



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 05:38 PM EDT

PDB ID : 3DMK  
Title : Crystal structure of Down Syndrome Cell Adhesion Molecule (DSCAM) iso-form 1.30.30, N-terminal eight Ig domains  
Authors : Sawaya, M.R.; Wojtowicz, W.M.; Eisenberg, D.; Zipursky, S.L.  
Deposited on : unknown  
Resolution : 4.19 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-20030345  
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-20030345

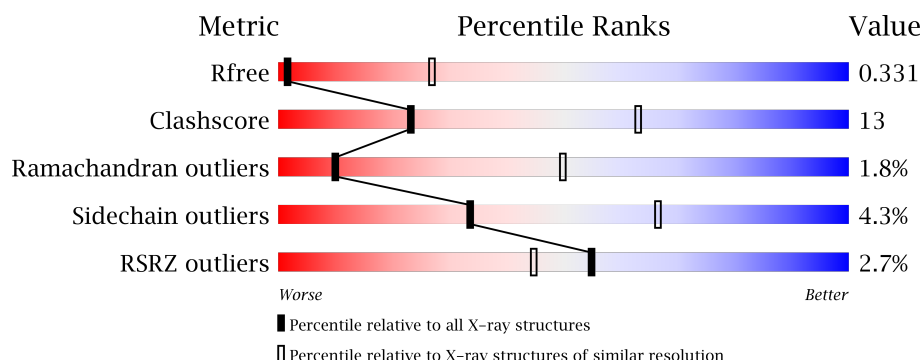
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.19 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	1177 (4.80-3.60)
Clashscore	112137	1025 (4.72-3.66)
Ramachandran outliers	110173	1024 (4.76-3.62)
Sidechain outliers	110143	1008 (4.76-3.62)
RSRZ outliers	101464	1188 (4.80-3.60)

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	816	<div> <div>5%</div> <div>67%</div> <div>26%</div> <div>• 5%</div> </div>
1	B	816	<div> <div>61%</div> <div>21%</div> <div>•</div> <div>17%</div> </div>
1	C	816	<div> <div>%</div> <div>60%</div> <div>22%</div> <div>•</div> <div>17%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	784	X	-	-	-
2	NAG	B	790	-	-	-	X
3	GOL	A	786	-	-	-	X
3	GOL	A	787	-	-	-	X
3	GOL	B	794	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16740 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 Down Syndrome Cell Adhesion Molecule (DSCAM) isoform 1.30.30, N-terminal eight Ig domains.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	775	Total	C	N	O	S	0	0	0
			5985	3778	1035	1147	25			
1	B	676	Total	C	N	O	S	0	0	0
			5223	3295	908	998	22			
1	C	676	Total	C	N	O	S	0	0	0
			5223	3295	908	998	22			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	776	HIS	-	EXPRESSION TAG	PDB 3DMK
A	777	HIS	-	EXPRESSION TAG	PDB 3DMK
A	778	HIS	-	EXPRESSION TAG	PDB 3DMK
A	779	HIS	-	EXPRESSION TAG	PDB 3DMK
A	780	HIS	-	EXPRESSION TAG	PDB 3DMK
A	781	HIS	-	EXPRESSION TAG	PDB 3DMK
B	776	HIS	-	EXPRESSION TAG	PDB 3DMK
B	777	HIS	-	EXPRESSION TAG	PDB 3DMK
B	778	HIS	-	EXPRESSION TAG	PDB 3DMK
B	779	HIS	-	EXPRESSION TAG	PDB 3DMK
B	780	HIS	-	EXPRESSION TAG	PDB 3DMK
B	781	HIS	-	EXPRESSION TAG	PDB 3DMK
C	776	HIS	-	EXPRESSION TAG	PDB 3DMK
C	777	HIS	-	EXPRESSION TAG	PDB 3DMK
C	778	HIS	-	EXPRESSION TAG	PDB 3DMK
C	779	HIS	-	EXPRESSION TAG	PDB 3DMK
C	780	HIS	-	EXPRESSION TAG	PDB 3DMK
C	781	HIS	-	EXPRESSION TAG	PDB 3DMK

- Molecule 2 is 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		
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		
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		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

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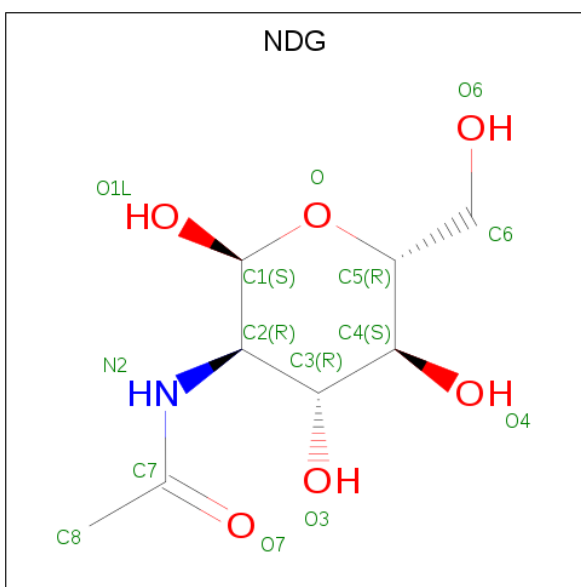
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

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



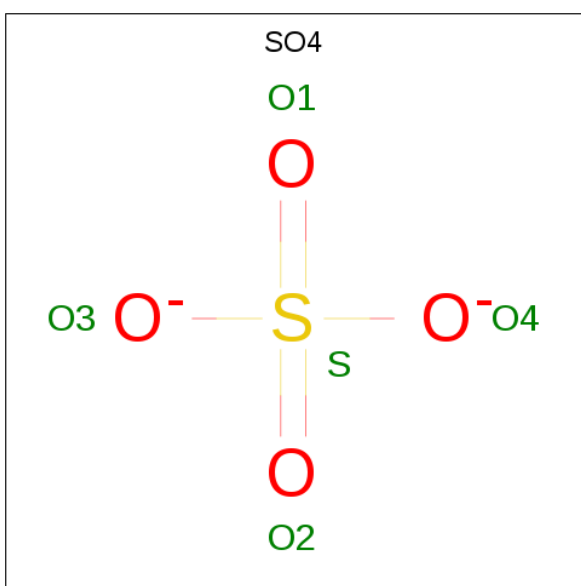
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

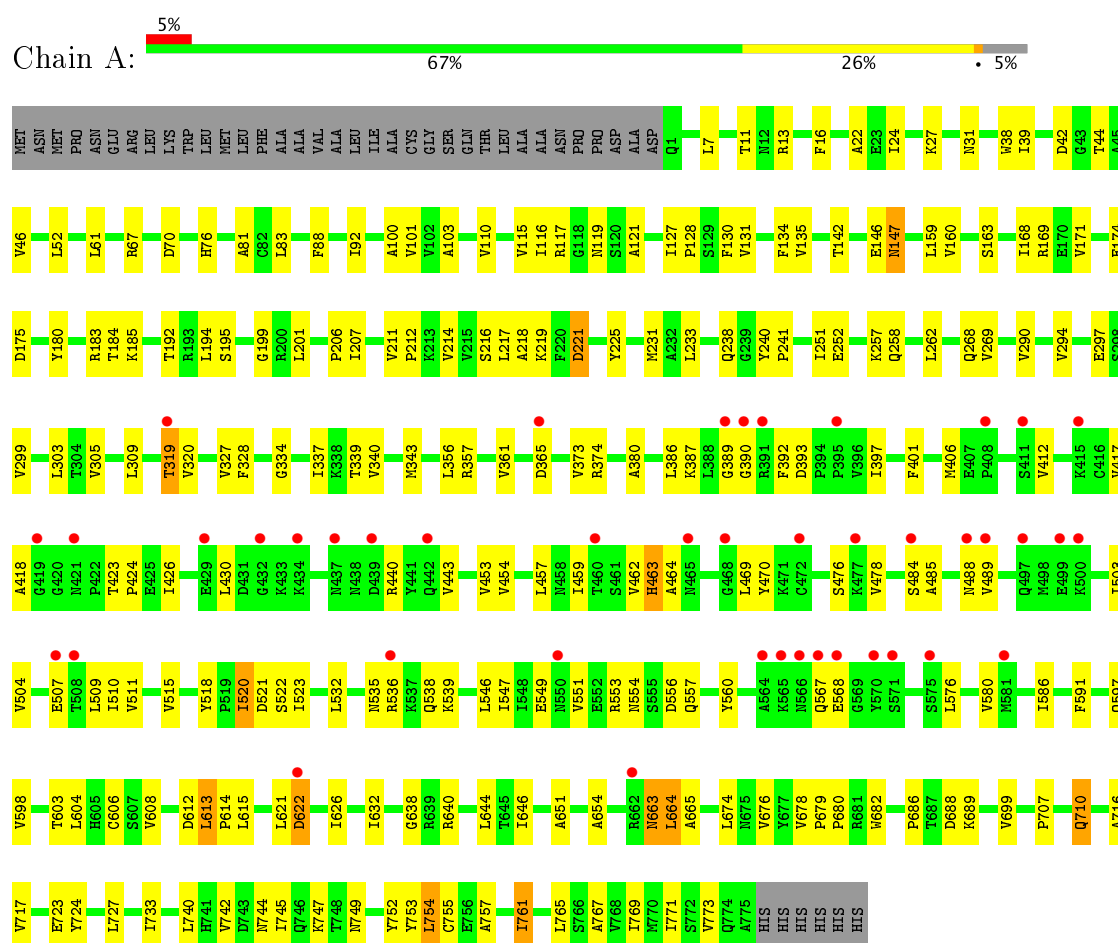


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		

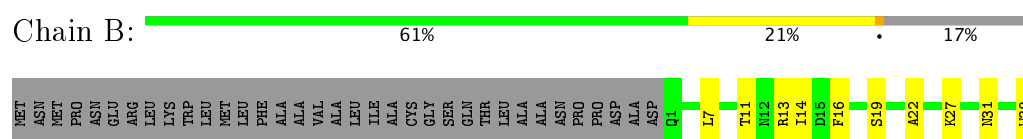
### 3 Residue-property plots

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.

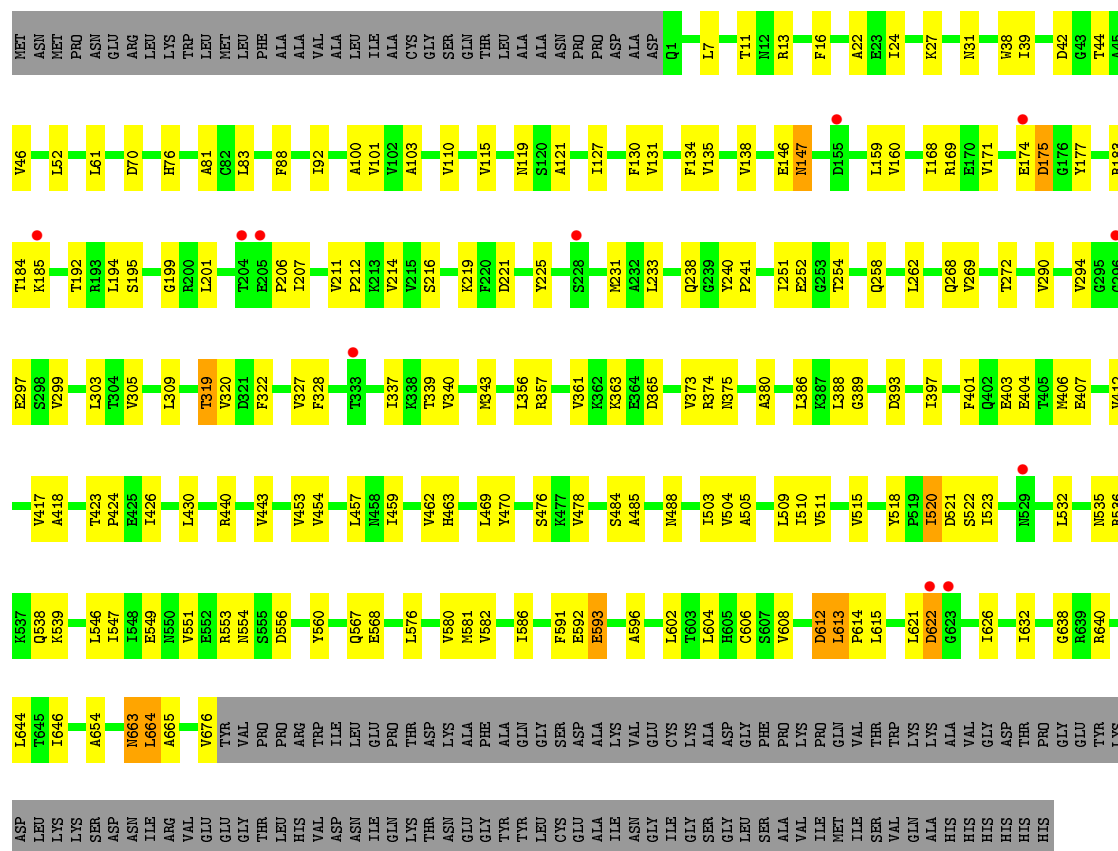
- Molecule 1: Down Syndrome Cell Adhesion Molecule (DSCAM) isoform 1.30.30, N-terminal eight Ig domains



- Molecule 1: Down Syndrome Cell Adhesion Molecule (DSCAM) isoform 1.30.30, N-terminal eight Ig domains







## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.46Å 177.61Å 434.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 4.19 11.99 – 4.19	Depositor EDS
% Data completeness (in resolution range)	99.4 (12.00-4.19) 99.4 (11.99-4.19)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.72 (at 4.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.280 , 0.327 0.283 , 0.331	Depositor DCC
$R_{free}$ test set	1618 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	99.4	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 2.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.69	EDS
Total number of atoms	16740	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, NDG, SO4

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	0.33	0/6113	0.52	0/8303
1	B	0.38	0/5334	0.54	0/7246
1	C	0.33	0/5334	0.52	0/7246
All	All	0.35	0/16781	0.53	0/22795

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5985	0	5928	174	0
1	B	5223	0	5172	128	1
1	C	5223	0	5174	131	1
2	A	56	0	50	3	0
2	B	126	0	112	1	0
2	C	70	0	62	1	0
3	A	12	0	16	0	0
3	B	12	0	16	0	0
4	B	14	0	12	0	0
4	C	14	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	5	0	0	0	0
All	All	16740	0	16554	425	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 13.

All (425) 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:654:ALA:HB2	1:A:676:VAL:HG12	1.38	1.00
1:A:733:ILE:HG23	1:A:742:VAL:HG22	1.46	0.97
1:B:412:VAL:HB	1:B:459:ILE:HG22	1.53	0.90
1:C:412:VAL:HB	1:C:459:ILE:HG22	1.56	0.87
1:C:504:VAL:HG12	1:C:581:MET:HB2	1.56	0.87
1:C:401:PHE:CE2	1:C:485:ALA:HB3	2.11	0.86
1:A:412:VAL:HB	1:A:459:ILE:HG22	1.58	0.85
1:B:654:ALA:HB2	1:B:676:VAL:HG12	1.59	0.85
1:A:654:ALA:HB2	1:A:676:VAL:CG1	2.08	0.84
1:B:320:VAL:HG21	1:B:361:VAL:HG21	1.61	0.82
1:A:320:VAL:HG21	1:A:361:VAL:HG21	1.62	0.82
1:A:401:PHE:CE2	1:A:485:ALA:HB3	2.14	0.82
1:B:401:PHE:CE2	1:B:485:ALA:HB3	2.15	0.81
1:C:320:VAL:HG21	1:C:361:VAL:HG21	1.62	0.81
1:A:217:LEU:HD23	1:B:217:LEU:HD23	1.62	0.81
1:A:218:ALA:HA	1:B:217:LEU:HD21	1.66	0.78
1:A:217:LEU:HD21	1:B:218:ALA:HA	1.64	0.78
1:C:417:VAL:HG22	1:C:454:VAL:HG22	1.65	0.77
1:A:699:VAL:HG13	1:A:740:LEU:HB3	1.65	0.77
1:C:596:ALA:HB2	1:C:602:LEU:HD21	1.65	0.77
1:A:417:VAL:HG22	1:A:454:VAL:HG22	1.68	0.76
1:C:504:VAL:HG11	1:C:665:ALA:HB3	1.67	0.75
1:B:503:ILE:HG21	1:B:551:VAL:HG21	1.70	0.74
1:A:217:LEU:CD2	1:B:217:LEU:HD23	2.18	0.74
1:A:217:LEU:HD23	1:B:217:LEU:CD2	2.17	0.74
1:B:417:VAL:HG22	1:B:454:VAL:HG22	1.70	0.74
1:C:373:VAL:HG23	1:C:380:ALA:HB3	1.69	0.74
1:B:76:HIS:HB3	1:B:100:ALA:HB3	1.68	0.74
1:C:532:LEU:HD23	1:C:546:LEU:HD13	1.68	0.73
1:A:373:VAL:HG23	1:A:380:ALA:HB3	1.70	0.73
1:B:127:ILE:HD13	1:B:135:VAL:HG12	1.71	0.72
1:A:651:ALA:HA	1:A:676:VAL:HG11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ILE:HG21	1:A:551:VAL:HG21	1.72	0.71
1:B:373:VAL:HG23	1:B:380:ALA:HB3	1.71	0.71
1:A:532:LEU:HD21	1:A:546:LEU:HD22	1.71	0.71
1:C:76:HIS:HB3	1:C:100:ALA:HB3	1.71	0.71
1:B:632:ILE:CG2	1:B:644:LEU:HD11	2.21	0.71
1:C:503:ILE:HG21	1:C:551:VAL:HG21	1.71	0.71
1:A:76:HIS:HB3	1:A:100:ALA:HB3	1.73	0.71
1:C:632:ILE:CG2	1:C:644:LEU:HD11	2.20	0.71
1:A:597:GLN:OE1	1:A:761:ILE:HG22	1.91	0.70
1:C:127:ILE:HD13	1:C:135:VAL:HG12	1.73	0.70
1:A:532:LEU:CD2	1:A:546:LEU:HD22	2.22	0.70
1:C:430:LEU:HD12	1:C:470:TYR:CZ	2.28	0.69
1:B:412:VAL:HB	1:B:459:ILE:CG2	2.22	0.69
1:A:612:ASP:O	1:A:614:PRO:HD2	1.93	0.69
1:A:225:TYR:HB2	1:A:231:MET:HE3	1.74	0.68
1:B:612:ASP:O	1:B:614:PRO:HD2	1.93	0.68
1:A:586:ILE:HA	1:A:608:VAL:HG22	1.76	0.67
1:B:586:ILE:HA	1:B:608:VAL:HG22	1.76	0.67
1:A:632:ILE:CG2	1:A:644:LEU:HD11	2.24	0.67
1:C:612:ASP:O	1:C:614:PRO:HD2	1.94	0.67
1:A:319:THR:HG22	1:A:389:GLY:CA	2.24	0.67
1:A:67:ARG:HH11	2:A:782:NAG:H81	1.60	0.67
1:A:127:ILE:HD13	1:A:135:VAL:HG12	1.76	0.66
1:B:476:SER:OG	1:B:478:VAL:HG12	1.96	0.66
1:C:532:LEU:CD2	1:C:546:LEU:HD13	2.26	0.65
1:B:535:ASN:C	1:B:535:ASN:HD22	2.00	0.65
1:A:532:LEU:HD21	1:A:546:LEU:CD2	2.27	0.64
1:A:430:LEU:HD12	1:A:470:TYR:CZ	2.33	0.64
1:B:225:TYR:HB2	1:B:231:MET:HE3	1.79	0.64
1:B:430:LEU:HD12	1:B:470:TYR:CZ	2.32	0.64
1:B:168:ILE:HD12	1:B:201:LEU:HD11	1.80	0.64
1:C:476:SER:OG	1:C:478:VAL:HG12	1.98	0.64
1:C:231:MET:CE	1:C:305:VAL:HG22	2.29	0.63
1:A:211:VAL:HG22	1:A:294:VAL:CG1	2.29	0.63
1:A:476:SER:OG	1:A:478:VAL:HG12	1.99	0.63
1:C:168:ILE:HD12	1:C:201:LEU:HD11	1.80	0.63
1:A:231:MET:CE	1:A:305:VAL:HG22	2.29	0.63
1:A:412:VAL:HB	1:A:459:ILE:CG2	2.28	0.63
1:A:532:LEU:O	1:A:538:GLN:OE1	2.17	0.63
1:A:676:VAL:HG13	1:A:676:VAL:O	1.99	0.62
1:B:211:VAL:HG22	1:B:294:VAL:CG1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:VAL:HB	1:C:459:ILE:CG2	2.27	0.62
1:B:251:ILE:HD11	1:B:258:GLN:HG3	1.81	0.61
1:A:110:VAL:HG12	1:A:199:GLY:HA3	1.82	0.61
1:C:110:VAL:HG12	1:C:199:GLY:HA3	1.83	0.61
1:C:211:VAL:HG22	1:C:294:VAL:CG1	2.30	0.61
1:A:423:THR:CG2	1:A:453:VAL:HG23	2.31	0.60
1:A:168:ILE:HD12	1:A:201:LEU:HD11	1.83	0.60
1:A:717:VAL:H	1:A:723:GLU:CD	2.03	0.60
1:B:110:VAL:HG12	1:B:199:GLY:HA3	1.83	0.60
1:C:251:ILE:HD11	1:C:258:GLN:HG3	1.82	0.59
1:C:592:GLU:O	1:C:593:GLU:C	2.40	0.59
1:A:251:ILE:HD11	1:A:258:GLN:HG3	1.84	0.59
1:A:747:LYS:HA	1:A:773:VAL:HG21	1.84	0.59
1:B:231:MET:CE	1:B:305:VAL:HG22	2.32	0.59
1:A:231:MET:HE1	1:A:305:VAL:HG22	1.84	0.59
1:C:423:THR:CG2	1:C:453:VAL:HG23	2.33	0.59
1:B:83:LEU:HD13	1:B:92:ILE:CG2	2.33	0.58
1:A:707:PRO:CD	1:A:761:ILE:HD11	2.33	0.58
1:A:591:PHE:CE1	1:A:604:LEU:HD13	2.39	0.58
1:B:340:VAL:HG22	1:B:373:VAL:HG12	1.86	0.58
1:B:231:MET:HE1	1:B:305:VAL:HG22	1.84	0.58
1:C:262:LEU:HD21	1:C:268:GLN:HB2	1.86	0.58
1:A:262:LEU:HD21	1:A:268:GLN:HB2	1.85	0.57
1:C:121:ALA:HB2	1:C:171:VAL:HG21	1.86	0.57
1:A:185:LYS:HB2	1:A:192:THR:HG22	1.87	0.57
1:B:121:ALA:HB2	1:B:171:VAL:HG21	1.87	0.57
1:A:678:VAL:HG13	1:A:679:PRO:HD2	1.87	0.57
1:B:146:GLU:C	1:B:147:ASN:HD22	2.08	0.57
1:B:262:LEU:HD21	1:B:268:GLN:HB2	1.87	0.56
1:B:488:ASN:HB3	1:B:518:TYR:HB2	1.86	0.56
1:B:532:LEU:CD2	1:B:546:LEU:HD22	2.36	0.56
1:B:423:THR:CG2	1:B:453:VAL:HG23	2.35	0.56
1:A:511:VAL:HG21	1:A:576:LEU:HD22	1.87	0.56
1:C:225:TYR:HB2	1:C:231:MET:HE3	1.86	0.56
1:C:551:VAL:HG12	1:C:580:VAL:HG13	1.87	0.56
1:C:586:ILE:HD11	1:C:606:CYS:SG	2.45	0.56
1:C:83:LEU:HD13	1:C:92:ILE:CG2	2.36	0.56
1:C:254:THR:HG22	1:C:593:GLU:O	2.05	0.56
1:A:121:ALA:HB2	1:A:171:VAL:HG21	1.88	0.56
1:A:504:VAL:HG11	1:A:665:ALA:O	2.06	0.56
1:C:511:VAL:HG21	1:C:576:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ASN:HB3	1:A:518:TYR:HB2	1.88	0.55
1:A:680:PRO:HB2	1:A:765:LEU:HD13	1.87	0.55
1:A:83:LEU:HB2	1:A:92:ILE:HG22	1.88	0.55
1:A:211:VAL:HG22	1:A:294:VAL:HG12	1.87	0.55
1:B:211:VAL:HG22	1:B:294:VAL:HG12	1.89	0.55
1:C:488:ASN:HB3	1:C:518:TYR:HB2	1.88	0.55
1:C:586:ILE:HA	1:C:608:VAL:HG22	1.87	0.55
1:A:83:LEU:HD13	1:A:92:ILE:CG2	2.37	0.55
1:A:340:VAL:HG22	1:A:373:VAL:HG12	1.89	0.55
1:A:654:ALA:CB	1:A:676:VAL:HG12	2.26	0.55
1:B:185:LYS:HB2	1:B:192:THR:HG22	1.89	0.55
1:B:83:LEU:HB2	1:B:92:ILE:HG22	1.88	0.55
1:A:146:GLU:C	1:A:147:ASN:HD22	2.09	0.54
1:B:591:PHE:CE1	1:B:604:LEU:HD13	2.43	0.54
1:A:418:ALA:CB	1:A:426:ILE:HD11	2.37	0.54
1:C:146:GLU:C	1:C:147:ASN:HD22	2.11	0.54
1:C:83:LEU:HB2	1:C:92:ILE:HG22	1.89	0.54
1:A:217:LEU:CD2	1:B:217:LEU:CD2	2.84	0.54
1:B:397:ILE:O	1:B:397:ILE:HD12	2.08	0.54
1:C:211:VAL:HG22	1:C:294:VAL:HG12	1.88	0.54
1:C:654:ALA:HB2	1:C:676:VAL:HG12	1.89	0.54
1:B:83:LEU:HD13	1:B:92:ILE:HG23	1.90	0.54
1:A:225:TYR:HD1	1:A:231:MET:HE2	1.73	0.54
1:C:322:PHE:O	1:C:478:VAL:HG23	2.08	0.54
1:B:418:ALA:CB	1:B:426:ILE:HD11	2.38	0.53
1:B:518:TYR:O	1:B:518:TYR:CD1	2.61	0.53
1:C:185:LYS:HB2	1:C:192:THR:HG22	1.90	0.53
1:C:212:PRO:HA	1:C:238:GLN:O	2.09	0.53
1:A:504:VAL:CG1	1:A:665:ALA:HB1	2.39	0.53
1:C:340:VAL:HG22	1:C:373:VAL:HG12	1.90	0.53
1:A:532:LEU:CD2	1:A:546:LEU:HD13	2.38	0.53
1:B:206:PRO:O	1:B:207:ILE:HD13	2.09	0.53
1:B:567:GLN:O	1:B:568:GLU:HG3	2.09	0.53
1:C:418:ALA:CB	1:C:426:ILE:HD11	2.39	0.52
1:C:532:LEU:CD2	1:C:546:LEU:HD22	2.38	0.52
1:A:397:ILE:HD12	1:A:397:ILE:O	2.09	0.52
1:B:212:PRO:HA	1:B:238:GLN:O	2.08	0.52
1:B:38:TRP:O	1:B:46:VAL:HG22	2.09	0.52
1:C:518:TYR:CD1	1:C:518:TYR:O	2.62	0.52
1:B:406:MET:SD	1:B:462:VAL:HG11	2.49	0.52
1:B:520:ILE:HD13	1:B:521:ASP:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:PHE:HD2	1:B:356:LEU:HD12	1.74	0.52
1:C:591:PHE:CZ	1:C:604:LEU:HD13	2.43	0.52
1:B:169:ARG:NH2	1:B:269:VAL:HG13	2.25	0.52
1:C:397:ILE:HD12	1:C:397:ILE:O	2.09	0.52
1:C:591:PHE:CE1	1:C:604:LEU:HD13	2.44	0.52
1:A:551:VAL:HG12	1:A:580:VAL:HG13	1.91	0.52
1:A:716:ALA:HA	1:A:723:GLU:CG	2.40	0.52
1:B:515:VAL:HG21	1:B:523:ILE:HD11	1.91	0.52
1:A:319:THR:HG22	1:A:389:GLY:N	2.24	0.52
1:A:212:PRO:HA	1:A:238:GLN:O	2.10	0.51
1:C:504:VAL:HG13	1:C:581:MET:HE3	1.92	0.51
1:C:101:VAL:HG21	1:C:134:PHE:CZ	2.46	0.51
1:C:520:ILE:HD13	1:C:521:ASP:N	2.25	0.51
1:A:598:VAL:CG1	1:A:678:VAL:HG22	2.40	0.51
1:C:225:TYR:HD1	1:C:231:MET:HE2	1.74	0.51
1:C:83:LEU:HD13	1:C:92:ILE:HG23	1.92	0.51
1:B:511:VAL:HG21	1:B:576:LEU:HD22	1.93	0.51
1:A:520:ILE:HD13	1:A:521:ASP:N	2.26	0.51
1:A:688:ASP:N	1:A:769:ILE:HD11	2.26	0.51
1:A:211:VAL:HG22	1:A:294:VAL:HG11	1.93	0.50
1:A:83:LEU:HD13	1:A:92:ILE:HG23	1.93	0.50
1:C:328:PHE:HD2	1:C:356:LEU:HD12	1.76	0.50
1:A:532:LEU:HD23	1:A:546:LEU:HD13	1.93	0.50
1:B:211:VAL:HG22	1:B:294:VAL:HG11	1.93	0.50
1:C:505:ALA:HB2	1:C:582:VAL:HA	1.93	0.50
1:C:231:MET:HE1	1:C:305:VAL:HG22	1.93	0.50
1:C:309:LEU:HD22	1:C:337:ILE:CD1	2.42	0.50
1:B:309:LEU:HD22	1:B:337:ILE:CD1	2.41	0.50
1:A:603:THR:HG21	1:B:607:SER:CB	2.42	0.50
1:A:257:LYS:HE3	2:A:785:NAG:H81	1.94	0.50
1:C:169:ARG:NH2	1:C:269:VAL:HG13	2.27	0.50
1:A:328:PHE:HD2	1:A:356:LEU:HD12	1.77	0.50
1:A:67:ARG:NH1	2:A:782:NAG:H81	2.26	0.50
1:A:7:LEU:HD12	1:A:27:LYS:HE3	1.94	0.50
1:B:7:LEU:HD12	1:B:27:LYS:HE3	1.93	0.50
1:A:309:LEU:HD22	1:A:337:ILE:CD1	2.41	0.49
1:B:42:ASP:OD1	1:B:44:THR:HG22	2.12	0.49
1:A:101:VAL:HG21	1:A:134:PHE:CZ	2.48	0.49
1:A:183:ARG:HG3	1:A:194:LEU:HD23	1.94	0.49
1:C:663:ASN:O	1:C:664:LEU:C	2.51	0.49
1:A:515:VAL:HG21	1:A:523:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:LEU:O	1:B:538:GLN:OE1	2.30	0.49
1:C:175:ASP:C	1:C:177:TYR:H	2.15	0.49
1:C:225:TYR:CD1	1:C:231:MET:HE2	2.46	0.49
1:A:327:VAL:HG22	1:A:357:ARG:CD	2.43	0.49
1:A:682:TRP:CD1	1:A:765:LEU:HD23	2.48	0.49
1:B:183:ARG:HG3	1:B:194:LEU:HD23	1.95	0.49
1:B:240:TYR:HA	1:B:241:PRO:C	2.32	0.49
1:C:505:ALA:CB	1:C:582:VAL:HA	2.43	0.49
1:A:753:TYR:CD2	1:A:771:ILE:HD12	2.48	0.49
1:B:101:VAL:HG21	1:B:134:PHE:CZ	2.47	0.49
1:B:532:LEU:HD12	1:B:532:LEU:O	2.13	0.49
1:A:689:LYS:O	1:A:771:ILE:HA	2.13	0.48
1:C:42:ASP:OD1	1:C:44:THR:HG22	2.13	0.48
1:C:38:TRP:O	1:C:46:VAL:HG22	2.13	0.48
1:C:632:ILE:HG23	1:C:646:ILE:HG12	1.93	0.48
1:B:663:ASN:O	1:B:664:LEU:C	2.51	0.48
1:A:169:ARG:NH2	1:A:269:VAL:HG13	2.27	0.48
1:A:42:ASP:OD1	1:A:44:THR:HG22	2.13	0.48
1:A:682:TRP:NE1	1:A:765:LEU:HD23	2.28	0.48
1:C:532:LEU:HD21	1:C:546:LEU:CD2	2.44	0.48
1:A:233:LEU:HD21	1:A:303:LEU:HD13	1.95	0.48
1:C:211:VAL:HG22	1:C:294:VAL:HG11	1.94	0.48
1:B:327:VAL:HG22	1:B:357:ARG:CD	2.44	0.48
1:B:615:LEU:HD13	1:B:640:ARG:HB2	1.94	0.48
1:C:327:VAL:HG22	1:C:357:ARG:CD	2.44	0.48
1:B:535:ASN:C	1:B:535:ASN:ND2	2.67	0.48
1:A:240:TYR:HA	1:A:241:PRO:C	2.34	0.47
1:C:532:LEU:HD21	1:C:546:LEU:HD22	1.95	0.47
1:A:214:VAL:HG13	1:A:297:GLU:HG2	1.95	0.47
1:A:632:ILE:HG23	1:A:646:ILE:HG12	1.96	0.47
1:A:686:PRO:HG2	1:A:769:ILE:HD13	1.96	0.47
1:B:92:ILE:HD11	1:B:343:MET:SD	2.54	0.47
1:C:363:LYS:HA	1:C:388:LEU:HD11	1.96	0.47
1:C:532:LEU:O	1:C:538:GLN:OE1	2.32	0.47
1:A:319:THR:CG2	1:A:389:GLY:O	2.62	0.47
1:A:761:ILE:CD1	1:A:761:ILE:N	2.78	0.47
1:B:532:LEU:HD23	1:B:546:LEU:HD13	1.95	0.47
1:B:214:VAL:HG13	1:B:297:GLU:HG2	1.97	0.47
1:B:632:ILE:HG23	1:B:646:ILE:HG12	1.95	0.47
1:C:7:LEU:HD12	1:C:27:LYS:HE3	1.94	0.47
1:A:319:THR:HG22	1:A:389:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:LEU:HD23	1:B:430:LEU:C	2.35	0.47
1:A:664:LEU:O	1:A:665:ALA:HB3	2.15	0.47
1:B:290:VAL:HG12	1:B:297:GLU:O	2.14	0.47
1:C:240:TYR:HA	1:C:241:PRO:C	2.35	0.47
1:A:551:VAL:HG12	1:A:580:VAL:CG1	2.45	0.47
1:A:733:ILE:HG12	1:A:742:VAL:HG13	1.96	0.47
1:B:418:ALA:HB2	1:B:426:ILE:HD11	1.97	0.47
1:B:457:LEU:C	1:B:457:LEU:HD12	2.35	0.47
1:B:365:ASP:O	1:B:386:LEU:HD23	2.15	0.47
1:B:469:LEU:HD11	1:B:484:SER:HB3	1.96	0.47
1:A:115:VAL:HG11	1:A:121:ALA:HB2	1.97	0.46
1:A:532:LEU:HD11	1:A:560:TYR:HE2	1.80	0.46
1:A:603:THR:HG21	1:B:607:SER:HB3	1.97	0.46
1:C:206:PRO:O	1:C:207:ILE:HD13	2.15	0.46
1:C:430:LEU:C	1:C:430:LEU:HD23	2.36	0.46
1:A:615:LEU:HD13	1:A:640:ARG:HB2	1.97	0.46
1:A:757:ALA:HB3	1:A:765:LEU:HB2	1.97	0.46
1:B:130:PHE:CD1	1:B:131:VAL:HG13	2.51	0.46
1:B:515:VAL:HG11	1:B:523:ILE:CD1	2.46	0.46
1:A:327:VAL:HG22	1:A:357:ARG:HD3	1.97	0.46
1:A:406:MET:SD	1:A:462:VAL:HG11	2.55	0.46
1:C:115:VAL:HG21	1:C:171:VAL:HG11	1.98	0.46
1:A:206:PRO:O	1:A:207:ILE:HD13	2.15	0.46
1:A:225:TYR:CD1	1:A:231:MET:HE2	2.49	0.46
1:A:567:GLN:O	1:A:568:GLU:HG3	2.15	0.46
1:A:591:PHE:CZ	1:A:674:LEU:HD12	2.51	0.46
1:C:613:LEU:CB	1:C:614:PRO:CD	2.94	0.46
1:C:621:LEU:HD23	1:C:622:ASP:N	2.31	0.46
1:B:225:TYR:HD1	1:B:231:MET:HE2	1.81	0.46
1:C:130:PHE:CD1	1:C:131:VAL:HG13	2.51	0.46
1:B:233:LEU:HD21	1:B:303:LEU:HD13	1.97	0.46
1:C:365:ASP:O	1:C:386:LEU:HD23	2.16	0.46
1:C:52:LEU:HD21	1:C:70:ASP:HB3	1.98	0.46
1:C:615:LEU:HD13	1:C:640:ARG:HB2	1.97	0.46
1:A:365:ASP:O	1:A:386:LEU:HD23	2.16	0.46
1:A:38:TRP:O	1:A:46:VAL:HG22	2.16	0.46
1:A:745:ILE:HD12	1:A:749:ASN:HD22	1.81	0.46
1:C:183:ARG:HG3	1:C:194:LEU:HD23	1.97	0.46
1:B:121:ALA:HB3	1:B:168:ILE:HB	1.98	0.46
1:B:83:LEU:HD13	1:B:92:ILE:HG22	1.98	0.46
1:C:532:LEU:HD11	1:C:560:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:GLN:HB2	1:A:580:VAL:HB	1.96	0.45
1:A:621:LEU:O	1:A:622:ASP:C	2.54	0.45
1:B:534:ILE:HD11	1:B:538:GLN:HE22	1.80	0.45
1:A:52:LEU:HD21	1:A:70:ASP:HB3	1.99	0.45
1:B:443:VAL:HG22	1:B:457:LEU:HD13	1.98	0.45
1:B:535:ASN:O	1:B:536:ARG:C	2.54	0.45
1:A:754:LEU:CD2	1:A:754:LEU:C	2.85	0.45
1:B:613:LEU:CB	1:B:614:PRO:CD	2.94	0.45
1:C:430:LEU:HD12	1:C:470:TYR:CE2	2.51	0.45
1:C:532:LEU:HD11	1:C:560:TYR:HE2	1.80	0.45
1:C:567:GLN:O	1:C:568:GLU:HG3	2.15	0.45
1:A:586:ILE:HD11	1:A:606:CYS:SG	2.57	0.45
1:A:613:LEU:CB	1:A:614:PRO:CD	2.94	0.45
1:B:535:ASN:O	1:B:535:ASN:ND2	2.49	0.45
1:A:621:LEU:HD23	1:A:622:ASP:N	2.32	0.45
1:C:233:LEU:HD21	1:C:303:LEU:HD13	1.97	0.45
1:C:327:VAL:HG22	1:C:357:ARG:HD3	1.99	0.45
1:A:443:VAL:HG22	1:A:457:LEU:HD13	1.98	0.45
1:C:92:ILE:HD11	1:C:343:MET:SD	2.57	0.45
1:C:621:LEU:O	1:C:622:ASP:C	2.55	0.45
1:A:231:MET:CE	1:A:303:LEU:HD21	2.47	0.45
1:A:430:LEU:HD23	1:A:430:LEU:C	2.37	0.45
1:B:327:VAL:HG22	1:B:357:ARG:HD3	1.99	0.45
1:B:591:PHE:CZ	1:B:674:LEU:HD12	2.51	0.45
1:C:214:VAL:HG13	1:C:297:GLU:HG2	1.99	0.45
1:C:539:LYS:HB2	1:C:547:ILE:HG23	1.99	0.45
1:A:707:PRO:HD2	1:A:761:ILE:HD11	1.99	0.45
1:B:290:VAL:HG13	1:B:290:VAL:O	2.17	0.45
1:A:518:TYR:O	1:A:518:TYR:CD1	2.69	0.45
1:A:663:ASN:O	1:A:664:LEU:C	2.55	0.45
1:B:52:LEU:HD21	1:B:70:ASP:HB3	1.98	0.45
1:B:309:LEU:HD11	1:B:375:ASN:ND2	2.32	0.44
1:A:539:LYS:HB2	1:A:547:ILE:HG23	1.99	0.44
1:C:373:VAL:CG2	1:C:380:ALA:HB3	2.44	0.44
1:C:418:ALA:HB2	1:C:426:ILE:HD11	2.00	0.44
1:A:130:PHE:CD1	1:A:131:VAL:HG13	2.52	0.44
1:B:116:ILE:O	1:B:117:ARG:C	2.55	0.44
1:C:469:LEU:HD11	1:C:484:SER:HB3	2.00	0.44
1:A:115:VAL:HG21	1:A:171:VAL:HG11	1.99	0.44
1:A:319:THR:HG22	1:A:389:GLY:HA2	1.98	0.44
1:A:518:TYR:C	1:A:520:ILE:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:MET:CE	1:B:303:LEU:HD21	2.47	0.44
1:B:664:LEU:O	1:B:665:ALA:HB3	2.17	0.44
1:A:24:ILE:HD11	1:A:61:LEU:HD23	2.00	0.44
1:A:551:VAL:CG1	1:A:580:VAL:HG13	2.48	0.44
1:A:119:ASN:N	1:A:119:ASN:HD22	2.16	0.44
1:A:184:THR:O	1:A:192:THR:HA	2.18	0.44
1:A:469:LEU:HD11	1:A:484:SER:HB3	1.99	0.44
1:B:119:ASN:N	1:B:119:ASN:HD22	2.16	0.44
1:B:621:LEU:HD23	1:B:622:ASP:N	2.33	0.44
1:A:319:THR:HG23	1:A:387:LYS:HB3	2.00	0.44
1:C:184:THR:O	1:C:192:THR:HA	2.18	0.43
1:C:219:LYS:HA	1:C:299:VAL:HG12	2.00	0.43
1:C:417:VAL:CG2	1:C:454:VAL:HG22	2.42	0.43
1:C:115:VAL:HG11	1:C:121:ALA:HB2	2.00	0.43
1:A:598:VAL:HG11	1:A:678:VAL:HG22	2.01	0.43
1:C:24:ILE:HD11	1:C:61:LEU:HD23	2.00	0.43
1:C:515:VAL:HG21	1:C:523:ILE:HD11	1.99	0.43
1:B:184:THR:O	1:B:192:THR:HA	2.18	0.43
1:C:363:LYS:HA	1:C:388:LEU:CD1	2.48	0.43
1:A:159:LEU:HD12	1:A:160:VAL:N	2.34	0.43
1:A:418:ALA:HB2	1:A:426:ILE:HD11	1.99	0.43
1:A:507:GLU:O	1:A:551:VAL:HG23	2.19	0.43
1:B:621:LEU:O	1:B:622:ASP:C	2.55	0.43
1:C:309:LEU:HD11	1:C:375:ASN:ND2	2.34	0.43
1:A:92:ILE:HD11	1:A:343:MET:SD	2.58	0.42
1:B:219:LYS:HA	1:B:299:VAL:HG12	2.00	0.42
1:B:586:ILE:HD11	1:B:606:CYS:SG	2.58	0.42
1:B:632:ILE:HG22	1:B:644:LEU:HD11	2.00	0.42
1:C:231:MET:CE	1:C:303:LEU:HD21	2.49	0.42
1:C:319:THR:HG22	1:C:389:GLY:CA	2.49	0.42
1:C:664:LEU:O	1:C:665:ALA:HB3	2.19	0.42
1:C:83:LEU:HD13	1:C:92:ILE:HG22	2.01	0.42
1:A:147:ASN:N	1:A:147:ASN:HD22	2.17	0.42
1:A:290:VAL:HG12	1:A:297:GLU:O	2.19	0.42
1:A:258:GLN:HE21	1:A:710:GLN:CD	2.22	0.42
1:B:225:TYR:CD1	1:B:231:MET:HE2	2.54	0.42
1:C:443:VAL:HG22	1:C:457:LEU:HD13	2.01	0.42
1:A:319:THR:HG23	1:A:387:LYS:CB	2.49	0.42
1:A:418:ALA:HB3	1:A:426:ILE:HD11	2.02	0.42
1:B:233:LEU:O	1:B:272:THR:HG23	2.20	0.42
1:B:518:TYR:C	1:B:520:ILE:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:VAL:HG22	1:A:478:VAL:O	2.19	0.42
1:B:373:VAL:CG2	1:B:380:ALA:HB3	2.44	0.42
1:B:507:GLU:O	1:B:551:VAL:HG23	2.19	0.42
1:C:632:ILE:HG22	1:C:644:LEU:HD11	2.00	0.42
1:B:159:LEU:HD12	1:B:160:VAL:N	2.35	0.42
1:C:119:ASN:HD22	1:C:119:ASN:N	2.17	0.42
1:C:290:VAL:O	1:C:290:VAL:HG13	2.20	0.42
1:A:424:PRO:O	1:A:453:VAL:HG21	2.19	0.42
1:B:231:MET:HE2	1:B:303:LEU:HD11	2.01	0.42
1:B:424:PRO:O	1:B:453:VAL:HG21	2.19	0.42
1:A:390:GLY:C	1:A:392:PHE:N	2.72	0.42
1:B:115:VAL:HG21	1:B:171:VAL:HG11	2.02	0.42
1:C:147:ASN:HD22	1:C:147:ASN:N	2.18	0.42
1:C:168:ILE:CD1	1:C:201:LEU:HD11	2.49	0.42
1:C:290:VAL:HG12	1:C:297:GLU:O	2.19	0.42
1:A:128:PRO:HB2	1:A:131:VAL:HG22	2.02	0.41
1:A:16:PHE:CG	1:A:22:ALA:HB2	2.55	0.41
1:A:231:MET:HE2	1:A:303:LEU:HD11	2.01	0.41
1:A:515:VAL:HG11	1:A:523:ILE:CD1	2.50	0.41
1:B:539:LYS:HB2	1:B:547:ILE:HG23	2.02	0.41
1:C:159:LEU:HD12	1:C:160:VAL:N	2.35	0.41
1:C:518:TYR:C	1:C:520:ILE:H	2.24	0.41
1:A:116:ILE:O	1:A:117:ARG:C	2.59	0.41
1:A:707:PRO:HD3	1:A:761:ILE:HD11	2.02	0.41
1:B:16:PHE:CG	1:B:22:ALA:HB2	2.54	0.41
1:A:221:ASP:HB2	1:B:217:LEU:HG	2.02	0.41
1:C:16:PHE:CG	1:C:22:ALA:HB2	2.56	0.41
1:C:457:LEU:C	1:C:457:LEU:HD12	2.40	0.41
1:A:258:GLN:NE2	1:A:710:GLN:OE1	2.53	0.41
1:C:101:VAL:HG21	1:C:134:PHE:CE2	2.55	0.41
1:C:138:VAL:HG21	1:C:185:LYS:HB2	2.02	0.41
1:A:463:HIS:O	1:A:489:VAL:HG11	2.20	0.41
1:B:551:VAL:CG1	1:B:580:VAL:HG22	2.50	0.41
1:C:406:MET:SD	1:C:462:VAL:HG11	2.60	0.41
1:A:754:LEU:HD23	1:A:767:ALA:O	2.20	0.41
1:B:19:SER:OG	2:B:782:NAG:N2	2.54	0.41
1:A:219:LYS:HA	1:A:299:VAL:HG12	2.02	0.41
1:A:290:VAL:HG13	1:A:290:VAL:O	2.20	0.41
1:A:423:THR:HA	1:A:424:PRO:HD3	1.96	0.41
1:B:14:ILE:HA	1:B:14:ILE:HD13	1.97	0.41
1:B:532:LEU:HD21	1:B:546:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LEU:HD12	1:B:273:LEU:HD23	2.03	0.41
1:B:403:GLU:HG3	1:B:404:GLU:N	2.36	0.41
1:C:478:VAL:HG22	1:C:478:VAL:O	2.20	0.41
1:C:39:ILE:HG13	1:C:81:ALA:HB3	2.02	0.41
1:A:727:LEU:HD23	1:A:733:ILE:HG21	2.03	0.41
1:C:322:PHE:CB	1:C:478:VAL:HG22	2.51	0.41
1:A:142:THR:HG22	1:A:180:TYR:HD1	1.86	0.40
1:A:83:LEU:HD13	1:A:92:ILE:HG22	2.02	0.40
1:C:322:PHE:HB3	1:C:478:VAL:HG22	2.02	0.40
1:C:424:PRO:O	1:C:453:VAL:HG21	2.22	0.40
1:A:417:VAL:CG2	1:A:454:VAL:HG22	2.45	0.40
1:B:478:VAL:O	1:B:478:VAL:HG22	2.21	0.40
1:C:518:TYR:CG	1:C:518:TYR:O	2.74	0.40
1:A:309:LEU:HD23	1:A:334:GLY:HA3	2.04	0.40
1:A:716:ALA:HA	1:A:723:GLU:HG3	2.03	0.40
1:A:752:TYR:HA	1:A:769:ILE:O	2.21	0.40
1:A:373:VAL:CG2	1:A:380:ALA:HB3	2.45	0.40
1:A:39:ILE:HG13	1:A:81:ALA:HB3	2.03	0.40
1:C:233:LEU:O	1:C:272:THR:HG23	2.20	0.40
1:C:403:GLU:HG3	1:C:404:GLU:N	2.35	0.40
1:B:147:ASN:HD22	1:B:147:ASN:N	2.17	0.40
1:B:251:ILE:O	1:B:252:GLU:C	2.60	0.40
1:B:430:LEU:HD12	1:B:470:TYR:CE2	2.57	0.40
2:C:782:NAG:O3	2:C:783:NAG:O5	2.33	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:492:LEU:N	1:C:407:GLU:OE1[8_455]	2.04	0.16

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	773/816 (95%)	696 (90%)	64 (8%)	13 (2%)	11	51
1	B	674/816 (83%)	605 (90%)	56 (8%)	13 (2%)	9	49
1	C	674/816 (83%)	600 (89%)	62 (9%)	12 (2%)	10	50
All	All	2121/2448 (87%)	1901 (90%)	182 (9%)	38 (2%)	10	50

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	613	LEU
1	A	626	ILE
1	B	613	LEU
1	B	626	ILE
1	C	613	LEU
1	C	626	ILE
1	A	216	SER
1	A	638	GLY
1	A	724	TYR
1	B	216	SER
1	B	392	PHE
1	B	638	GLY
1	C	216	SER
1	C	638	GLY
1	A	103	ALA
1	A	174	GLU
1	A	252	GLU
1	A	622	ASP
1	A	664	LEU
1	B	103	ALA
1	B	252	GLU
1	B	622	ASP
1	B	664	LEU
1	C	103	ALA
1	C	174	GLU
1	C	252	GLU
1	C	593	GLU
1	C	622	ASP
1	C	664	LEU
1	A	744	ASN
1	B	174	GLU
1	B	464	ALA

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Mol	Chain	Res	Type
1	B	612	ASP
1	C	612	ASP
1	A	464	ALA
1	A	553	ARG
1	B	553	ARG
1	C	553	ARG

### 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	654/687 (95%)	625 (96%)	29 (4%)	33	66
1	B	572/687 (83%)	548 (96%)	24 (4%)	34	67
1	C	572/687 (83%)	548 (96%)	24 (4%)	34	67
All	All	1798/2061 (87%)	1721 (96%)	77 (4%)	33	66

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	13	ARG
1	A	31	ASN
1	A	88	PHE
1	A	147	ASN
1	A	163	SER
1	A	175	ASP
1	A	195	SER
1	A	221	ASP
1	A	319	THR
1	A	339	THR
1	A	374	ARG
1	A	393	ASP
1	A	440	ARG
1	A	463	HIS
1	A	509	LEU

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Mol	Chain	Res	Type
1	A	510	ILE
1	A	520	ILE
1	A	522	SER
1	A	535	ASN
1	A	536	ARG
1	A	549	GLU
1	A	554	ASN
1	A	556	ASP
1	A	663	ASN
1	A	710	GLN
1	A	754	LEU
1	A	755	CYS
1	A	761	ILE
1	B	11	THR
1	B	13	ARG
1	B	31	ASN
1	B	88	PHE
1	B	147	ASN
1	B	175	ASP
1	B	195	SER
1	B	221	ASP
1	B	319	THR
1	B	339	THR
1	B	374	ARG
1	B	393	ASP
1	B	440	ARG
1	B	463	HIS
1	B	509	LEU
1	B	510	ILE
1	B	520	ILE
1	B	522	SER
1	B	535	ASN
1	B	536	ARG
1	B	549	GLU
1	B	554	ASN
1	B	556	ASP
1	B	663	ASN
1	C	11	THR
1	C	13	ARG
1	C	31	ASN
1	C	88	PHE
1	C	147	ASN

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Mol	Chain	Res	Type
1	C	175	ASP
1	C	195	SER
1	C	221	ASP
1	C	319	THR
1	C	339	THR
1	C	374	ARG
1	C	393	ASP
1	C	440	ARG
1	C	463	HIS
1	C	509	LEU
1	C	510	ILE
1	C	520	ILE
1	C	522	SER
1	C	535	ASN
1	C	536	ARG
1	C	549	GLU
1	C	554	ASN
1	C	556	ASP
1	C	663	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	147	ASN
1	A	258	GLN
1	A	402	GLN
1	A	554	ASN
1	A	732	ASN
1	B	31	ASN
1	B	147	ASN
1	B	402	GLN
1	B	535	ASN
1	B	554	ASN
1	B	579	GLN
1	C	31	ASN
1	C	147	ASN
1	C	167	HIS
1	C	402	GLN
1	C	554	ASN
1	C	579	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

25 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	782	1,2	14,14,15	0.41	0	15,19,21	1.73	2 (13%)
2	NAG	A	783	2	14,14,15	0.50	0	15,19,21	0.78	0
2	NAG	A	784	1,2	14,14,15	0.67	1 (7%)	15,19,21	1.98	3 (20%)
2	NAG	A	785	2	14,14,15	0.49	0	15,19,21	0.83	1 (6%)
3	GOL	A	786	-	5,5,5	0.34	0	5,5,5	0.33	0
3	GOL	A	787	-	5,5,5	0.36	0	5,5,5	0.27	0
2	NAG	B	782	1,2	14,14,15	0.57	0	15,19,21	1.50	1 (6%)
2	NAG	B	783	2	14,14,15	0.76	0	15,19,21	1.18	1 (6%)
2	NAG	B	784	1,2	14,14,15	0.54	0	15,19,21	1.33	2 (13%)
2	NAG	B	785	2	14,14,15	0.46	0	15,19,21	1.32	2 (13%)
2	NAG	B	786	2	14,14,15	0.55	0	15,19,21	0.83	0
4	NDG	B	787	1,2	14,14,15	0.78	0	15,19,21	2.03	4 (26%)
2	NAG	B	788	2,4	14,14,15	0.71	0	15,19,21	1.50	3 (20%)
2	NAG	B	789	2	14,14,15	0.56	0	15,19,21	0.81	0
2	NAG	B	790	1,2	14,14,15	0.78	1 (7%)	15,19,21	1.46	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	791	2	14,14,15	0.59	0	15,19,21	0.75	0
5	SO4	B	792	-	4,4,4	0.12	0	6,6,6	0.13	0
3	GOL	B	793	-	5,5,5	0.37	0	5,5,5	0.16	0
3	GOL	B	794	-	5,5,5	0.40	0	5,5,5	0.25	0
2	NAG	C	782	1,2	14,14,15	0.33	0	15,19,21	1.65	2 (13%)
2	NAG	C	783	2	14,14,15	0.57	0	15,19,21	0.70	0
2	NAG	C	784	2	14,14,15	0.51	0	15,19,21	0.88	0
4	NDG	C	785	1,2	14,14,15	0.42	0	15,19,21	1.57	2 (13%)
2	NAG	C	786	2,4	14,14,15	0.60	0	15,19,21	1.16	1 (6%)
2	NAG	C	787	2	14,14,15	0.64	0	15,19,21	1.08	2 (13%)

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	782	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	783	2	-	0/6/23/26	0/1/1/1
2	NAG	A	784	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	785	2	-	2/6/23/26	0/1/1/1
3	GOL	A	786	-	-	0/4/4/4	0/0/0/0
3	GOL	A	787	-	-	0/4/4/4	0/0/0/0
2	NAG	B	782	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	783	2	-	0/6/23/26	0/1/1/1
2	NAG	B	784	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	785	2	-	0/6/23/26	0/1/1/1
2	NAG	B	786	2	-	0/6/23/26	0/1/1/1
4	NDG	B	787	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	788	2,4	-	0/6/23/26	0/1/1/1
2	NAG	B	789	2	-	0/6/23/26	0/1/1/1
2	NAG	B	790	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	791	2	-	0/6/23/26	0/1/1/1
5	SO4	B	792	-	-	0/0/0/0	0/0/0/0
3	GOL	B	793	-	-	0/4/4/4	0/0/0/0
3	GOL	B	794	-	-	0/4/4/4	0/0/0/0
2	NAG	C	782	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	783	2	-	0/6/23/26	0/1/1/1
2	NAG	C	784	2	-	0/6/23/26	0/1/1/1
4	NDG	C	785	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	786	2,4	-	0/6/23/26	0/1/1/1
2	NAG	C	787	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	784	NAG	C1-C2	2.05	1.55	1.52
2	B	790	NAG	C1-C2	2.11	1.55	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	784	NAG	O5-C1-C2	-6.12	102.95	111.47
2	A	782	NAG	O5-C1-C2	-5.00	104.51	111.47
2	B	782	NAG	O5-C1-C2	-4.96	104.58	111.47
4	C	785	NDG	O-C1-C2	-4.33	105.44	111.47
2	C	782	NAG	C4-C3-C2	-3.37	106.08	111.02
2	B	785	NAG	O5-C1-C2	-3.35	106.82	111.47
2	B	785	NAG	C2-N2-C7	-2.87	118.75	122.94
2	B	790	NAG	O5-C1-C2	-2.71	107.70	111.47
2	B	788	NAG	C1-O5-C5	-2.56	108.64	112.17
2	C	787	NAG	O5-C1-C2	-2.19	108.43	111.47
2	B	788	NAG	C1-C2-N2	-2.02	107.04	110.49
2	A	785	NAG	C1-O5-C5	2.01	114.94	112.17
4	B	787	NDG	O7-C7-N2	2.02	125.81	121.92
2	C	787	NAG	C4-C3-C2	2.05	114.02	111.02
2	A	784	NAG	C1-O5-C5	2.10	115.06	112.17
2	B	784	NAG	C1-C2-N2	2.32	114.45	110.49
2	B	784	NAG	C1-O5-C5	2.90	116.17	112.17
2	A	784	NAG	C1-C2-N2	3.03	115.66	110.49
2	A	782	NAG	C1-O5-C5	3.28	116.68	112.17
2	B	783	NAG	C4-C3-C2	3.46	116.09	111.02
4	B	787	NDG	C3-C4-C5	3.47	116.33	110.22
4	B	787	NDG	C2-N2-C7	3.48	128.02	122.94
2	C	786	NAG	C4-C3-C2	3.48	116.12	111.02
4	C	785	NDG	C1-O-C5	3.74	117.32	112.17
2	B	788	NAG	C4-C3-C2	4.12	117.05	111.02
2	B	790	NAG	C4-C3-C2	4.37	117.42	111.02
2	C	782	NAG	C1-O5-C5	4.67	118.61	112.17
4	B	787	NDG	C4-C3-C2	4.71	117.92	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	784	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	785	NAG	C8-C7-N2-C2
2	A	785	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	782	NAG	2	0
2	A	785	NAG	1	0
2	B	782	NAG	1	0
2	C	782	NAG	1	0
2	C	783	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	775/816 (94%)	0.33	43 (5%)	26 20	27, 55, 89, 101	0
1	B	676/816 (82%)	-0.19	4 (0%)	89 84	16, 42, 82, 93	0
1	C	676/816 (82%)	0.26	11 (1%)	72 63	25, 53, 101, 108	0
All	All	2127/2448 (86%)	0.14	58 (2%)	55 45	16, 50, 93, 108	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	390	GLY	4.3
1	C	622	ASP	4.0
1	A	567	GLN	3.7
1	A	550	ASN	3.4
1	A	571	SER	3.4
1	A	468	GLY	3.2
1	A	575	SER	3.0
1	A	389	GLY	3.0
1	A	484	SER	2.8
1	A	488	ASN	2.7
1	A	429	GLU	2.6
1	A	622	ASP	2.6
1	A	565	LYS	2.6
1	C	296	GLY	2.6
1	A	421	ASN	2.6
1	B	594	GLY	2.5
1	A	419	GLY	2.5
1	A	415	LYS	2.5
1	A	581	MET	2.5
1	A	391	ARG	2.5
1	A	536	ARG	2.5
1	A	432	GLY	2.5
1	A	437	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	228	SER	2.4
1	A	442	GLN	2.4
1	C	174	GLU	2.4
1	B	599	GLY	2.4
1	C	529	ASN	2.4
1	A	408	PRO	2.3
1	A	477	LYS	2.3
1	C	205	GLU	2.3
1	A	411	SER	2.3
1	A	500	LYS	2.3
1	A	434	LYS	2.3
1	A	489	VAL	2.3
1	A	460	THR	2.3
1	B	656	ASN	2.3
1	A	439	ASP	2.3
1	A	365	ASP	2.2
1	B	629	ASP	2.2
1	A	570	TYR	2.2
1	A	662	ARG	2.2
1	A	499	GLU	2.2
1	C	185	LYS	2.1
1	C	333	THR	2.1
1	A	472	CYS	2.1
1	C	623	GLY	2.1
1	A	507	GLU	2.1
1	A	564	ALA	2.1
1	A	568	GLU	2.1
1	A	465	ASN	2.1
1	A	319	THR	2.0
1	A	508	THR	2.0
1	A	566	ASN	2.0
1	C	155	ASP	2.0
1	A	395	PRO	2.0
1	A	497	GLN	2.0
1	C	204	THR	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 [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	787	6/6	0.71	0.41	4.36	22,22,22,23	0
3	GOL	B	794	6/6	0.78	0.45	2.95	41,41,42,44	0
2	NAG	B	790	14/15	0.76	0.46	2.69	64,66,68,70	0
3	GOL	A	786	6/6	0.88	0.32	2.44	25,27,27,27	0
2	NAG	A	784	14/15	0.83	0.39	1.43	62,65,66,66	0
3	GOL	B	793	6/6	0.87	0.33	1.13	23,23,24,24	0
2	NAG	B	782	14/15	0.84	0.27	0.42	46,47,49,51	0
2	NAG	A	782	14/15	0.86	0.29	-0.14	50,52,52,53	0
4	NDG	B	787	14/15	0.83	0.29	-0.54	60,64,68,72	0
2	NAG	C	782	14/15	0.92	0.22	-1.09	42,45,46,46	0
5	SO4	B	792	5/5	0.91	0.20	-1.15	20,21,21,24	0
2	NAG	B	789	14/15	0.71	0.51	-	83,84,85,86	0
2	NAG	C	784	14/15	0.69	0.50	-	53,53,55,55	0
2	NAG	B	791	14/15	0.81	0.38	-	71,72,73,73	0
2	NAG	C	783	14/15	0.91	0.20	-	46,49,50,51	0
2	NAG	B	783	14/15	0.84	0.47	-	54,56,59,59	0
2	NAG	C	786	14/15	0.80	0.33	-	66,66,67,67	0
2	NAG	A	783	14/15	0.79	0.37	-	52,53,53,54	0
2	NAG	C	787	14/15	0.82	0.37	-	66,67,67,67	0
2	NAG	A	785	14/15	0.83	0.31	-	66,66,67,67	0
2	NAG	B	786	14/15	0.77	0.55	-	52,53,54,54	0
2	NAG	B	784	14/15	0.89	0.24	-	38,44,48,48	0
2	NAG	B	785	14/15	0.79	0.29	-	44,50,51,51	0
4	NDG	C	785	14/15	0.81	0.29	-	63,64,67,67	0
2	NAG	B	788	14/15	0.75	0.37	-	77,80,81,81	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.