Full wwPDB EM Validation Report ⓘ

Mar 3, 2025 – 12:37 pm GMT

PDB ID	:	8S50
EMDB ID	:	EMD-19717
Title	:	Cryo-EM structure of the C terminal region of PTX3 with a section of coiled-coil
Authors	:	Snee, M.; Shah, A.; Lockhart-Cairns, M.; Collins, R.; Levy, C.; Baldock, C.; Day, A.
Deposited on	:	2024-02-22
Resolution	:	3.33 Å(reported)
Based on initial model	:	8PVQ

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

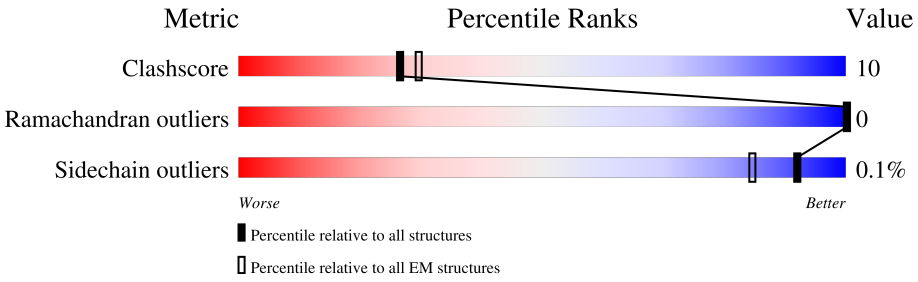
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	364	51% 12% 37%
1	B	364	52% 12% 37%
1	C	364	51% 13% 37%
1	D	364	50% 13% 37%
1	F	364	52% 11% 37%
1	G	364	51% 13% 37%
1	J	364	52% 12% 37%
1	K	364	50% 13% 37%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 28718 atoms, of which 14080 are hydrogens and 0 are deuteriums.

In the tables below, 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.

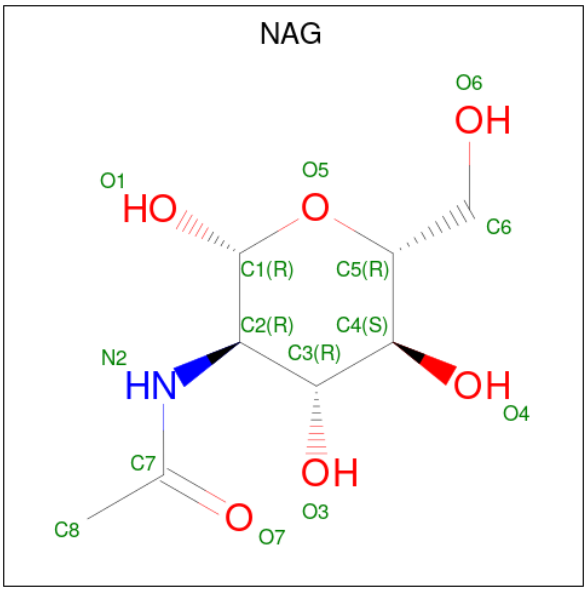
- Molecule 1 is a protein called Pentraxin-related protein PTX3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	231	Total	C	H	N	O	S	2	0
			3541	1134	1752	314	331	10		
1	A	231	Total	C	H	N	O	S	2	0
			3541	1134	1752	314	331	10		
1	C	231	Total	C	H	N	O	S	2	0
			3541	1134	1752	314	331	10		
1	D	231	Total	C	H	N	O	S	2	0
			3541	1134	1752	314	331	10		
1	F	231	Total	C	H	N	O	S	2	0
			3541	1134	1752	314	331	10		
1	G	231	Total	C	H	N	O	S	2	0
			3541	1134	1752	314	331	10		
1	J	231	Total	C	H	N	O	S	2	0
			3541	1134	1752	314	331	10		
1	K	231	Total	C	H	N	O	S	2	0
			3541	1134	1752	314	331	10		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	48	ASP	ALA	variant	UNP P26022
A	48	ASP	ALA	variant	UNP P26022
C	48	ASP	ALA	variant	UNP P26022
D	48	ASP	ALA	variant	UNP P26022
F	48	ASP	ALA	variant	UNP P26022
G	48	ASP	ALA	variant	UNP P26022
J	48	ASP	ALA	variant	UNP P26022
K	48	ASP	ALA	variant	UNP P26022

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	H	N	O	0
			22	8	8	1	5	
2	A	1	Total	C	H	N	O	0
			22	8	8	1	5	
2	C	1	Total	C	H	N	O	0
			22	8	8	1	5	
2	D	1	Total	C	H	N	O	0
			22	8	8	1	5	
2	F	1	Total	C	H	N	O	0
			22	8	8	1	5	
2	G	1	Total	C	H	N	O	0
			22	8	8	1	5	
2	J	1	Total	C	H	N	O	0
			22	8	8	1	5	
2	K	1	Total	C	H	N	O	0
			22	8	8	1	5	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	B	28	Total	O	0
			28	28	
3	A	27	Total	O	0
			27	27	
3	C	28	Total	O	0
			28	28	
3	D	24	Total	O	0
			24	24	

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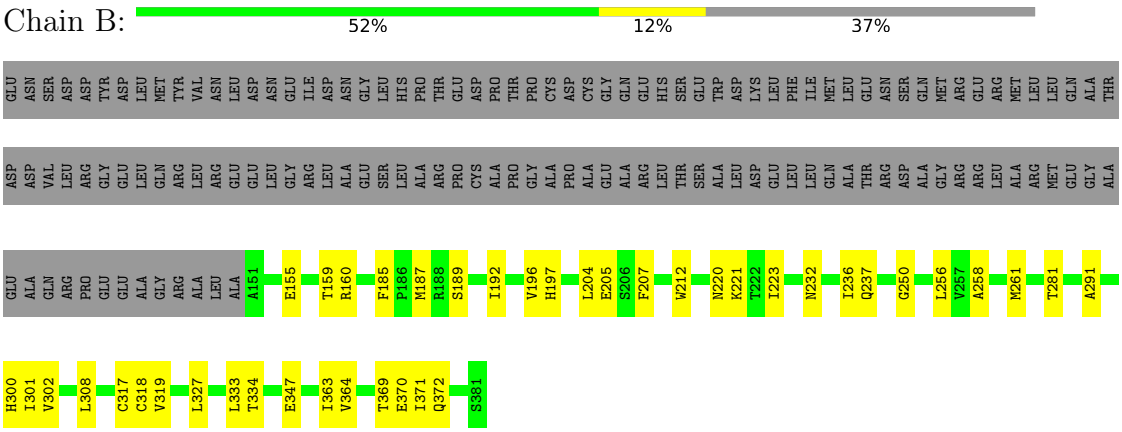
Mol	Chain	Residues	Atoms	AltConf
3	F	28	Total O 28 28	0
3	G	25	Total O 25 25	0
3	J	28	Total O 28 28	0
3	K	26	Total O 26 26	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

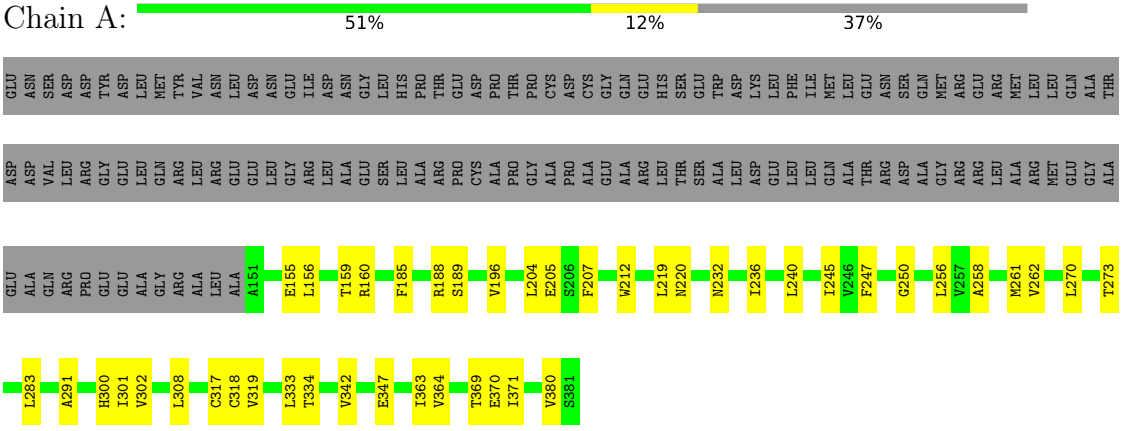
• Molecule 1: Pentraxin-related protein PTX3

Chain B:



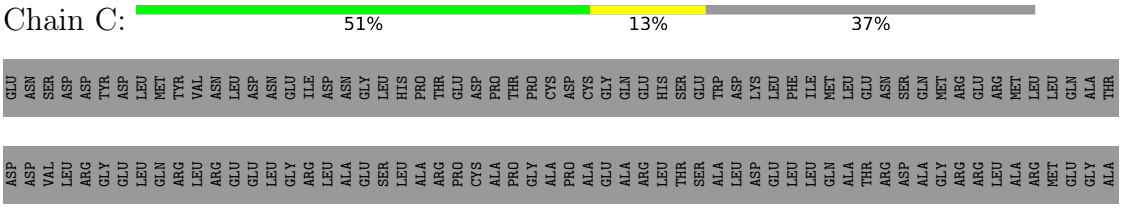
• Molecule 1: Pentraxin-related protein PTX3

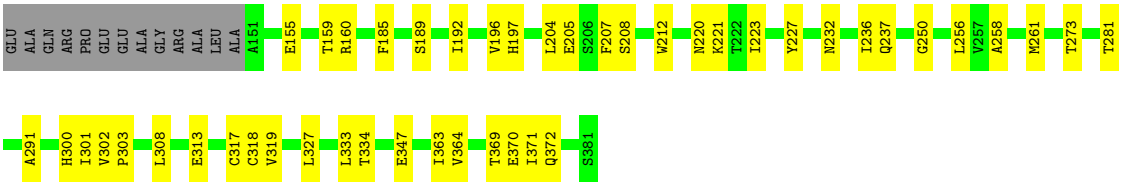
Chain A:



• Molecule 1: Pentraxin-related protein PTX3

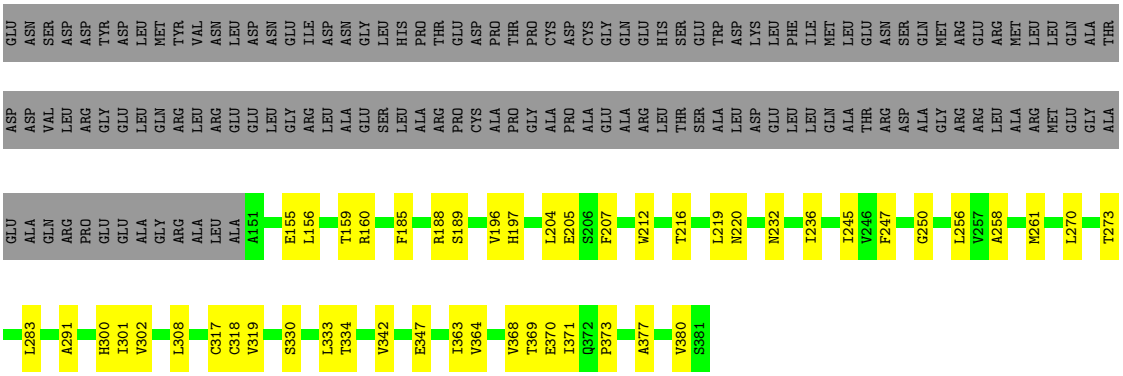
Chain C:





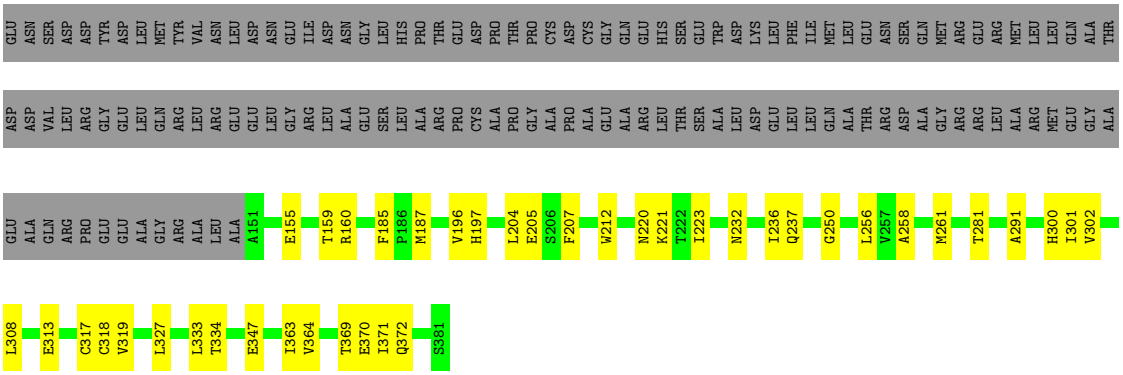
• Molecule 1: Pentraxin-related protein PTX3

Chain D:



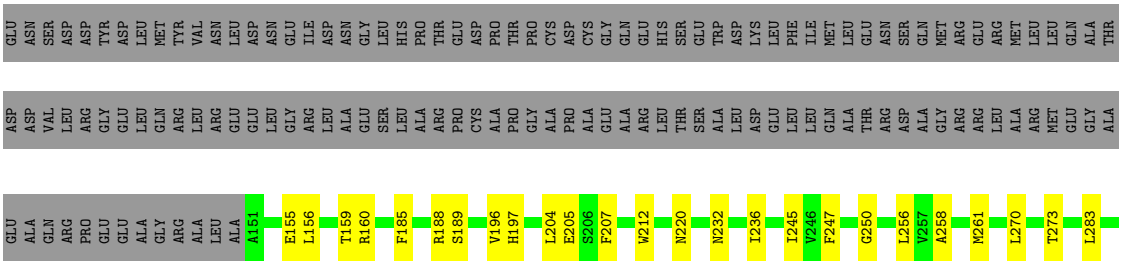
• Molecule 1: Pentraxin-related protein PTX3

Chain F:



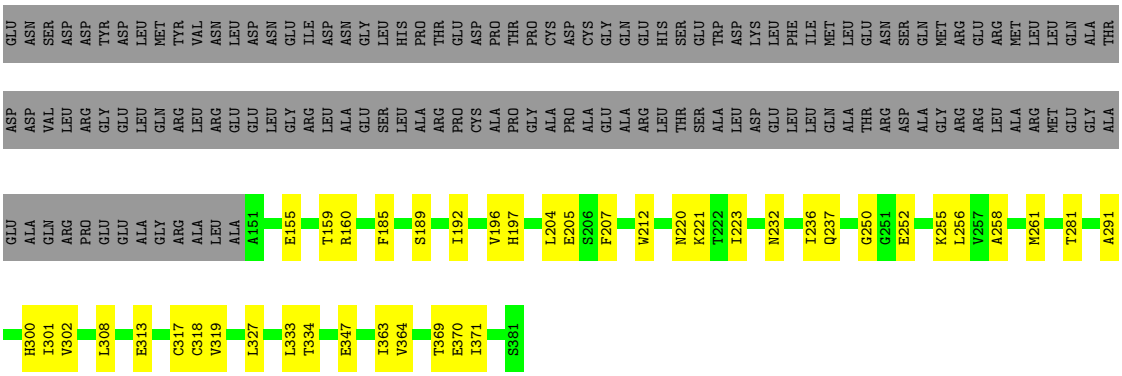
• Molecule 1: Pentraxin-related protein PTX3

Chain G:



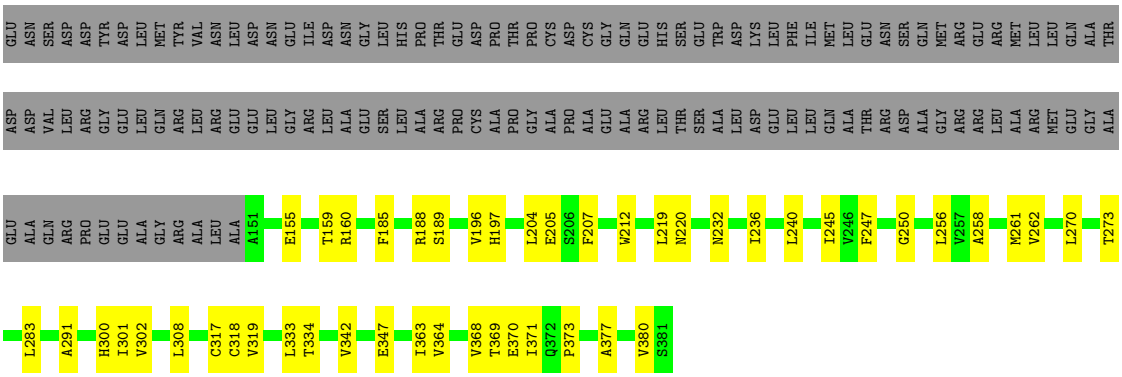
• Molecule 1: Pentraxin-related protein PTX3

Chain J:



• Molecule 1: Pentraxin-related protein PTX3

Chain K:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D4	Depositor
Number of particles used	23457	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/1836	0.51	0/2490
1	B	0.26	0/1836	0.51	0/2490
1	C	0.26	0/1836	0.51	0/2490
1	D	0.26	0/1836	0.51	0/2490
1	F	0.26	0/1836	0.51	0/2490
1	G	0.26	0/1836	0.51	0/2490
1	J	0.26	0/1836	0.51	0/2490
1	K	0.26	0/1836	0.51	0/2490
All	All	0.26	0/14688	0.51	0/19920

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	1789	1752	1752	41	0
1	B	1789	1752	1752	34	0
1	C	1789	1752	1752	37	0
1	D	1789	1752	1752	44	0
1	F	1789	1752	1752	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1789	1752	1752	42	0
1	J	1789	1752	1752	39	0
1	K	1789	1752	1752	42	0
2	A	14	8	13	1	0
2	B	14	8	13	1	0
2	C	14	8	13	1	0
2	D	14	8	13	1	0
2	F	14	8	13	1	0
2	G	14	8	13	1	0
2	J	14	8	13	1	0
2	K	14	8	13	1	0
3	A	27	0	0	0	0
3	B	28	0	0	0	0
3	C	28	0	0	0	0
3	D	24	0	0	0	0
3	F	28	0	0	0	0
3	G	25	0	0	0	0
3	J	28	0	0	0	0
3	K	26	0	0	0	0
All	All	14638	14080	14120	280	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 10.

All (280) 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:370:GLU:OE1	1:D:189:SER:OG	1.88	0.90
1:G:370:GLU:OE1	1:K:189:SER:OG	1.91	0.89
1:B:370:GLU:OE1	1:J:189:SER:OG	1.90	0.88
1:D:370:GLU:OE1	1:G:189:SER:OG	1.90	0.87
1:A:189:SER:OG	1:K:370:GLU:OE1	1.91	0.87
1:A:159:THR:HG22	1:K:160:ARG:HD3	1.72	0.71
1:F:159:THR:HG22	1:J:160:ARG:HD3	1.72	0.71
1:D:160:ARG:HD3	1:G:159:THR:HG22	1.73	0.70
1:D:364:VAL:HG13	1:D:369:THR:HG21	1.73	0.70
1:G:364:VAL:HG13	1:G:369:THR:HG21	1.73	0.70
1:A:364:VAL:HG13	1:A:369:THR:HG21	1.73	0.70
1:G:247:PHE:HB2	1:G:283:LEU:HD21	1.74	0.70
1:C:159:THR:HG22	1:F:160:ARG:HD3	1.72	0.69
1:G:160:ARG:HD3	1:K:159:THR:HG22	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:GLU:OE2	1:B:372:GLN:NE2	2.23	0.69
1:D:247:PHE:HB2	1:D:283:LEU:HD21	1.75	0.69
1:A:247:PHE:HB2	1:A:283:LEU:HD21	1.74	0.69
1:K:247:PHE:HB2	1:K:283:LEU:HD21	1.75	0.69
1:D:155:GLU:O	1:D:159:THR:HG23	1.93	0.69
1:A:160:ARG:HD3	1:D:159:THR:HG22	1.75	0.69
1:G:155:GLU:O	1:G:159:THR:HG23	1.93	0.68
1:K:256:LEU:HD21	1:K:291:ALA:HB3	1.75	0.68
1:A:256:LEU:HD21	1:A:291:ALA:HB3	1.76	0.68
1:K:364:VAL:HG13	1:K:369:THR:HG21	1.74	0.68
1:B:160:ARG:HD3	1:J:159:THR:HG22	1.76	0.68
1:J:155:GLU:O	1:J:159:THR:HG23	1.95	0.67
1:D:256:LEU:HD21	1:D:291:ALA:HB3	1.75	0.67
1:B:205:GLU:HG3	1:B:301:ILE:HD12	1.78	0.66
1:F:205:GLU:HG3	1:F:301:ILE:HD12	1.77	0.66
1:G:256:LEU:HD21	1:G:291:ALA:HB3	1.75	0.66
1:J:205:GLU:HG3	1:J:301:ILE:HD12	1.77	0.66
1:G:205:GLU:HG3	1:G:301:ILE:HD12	1.78	0.66
1:C:205:GLU:HG3	1:C:301:ILE:HD12	1.77	0.66
1:F:155:GLU:O	1:F:159:THR:HG23	1.96	0.65
1:D:205:GLU:HG3	1:D:301:ILE:HD12	1.79	0.65
1:C:155:GLU:O	1:C:159:THR:HG23	1.96	0.65
1:K:205:GLU:HG3	1:K:301:ILE:HD12	1.79	0.65
1:A:155:GLU:O	1:A:159:THR:HG23	1.97	0.64
1:A:205:GLU:HG3	1:A:301:ILE:HD12	1.79	0.64
1:K:155:GLU:O	1:K:159:THR:HG23	1.97	0.63
1:B:155:GLU:O	1:B:159:THR:HG23	1.98	0.63
1:B:159:THR:HG22	1:C:160:ARG:HD3	1.80	0.63
1:B:364:VAL:HG13	1:B:369:THR:HG21	1.81	0.63
1:C:204:LEU:HD13	1:C:207:PHE:HB3	1.81	0.63
1:D:156:LEU:HD11	1:G:159:THR:HG21	1.81	0.62
1:J:364:VAL:HG13	1:J:369:THR:HG21	1.79	0.62
1:B:204:LEU:HD13	1:B:207:PHE:HB3	1.82	0.62
1:J:204:LEU:HD13	1:J:207:PHE:HB3	1.81	0.62
1:C:364:VAL:HG13	1:C:369:THR:HG21	1.82	0.62
1:F:364:VAL:HG13	1:F:369:THR:HG21	1.82	0.62
1:F:204:LEU:HD13	1:F:207:PHE:HB3	1.81	0.61
1:G:380:VAL:HG23	1:G:380:VAL:O	2.02	0.60
1:F:300:HIS:O	1:F:301:ILE:HD13	2.02	0.60
1:G:319:VAL:O	1:G:319:VAL:HG22	2.02	0.60
1:D:380:VAL:HG23	1:D:380:VAL:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LEU:HD21	1:A:291:ALA:CB	2.32	0.60
1:K:380:VAL:HG23	1:K:380:VAL:O	2.01	0.60
1:J:300:HIS:O	1:J:301:ILE:HD13	2.02	0.59
1:C:212:TRP:HB2	1:C:334:THR:HG23	1.84	0.59
1:D:204:LEU:HD13	1:D:207:PHE:HB3	1.85	0.59
1:K:300:HIS:O	1:K:301:ILE:HD13	2.03	0.59
1:G:204:LEU:HD13	1:G:207:PHE:HB3	1.85	0.59
1:A:204:LEU:HD13	1:A:207:PHE:HB3	1.84	0.59
1:C:300:HIS:O	1:C:301:ILE:HD13	2.03	0.59
1:D:319:VAL:O	1:D:319:VAL:HG22	2.02	0.59
1:J:212:TRP:HB2	1:J:334:THR:HG23	1.85	0.59
1:B:300:HIS:O	1:B:301:ILE:HD13	2.02	0.59
1:D:256:LEU:HD21	1:D:291:ALA:CB	2.32	0.59
1:G:256:LEU:HD21	1:G:291:ALA:CB	2.33	0.59
1:K:256:LEU:HD21	1:K:291:ALA:CB	2.32	0.59
1:A:300:HIS:O	1:A:301:ILE:HD13	2.03	0.59
1:G:300:HIS:O	1:G:301:ILE:HD13	2.03	0.59
1:K:319:VAL:HG22	1:K:319:VAL:O	2.02	0.59
1:A:319:VAL:HG22	1:A:319:VAL:O	2.03	0.59
1:G:156:LEU:HD11	1:K:159:THR:HG21	1.85	0.59
1:B:212:TRP:HB2	1:B:334:THR:HG23	1.85	0.58
1:F:212:TRP:HB2	1:F:334:THR:HG23	1.85	0.58
1:D:300:HIS:O	1:D:301:ILE:HD13	2.03	0.58
1:K:204:LEU:HD13	1:K:207:PHE:HB3	1.85	0.58
1:A:380:VAL:HG23	1:A:380:VAL:O	2.02	0.58
1:A:273:THR:HG21	1:A:342:VAL:HG13	1.86	0.58
1:J:319:VAL:HG22	1:J:319:VAL:O	2.04	0.58
1:D:273:THR:HG21	1:D:342:VAL:HG13	1.86	0.57
1:F:319:VAL:HG22	1:F:319:VAL:O	2.04	0.57
1:C:256:LEU:HD21	1:C:291:ALA:HB3	1.86	0.57
1:B:221:LYS:HG2	1:B:327:LEU:HD22	1.87	0.57
1:C:319:VAL:HG22	1:C:319:VAL:O	2.04	0.57
1:B:319:VAL:O	1:B:319:VAL:HG22	2.04	0.57
1:K:236:ILE:HD11	1:K:302:VAL:HG11	1.87	0.57
1:F:256:LEU:HD12	1:F:281:THR:HG23	1.87	0.56
1:C:256:LEU:HD12	1:C:281:THR:HG23	1.88	0.56
1:G:273:THR:HG21	1:G:342:VAL:HG13	1.86	0.56
1:K:273:THR:HG21	1:K:342:VAL:HG13	1.86	0.56
1:B:256:LEU:HD21	1:B:291:ALA:HB3	1.87	0.56
1:C:221:LYS:HG2	1:C:327:LEU:HD22	1.87	0.56
1:G:236:ILE:HD11	1:G:302:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:LEU:HD12	1:B:281:THR:HG23	1.88	0.56
1:J:256:LEU:HD12	1:J:281:THR:HG23	1.87	0.55
1:D:236:ILE:HD11	1:D:302:VAL:HG11	1.87	0.55
1:J:256:LEU:HD21	1:J:291:ALA:HB3	1.87	0.55
1:A:236:ILE:HD11	1:A:302:VAL:HG11	1.87	0.55
1:G:212:TRP:HB2	1:G:334:THR:HG23	1.89	0.54
1:B:318:CYS:SG	1:A:317:CYS:N	2.80	0.54
1:F:318:CYS:SG	1:G:317:CYS:N	2.81	0.54
1:C:318:CYS:SG	1:D:317:CYS:N	2.80	0.54
1:K:369:THR:HG23	1:K:371:ILE:HG13	1.90	0.54
1:B:236:ILE:HD11	1:B:302:VAL:HG11	1.91	0.53
1:K:212:TRP:HB2	1:K:334:THR:HG23	1.90	0.53
1:D:212:TRP:HB2	1:D:334:THR:HG23	1.90	0.53
1:J:221:LYS:HG2	1:J:327:LEU:HD22	1.90	0.53
1:A:212:TRP:HB2	1:A:334:THR:HG23	1.90	0.53
1:F:221:LYS:HG2	1:F:327:LEU:HD22	1.91	0.53
1:A:156:LEU:HD12	1:A:159:THR:OG1	2.09	0.53
1:B:223:ILE:HD12	1:B:237:GLN:HE21	1.74	0.53
1:G:369:THR:HG23	1:G:371:ILE:HG13	1.91	0.53
1:J:318:CYS:SG	1:K:317:CYS:N	2.82	0.53
1:J:236:ILE:HD11	1:J:302:VAL:HG11	1.90	0.52
1:C:236:ILE:HD11	1:C:302:VAL:HG11	1.91	0.52
1:B:197:HIS:CD2	1:A:319:VAL:HG23	2.44	0.52
1:D:369:THR:HG23	1:D:371:ILE:HG13	1.91	0.52
1:C:197:HIS:ND1	1:C:370:GLU:OE1	2.42	0.52
1:J:197:HIS:ND1	1:J:370:GLU:OE1	2.42	0.52
1:K:196:VAL:HB	1:K:308:LEU:HD22	1.92	0.52
1:F:204:LEU:O	1:F:204:LEU:HD12	2.10	0.52
1:J:223:ILE:HD12	1:J:237:GLN:HE21	1.74	0.52
1:F:236:ILE:HD11	1:F:302:VAL:HG11	1.90	0.52
1:F:256:LEU:HD21	1:F:291:ALA:HB3	1.91	0.52
1:K:204:LEU:HD12	1:K:204:LEU:O	2.09	0.52
1:J:204:LEU:HD12	1:J:204:LEU:O	2.10	0.52
1:A:204:LEU:O	1:A:204:LEU:HD12	2.09	0.52
1:G:204:LEU:HD12	1:G:204:LEU:O	2.10	0.52
1:C:204:LEU:HD12	1:C:204:LEU:O	2.09	0.52
1:F:223:ILE:HD12	1:F:237:GLN:HE21	1.74	0.52
1:B:196:VAL:HB	1:B:308:LEU:HD22	1.92	0.51
1:C:223:ILE:HD12	1:C:237:GLN:HE21	1.74	0.51
1:J:197:HIS:CD2	1:K:319:VAL:HG23	2.45	0.51
1:D:204:LEU:HD12	1:D:204:LEU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:VAL:HB	1:A:308:LEU:HD22	1.93	0.51
1:D:185:PHE:CE1	1:D:333:LEU:HD12	2.46	0.51
1:F:197:HIS:ND1	1:F:370:GLU:OE1	2.44	0.51
1:C:197:HIS:CD2	1:D:319:VAL:HG23	2.46	0.50
1:D:196:VAL:HB	1:D:308:LEU:HD22	1.93	0.50
1:F:197:HIS:CD2	1:G:319:VAL:HG23	2.46	0.50
1:G:185:PHE:CE1	1:G:333:LEU:HD12	2.46	0.50
1:G:196:VAL:HB	1:G:308:LEU:HD22	1.92	0.50
1:A:185:PHE:CE1	1:A:333:LEU:HD12	2.46	0.50
1:B:204:LEU:HD12	1:B:204:LEU:O	2.11	0.50
1:B:185:PHE:CE1	1:B:333:LEU:HD12	2.47	0.50
1:C:196:VAL:HB	1:C:308:LEU:HD22	1.94	0.50
1:C:258:ALA:HB1	1:C:261:MET:HE1	1.94	0.49
1:F:196:VAL:HB	1:F:308:LEU:HD22	1.94	0.49
1:K:347:GLU:N	1:K:347:GLU:OE1	2.45	0.49
1:A:347:GLU:OE1	1:A:347:GLU:N	2.45	0.49
1:J:185:PHE:CE1	1:J:333:LEU:HD12	2.48	0.49
1:A:156:LEU:HD11	1:D:159:THR:HG21	1.94	0.49
1:D:347:GLU:N	1:D:347:GLU:OE1	2.45	0.49
1:G:347:GLU:N	1:G:347:GLU:OE1	2.45	0.49
1:C:317:CYS:N	1:D:318:CYS:SG	2.86	0.49
1:J:196:VAL:HB	1:J:308:LEU:HD22	1.94	0.49
1:J:258:ALA:HB1	1:J:261:MET:HE1	1.94	0.49
1:K:185:PHE:CE1	1:K:333:LEU:HD12	2.48	0.49
1:F:185:PHE:CE1	1:F:333:LEU:HD12	2.48	0.48
1:C:185:PHE:CE1	1:C:333:LEU:HD12	2.48	0.48
1:A:369:THR:HG23	1:A:371:ILE:HG13	1.95	0.48
1:F:258:ALA:HB1	1:F:261:MET:HE1	1.93	0.48
1:A:245:ILE:HD13	1:A:270:LEU:HD22	1.96	0.48
1:B:317:CYS:N	1:A:318:CYS:SG	2.87	0.48
1:F:317:CYS:N	1:G:318:CYS:SG	2.86	0.48
1:B:258:ALA:HB1	1:B:261:MET:HE1	1.96	0.48
1:G:363:ILE:HG22	1:G:364:VAL:HG23	1.96	0.48
1:K:245:ILE:HD13	1:K:270:LEU:HD22	1.95	0.48
1:J:252:GLU:HA	1:J:252:GLU:OE1	2.14	0.48
1:D:245:ILE:HD13	1:D:270:LEU:HD22	1.96	0.48
1:J:317:CYS:N	1:K:318:CYS:SG	2.86	0.47
1:K:232:ASN:ND2	1:K:250:GLY:O	2.47	0.47
1:A:363:ILE:HG22	1:A:364:VAL:HG23	1.96	0.47
1:F:347:GLU:OE1	1:F:347:GLU:N	2.47	0.47
1:B:369:THR:HG23	1:B:371:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:ILE:HG22	1:D:364:VAL:HG23	1.96	0.47
1:J:347:GLU:N	1:J:347:GLU:OE1	2.47	0.47
1:K:363:ILE:HG22	1:K:364:VAL:HG23	1.96	0.47
1:B:347:GLU:N	1:B:347:GLU:OE1	2.47	0.47
1:A:220:ASN:OD1	2:A:401:NAG:H2	2.15	0.47
1:C:347:GLU:OE1	1:C:347:GLU:N	2.48	0.47
1:C:220:ASN:OD1	2:C:401:NAG:H2	2.15	0.46
1:G:207:PHE:CZ	1:G:236:ILE:HD12	2.50	0.46
1:F:237:GLN:NE2	1:F:313:GLU:OE2	2.43	0.46
1:K:373:PRO:HB3	1:K:377:ALA:HB3	1.97	0.46
1:B:220:ASN:OD1	2:B:401:NAG:H2	2.15	0.46
1:D:207:PHE:CZ	1:D:236:ILE:HD12	2.50	0.46
1:J:237:GLN:NE2	1:J:313:GLU:OE2	2.43	0.46
1:D:220:ASN:OD1	2:D:401:NAG:H2	2.15	0.46
1:D:156:LEU:HD12	1:D:159:THR:OG1	2.16	0.46
1:A:207:PHE:CZ	1:A:236:ILE:HD12	2.50	0.46
1:J:232:ASN:ND2	1:J:250:GLY:O	2.43	0.46
1:J:189:SER:HB2	1:J:192:ILE:HB	1.98	0.46
1:K:220:ASN:OD1	2:K:401:NAG:H2	2.16	0.46
1:F:258:ALA:HB1	1:F:261:MET:CE	2.46	0.46
1:A:205:GLU:CG	1:A:301:ILE:HD12	2.45	0.45
1:B:258:ALA:HB1	1:B:261:MET:CE	2.46	0.45
1:K:207:PHE:CZ	1:K:236:ILE:HD12	2.51	0.45
1:D:205:GLU:CG	1:D:301:ILE:HD12	2.46	0.45
1:J:258:ALA:HB1	1:J:261:MET:CE	2.46	0.45
1:C:369:THR:HG23	1:C:371:ILE:HG13	1.98	0.45
1:F:220:ASN:OD1	2:F:401:NAG:H2	2.16	0.45
1:D:232:ASN:ND2	1:D:250:GLY:O	2.46	0.45
1:C:258:ALA:HB1	1:C:261:MET:CE	2.46	0.45
1:G:220:ASN:OD1	2:G:401:NAG:H2	2.16	0.44
1:K:205:GLU:CG	1:K:301:ILE:HD12	2.46	0.44
1:J:220:ASN:OD1	2:J:401:NAG:H2	2.17	0.44
1:B:232:ASN:ND2	1:B:250:GLY:O	2.46	0.44
1:C:232:ASN:ND2	1:C:250:GLY:O	2.47	0.44
1:F:232:ASN:ND2	1:F:250:GLY:O	2.47	0.44
1:G:232:ASN:ND2	1:G:250:GLY:O	2.46	0.44
1:B:205:GLU:CG	1:B:301:ILE:HD12	2.48	0.43
1:G:245:ILE:HD13	1:G:270:LEU:HD22	1.99	0.43
1:C:237:GLN:NE2	1:C:313:GLU:OE2	2.44	0.43
1:F:369:THR:HG23	1:F:371:ILE:HG13	2.00	0.43
1:J:363:ILE:HG22	1:J:364:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:PHE:CZ	1:B:236:ILE:HD12	2.54	0.43
1:D:216:THR:OG1	1:D:330:SER:O	2.29	0.43
1:A:232:ASN:ND2	1:A:250:GLY:O	2.46	0.43
1:G:205:GLU:CG	1:G:301:ILE:HD12	2.45	0.43
1:D:185:PHE:HE1	1:D:333:LEU:HD12	1.84	0.42
1:J:319:VAL:HG23	1:K:197:HIS:CD2	2.54	0.42
1:F:363:ILE:HG22	1:F:364:VAL:HG23	2.02	0.42
1:D:302:VAL:HG23	1:D:302:VAL:O	2.19	0.42
1:J:369:THR:HG23	1:J:371:ILE:HG13	2.00	0.42
1:F:207:PHE:CZ	1:F:236:ILE:HD12	2.53	0.42
1:J:364:VAL:CG1	1:J:369:THR:HG21	2.49	0.42
1:K:258:ALA:HB1	1:K:261:MET:CE	2.49	0.42
1:A:258:ALA:HB1	1:A:261:MET:CE	2.50	0.42
1:A:302:VAL:O	1:A:302:VAL:HG23	2.19	0.42
1:G:302:VAL:HG23	1:G:302:VAL:O	2.19	0.42
1:F:205:GLU:CG	1:F:301:ILE:HD12	2.49	0.42
1:A:185:PHE:HE1	1:A:333:LEU:HD12	1.85	0.42
1:C:302:VAL:HG23	1:C:302:VAL:O	2.20	0.42
1:C:319:VAL:HG23	1:D:197:HIS:CD2	2.55	0.42
1:D:258:ALA:HB1	1:D:261:MET:CE	2.50	0.42
1:F:302:VAL:HG23	1:F:302:VAL:O	2.20	0.41
1:J:302:VAL:HG23	1:J:302:VAL:O	2.20	0.41
1:K:302:VAL:O	1:K:302:VAL:HG23	2.19	0.41
1:C:363:ILE:HG22	1:C:364:VAL:HG23	2.02	0.41
1:G:185:PHE:HE1	1:G:333:LEU:HD12	1.85	0.41
1:C:189:SER:HB2	1:C:192:ILE:HB	2.03	0.41
1:G:258:ALA:HB1	1:G:261:MET:CE	2.50	0.41
1:J:207:PHE:CZ	1:J:236:ILE:HD12	2.55	0.41
1:D:188:ARG:CZ	1:D:219:LEU:HD11	2.50	0.41
1:B:302:VAL:HG23	1:B:302:VAL:O	2.20	0.41
1:C:207:PHE:CZ	1:C:236:ILE:HD12	2.55	0.41
1:C:370:GLU:OE2	1:C:372:GLN:NE2	2.52	0.41
1:F:185:PHE:HE1	1:F:333:LEU:HD12	1.85	0.41
1:F:319:VAL:HG23	1:G:197:HIS:CD2	2.55	0.41
1:C:227:TYR:OH	1:C:303:PRO:O	2.29	0.41
1:K:188:ARG:CZ	1:K:219:LEU:HD11	2.51	0.41
1:A:261:MET:SD	1:A:261:MET:N	2.94	0.41
1:B:363:ILE:HG22	1:B:364:VAL:HG23	2.02	0.41
1:A:188:ARG:NH1	1:K:368:VAL:HG13	2.35	0.41
1:C:208:SER:CB	1:C:273:THR:HG22	2.51	0.41
1:D:261:MET:SD	1:D:261:MET:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:VAL:HG13	1:G:188:ARG:NH1	2.36	0.41
1:G:256:LEU:C	1:G:256:LEU:HD23	2.41	0.41
1:G:373:PRO:HB3	1:G:377:ALA:HB3	2.03	0.41
1:K:256:LEU:HD23	1:K:256:LEU:C	2.41	0.41
1:F:187:MET:HG3	1:J:370:GLU:HA	2.03	0.41
1:J:185:PHE:HE1	1:J:333:LEU:HD12	1.86	0.41
1:B:189:SER:HB2	1:B:192:ILE:HB	2.03	0.40
1:A:256:LEU:C	1:A:256:LEU:HD23	2.41	0.40
1:D:256:LEU:C	1:D:256:LEU:HD23	2.41	0.40
1:D:373:PRO:HB3	1:D:377:ALA:HB3	2.03	0.40
1:G:261:MET:SD	1:G:261:MET:N	2.94	0.40
1:G:368:VAL:HG13	1:K:188:ARG:NH1	2.36	0.40
1:A:188:ARG:CZ	1:A:219:LEU:HD11	2.52	0.40
1:C:261:MET:SD	1:C:261:MET:N	2.95	0.40
1:K:240:LEU:HD21	1:K:262:VAL:HG21	2.03	0.40
1:B:261:MET:SD	1:B:261:MET:N	2.95	0.40
1:A:240:LEU:HD21	1:A:262:VAL:HG21	2.03	0.40
1:F:370:GLU:OE2	1:F:372:GLN:NE2	2.55	0.40
1:J:261:MET:N	1:J:261:MET:SD	2.95	0.40
1:K:261:MET:N	1:K:261:MET:SD	2.94	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 PDB entries followed by that with respect to all EM entries.

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	231/364 (64%)	211 (91%)	20 (9%)	0	100	100
1	B	231/364 (64%)	212 (92%)	19 (8%)	0	100	100
1	C	231/364 (64%)	211 (91%)	20 (9%)	0	100	100
1	D	231/364 (64%)	211 (91%)	20 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	231/364 (64%)	210 (91%)	21 (9%)	0	100	100
1	G	231/364 (64%)	210 (91%)	21 (9%)	0	100	100
1	J	231/364 (64%)	211 (91%)	20 (9%)	0	100	100
1	K	231/364 (64%)	211 (91%)	20 (9%)	0	100	100
All	All	1848/2912 (64%)	1687 (91%)	161 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	188/296 (64%)	188 (100%)	0	100	100
1	B	188/296 (64%)	187 (100%)	1 (0%)	86	91
1	C	188/296 (64%)	188 (100%)	0	100	100
1	D	188/296 (64%)	188 (100%)	0	100	100
1	F	188/296 (64%)	188 (100%)	0	100	100
1	G	188/296 (64%)	188 (100%)	0	100	100
1	J	188/296 (64%)	187 (100%)	1 (0%)	86	91
1	K	188/296 (64%)	188 (100%)	0	100	100
All	All	1504/2368 (64%)	1502 (100%)	2 (0%)	92	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	187	MET
1	J	255	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	HIS
1	A	372	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	J	401	1	14,14,15	0.30	0	17,19,21	0.46	0
2	NAG	C	401	1	14,14,15	0.29	0	17,19,21	0.46	0
2	NAG	A	401	1	14,14,15	0.29	0	17,19,21	0.46	0
2	NAG	D	401	1	14,14,15	0.30	0	17,19,21	0.46	0
2	NAG	K	401	1	14,14,15	0.29	0	17,19,21	0.46	0
2	NAG	B	401	1	14,14,15	0.29	0	17,19,21	0.46	0
2	NAG	G	401	1	14,14,15	0.30	0	17,19,21	0.46	0
2	NAG	F	401	1	14,14,15	0.29	0	17,19,21	0.46	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	J	401	1	-	3/6/23/26	0/1/1/1
2	NAG	C	401	1	-	3/6/23/26	0/1/1/1
2	NAG	A	401	1	-	2/6/23/26	0/1/1/1
2	NAG	D	401	1	-	2/6/23/26	0/1/1/1
2	NAG	K	401	1	-	2/6/23/26	0/1/1/1
2	NAG	B	401	1	-	3/6/23/26	0/1/1/1
2	NAG	G	401	1	-	3/6/23/26	0/1/1/1
2	NAG	F	401	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	NAG	C8-C7-N2-C2
2	B	401	NAG	O7-C7-N2-C2
2	A	401	NAG	C8-C7-N2-C2
2	A	401	NAG	O7-C7-N2-C2
2	C	401	NAG	C8-C7-N2-C2
2	C	401	NAG	O7-C7-N2-C2
2	D	401	NAG	C8-C7-N2-C2
2	D	401	NAG	O7-C7-N2-C2
2	F	401	NAG	C8-C7-N2-C2
2	F	401	NAG	O7-C7-N2-C2
2	G	401	NAG	C8-C7-N2-C2
2	G	401	NAG	O7-C7-N2-C2
2	J	401	NAG	C8-C7-N2-C2
2	J	401	NAG	O7-C7-N2-C2
2	K	401	NAG	C8-C7-N2-C2
2	K	401	NAG	O7-C7-N2-C2
2	J	401	NAG	O5-C5-C6-O6
2	B	401	NAG	O5-C5-C6-O6
2	F	401	NAG	O5-C5-C6-O6
2	C	401	NAG	O5-C5-C6-O6
2	G	401	NAG	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	401	NAG	1	0
2	C	401	NAG	1	0
2	A	401	NAG	1	0
2	D	401	NAG	1	0
2	K	401	NAG	1	0
2	B	401	NAG	1	0
2	G	401	NAG	1	0
2	F	401	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.