



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:26 PM GMT

PDB ID : 1K9I  
Title : Complex of DC-SIGN and GlcNAc2Man3  
Authors : Feinberg, H.; Mitchell, D.A.; Drickamer, K.; Weis, W.I.  
Deposited on : 2001-10-29  
Resolution : 2.50 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

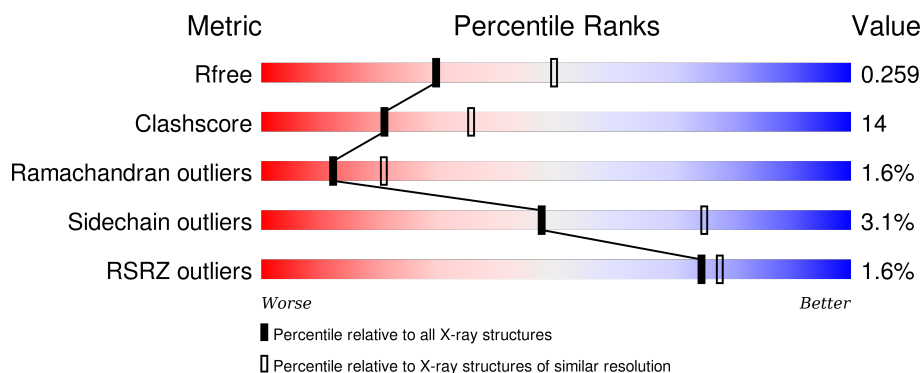
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	156	<div> <div>4%</div> <div>52%</div> <div>28%</div> <div>•</div> <div>18%</div> </div>
1	B	156	<div> <div>%</div> <div>61%</div> <div>20%</div> <div>•</div> <div>18%</div> </div>
1	C	156	<div> <div>61%</div> <div>19%</div> <div>•</div> <div>18%</div> </div>
1	D	156	<div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
1	E	156	<div> <div>59%</div> <div>22%</div> <div>•</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	156	
1	G	156	
1	H	156	
1	I	156	
1	J	156	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11035 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 mDC-SIGN1B type I isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	128	Total	C	N	O	S	0	0	0
			1042	658	179	197	8			
1	B	128	Total	C	N	O	S	0	0	0
			1042	658	179	197	8			
1	C	128	Total	C	N	O	S	0	0	0
			1042	658	179	197	8			
1	D	132	Total	C	N	O	S	0	0	0
			1070	673	185	202	10			
1	E	128	Total	C	N	O	S	0	0	0
			1042	658	179	197	8			
1	F	128	Total	C	N	O	S	0	0	0
			1042	658	179	197	8			
1	G	128	Total	C	N	O	S	0	0	0
			1042	658	179	197	8			
1	H	127	Total	C	N	O	S	0	0	0
			1037	655	178	196	8			
1	I	128	Total	C	N	O	S	0	0	0
			1042	658	179	197	8			
1	J	128	Total	C	N	O	S	0	0	0
			1042	658	179	197	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	249	ALA	-	see remark 999	GB 15281089
B	249	ALA	-	see remark 999	GB 15281089
C	249	ALA	-	see remark 999	GB 15281089
D	249	ALA	-	see remark 999	GB 15281089
E	249	ALA	-	see remark 999	GB 15281089
F	249	ALA	-	see remark 999	GB 15281089
G	249	ALA	-	see remark 999	GB 15281089
H	249	ALA	-	see remark 999	GB 15281089
I	249	ALA	-	see remark 999	GB 15281089

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Chain	Residue	Modelled	Actual	Comment	Reference
J	249	ALA	-	see remark 999	GB 15281089

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			62	34	2	26		
2	C	5	Total	C	N	O	0	0
			62	34	2	26		
2	D	5	Total	C	N	O	0	0
			62	34	2	26		
2	E	5	Total	C	N	O	0	0
			62	34	2	26		
2	H	5	Total	C	N	O	0	0
			62	34	2	26		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	3	Total	Ca	0	0
			3	3		
3	J	3	Total	Ca	0	0
			3	3		
3	D	3	Total	Ca	0	0
			3	3		
3	E	3	Total	Ca	0	0
			3	3		
3	H	3	Total	Ca	0	0
			3	3		
3	B	3	Total	Ca	0	0
			3	3		
3	I	3	Total	Ca	0	0
			3	3		
3	C	3	Total	Ca	0	0
			3	3		
3	A	3	Total	Ca	0	0
			3	3		
3	F	3	Total	Ca	0	0
			3	3		

- Molecule 4 is water.

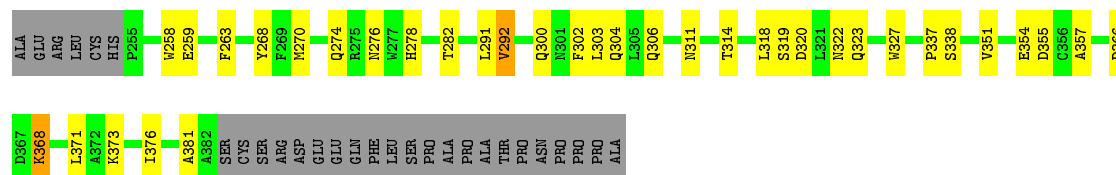
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total 13	O 13	0	0
4	B	29	Total 29	O 29	0	0
4	C	36	Total 36	O 36	0	0
4	D	38	Total 38	O 38	0	0
4	E	31	Total 31	O 31	0	0
4	F	30	Total 30	O 30	0	0
4	G	25	Total 25	O 25	0	0
4	H	23	Total 23	O 23	0	0
4	I	15	Total 15	O 15	0	0
4	J	12	Total 12	O 12	0	0



ASP  
GLU  
GLN  
GLN  
PHE  
LEU  
SER  
PRO  
ALA  
ALA  
ALA  
THR  
ASN  
PRO  
PRO  
PRO  
PRO  
ALA

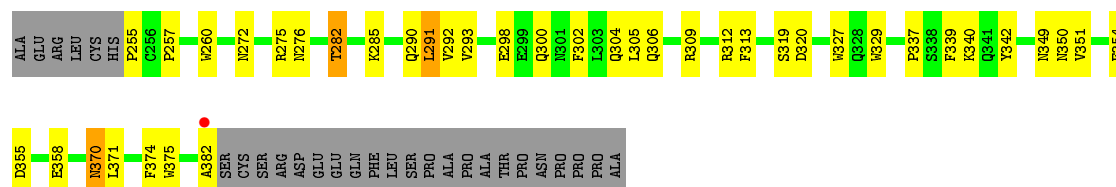
- Molecule 1: mDC-SIGN1B type I isoform

Chain E: 



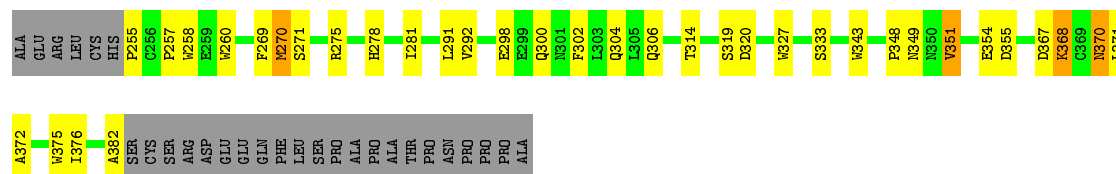
- Molecule 1: mDC-SIGN1B type I isoform

Chain F: 



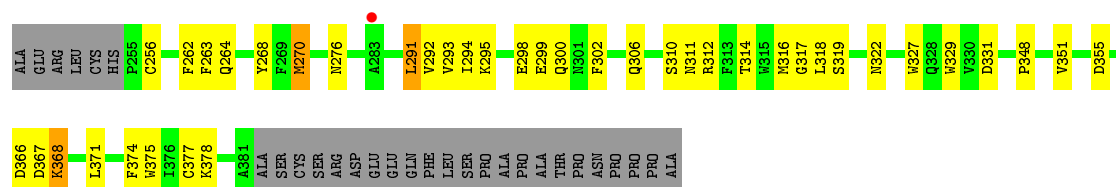
- Molecule 1: mDC-SIGN1B type I isoform

Chain G: 



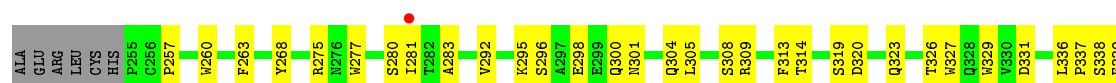
- Molecule 1: mDC-SIGN1B type I isoform

Chain H: 

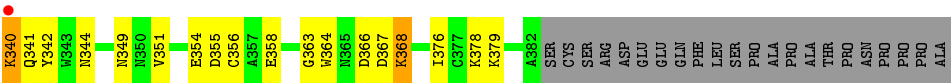


- Molecule 1: mDC-SIGN1B type I isoform

Chain I: 







● Molecule 1: mDC-SIGN1B type I isoform



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.81Å 148.16Å 112.99Å 90.00° 91.03° 90.00°	Depositor
Resolution (Å)	26.68 – 2.50 48.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (26.68-2.50) 94.6 (48.61-2.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.27 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.213 , 0.258 0.214 , 0.259	Depositor DCC
$R_{free}$ test set	3585 reflections (6.65%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.8	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.8	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 59357 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, MAN

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	0.36	0/1075	0.57	0/1458
1	B	0.41	0/1075	0.63	0/1458
1	C	0.41	0/1075	0.59	0/1458
1	D	0.41	0/1104	0.62	0/1498
1	E	0.41	0/1075	0.60	0/1458
1	F	0.44	0/1075	0.64	0/1458
1	G	0.39	0/1075	0.59	0/1458
1	H	0.42	0/1070	0.62	0/1451
1	I	0.37	0/1075	0.56	0/1458
1	J	0.37	0/1075	0.57	0/1458
All	All	0.40	0/10774	0.60	0/14613

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

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	1042	0	945	36	0
1	B	1042	0	945	21	0
1	C	1042	0	945	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1070	0	964	20	0
1	E	1042	0	945	26	0
1	F	1042	0	945	31	0
1	G	1042	0	945	26	0
1	H	1037	0	940	29	0
1	I	1042	0	945	45	0
1	J	1042	0	945	37	0
2	A	62	0	52	1	0
2	C	62	0	51	2	0
2	D	62	0	50	3	0
2	E	62	0	50	2	0
2	H	62	0	51	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	0	0
4	A	13	0	0	0	0
4	B	29	0	0	0	0
4	C	36	0	0	2	0
4	D	38	0	0	5	0
4	E	31	0	0	0	0
4	F	30	0	0	1	0
4	G	25	0	0	1	0
4	H	23	0	0	1	0
4	I	15	0	0	4	0
4	J	12	0	0	0	0
All	All	11035	0	9718	296	0

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 14.

All (296) 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:J:370:ASN:HD22	1:J:370:ASN:H	1.12	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LYS:H	1:A:368:LYS:HD2	1.40	0.87
1:F:305:LEU:HD13	1:F:309:ARG:HH21	1.43	0.84
1:I:368:LYS:HD2	1:I:368:LYS:H	1.43	0.84
1:D:311:ASN:HA	2:D:5:NAG:O4	1.80	0.81
1:I:354:GLU:HG2	1:I:368:LYS:HE2	1.62	0.79
1:H:368:LYS:H	1:H:368:LYS:HD2	1.49	0.77
1:A:311:ASN:HA	2:A:5:NAG:O4	1.85	0.77
1:A:318:LEU:HD11	1:A:327:TRP:HB3	1.68	0.75
1:F:290:GLN:HE22	1:F:293:VAL:HB	1.52	0.75
1:A:339:PHE:HD1	1:A:342:TYR:HE1	1.35	0.75
1:J:370:ASN:N	1:J:370:ASN:HD22	1.83	0.75
1:I:304:GLN:O	1:I:308:SER:HB2	1.89	0.73
1:C:368:LYS:HD2	1:C:368:LYS:N	2.04	0.73
1:A:368:LYS:N	1:A:368:LYS:HD2	2.04	0.72
1:E:311:ASN:HA	2:E:5:NAG:O4	1.90	0.71
1:D:309:ARG:NH1	1:E:337:PRO:HD3	2.07	0.69
1:H:263:PHE:HB3	1:H:268:TYR:CE1	2.27	0.69
1:J:338:SER:O	1:J:341:GLN:HG2	1.93	0.68
1:J:368:LYS:HD2	1:J:368:LYS:H	1.60	0.66
1:B:298:GLU:CD	1:B:298:GLU:H	1.97	0.66
1:I:337:PRO:HA	1:I:340:LYS:HE3	1.77	0.66
1:H:263:PHE:HB3	1:H:268:TYR:HE1	1.61	0.65
1:J:349:ASN:OD1	1:J:351:VAL:HG23	1.95	0.65
1:G:298:GLU:CD	1:G:298:GLU:H	1.99	0.65
1:C:354:GLU:HG2	1:C:368:LYS:HD2	1.78	0.65
1:B:276:ASN:HA	1:B:371:LEU:O	1.96	0.65
1:A:339:PHE:HD1	1:A:342:TYR:CE1	2.15	0.64
1:I:337:PRO:HA	1:I:340:LYS:CE	2.28	0.64
1:F:300:GLN:NE2	1:F:304:GLN:HB2	2.13	0.64
1:G:370:ASN:HD22	1:G:371:LEU:N	1.96	0.64
1:F:305:LEU:O	1:F:309:ARG:HG3	1.97	0.63
1:C:319:SER:HA	1:C:327:TRP:CZ3	2.34	0.63
1:C:370:ASN:ND2	1:C:370:ASN:H	1.97	0.63
1:J:370:ASN:ND2	1:J:370:ASN:H	1.91	0.63
1:J:301:ASN:O	1:J:305:LEU:HG	1.99	0.62
1:D:307:SER:HB3	4:D:708:HOH:O	1.99	0.62
1:I:339:PHE:HD1	1:I:342:TYR:HE1	1.47	0.62
1:J:368:LYS:HB3	1:J:370:ASN:HD21	1.63	0.62
1:F:255:PRO:HA	1:F:382:ALA:HB3	1.81	0.62
1:G:368:LYS:HD2	1:G:368:LYS:N	2.16	0.61
1:A:310:SER:O	1:A:312:ARG:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:368:LYS:HB3	1:J:370:ASN:ND2	2.14	0.61
1:C:257:PRO:HB2	1:C:260:TRP:CD1	2.35	0.61
1:H:302:PHE:O	1:H:306:GLN:HG2	2.02	0.60
1:I:301:ASN:O	1:I:305:LEU:HG	2.02	0.60
1:A:302:PHE:O	1:A:306:GLN:HG2	2.01	0.60
1:J:378:LYS:HG2	1:J:379:LYS:N	2.17	0.60
1:I:309:ARG:HB2	4:I:1215:HOH:O	2.02	0.60
1:G:368:LYS:HD2	1:G:368:LYS:H	1.67	0.59
1:A:314:THR:HG21	1:A:376:ILE:HG13	1.84	0.59
1:H:276:ASN:HA	1:H:371:LEU:O	2.02	0.59
1:C:311:ASN:HA	2:C:5:NAG:O4	2.03	0.59
1:C:305:LEU:O	1:C:309:ARG:HG3	2.03	0.58
1:C:368:LYS:HD2	1:C:368:LYS:H	1.67	0.58
1:E:276:ASN:HA	1:E:371:LEU:O	2.04	0.58
1:G:255:PRO:HA	1:G:382:ALA:HB3	1.86	0.58
1:B:350:ASN:OD1	1:B:353:GLU:HA	2.01	0.58
4:D:709:HOH:O	1:E:337:PRO:HD2	2.02	0.58
1:I:277:TRP:CZ3	1:I:281:ILE:HD11	2.38	0.58
1:H:298:GLU:CD	1:H:298:GLU:H	2.07	0.58
1:C:276:ASN:HA	1:C:371:LEU:O	2.04	0.57
1:I:368:LYS:N	1:I:368:LYS:HD2	2.17	0.57
1:F:339:PHE:HD1	1:F:342:TYR:CE1	2.23	0.57
1:I:367:ASP:OD1	1:I:368:LYS:HD2	2.05	0.56
1:F:275:ARG:HG3	1:F:375:TRP:CZ3	2.40	0.56
1:C:368:LYS:HB3	1:C:370:ASN:HD21	1.69	0.56
1:A:301:ASN:O	1:A:305:LEU:HG	2.05	0.56
1:J:291:LEU:HD22	1:J:317:GLY:N	2.21	0.56
1:G:302:PHE:O	1:G:306:GLN:HG2	2.05	0.56
1:J:263:PHE:HB3	1:J:268:TYR:HE1	1.69	0.56
1:I:319:SER:HB2	1:I:355:ASP:O	2.06	0.56
1:C:270:MET:HE2	4:C:618:HOH:O	2.04	0.56
1:F:282:THR:O	1:F:285:LYS:HB3	2.06	0.56
1:I:300:GLN:NE2	1:I:304:GLN:HB2	2.21	0.56
1:C:314:THR:HG21	1:C:376:ILE:HG13	1.88	0.56
1:D:333:SER:HB2	4:D:713:HOH:O	2.06	0.55
1:J:299:GLU:O	1:J:303:LEU:HG	2.06	0.55
1:A:368:LYS:H	1:A:368:LYS:CD	2.17	0.55
1:A:338:SER:O	1:A:341:GLN:HG2	2.07	0.55
1:A:319:SER:HB2	1:A:355:ASP:O	2.07	0.55
1:E:368:LYS:HD2	1:E:368:LYS:H	1.72	0.55
1:A:276:ASN:HA	1:A:371:LEU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:319:SER:HB2	1:J:355:ASP:O	2.06	0.55
1:G:257:PRO:HB2	1:G:260:TRP:CD1	2.42	0.55
1:C:298:GLU:CD	1:C:298:GLU:H	2.09	0.54
1:E:320:ASP:OD1	1:E:355:ASP:HA	2.07	0.54
1:E:354:GLU:HG2	1:E:368:LYS:HE2	1.89	0.54
1:H:319:SER:HB2	1:H:355:ASP:O	2.08	0.54
1:A:305:LEU:O	1:A:309:ARG:HG3	2.08	0.54
1:E:319:SER:HA	1:E:327:TRP:CZ3	2.42	0.54
1:B:300:GLN:NE2	1:B:304:GLN:HB2	2.22	0.54
1:E:314:THR:HG21	1:E:376:ILE:HG13	1.89	0.54
1:J:349:ASN:CG	1:J:351:VAL:HG23	2.29	0.53
1:H:291:LEU:HD13	1:H:316:MET:C	2.29	0.53
1:B:257:PRO:HB2	1:B:260:TRP:CD1	2.42	0.53
1:B:320:ASP:OD1	1:B:355:ASP:HA	2.08	0.53
1:I:349:ASN:CG	1:I:351:VAL:HG23	2.28	0.53
1:C:319:SER:HB2	1:C:355:ASP:O	2.08	0.53
1:C:278:HIS:O	1:C:282:THR:HG23	2.08	0.53
1:E:278:HIS:O	1:E:282:THR:HG23	2.09	0.53
1:A:339:PHE:CD1	1:A:342:TYR:HE1	2.22	0.53
1:A:270:MET:CE	1:A:306:GLN:HB3	2.38	0.53
1:D:276:ASN:HA	1:D:371:LEU:O	2.09	0.53
1:I:354:GLU:HB2	1:I:366:ASP:OD2	2.09	0.52
1:F:298:GLU:H	1:F:298:GLU:CD	2.12	0.52
1:J:269:PHE:O	1:J:376:ILE:HA	2.08	0.52
1:J:266:ASN:HA	1:J:380:SER:HA	1.90	0.52
1:A:337:PRO:HA	1:A:340:LYS:HD2	1.92	0.52
1:B:293:VAL:HG11	1:B:331:ASP:OD2	2.10	0.52
1:F:349:ASN:CG	1:F:351:VAL:HG23	2.30	0.52
1:H:318:LEU:HD13	1:H:329:TRP:CD2	2.44	0.52
1:J:298:GLU:H	1:J:298:GLU:CD	2.13	0.52
1:E:258:TRP:CD2	1:J:287:VAL:HG11	2.45	0.52
1:F:302:PHE:O	1:F:306:GLN:HG2	2.09	0.52
1:C:368:LYS:CD	1:C:368:LYS:H	2.23	0.52
1:A:270:MET:HE3	1:A:306:GLN:HB3	1.91	0.52
1:H:256:CYS:SG	1:H:262:PHE:HB2	2.50	0.51
1:J:368:LYS:HD2	1:J:368:LYS:N	2.23	0.51
1:H:291:LEU:HD13	1:H:317:GLY:N	2.25	0.51
1:H:293:VAL:HG11	1:H:295:LYS:NZ	2.26	0.51
1:G:270:MET:HE3	1:G:306:GLN:HG3	1.93	0.51
1:A:320:ASP:OD1	1:A:355:ASP:HA	2.11	0.51
1:H:319:SER:HA	1:H:327:TRP:CZ3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:302:PHE:O	1:J:306:GLN:HG2	2.11	0.50
1:B:349:ASN:CG	1:B:351:VAL:HG23	2.32	0.50
1:I:263:PHE:HB3	1:I:268:TYR:CE1	2.46	0.50
1:D:368:LYS:HD2	1:D:368:LYS:N	2.26	0.50
1:A:290:GLN:HE22	1:A:331:ASP:HB3	1.76	0.50
1:F:275:ARG:HG3	1:F:375:TRP:HZ3	1.77	0.50
2:D:1:NAG:H61	4:D:731:HOH:O	2.10	0.50
1:F:313:PHE:HB3	1:F:358:GLU:OE2	2.12	0.50
1:F:319:SER:HB2	1:F:355:ASP:O	2.11	0.50
1:G:269:PHE:CE2	1:G:271:SER:HA	2.46	0.50
1:A:362:ASN:HD22	1:A:362:ASN:N	2.10	0.50
1:D:278:HIS:O	1:D:282:THR:HG23	2.12	0.49
1:A:320:ASP:HB3	1:A:327:TRP:CD2	2.47	0.49
1:G:260:TRP:CE2	1:G:269:PHE:HB2	2.47	0.49
1:J:378:LYS:O	1:J:379:LYS:HB3	2.12	0.49
1:F:337:PRO:O	1:F:340:LYS:HG3	2.11	0.49
1:A:293:VAL:HG13	1:A:329:TRP:CD2	2.47	0.49
1:D:336:LEU:HG	4:D:730:HOH:O	2.13	0.49
1:G:319:SER:HB2	1:G:355:ASP:O	2.13	0.49
1:A:281:ILE:HG12	1:A:291:LEU:HD12	1.94	0.49
1:J:339:PHE:O	1:J:341:GLN:N	2.45	0.49
1:J:354:GLU:HB3	1:J:367:ASP:CA	2.42	0.49
1:H:311:ASN:HA	2:H:5:NAG:O4	2.13	0.49
1:G:320:ASP:OD1	1:G:355:ASP:HA	2.13	0.49
1:J:331:ASP:OD1	1:J:332:GLY:N	2.46	0.49
1:J:277:TRP:O	1:J:281:ILE:HG13	2.12	0.49
1:J:263:PHE:HB3	1:J:268:TYR:CE1	2.47	0.48
1:B:313:PHE:HE2	1:B:360:SER:HG	1.60	0.48
1:A:327:TRP:HB2	1:A:335:LEU:HD22	1.95	0.48
1:B:370:ASN:HD22	1:B:370:ASN:N	2.12	0.48
1:H:375:TRP:HZ3	1:H:377:CYS:SG	2.36	0.48
1:I:280:SER:O	1:I:283:ALA:HB3	2.13	0.48
1:I:337:PRO:HA	1:I:340:LYS:CD	2.43	0.48
1:B:275:ARG:HG3	1:B:375:TRP:CZ3	2.49	0.48
1:C:368:LYS:N	1:C:368:LYS:CD	2.74	0.48
1:E:302:PHE:O	1:E:306:GLN:HG2	2.14	0.48
1:D:320:ASP:OD1	1:D:355:ASP:HA	2.14	0.48
1:I:296:SER:HB2	1:I:298:GLU:OE2	2.14	0.48
1:D:314:THR:HG21	1:D:376:ILE:HG13	1.96	0.48
1:I:323:GLN:HB3	1:I:326:THR:HB	1.95	0.48
1:A:275:ARG:HG3	1:A:375:TRP:CZ3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:SER:OG	1:C:375:TRP:CH2	2.67	0.47
1:E:258:TRP:O	1:E:259:GLU:HB2	2.14	0.47
1:D:319:SER:HB2	1:D:355:ASP:O	2.14	0.47
1:G:368:LYS:CD	1:G:368:LYS:H	2.25	0.47
1:C:348:PRO:HD2	4:C:612:HOH:O	2.14	0.47
1:E:323:GLN:HG3	1:E:323:GLN:O	2.12	0.47
1:F:276:ASN:HA	1:F:371:LEU:O	2.14	0.47
1:D:368:LYS:HD2	1:D:368:LYS:H	1.80	0.47
1:B:370:ASN:HD22	1:B:370:ASN:H	1.62	0.47
1:J:300:GLN:HG2	1:J:342:TYR:CE1	2.50	0.47
1:E:292:VAL:HG21	1:E:303:LEU:CD1	2.45	0.47
1:D:313:PHE:HB3	1:D:358:GLU:OE2	2.15	0.47
1:J:370:ASN:N	1:J:370:ASN:ND2	2.56	0.46
1:C:368:LYS:HB3	1:C:370:ASN:ND2	2.29	0.46
1:F:290:GLN:NE2	1:F:293:VAL:HB	2.26	0.46
1:I:320:ASP:OD1	1:I:355:ASP:HA	2.16	0.46
1:A:257:PRO:HB2	1:A:260:TRP:CD1	2.50	0.46
1:F:319:SER:HA	1:F:327:TRP:CZ3	2.51	0.46
1:D:275:ARG:HG2	1:D:275:ARG:HH11	1.79	0.46
1:I:275:ARG:HH11	1:I:275:ARG:HG2	1.80	0.46
1:G:278:HIS:O	1:G:281:ILE:HB	2.15	0.46
1:E:300:GLN:NE2	1:E:304:GLN:HB2	2.31	0.46
1:F:339:PHE:HD1	1:F:342:TYR:HE1	1.63	0.46
1:F:320:ASP:OD1	1:F:355:ASP:HA	2.16	0.46
1:A:323:GLN:HB3	1:A:326:THR:HB	1.98	0.46
1:C:354:GLU:OE2	2:C:2:MAN:O4	2.34	0.46
1:F:291:LEU:HA	1:F:291:LEU:HD23	1.80	0.46
1:B:290:GLN:HE22	1:B:331:ASP:HB3	1.81	0.45
1:G:319:SER:HA	1:G:327:TRP:CZ3	2.52	0.45
1:G:300:GLN:NE2	1:G:304:GLN:HB2	2.32	0.45
1:H:293:VAL:HG11	1:H:295:LYS:HZ3	1.80	0.45
1:I:295:LYS:NZ	1:I:331:ASP:OD2	2.49	0.45
1:H:299:GLU:OE1	1:H:378:LYS:NZ	2.47	0.45
1:D:269:PHE:O	1:D:376:ILE:HA	2.16	0.45
1:A:339:PHE:HA	1:A:342:TYR:CE1	2.52	0.45
1:H:310:SER:O	1:H:312:ARG:HG3	2.16	0.45
1:C:276:ASN:HB2	1:C:369:CYS:O	2.17	0.45
1:E:274:GLN:HA	1:E:373:LYS:O	2.17	0.45
1:E:318:LEU:HB3	1:E:357:ALA:HB3	1.99	0.45
1:F:257:PRO:HB2	1:F:260:TRP:CD1	2.52	0.45
1:C:370:ASN:H	1:C:370:ASN:HD22	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:354:GLU:HB3	1:G:367:ASP:CA	2.47	0.44
1:I:339:PHE:HD1	1:I:342:TYR:CE1	2.29	0.44
1:F:370:ASN:HD22	1:F:371:LEU:N	2.14	0.44
1:G:351:VAL:HG11	1:H:351:VAL:CG1	2.47	0.44
1:G:314:THR:HG21	1:G:376:ILE:HG13	1.99	0.44
1:C:291:LEU:HD23	1:C:291:LEU:HA	1.85	0.44
1:I:368:LYS:HA	4:I:1213:HOH:O	2.16	0.44
1:F:312:ARG:HB3	1:F:374:PHE:CD1	2.53	0.44
1:I:349:ASN:OD1	1:I:351:VAL:HG23	2.17	0.44
1:I:314:THR:HG21	1:I:376:ILE:HG13	2.00	0.44
1:J:337:PRO:HA	1:J:340:LYS:HG3	1.98	0.44
1:B:319:SER:HA	1:B:327:TRP:CZ3	2.52	0.44
1:E:319:SER:HB2	1:E:355:ASP:O	2.18	0.44
1:D:320:ASP:HB3	1:D:327:TRP:CE2	2.53	0.44
1:C:298:GLU:CD	1:C:298:GLU:N	2.71	0.43
1:G:368:LYS:CD	1:G:368:LYS:N	2.81	0.43
1:J:291:LEU:O	1:J:292:VAL:C	2.57	0.43
1:E:354:GLU:OE2	2:E:2:MAN:O4	2.35	0.43
1:A:292:VAL:O	1:A:292:VAL:HG13	2.18	0.43
1:H:314:THR:HG23	1:H:374:PHE:C	2.38	0.43
1:H:348:PRO:HA	1:H:366:ASP:OD1	2.18	0.43
1:F:339:PHE:CD1	1:F:342:TYR:HE1	2.36	0.43
1:E:292:VAL:HG21	1:E:303:LEU:HD11	2.00	0.43
1:A:274:GLN:HA	1:A:373:LYS:O	2.18	0.43
1:I:336:LEU:C	1:I:338:SER:N	2.72	0.43
1:C:351:VAL:HG12	1:I:351:VAL:HG21	2.00	0.43
1:G:275:ARG:O	1:G:372:ALA:HA	2.17	0.43
1:I:300:GLN:HE22	1:I:304:GLN:HB2	1.81	0.43
1:A:293:VAL:HG13	1:A:329:TRP:CE3	2.54	0.43
1:I:313:PHE:HB2	4:I:1217:HOH:O	2.19	0.43
1:F:293:VAL:HA	1:F:329:TRP:CE3	2.54	0.43
1:F:305:LEU:HD13	1:F:309:ARG:NH2	2.23	0.43
1:G:258:TRP:HB3	4:G:80:HOH:O	2.18	0.43
1:D:319:SER:HA	1:D:327:TRP:CZ3	2.53	0.42
1:H:294:ILE:HG21	1:H:300:GLN:HB2	1.99	0.42
1:G:343:TRP:CD2	1:G:348:PRO:HD3	2.54	0.42
1:C:259:GLU:OE2	1:F:275:ARG:NH2	2.51	0.42
1:A:258:TRP:O	1:A:259:GLU:HB2	2.18	0.42
1:A:320:ASP:HB3	1:A:327:TRP:CE2	2.53	0.42
1:C:314:THR:HA	1:C:374:PHE:O	2.19	0.42
1:J:321:LEU:CD2	1:J:355:ASP:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:339:PHE:O	1:I:341:GLN:N	2.51	0.42
1:I:257:PRO:HB2	1:I:260:TRP:CD1	2.55	0.42
1:I:309:ARG:HD2	4:I:1215:HOH:O	2.19	0.42
1:I:319:SER:O	1:I:327:TRP:HA	2.19	0.42
1:E:366:ASP:OD1	1:E:366:ASP:N	2.51	0.42
1:I:275:ARG:NH1	1:I:275:ARG:HG2	2.35	0.42
1:D:302:PHE:CE2	1:E:338:SER:HB3	2.55	0.42
1:B:293:VAL:HA	1:B:329:TRP:CE3	2.55	0.42
1:B:269:PHE:O	1:B:376:ILE:HA	2.19	0.42
1:I:344:ASN:OD1	1:I:363:GLY:HA3	2.20	0.42
1:I:378:LYS:O	1:I:379:LYS:HB3	2.20	0.42
1:I:378:LYS:HG2	1:I:379:LYS:N	2.34	0.42
1:H:298:GLU:CD	1:H:298:GLU:N	2.72	0.42
1:B:300:GLN:HG2	1:B:342:TYR:CE2	2.55	0.42
1:B:368:LYS:HB3	1:B:370:ASN:ND2	2.35	0.41
1:I:336:LEU:C	1:I:338:SER:H	2.23	0.41
1:B:331:ASP:C	1:B:331:ASP:OD1	2.59	0.41
1:I:329:TRP:HB2	1:I:331:ASP:OD1	2.19	0.41
1:J:274:GLN:HA	1:J:373:LYS:O	2.20	0.41
1:E:263:PHE:HB3	1:E:268:TYR:CE1	2.55	0.41
1:E:354:GLU:CG	1:E:368:LYS:HE2	2.50	0.41
1:H:367:ASP:OD1	1:H:368:LYS:HD2	2.20	0.41
1:D:275:ARG:HG3	1:D:375:TRP:CZ3	2.55	0.41
1:B:295:LYS:NZ	1:B:331:ASP:OD2	2.53	0.41
1:H:375:TRP:N	1:H:375:TRP:CD1	2.89	0.41
1:H:322:ASN:HB3	4:H:131:HOH:O	2.20	0.41
1:I:341:GLN:HG3	1:I:342:TYR:CD2	2.55	0.41
1:I:277:TRP:CG	1:I:356:CYS:SG	3.13	0.41
1:G:349:ASN:OD1	1:G:351:VAL:HG22	2.21	0.41
1:J:317:GLY:O	1:J:329:TRP:HE3	2.04	0.41
1:I:319:SER:HA	1:I:327:TRP:CZ3	2.56	0.41
1:H:295:LYS:NZ	1:H:331:ASP:OD2	2.53	0.41
1:G:333:SER:H	1:G:333:SER:HG	1.66	0.41
1:H:270:MET:N	1:H:270:MET:SD	2.94	0.41
1:D:257:PRO:HB2	1:D:260:TRP:CD1	2.56	0.41
1:B:319:SER:HB2	1:B:355:ASP:O	2.21	0.41
1:F:351:VAL:O	1:F:354:GLU:HG3	2.20	0.41
1:I:344:ASN:ND2	1:I:364:TRP:O	2.54	0.41
1:E:351:VAL:O	1:E:354:GLU:HG3	2.21	0.40
1:J:354:GLU:HB3	1:J:367:ASP:C	2.41	0.40
1:H:368:LYS:N	1:H:368:LYS:HD2	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:298:GLU:HA	1:J:301:ASN:HD22	1.86	0.40
1:A:336:LEU:HA	1:A:337:PRO:HD3	1.94	0.40
1:G:275:ARG:HD2	1:G:375:TRP:CZ3	2.56	0.40
1:C:323:GLN:O	1:C:324:GLU:C	2.59	0.40
2:D:1:NAG:O4	1:F:354:GLU:OE2	2.39	0.40
1:C:318:LEU:HD13	1:C:329:TRP:CD2	2.57	0.40
1:J:378:LYS:CG	1:J:379:LYS:N	2.84	0.40
1:F:350:ASN:HB2	4:F:17:HOH:O	2.22	0.40

There are no symmetry-related clashes.

## 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	126/156 (81%)	110 (87%)	13 (10%)	3 (2%)	7	11
1	B	126/156 (81%)	117 (93%)	8 (6%)	1 (1%)	24	41
1	C	126/156 (81%)	116 (92%)	9 (7%)	1 (1%)	24	41
1	D	130/156 (83%)	126 (97%)	2 (2%)	2 (2%)	13	22
1	E	126/156 (81%)	119 (94%)	5 (4%)	2 (2%)	12	21
1	F	126/156 (81%)	121 (96%)	4 (3%)	1 (1%)	24	41
1	G	126/156 (81%)	116 (92%)	9 (7%)	1 (1%)	24	41
1	H	125/156 (80%)	119 (95%)	4 (3%)	2 (2%)	12	21
1	I	126/156 (81%)	115 (91%)	9 (7%)	2 (2%)	12	21
1	J	126/156 (81%)	109 (86%)	12 (10%)	5 (4%)	4	4
All	All	1263/1560 (81%)	1168 (92%)	75 (6%)	20 (2%)	12	21

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	381	ALA
1	I	292	VAL
1	A	292	VAL
1	A	381	ALA
1	D	292	VAL
1	E	292	VAL
1	F	292	VAL
1	G	292	VAL
1	H	292	VAL
1	I	340	LYS
1	J	292	VAL
1	J	340	LYS
1	H	264	GLN
1	J	379	LYS
1	J	264	GLN
1	B	292	VAL
1	D	353	GLU
1	J	381	ALA
1	C	292	VAL
1	A	334	PRO

### 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	112/136 (82%)	110 (98%)	2 (2%)	66	88
1	B	112/136 (82%)	107 (96%)	5 (4%)	34	59
1	C	112/136 (82%)	107 (96%)	5 (4%)	34	59
1	D	116/136 (85%)	114 (98%)	2 (2%)	68	89
1	E	112/136 (82%)	108 (96%)	4 (4%)	42	69
1	F	112/136 (82%)	108 (96%)	4 (4%)	42	69
1	G	112/136 (82%)	107 (96%)	5 (4%)	34	59
1	H	112/136 (82%)	109 (97%)	3 (3%)	52	79
1	I	112/136 (82%)	110 (98%)	2 (2%)	66	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	112/136 (82%)	109 (97%)	3 (3%)	52 79
All	All	1124/1360 (83%)	1089 (97%)	35 (3%)	47 75

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	MET
1	A	368	LYS
1	B	282	THR
1	B	291	LEU
1	B	323	GLN
1	B	368	LYS
1	B	370	ASN
1	C	272	ASN
1	C	282	THR
1	C	291	LEU
1	C	368	LYS
1	C	370	ASN
1	D	291	LEU
1	D	362	ASN
1	E	270	MET
1	E	291	LEU
1	E	322	ASN
1	E	368	LYS
1	F	272	ASN
1	F	282	THR
1	F	291	LEU
1	F	370	ASN
1	G	270	MET
1	G	291	LEU
1	G	351	VAL
1	G	368	LYS
1	G	370	ASN
1	H	270	MET
1	H	291	LEU
1	H	368	LYS
1	I	358	GLU
1	I	368	LYS
1	J	291	LEU
1	J	368	LYS
1	J	370	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	ASN
1	A	290	GLN
1	A	301	ASN
1	A	362	ASN
1	B	272	ASN
1	B	290	GLN
1	B	306	GLN
1	B	323	GLN
1	B	328	GLN
1	B	370	ASN
1	C	370	ASN
1	D	306	GLN
1	D	362	ASN
1	D	370	ASN
1	E	322	ASN
1	E	328	GLN
1	E	370	ASN
1	F	272	ASN
1	F	290	GLN
1	F	328	GLN
1	F	370	ASN
1	G	328	GLN
1	G	370	ASN
1	H	301	ASN
1	H	328	GLN
1	I	301	ASN
1	I	370	ASN
1	J	301	ASN
1	J	328	GLN
1	J	370	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

25 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	1	3,2	14,14,15	0.51	0	15,19,21	0.82	0
2	MAN	A	2	3,2	11,11,12	0.49	0	14,15,17	0.86	1 (7%)
2	MAN	A	3	2	12,12,12	0.37	0	17,17,17	0.54	0
2	MAN	A	4	2	11,11,12	0.56	0	14,15,17	0.59	0
2	NAG	A	5	2	14,14,15	0.44	0	15,19,21	1.11	2 (13%)
2	NAG	C	1	3,2	14,14,15	0.53	0	15,19,21	1.03	1 (6%)
2	MAN	C	2	3,2	11,11,12	0.56	0	14,15,17	0.79	1 (7%)
2	MAN	C	3	2	12,12,12	0.44	0	17,17,17	0.52	0
2	MAN	C	4	2	11,11,12	0.60	0	14,15,17	0.70	0
2	NAG	C	5	2	14,14,15	0.48	0	15,19,21	0.72	1 (6%)
2	NAG	D	1	3,2	14,14,15	0.37	0	15,19,21	0.86	1 (6%)
2	MAN	D	2	3,2	11,11,12	0.52	0	14,15,17	0.72	1 (7%)
2	MAN	D	3	2	12,12,12	0.38	0	17,17,17	0.44	0
2	MAN	D	4	2	11,11,12	0.51	0	14,15,17	0.66	0
2	NAG	D	5	2	14,14,15	0.54	0	15,19,21	0.65	0
2	NAG	E	1	3,2	14,14,15	0.46	0	15,19,21	0.84	1 (6%)
2	MAN	E	2	3,2	11,11,12	0.48	0	14,15,17	0.77	1 (7%)
2	MAN	E	3	2	12,12,12	0.56	0	17,17,17	0.62	0
2	MAN	E	4	2	11,11,12	0.43	0	14,15,17	0.83	1 (7%)
2	NAG	E	5	2	14,14,15	0.51	0	15,19,21	0.86	1 (6%)
2	NAG	H	1	3,2	14,14,15	0.42	0	15,19,21	0.77	0
2	MAN	H	2	3,2	11,11,12	0.50	0	14,15,17	0.72	1 (7%)
2	MAN	H	3	2	12,12,12	0.38	0	17,17,17	0.53	0
2	MAN	H	4	2	11,11,12	0.53	0	14,15,17	0.76	1 (7%)
2	NAG	H	5	2	14,14,15	0.48	0	15,19,21	0.79	1 (6%)

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	1	3,2	-	0/6/23/26	0/1/1/1
2	MAN	A	2	3,2	-	0/2/19/22	0/1/1/1
2	MAN	A	3	2	-	0/2/22/22	0/1/1/1
2	MAN	A	4	2	-	0/2/19/22	0/1/1/1
2	NAG	A	5	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1	3,2	-	0/6/23/26	0/1/1/1
2	MAN	C	2	3,2	-	0/2/19/22	0/1/1/1
2	MAN	C	3	2	-	0/2/22/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	NAG	C	5	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	3,2	-	0/6/23/26	0/1/1/1
2	MAN	D	2	3,2	-	0/2/19/22	0/1/1/1
2	MAN	D	3	2	-	0/2/22/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	NAG	D	5	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	3,2	-	0/6/23/26	0/1/1/1
2	MAN	E	2	3,2	-	0/2/19/22	0/1/1/1
2	MAN	E	3	2	-	0/2/22/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	NAG	E	5	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	3,2	-	0/6/23/26	0/1/1/1
2	MAN	H	2	3,2	-	0/2/19/22	0/1/1/1
2	MAN	H	3	2	-	0/2/22/22	0/1/1/1
2	MAN	H	4	2	-	0/2/19/22	0/1/1/1
2	NAG	H	5	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C2-N2-C7	-2.84	119.39	123.04
2	E	1	NAG	C2-N2-C7	-2.80	119.44	123.04
2	A	5	NAG	C2-N2-C7	-2.69	119.58	123.04
2	A	5	NAG	C4-C3-C2	-2.64	107.13	111.23
2	E	5	NAG	C2-N2-C7	-2.59	119.72	123.04
2	D	1	NAG	C2-N2-C7	-2.43	119.91	123.04
2	C	5	NAG	C2-N2-C7	-2.17	120.25	123.04
2	H	5	NAG	C2-N2-C7	-2.11	120.32	123.04
2	D	2	MAN	C1-O5-C5	2.10	114.92	112.25
2	E	2	MAN	C1-O5-C5	2.13	114.96	112.25
2	H	2	MAN	C1-O5-C5	2.18	115.01	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	MAN	C1-O5-C5	2.39	115.28	112.25
2	H	4	MAN	C1-O5-C5	2.41	115.31	112.25
2	C	2	MAN	C1-O5-C5	2.55	115.49	112.25
2	A	2	MAN	C1-O5-C5	2.66	115.63	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5	NAG	1	0
2	C	2	MAN	1	0
2	C	5	NAG	1	0
2	D	1	NAG	2	0
2	D	5	NAG	1	0
2	E	2	MAN	1	0
2	E	5	NAG	1	0
2	H	5	NAG	1	0

## 5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 30 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

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	128/156 (82%)	0.44	7 (5%) 29 32	39, 66, 81, 87	0
1	B	128/156 (82%)	-0.08	1 (0%) 87 89	27, 43, 59, 77	0
1	C	128/156 (82%)	-0.01	0 100 100	26, 42, 56, 68	0
1	D	132/156 (84%)	0.02	0 100 100	25, 43, 57, 74	0
1	E	128/156 (82%)	0.11	0 100 100	26, 44, 57, 67	0
1	F	128/156 (82%)	0.00	1 (0%) 87 89	26, 38, 54, 69	0
1	G	128/156 (82%)	-0.07	0 100 100	30, 45, 64, 83	0
1	H	127/156 (81%)	0.17	1 (0%) 87 89	31, 47, 60, 68	0
1	I	128/156 (82%)	0.28	2 (1%) 74 78	43, 62, 81, 84	0
1	J	128/156 (82%)	0.40	8 (6%) 23 26	43, 62, 76, 83	0
All	All	1283/1560 (82%)	0.13	20 (1%) 74 78	25, 48, 74, 87	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	382	ALA	3.8
1	A	256	CYS	3.4
1	A	292	VAL	3.3
1	A	267	CYS	3.1
1	J	321	LEU	3.0
1	J	282	THR	2.7
1	F	382	ALA	2.6
1	B	309	ARG	2.6
1	A	262	PHE	2.4
1	A	330	VAL	2.3
1	I	340	LYS	2.3
1	H	283	ALA	2.3
1	J	263	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	268	TYR	2.2
1	J	382	ALA	2.2
1	J	381	ALA	2.1
1	J	256	CYS	2.1
1	I	281	ILE	2.1
1	J	267	CYS	2.0
1	A	268	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	5	14/15	0.89	0.22	1.92	68,71,73,73	0
2	MAN	D	3	12/12	0.95	0.17	0.93	31,39,42,48	0
2	MAN	C	4	11/12	0.96	0.19	0.54	47,49,51,55	0
2	NAG	A	1	14/15	0.96	0.17	0.52	48,50,52,52	0
2	MAN	D	2	11/12	0.98	0.15	0.45	23,27,30,33	0
2	MAN	A	3	12/12	0.93	0.14	0.35	49,55,59,62	0
2	NAG	H	1	14/15	0.95	0.15	0.19	33,38,46,47	0
2	NAG	C	1	14/15	0.96	0.15	0.14	41,42,46,50	0
2	MAN	E	4	11/12	0.96	0.17	-0.02	39,44,46,47	0
2	MAN	D	4	11/12	0.97	0.16	-0.04	36,38,40,42	0
2	NAG	C	5	14/15	0.95	0.17	-0.08	42,46,48,49	0
2	NAG	E	5	14/15	0.93	0.16	-0.08	47,49,51,54	0
2	MAN	C	2	11/12	0.97	0.15	-0.20	30,37,41,45	0
2	NAG	D	5	14/15	0.94	0.16	-0.25	32,41,42,43	0
2	MAN	E	3	12/12	0.93	0.16	-0.26	38,41,44,45	0
2	MAN	A	2	11/12	0.95	0.13	-0.27	39,45,49,50	0
2	NAG	E	1	14/15	0.97	0.15	-0.42	31,35,39,42	0
2	NAG	D	1	14/15	0.98	0.14	-0.64	25,27,31,34	0
2	NAG	H	5	14/15	0.92	0.14	-0.76	51,52,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAN	E	2	11/12	0.98	0.15	-0.85	29,33,38,39	0
2	MAN	H	2	11/12	0.97	0.14	-0.92	28,33,36,36	0
2	MAN	A	4	11/12	0.94	0.11	-1.53	61,63,66,66	0
2	MAN	H	4	11/12	0.95	0.12	-3.74	42,46,48,53	0
2	MAN	H	3	12/12	0.97	0.12	-5.21	35,40,42,44	0
2	MAN	C	3	12/12	0.96	0.15	-	44,48,50,50	0

## 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	A	406	1/1	0.98	0.15	0.51	41,41,41,41	0
3	CA	H	1101	1/1	0.98	0.17	0.13	37,37,37,37	0
3	CA	I	1202	1/1	0.98	0.14	-0.02	43,43,43,43	0
3	CA	E	802	1/1	0.99	0.16	-0.15	31,31,31,31	0
3	CA	E	801	1/1	0.99	0.16	-0.28	33,33,33,33	0
3	CA	D	702	1/1	0.99	0.13	-0.36	32,32,32,32	0
3	CA	H	1102	1/1	0.97	0.15	-0.54	33,33,33,33	0
3	CA	F	901	1/1	0.99	0.12	-0.68	29,29,29,29	0
3	CA	C	602	1/1	0.98	0.12	-0.75	34,34,34,34	0
3	CA	B	501	1/1	0.99	0.13	-0.76	32,32,32,32	0
3	CA	J	1302	1/1	0.99	0.14	-0.84	39,39,39,39	0
3	CA	G	1002	1/1	0.99	0.12	-0.87	30,30,30,30	0
3	CA	B	502	1/1	0.99	0.13	-1.05	27,27,27,27	0
3	CA	D	701	1/1	0.99	0.11	-1.11	37,37,37,37	0
3	CA	J	1303	1/1	0.93	0.06	-1.12	53,53,53,53	0
3	CA	F	902	1/1	0.99	0.12	-1.37	28,28,28,28	0
3	CA	G	1001	1/1	0.96	0.11	-1.73	32,32,32,32	0
3	CA	J	1301	1/1	0.98	0.10	-1.76	46,46,46,46	0
3	CA	I	1201	1/1	0.97	0.10	-2.24	44,44,44,44	0
3	CA	A	405	1/1	0.96	0.09	-3.80	56,56,56,56	0
3	CA	C	601	1/1	0.96	0.08	-4.92	54,54,54,54	0
3	CA	D	703	1/1	0.97	0.08	-	50,50,50,50	0
3	CA	F	903	1/1	0.96	0.09	-	48,48,48,48	0
3	CA	A	407	1/1	0.91	0.13	-	64,64,64,64	0
3	CA	I	1203	1/1	0.98	0.13	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	G	1003	1/1	0.96	0.13	-	43,43,43,43	0
3	CA	B	503	1/1	0.99	0.07	-	49,49,49,49	0
3	CA	E	803	1/1	0.98	0.09	-	40,40,40,40	0
3	CA	H	1103	1/1	0.99	0.20	-	51,51,51,51	0
3	CA	C	603	1/1	0.97	0.12	-	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.