAL:HG21	1.89	0.54
1:A:51:GLY:O	1:A:52:LEU:HD23	2.08	0.53
1:B:51:GLY:O	1:B:52:LEU:HD23	2.08	0.53
1:A:53:ARG:HB2	1:A:75:VAL:HG13	1.91	0.53
1:B:313:ALA:HB2	1:B:375:VAL:HG22	1.90	0.53
1:B:342:VAL:HG22	1:B:375:VAL:HG12	1.91	0.53
1:B:175:PRO:HA	1:B:205:ILE:HG12	1.90	0.53
1:B:131:VAL:O	1:B:135:VAL:HG23	2.09	0.53
1:B:175:PRO:C	1:B:177:ASP:H	2.11	0.53
1:A:334:TYR:O	1:A:334:TYR:HD2	1.90	0.53
1:B:40:ARG:HD3	1:B:46:VAL:HG12	1.91	0.53
1:B:1:GLN:HB2	1:B:31:ASN:CG	2.29	0.53
1:B:229:LEU:HD23	1:B:230:ALA:CB	2.38	0.53
1:A:175:PRO:C	1:A:177:ASP:H	2.11	0.53
1:A:370:MET:SD	1:A:387:GLU:HB3	2.48	0.53
1:B:340:LYS:HB3	1:B:377:ASN:HA	1.91	0.53
1:A:340:LYS:HB3	1:A:377:ASN:HA	1.90	0.53
1:A:313:ALA:HB2	1:A:375:VAL:HG22	1.90	0.53
1:B:213:ARG:HH22	1:B:215:LYS:HE3	1.74	0.53
1:A:104:GLN:HG2	1:A:105:SER:H	1.74	0.52
1:B:52:LEU:O	1:B:64:PRO:CD	2.50	0.52
1:A:48:ASP:OD2	1:A:54:GLN:HG2	2.09	0.52
1:A:28:ALA:N	1:A:36:ILE:HD11	2.25	0.52
1:B:331:THR:HA	1:B:357:VAL:HG22	1.91	0.52
1:A:364:LYS:HG2	1:A:366:GLU:CD	2.30	0.52
1:A:1:GLN:HB2	1:A:31:ASN:CG	2.29	0.52
1:A:135:VAL:HG12	1:A:186:THR:HB	1.91	0.52
1:A:229:LEU:HD23	1:A:230:ALA:CB	2.39	0.52
1:B:315:ILE:HG22	1:B:316:ASP:H	1.75	0.52
1:A:211:SER:HB3	1:A:296:VAL:HG21	1.91	0.52
1:A:40:ARG:HD3	1:A:46:VAL:HG12	1.91	0.52
1:B:326:ARG:HB3	1:B:327:PRO:CD	2.40	0.52
1:B:13:ARG:NH1	1:B:99:ARG:NH2	2.57	0.52
1:A:334:TYR:O	1:A:335:THR:HG23	2.10	0.52
1:A:48:ASP:OD1	1:A:54:GLN:HA	2.09	0.52
1:B:364:LYS:HG2	1:B:366:GLU:CD	2.29	0.52
1:A:36:ILE:HG23	1:A:82:CYS:SG	2.50	0.52
1:A:227:VAL:HG11	1:A:233:TYR:CB	2.40	0.52
1:B:390:LEU:HD22	1:B:391:GLY:H	1.74	0.52
1:A:180:LYS:H	1:A:202:ARG:HH22	1.58	0.52
1:A:23:GLU:HB3	1:A:62:VAL:HA	1.92	0.51
1:B:106:TYR:CE1	1:B:188:HIS:CD2	2.82	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:37:ILE:HB	1:A:83:LEU:CB	2.39	0.51
1:A:326:ARG:HB3	1:A:327:PRO:CD	2.39	0.51
1:B:28:ALA:N	1:B:36:ILE:HD11	2.25	0.51
1:A:29:SER:O	1:A:34:PRO:HG2	2.10	0.51
1:B:37:ILE:HB	1:B:83:LEU:CB	2.40	0.51
1:A:369:GLY:O	1:A:387:GLU:HA	2.10	0.51
1:B:29:SER:O	1:B:34:PRO:HG2	2.10	0.51
1:A:212:VAL:CG2	1:A:213:ARG:N	2.72	0.51
1:B:227:VAL:HG11	1:B:233:TYR:CB	2.40	0.51
1:A:13:ARG:NH1	1:A:99:ARG:NH2	2.57	0.51
1:B:57:SER:O	1:B:59:GLY:N	2.44	0.51
1:B:53:ARG:HB2	1:B:75:VAL:HG13	1.91	0.51
1:B:48:ASP:OD2	1:B:54:GLN:HG2	2.10	0.51
1:A:342:VAL:HG22	1:A:375:VAL:HG12	1.91	0.51
1:A:84:ALA:HB3	1:A:91:ILE:HG12	1.93	0.51
1:A:9:GLU:HG2	1:A:10:PRO:HD2	1.91	0.51
1:A:213:ARG:HH12	1:A:215:LYS:HD2	1.76	0.51
1:A:326:ARG:CD	1:A:327:PRO:HD2	2.41	0.51
1:B:15:ASP:CG	1:B:99:ARG:HH21	2.14	0.51
1:A:331:THR:HA	1:A:357:VAL:HG22	1.91	0.51
1:B:104:GLN:HG2	1:B:105:SER:H	1.76	0.50
1:B:369:GLY:O	1:B:387:GLU:HA	2.11	0.50
1:B:351:ILE:HG13	1:B:352:GLY:H	1.76	0.50
1:A:315:ILE:HG22	1:A:316:ASP:H	1.76	0.50
1:B:84:ALA:HB3	1:B:91:ILE:HG12	1.92	0.50
1:A:351:ILE:HG13	1:A:352:GLY:H	1.76	0.50
1:A:227:VAL:HG11	1:A:233:TYR:HB3	1.92	0.50
1:B:262:VAL:HG11	1:B:275:LEU:HD21	1.92	0.50
1:B:135:VAL:HG12	1:B:186:THR:HB	1.93	0.50
1:B:23:GLU:HB3	1:B:62:VAL:HA	1.93	0.50
1:A:325:GLY:N	1:A:363:VAL:HG12	2.27	0.50
1:A:15:ASP:CG	1:A:99:ARG:HH21	2.15	0.50
1:B:380:GLU:O	1:B:381:SER:HB3	2.12	0.49
1:B:205:ILE:HD12	1:B:205:ILE:N	2.27	0.49
1:B:111:ASP:OD2	3:B:1392:GOL:H2	2.12	0.49
1:B:241:SER:HB3	1:B:245:PRO:HD3	1.95	0.49
1:A:57:SER:O	1:A:59:GLY:N	2.44	0.49
1:B:16:PHE:CE1	1:B:100:ALA:HB2	2.48	0.49
1:A:12:ASN:OD1	1:A:97:HIS:CD2	2.63	0.49
1:B:326:ARG:CD	1:B:327:PRO:HD2	2.41	0.49
1:B:72:ARG:HH22	1:B:75:VAL:CG2	2.24	0.49
1:B:180:LYS:H	1:B:202:ARG:HH22	1.57	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:205:ILE:HD12	1:A:205:ILE:N	2.26	0.49
1:B:227:VAL:HG11	1:B:233:TYR:HB3	1.93	0.49
1:A:390:LEU:HD22	1:A:391:GLY:H	1.76	0.49
2:A:1392:NAG:C4	2:A:1393:NAG:C1	2.90	0.49
1:B:9:GLU:HG2	1:B:10:PRO:HD2	1.93	0.49
1:B:325:GLY:N	1:B:363:VAL:HG12	2.27	0.49
1:A:17:SER:CB	1:A:101:VAL:O	2.61	0.49
1:B:121:VAL:HG22	1:B:122:VAL:N	2.28	0.49
1:A:241:SER:HB3	1:A:245:PRO:HD3	1.93	0.49
1:A:219:GLN:H	1:A:219:GLN:HE21	1.57	0.49
1:A:136:PHE:CD2	1:A:189:ARG:CZ	2.95	0.49
1:B:12:ASN:OD1	1:B:97:HIS:CD2	2.63	0.49
1:B:354:SER:O	1:B:355:GLU:HG2	2.13	0.49
1:A:171:ARG:NE	1:A:172:GLU:OE2	2.31	0.49
1:A:380:GLU:O	1:A:381:SER:HB3	2.13	0.49
1:A:131:VAL:O	1:A:135:VAL:HG23	2.13	0.49
1:A:326:ARG:HD2	1:A:327:PRO:HD2	1.94	0.49
1:B:246:SER:O	1:B:292:VAL:HA	2.13	0.49
1:B:52:LEU:HD13	1:B:76:HIS:NE2	2.28	0.48
1:A:104:GLN:HG2	1:A:105:SER:N	2.28	0.48
1:B:270:GLN:HE21	1:B:272:SER:CB	2.26	0.48
1:B:126:GLU:O	1:B:128:PRO:HD3	2.13	0.48
1:A:52:LEU:HD13	1:A:76:HIS:NE2	2.28	0.48
1:A:121:VAL:HG22	1:A:122:VAL:N	2.28	0.48
1:A:364:LYS:NZ	1:A:364:LYS:HB2	2.29	0.48
1:A:39:ILE:CA	1:A:45:ALA:HA	2.38	0.48
1:A:176:GLU:HG3	1:A:176:GLU:H	1.22	0.48
1:A:24:ILE:HD11	1:A:63:PHE:HE2	1.78	0.48
2:B:1393:NAG:C4	2:B:1394:NAG:C1	2.91	0.48
1:A:16:PHE:CE1	1:A:100:ALA:HB2	2.49	0.48
1:A:321:THR:HB	1:A:389:LYS:CG	2.41	0.48
1:B:25:GLU:HA	1:B:59:GLY:O	2.14	0.48
1:A:125:CYS:SG	1:A:137:VAL:HG22	2.53	0.48
1:B:326:ARG:HD2	1:B:327:PRO:HD2	1.95	0.48
1:B:334:TYR:O	1:B:335:THR:HG23	2.13	0.48
1:A:25:GLU:HA	1:A:59:GLY:O	2.14	0.48
1:A:370:MET:HA	1:A:386:ALA:O	2.14	0.47
1:B:136:PHE:CD2	1:B:189:ARG:CZ	2.96	0.47
1:A:111:ASP:OD2	3:B:1397:GOL:H2	2.14	0.47
1:B:24:ILE:HD11	1:B:63:PHE:HE2	1.78	0.47
1:A:354:SER:O	1:A:355:GLU:HG2	2.13	0.47
1:A:51:GLY:H	1:A:54:GLN:NE2	2.13	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:379:ARG:O	1:A:380:GLU:HB2	2.14	0.47
1:B:104:GLN:HG2	1:B:105:SER:N	2.29	0.47
1:A:249:TRP:CD2	1:A:275:LEU:HD22	2.50	0.47
1:B:51:GLY:H	1:B:54:GLN:NE2	2.13	0.47
1:A:4:PRO:O	1:A:5:VAL:CB	2.62	0.47
1:B:39:ILE:CA	1:B:45:ALA:HA	2.39	0.47
1:B:25:GLU:HG3	1:B:27:LYS:NZ	2.30	0.47
1:A:25:GLU:HG3	1:A:27:LYS:NZ	2.30	0.47
1:B:379:ARG:O	1:B:380:GLU:HB2	2.15	0.47
1:A:39:ILE:CG1	1:A:81:ALA:HB3	2.45	0.47
1:B:4:PRO:O	1:B:5:VAL:CB	2.62	0.47
1:A:244:THR:HA	1:A:245:PRO:HD2	1.71	0.47
1:B:126:GLU:OE2	3:B:1392:GOL:H12	2.14	0.47
1:A:9:GLU:OE1	1:A:94:ARG:HG3	2.15	0.47
1:B:17:SER:CB	1:B:101:VAL:O	2.62	0.47
1:B:364:LYS:NZ	1:B:364:LYS:HB2	2.29	0.47
1:A:219:GLN:N	1:A:219:GLN:HE21	2.12	0.47
1:A:323:ASP:HB2	1:A:326:ARG:CG	2.45	0.47
1:A:24:ILE:HD13	1:A:24:ILE:N	2.29	0.46
1:B:71:TYR:HA	1:B:76:HIS:CD2	2.50	0.46
1:A:108:SER:O	1:A:197:SER:HB2	2.15	0.46
1:A:19:SER:OG	2:A:1392:NAG:H3	2.15	0.46
1:B:19:SER:OG	2:B:1393:NAG:H3	2.15	0.46
1:B:314:LYS:O	1:B:332:CYS:HA	2.15	0.46
1:B:9:GLU:OE1	1:B:94:ARG:HG3	2.15	0.46
1:B:24:ILE:N	1:B:24:ILE:HD13	2.30	0.46
1:B:370:MET:HA	1:B:386:ALA:O	2.15	0.46
1:B:321:THR:HB	1:B:389:LYS:CG	2.40	0.46
1:A:13:ARG:O	1:A:14:ILE:HD13	2.16	0.46
1:A:14:ILE:HA	1:A:14:ILE:HD13	1.74	0.46
1:A:35:GLU:HG2	1:A:85:ARG:O	2.16	0.46
1:B:39:ILE:CG1	1:B:81:ALA:HB3	2.46	0.46
1:A:340:LYS:CB	1:A:377:ASN:HA	2.46	0.46
1:B:342:VAL:CG1	1:B:373:CYS:SG	3.04	0.46
1:B:173:VAL:HG12	1:B:205:ILE:HG13	1.98	0.45
1:B:333:GLN:HA	1:B:333:GLN:HE21	1.81	0.45
1:A:71:TYR:HA	1:A:76:HIS:CD2	2.51	0.45
1:A:72:ARG:HH22	1:A:75:VAL:CG2	2.23	0.45
1:B:370:MET:SD	1:B:387:GLU:CB	3.04	0.45
1:A:370:MET:SD	1:A:387:GLU:CB	3.05	0.45
1:B:181:SER:OG	1:B:200:LYS:HD2	2.17	0.45
1:B:323:ASP:HB2	1:B:326:ARG:CG	2.44	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:314:LYS:O	1:A:332:CYS:HA	2.16	0.45
1:A:173:VAL:HG12	1:A:205:ILE:HG13	1.99	0.45
1:A:333:GLN:HA	1:A:333:GLN:HE21	1.80	0.45
1:B:298:GLY:O	1:B:299:GLU:HB2	2.17	0.45
1:B:131:VAL:HB	1:B:135:VAL:HG21	1.99	0.45
1:B:219:GLN:H	1:B:219:GLN:CD	2.20	0.45
1:A:253:ILE:H	1:A:253:ILE:HG12	1.50	0.45
1:A:246:SER:O	1:A:292:VAL:HA	2.17	0.45
1:B:212:VAL:HG13	1:B:242:TYR:N	2.18	0.45
1:A:389:LYS:HG2	1:A:389:LYS:H	1.51	0.45
1:A:323:ASP:CB	1:A:326:ARG:HG3	2.46	0.45
1:B:13:ARG:O	1:B:14:ILE:HD13	2.16	0.45
1:A:32:PRO:HG2	1:A:86:ASN:HD22	1.82	0.45
1:A:262:VAL:HG11	1:A:275:LEU:HD21	1.99	0.45
1:B:32:PRO:HB2	1:B:33:MET:H	1.59	0.45
1:B:108:SER:O	1:B:197:SER:HB2	2.17	0.45
1:B:171:ARG:NH2	1:B:172:GLU:OE1	2.46	0.45
1:A:131:VAL:HB	1:A:135:VAL:CG2	2.47	0.44
1:B:24:ILE:HD11	1:B:63:PHE:CE2	2.53	0.44
1:B:340:LYS:CB	1:B:377:ASN:HA	2.46	0.44
1:B:281:VAL:HG23	1:B:283:GLU:H	1.82	0.44
1:B:32:PRO:HG2	1:B:86:ASN:HD22	1.82	0.44
1:B:13:ARG:HH12	1:B:99:ARG:CZ	2.31	0.44
1:B:116:ILE:O	1:B:117:ARG:C	2.55	0.44
1:A:219:GLN:CD	1:A:219:GLN:H	2.21	0.44
1:A:270:GLN:HE21	1:A:272:SER:CB	2.30	0.44
1:A:342:VAL:CG1	1:A:373:CYS:SG	3.06	0.44
1:B:152:ASN:O	1:B:153:ALA:HB3	2.18	0.44
1:B:35:GLU:HG2	1:B:85:ARG:O	2.18	0.44
1:B:368:LYS:NZ	1:B:390:LEU:HD12	2.33	0.44
1:A:289:LEU:HD11	1:A:300:SER:HB2	1.99	0.44
1:A:23:GLU:CB	1:A:62:VAL:HA	2.48	0.44
1:A:56:SER:HB2	1:A:62:VAL:HG23	2.00	0.44
1:A:328:ALA:CB	1:A:359:ARG:HA	2.43	0.44
1:A:39:ILE:HG22	1:A:45:ALA:HB2	2.00	0.44
1:B:131:VAL:HB	1:B:135:VAL:CG2	2.48	0.44
1:A:131:VAL:HB	1:A:135:VAL:HG21	2.00	0.44
1:B:14:ILE:HA	1:B:14:ILE:HD13	1.73	0.44
1:B:2:LYS:HB3	1:B:30:GLY:HA2	2.00	0.44
1:B:23:GLU:CB	1:B:62:VAL:HA	2.48	0.44
1:B:56:SER:HB2	1:B:62:VAL:HG23	2.00	0.44
1:A:376:ARG:O	1:A:377:ASN:HB3	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:16:PHE:CZ	1:B:100:ALA:HB2	2.53	0.43
1:A:40:ARG:NH1	1:A:46:VAL:HA	2.33	0.43
1:A:32:PRO:HB2	1:A:33:MET:H	1.60	0.43
1:A:1:GLN:N	1:A:31:ASN:HD21	2.16	0.43
1:B:326:ARG:N	1:B:363:VAL:HG23	2.32	0.43
1:A:82:CYS:HB3	1:A:93:SER:HB3	1.99	0.43
1:A:313:ALA:C	1:A:384:ALA:HB2	2.38	0.43
1:A:16:PHE:CZ	1:A:100:ALA:HB2	2.53	0.43
1:B:40:ARG:NH1	1:B:46:VAL:HA	2.33	0.43
1:B:125:CYS:SG	1:B:137:VAL:HG22	2.58	0.43
1:B:323:ASP:CB	1:B:326:ARG:HG3	2.46	0.43
1:A:13:ARG:HH12	1:A:99:ARG:CZ	2.31	0.43
1:A:346:LYS:HA	1:A:370:MET:O	2.19	0.43
1:A:181:SER:OG	1:A:200:LYS:HD2	2.18	0.43
1:A:368:LYS:NZ	1:A:390:LEU:HD12	2.34	0.43
1:B:272:SER:HA	1:B:273:GLY:HA2	1.45	0.43
1:B:344:TRP:HB3	1:B:351:ILE:HD11	2.00	0.43
1:A:344:TRP:HB3	1:A:351:ILE:HD11	2.01	0.43
1:B:270:GLN:HE21	1:B:272:SER:HA	1.84	0.43
1:B:313:ALA:C	1:B:384:ALA:HB2	2.39	0.43
1:A:11:THR:HA	1:A:94:ARG:NH2	2.33	0.43
1:B:39:ILE:HG13	1:B:40:ARG:O	2.17	0.43
1:B:182:TYR:O	1:B:200:LYS:HB2	2.19	0.43
1:B:126:GLU:OE1	1:B:126:GLU:HA	2.18	0.43
1:B:380:GLU:CG	1:B:381:SER:N	2.79	0.43
1:A:116:ILE:O	1:A:117:ARG:C	2.57	0.43
1:A:24:ILE:HD11	1:A:63:PHE:CE2	2.53	0.43
1:A:37:ILE:O	1:A:83:LEU:N	2.45	0.43
1:B:249:TRP:CD2	1:B:275:LEU:HD22	2.53	0.43
1:B:346:LYS:HA	1:B:370:MET:O	2.18	0.43
1:B:82:CYS:HB3	1:B:93:SER:HB3	2.00	0.43
1:A:2:LYS:HB3	1:A:30:GLY:HA2	2.01	0.43
1:A:94:ARG:HG3	1:A:94:ARG:H	1.64	0.43
1:A:328:ALA:HB3	1:A:359:ARG:CA	2.44	0.43
1:A:39:ILE:HG13	1:A:40:ARG:O	2.19	0.43
1:B:63:PHE:CZ	1:B:98:VAL:HG21	2.54	0.42
1:B:161:LEU:HD23	1:B:161:LEU:HA	1.80	0.42
1:A:142:ASP:OD2	1:A:146:ARG:NH1	2.52	0.42
1:A:50:PRO:HA	1:A:54:GLN:HE21	1.85	0.42
1:A:270:GLN:HB2	1:A:275:LEU:HD12	2.00	0.42
1:A:353:HIS:CE1	1:A:355:GLU:HB2	2.54	0.42
1:B:281:VAL:O	1:B:284:ASP:HB2	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:313:ALA:HB2	1:B:375:VAL:CG2	2.50	0.42
1:A:298:GLY:O	1:A:299:GLU:HB2	2.18	0.42
1:B:342:VAL:HG11	1:B:373:CYS:SG	2.59	0.42
1:A:126:GLU:OE2	3:B:1397:GOL:H12	2.18	0.42
1:B:217:ASN:HB3	1:B:219:GLN:HE22	1.84	0.42
1:B:328:ALA:CB	1:B:359:ARG:HA	2.43	0.42
1:B:105:SER:CB	2:B:1395:NAG:H81	2.40	0.42
1:A:182:TYR:O	1:A:200:LYS:HB2	2.19	0.42
1:B:137:VAL:HA	1:B:186:THR:HA	2.02	0.42
1:B:376:ARG:O	1:B:377:ASN:HB3	2.19	0.42
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.79	0.42
1:B:39:ILE:HG22	1:B:45:ALA:HB2	2.01	0.42
1:B:142:ASP:OD2	1:B:146:ARG:NH1	2.52	0.42
1:B:37:ILE:O	1:B:83:LEU:N	2.45	0.42
1:A:270:GLN:HE21	1:A:272:SER:HA	1.84	0.42
1:A:2:LYS:HB3	1:A:3:GLY:O	2.19	0.42
1:B:142:ASP:HB3	1:B:144:GLU:H	1.84	0.42
1:B:176:GLU:H	1:B:176:GLU:HG3	1.20	0.42
1:A:216:VAL:HG22	1:A:238:MET:O	2.20	0.42
1:A:152:ASN:O	1:A:153:ALA:HB3	2.19	0.42
1:A:127:ILE:CG2	1:A:135:VAL:HB	2.49	0.42
1:B:7:LEU:HD22	1:B:8:LYS:HD2	2.01	0.42
1:A:106:TYR:CD2	1:A:106:TYR:C	2.92	0.42
1:A:342:VAL:HG11	1:A:373:CYS:SG	2.60	0.42
1:B:72:ARG:NH1	1:B:72:ARG:HG3	2.19	0.41
1:B:23:GLU:OE2	1:B:62:VAL:HG22	2.20	0.41
1:A:368:LYS:CB	1:A:388:LEU:HD23	2.50	0.41
1:A:63:PHE:CZ	1:A:98:VAL:HG21	2.54	0.41
1:B:66:PHE:CE2	1:B:71:TYR:HB2	2.54	0.41
1:A:66:PHE:CE2	1:A:71:TYR:HB2	2.55	0.41
1:B:240:GLN:O	1:B:241:SER:CB	2.68	0.41
1:B:331:THR:HG22	1:B:332:CYS:H	1.85	0.41
1:B:84:ALA:HB3	1:B:91:ILE:CG1	2.50	0.41
1:A:142:ASP:HB3	1:A:144:GLU:H	1.84	0.41
1:B:289:LEU:HD11	1:B:300:SER:HB2	2.02	0.41
1:A:251:LYS:HD2	1:A:288:TYR:CZ	2.55	0.41
1:A:52:LEU:O	1:A:64:PRO:CD	2.53	0.41
1:B:1:GLN:N	1:B:31:ASN:HD21	2.18	0.41
1:B:114:TYR:CD1	1:B:204:VAL:CB	3.03	0.41
1:B:241:SER:CB	1:B:245:PRO:HD3	2.50	0.41
1:B:331:THR:HG22	1:B:332:CYS:N	2.36	0.41
1:A:84:ALA:HB3	1:A:91:ILE:CG1	2.50	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:111:ASP:O	1:A:201:GLY:HA3	2.21	0.41
1:A:142:ASP:C	1:A:144:GLU:H	2.24	0.41
1:B:251:LYS:HD2	1:B:288:TYR:CZ	2.55	0.41
1:A:240:GLN:O	1:A:241:SER:CB	2.69	0.41
1:A:241:SER:CB	1:A:245:PRO:HD3	2.51	0.41
1:B:353:HIS:CE1	1:B:355:GLU:HB2	2.56	0.41
1:A:371:TYR:CD2	1:A:371:TYR:N	2.88	0.41
1:B:55:ILE:HG22	1:B:55:ILE:O	2.19	0.41
1:A:376:ARG:HB3	1:A:377:ASN:H	1.60	0.41
1:B:278:LYS:O	1:B:279:ASP:HB2	2.21	0.41
1:B:368:LYS:HB2	1:B:388:LEU:O	2.20	0.41
1:A:331:THR:HG22	1:A:332:CYS:N	2.35	0.41
1:B:16:PHE:CD2	1:B:16:PHE:N	2.89	0.41
1:B:368:LYS:HZ2	1:B:390:LEU:HD12	1.86	0.41
1:A:368:LYS:HB2	1:A:388:LEU:O	2.20	0.41
1:B:2:LYS:HB3	1:B:3:GLY:O	2.20	0.41
1:A:105:SER:CB	2:A:1394:NAG:H81	2.40	0.41
1:A:39:ILE:HG22	1:A:45:ALA:HA	2.03	0.41
1:B:142:ASP:C	1:B:144:GLU:H	2.25	0.41
1:A:98:VAL:HG13	1:A:98:VAL:O	2.21	0.41
1:B:270:GLN:HB2	1:B:275:LEU:HD12	2.02	0.41
1:A:55:ILE:O	1:A:55:ILE:HG22	2.20	0.41
1:B:11:THR:HA	1:B:94:ARG:NH2	2.35	0.40
1:B:242:TYR:HA	1:B:243:PRO:C	2.40	0.40
1:A:212:VAL:HG13	1:A:242:TYR:N	2.19	0.40
1:B:244:THR:HA	1:B:245:PRO:HD2	1.70	0.40
1:A:313:ALA:HB2	1:A:375:VAL:CG2	2.50	0.40
1:A:7:LEU:HD22	1:A:8:LYS:HD2	2.02	0.40
1:B:371:TYR:CD2	1:B:371:TYR:N	2.89	0.40
1:B:50:PRO:HA	1:B:54:GLN:HE21	1.85	0.40
1:B:52:LEU:CD1	1:B:72:ARG:NH1	2.84	0.40
1:B:106:TYR:CD2	1:B:106:TYR:C	2.94	0.40
1:A:331:THR:HG22	1:A:332:CYS:H	1.85	0.40
1:A:114:TYR:CD1	1:A:204:VAL:CB	3.04	0.40
1:B:139:LEU:CD2	1:B:140:TRP:H	2.32	0.40
2:A:1395:NAG:H2	2:A:1395:NAG:H82	1.92	0.40
1:A:272:SER:HA	1:A:273:GLY:HA2	1.44	0.40
1:A:141:LEU:O	1:A:182:TYR:HA	2.21	0.40
1:B:55:ILE:HA	1:B:61:LEU:HD12	2.03	0.40
1:B:111:ASP:O	1:B:201:GLY:HA3	2.20	0.40
1:A:217:ASN:HA	1:A:218:PRO:HD3	1.95	0.40
1:A:80:TYR:O	1:A:96:VAL:HG23	2.22	0.40



There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	389/391 (100%)	310 (80%)	54 (14%)	25 (6%)	2	11
1	B	389/391 (100%)	313 (80%)	51 (13%)	25 (6%)	2	11
All	All	778/782 (100%)	623 (80%)	105 (14%)	50 (6%)	2	11

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	32	PRO
1	A	58	ASP
1	A	176	GLU
1	A	180	LYS
1	A	212	VAL
1	A	280	ALA
1	A	377	ASN
1	B	5	VAL
1	B	32	PRO
1	B	58	ASP
1	B	176	GLU
1	B	180	LYS
1	B	212	VAL
1	B	280	ALA
1	B	377	ASN
1	A	12	ASN
1	A	56	SER
1	A	241	SER
1	A	341	THR
1	B	12	ASN
1	B	56	SER
1	B	241	SER
1	B	341	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	20	THR
1	A	381	SER
1	B	20	THR
1	B	381	SER
1	A	33	MET
1	A	324	PHE
1	A	376	ARG
1	A	380	GLU
1	B	33	MET
1	B	324	PHE
1	B	376	ARG
1	A	4	PRO
1	A	127	ILE
1	B	4	PRO
1	B	380	GLU
1	B	18	ASN
1	A	31	ASN
1	A	210	GLY
1	A	322	VAL
1	B	31	ASN
1	B	322	VAL
1	A	327	PRO
1	A	337	ASN
1	B	210	GLY
1	B	327	PRO
1	B	337	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	339/339 (100%)	283 (84%)	56 (16%)	3	16
1	B	339/339 (100%)	284 (84%)	55 (16%)	3	17
All	All	678/678 (100%)	567 (84%)	111 (16%)	3	16

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	14	ILE
1	A	24	ILE
1	A	31	ASN
1	A	33	MET
1	A	40	ARG
1	A	58	ASP
1	A	72	ARG
1	A	73	GLN
1	A	74	GLU
1	A	79	VAL
1	A	83	LEU
1	A	94	ARG
1	A	96	VAL
1	A	103	ILE
1	A	104	GLN
1	A	106	TYR
1	A	109	GLU
1	A	117	ARG
1	A	129	SER
1	A	134	PHE
1	A	138	ASP
1	A	139	LEU
1	A	161	LEU
1	A	163	LEU
1	A	176	GLU
1	A	179	TYR
1	A	189	ARG
1	A	195	ARG
1	A	219	GLN
1	A	221	LYS
1	A	238	MET
1	A	244	THR
1	A	253	ILE
1	A	256	THR
1	A	257	THR
1	A	258	ARG
1	A	275	LEU
1	A	278	LYS
1	A	292	VAL
1	A	303	THR
1	A	306	THR
1	A	311	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	315	ILE
1	A	321	THR
1	A	322	VAL
1	A	324	PHE
1	A	330	PHE
1	A	333	GLN
1	A	334	TYR
1	A	341	THR
1	A	363	VAL
1	A	364	LYS
1	A	373	CYS
1	A	389	LYS
1	A	390	LEU
1	B	5	VAL
1	B	14	ILE
1	B	24	ILE
1	B	31	ASN
1	B	33	MET
1	B	40	ARG
1	B	58	ASP
1	B	72	ARG
1	B	73	GLN
1	B	74	GLU
1	B	79	VAL
1	B	83	LEU
1	B	94	ARG
1	B	96	VAL
1	B	103	ILE
1	B	104	GLN
1	B	106	TYR
1	B	109	GLU
1	B	117	ARG
1	B	129	SER
1	B	134	PHE
1	B	138	ASP
1	B	139	LEU
1	B	161	LEU
1	B	163	LEU
1	B	176	GLU
1	B	179	TYR
1	B	189	ARG
1	B	195	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	221	LYS
1	B	238	MET
1	B	244	THR
1	B	253	ILE
1	B	256	THR
1	B	257	THR
1	B	258	ARG
1	B	275	LEU
1	B	278	LYS
1	B	292	VAL
1	B	303	THR
1	B	306	THR
1	B	311	LEU
1	B	315	ILE
1	B	321	THR
1	B	322	VAL
1	B	324	PHE
1	B	330	PHE
1	B	333	GLN
1	B	334	TYR
1	B	341	THR
1	B	363	VAL
1	B	364	LYS
1	B	373	CYS
1	B	389	LYS
1	B	390	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	54	GLN
1	A	76	HIS
1	A	87	GLN
1	A	97	HIS
1	A	188	HIS
1	A	219	GLN
1	A	270	GLN
1	A	293	ASN
1	A	320	GLN
1	A	333	GLN
1	A	353	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	372	GLN
1	B	31	ASN
1	B	54	GLN
1	B	76	HIS
1	B	87	GLN
1	B	97	HIS
1	B	188	HIS
1	B	270	GLN
1	B	293	ASN
1	B	320	GLN
1	B	333	GLN
1	B	353	HIS
1	B	372	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
2	NAG	A	1392	-	12,14,15	0.65	0	15,19,21	1.96	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	1393	-	12,14,15	0.60	0	15,19,21	1.51	2 (13%)
2	NAG	A	1394	-	12,14,15	0.70	0	15,19,21	1.55	2 (13%)
2	NAG	A	1395	-	12,14,15	0.60	0	15,19,21	1.69	3 (20%)
3	GOL	B	1392	-	5,5,5	0.37	0	5,5,5	0.28	0
2	NAG	B	1393	-	12,14,15	0.63	0	15,19,21	1.97	2 (13%)
2	NAG	B	1394	-	12,14,15	0.60	0	15,19,21	1.50	2 (13%)
2	NAG	B	1395	-	12,14,15	0.70	0	15,19,21	1.59	3 (20%)
2	NAG	B	1396	-	12,14,15	0.61	0	15,19,21	1.71	3 (20%)
3	GOL	B	1397	-	5,5,5	0.35	0	5,5,5	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1392	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1393	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1394	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1395	-	-	0/6/23/26	0/1/1/1
3	GOL	B	1392	-	-	0/4/4/4	0/0/0/0
2	NAG	B	1393	-	-	0/6/23/26	0/1/1/1
2	NAG	B	1394	-	-	0/6/23/26	0/1/1/1
2	NAG	B	1395	-	-	0/6/23/26	0/1/1/1
2	NAG	B	1396	-	-	0/6/23/26	0/1/1/1
3	GOL	B	1397	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1392	NAG	O5-C5-C4	5.87	118.11	110.65
2	B	1393	NAG	O5-C5-C4	5.87	118.10	110.65
2	B	1396	NAG	O5-C5-C4	4.77	116.71	110.65
2	A	1395	NAG	O5-C5-C4	4.74	116.67	110.65
2	B	1395	NAG	C3-C4-C5	4.23	117.77	110.20
2	A	1394	NAG	C3-C4-C5	4.08	117.49	110.20
2	A	1393	NAG	O5-C5-C4	4.03	115.77	110.65
2	B	1393	NAG	C3-C4-C5	4.00	117.34	110.20
2	A	1392	NAG	C3-C4-C5	3.93	117.22	110.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1394	NAG	O5-C5-C4	3.86	115.55	110.65
2	A	1393	NAG	C3-C4-C5	3.36	116.20	110.20
2	B	1394	NAG	C3-C4-C5	3.28	116.06	110.20
2	B	1396	NAG	C3-C4-C5	3.27	116.04	110.20
2	A	1394	NAG	O5-C5-C4	3.20	114.72	110.65
2	A	1395	NAG	C3-C4-C5	3.08	115.70	110.20
2	B	1395	NAG	O5-C5-C4	3.06	114.54	110.65
2	B	1396	NAG	C6-C5-C4	-2.28	107.50	113.00
2	A	1395	NAG	C6-C5-C4	-2.23	107.62	113.00
2	B	1395	NAG	O5-C5-C6	2.14	109.22	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	391/391 (100%)	-0.25	0 100 100	9, 67, 134, 163	0
1	B	391/391 (100%)	-0.25	2 (0%) 88 36	8, 69, 132, 168	0
All	All	782/782 (100%)	-0.25	2 (0%) 91 48	8, 68, 133, 168	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	34	PRO	3.0
1	B	35	GLU	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	B	1397	6/6	0.20	2.07	63,63,63,63	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	1392	6/6	0.16	0.36	64,64,64,64	0
2	NAG	B	1396	14/15	0.17	0.34	51,51,51,51	0
2	NAG	A	1395	14/15	0.17	0.19	53,53,53,53	0
2	NAG	A	1394	14/15	0.15	-0.15	97,97,97,97	0
2	NAG	B	1393	14/15	0.14	-0.85	62,62,62,62	0
2	NAG	B	1395	14/15	0.16	-0.90	95,95,95,95	0
2	NAG	A	1392	14/15	0.14	-0.99	54,54,54,54	0
2	NAG	B	1394	14/15	0.14	-7.38	75,75,75,75	0
2	NAG	A	1393	14/15	0.17	-11.00	74,74,74,74	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.