Full wwPDB EM Validation Report

Mar 3, 2025 – 03:04 pm GMT

PDB ID	:	8S7I
EMDB ID	:	EMD-19773
Title	:	Fructose 6-phosphate aldolase, L107C/A129G/R134V/L163C/S166G mutant
Authors	:	Hebert, H.; Widersten, M.
Deposited on	:	2024-03-01
Resolution	:	3.20 Å(reported)
Based on initial model	:	3wnq

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:

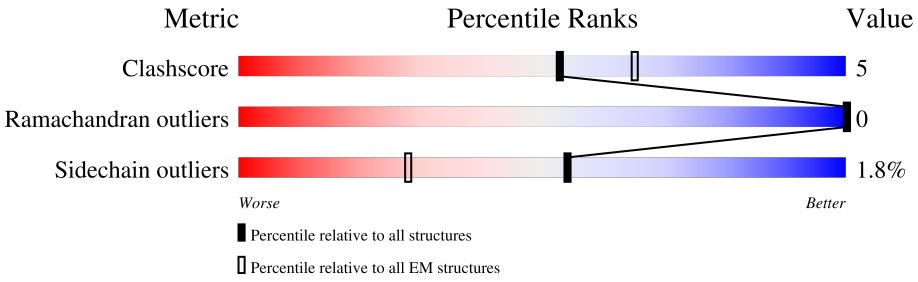
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	227	81% 14% • •
1	B	227	85% 11% • •
1	C	227	87% 8% • •
1	D	227	87% 8% • •
1	E	227	83% 12% • •
1	F	227	85% 11% • •
1	G	227	84% 12% • •
1	H	227	85% 11% • •
1	I	227	84% 11% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	227	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 32982 atoms, of which 16610 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 Fructose-6-phosphate aldolase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	220	Total	C	H	N	O	S	0	0
			3271	1028	1661	269	302	11		
1	B	220	Total	C	H	N	O	S	0	0
			3271	1028	1661	269	302	11		
1	C	220	Total	C	H	N	O	S	0	0
			3271	1028	1661	269	302	11		
1	D	220	Total	C	H	N	O	S	0	0
			3271	1028	1661	269	302	11		
1	E	220	Total	C	H	N	O	S	0	0
			3271	1028	1661	269	302	11		
1	F	220	Total	C	H	N	O	S	0	0
			3271	1028	1661	269	302	11		
1	G	220	Total	C	H	N	O	S	0	0
			3271	1028	1661	269	302	11		
1	H	220	Total	C	H	N	O	S	0	0
			3271	1028	1661	269	302	11		
1	I	220	Total	C	H	N	O	S	0	0
			3271	1028	1661	269	302	11		
1	J	220	Total	C	H	N	O	S	0	0
			3271	1028	1661	269	302	11		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	CYS	LEU	engineered mutation	UNP P78055
A	129	GLY	ALA	engineered mutation	UNP P78055
A	134	VAL	ARG	engineered mutation	UNP P78055
A	163	CYS	LEU	engineered mutation	UNP P78055
A	166	GLY	SER	engineered mutation	UNP P78055
A	221	THR	-	expression tag	UNP P78055
A	222	SER	-	expression tag	UNP P78055
A	223	HIS	-	expression tag	UNP P78055
A	224	HIS	-	expression tag	UNP P78055
A	225	HIS	-	expression tag	UNP P78055

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	226	HIS	-	expression tag	UNP P78055
A	227	HIS	-	expression tag	UNP P78055
B	107	CYS	LEU	engineered mutation	UNP P78055
B	129	GLY	ALA	engineered mutation	UNP P78055
B	134	VAL	ARG	engineered mutation	UNP P78055
B	163	CYS	LEU	engineered mutation	UNP P78055
B	166	GLY	SER	engineered mutation	UNP P78055
B	221	THR	-	expression tag	UNP P78055
B	222	SER	-	expression tag	UNP P78055
B	223	HIS	-	expression tag	UNP P78055
B	224	HIS	-	expression tag	UNP P78055
B	225	HIS	-	expression tag	UNP P78055
B	226	HIS	-	expression tag	UNP P78055
B	227	HIS	-	expression tag	UNP P78055
C	107	CYS	LEU	engineered mutation	UNP P78055
C	129	GLY	ALA	engineered mutation	UNP P78055
C	134	VAL	ARG	engineered mutation	UNP P78055
C	163	CYS	LEU	engineered mutation	UNP P78055
C	166	GLY	SER	engineered mutation	UNP P78055
C	221	THR	-	expression tag	UNP P78055
C	222	SER	-	expression tag	UNP P78055
C	223	HIS	-	expression tag	UNP P78055
C	224	HIS	-	expression tag	UNP P78055
C	225	HIS	-	expression tag	UNP P78055
C	226	HIS	-	expression tag	UNP P78055
C	227	HIS	-	expression tag	UNP P78055
D	107	CYS	LEU	engineered mutation	UNP P78055
D	129	GLY	ALA	engineered mutation	UNP P78055
D	134	VAL	ARG	engineered mutation	UNP P78055
D	163	CYS	LEU	engineered mutation	UNP P78055
D	166	GLY	SER	engineered mutation	UNP P78055
D	221	THR	-	expression tag	UNP P78055
D	222	SER	-	expression tag	UNP P78055
D	223	HIS	-	expression tag	UNP P78055
D	224	HIS	-	expression tag	UNP P78055
D	225	HIS	-	expression tag	UNP P78055
D	226	HIS	-	expression tag	UNP P78055
D	227	HIS	-	expression tag	UNP P78055
E	107	CYS	LEU	engineered mutation	UNP P78055
E	129	GLY	ALA	engineered mutation	UNP P78055
E	134	VAL	ARG	engineered mutation	UNP P78055
E	163	CYS	LEU	engineered mutation	UNP P78055

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	166	GLY	SER	engineered mutation	UNP P78055
E	221	THR	-	expression tag	UNP P78055
E	222	SER	-	expression tag	UNP P78055
E	223	HIS	-	expression tag	UNP P78055
E	224	HIS	-	expression tag	UNP P78055
E	225	HIS	-	expression tag	UNP P78055
E	226	HIS	-	expression tag	UNP P78055
E	227	HIS	-	expression tag	UNP P78055
F	107	CYS	LEU	engineered mutation	UNP P78055
F	129	GLY	ALA	engineered mutation	UNP P78055
F	134	VAL	ARG	engineered mutation	UNP P78055
F	163	CYS	LEU	engineered mutation	UNP P78055
F	166	GLY	SER	engineered mutation	UNP P78055
F	221	THR	-	expression tag	UNP P78055
F	222	SER	-	expression tag	UNP P78055
F	223	HIS	-	expression tag	UNP P78055
F	224	HIS	-	expression tag	UNP P78055
F	225	HIS	-	expression tag	UNP P78055
F	226	HIS	-	expression tag	UNP P78055
F	227	HIS	-	expression tag	UNP P78055
G	107	CYS	LEU	engineered mutation	UNP P78055
G	129	GLY	ALA	engineered mutation	UNP P78055
G	134	VAL	ARG	engineered mutation	UNP P78055
G	163	CYS	LEU	engineered mutation	UNP P78055
G	166	GLY	SER	engineered mutation	UNP P78055
G	221	THR	-	expression tag	UNP P78055
G	222	SER	-	expression tag	UNP P78055
G	223	HIS	-	expression tag	UNP P78055
G	224	HIS	-	expression tag	UNP P78055
G	225	HIS	-	expression tag	UNP P78055
G	226	HIS	-	expression tag	UNP P78055
G	227	HIS	-	expression tag	UNP P78055
H	107	CYS	LEU	engineered mutation	UNP P78055
H	129	GLY	ALA	engineered mutation	UNP P78055
H	134	VAL	ARG	engineered mutation	UNP P78055
H	163	CYS	LEU	engineered mutation	UNP P78055
H	166	GLY	SER	engineered mutation	UNP P78055
H	221	THR	-	expression tag	UNP P78055
H	222	SER	-	expression tag	UNP P78055
H	223	HIS	-	expression tag	UNP P78055
H	224	HIS	-	expression tag	UNP P78055
H	225	HIS	-	expression tag	UNP P78055

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	226	HIS	-	expression tag	UNP P78055
H	227	HIS	-	expression tag	UNP P78055
I	107	CYS	LEU	engineered mutation	UNP P78055
I	129	GLY	ALA	engineered mutation	UNP P78055
I	134	VAL	ARG	engineered mutation	UNP P78055
I	163	CYS	LEU	engineered mutation	UNP P78055
I	166	GLY	SER	engineered mutation	UNP P78055
I	221	THR	-	expression tag	UNP P78055
I	222	SER	-	expression tag	UNP P78055
I	223	HIS	-	expression tag	UNP P78055
I	224	HIS	-	expression tag	UNP P78055
I	225	HIS	-	expression tag	UNP P78055
I	226	HIS	-	expression tag	UNP P78055
I	227	HIS	-	expression tag	UNP P78055
J	107	CYS	LEU	engineered mutation	UNP P78055
J	129	GLY	ALA	engineered mutation	UNP P78055
J	134	VAL	ARG	engineered mutation	UNP P78055
J	163	CYS	LEU	engineered mutation	UNP P78055
J	166	GLY	SER	engineered mutation	UNP P78055
J	221	THR	-	expression tag	UNP P78055
J	222	SER	-	expression tag	UNP P78055
J	223	HIS	-	expression tag	UNP P78055
J	224	HIS	-	expression tag	UNP P78055
J	225	HIS	-	expression tag	UNP P78055
J	226	HIS	-	expression tag	UNP P78055
J	227	HIS	-	expression tag	UNP P78055

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	AltConf
2	A	35	Total O 35 35	0
2	B	26	Total O 26 26	0
2	C	17	Total O 17 17	0
2	D	28	Total O 28 28	0
2	E	26	Total O 26 26	0
2	F	28	Total O 28 28	0

Continued on next page...

Continued from previous page...

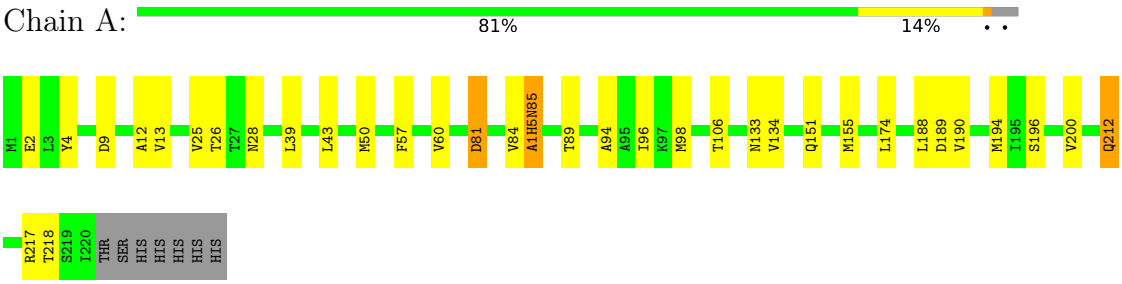
Mol	Chain	Residues	Atoms	AltConf
2	G	33	Total O 33 33	0
2	H	26	Total O 26 26	0
2	I	30	Total O 30 30	0
2	J	23	Total O 23 23	0

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.

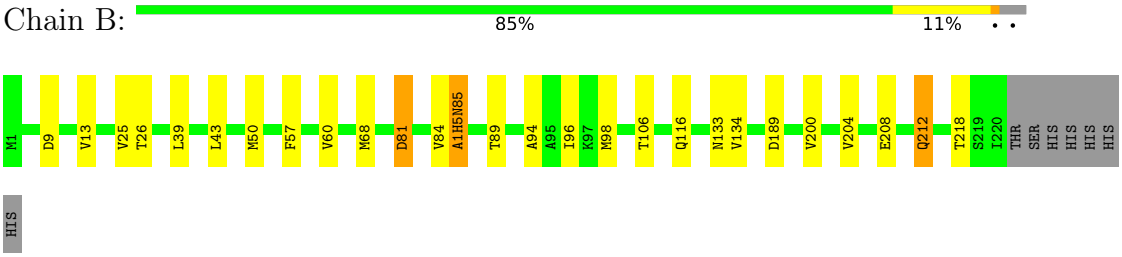
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain A:



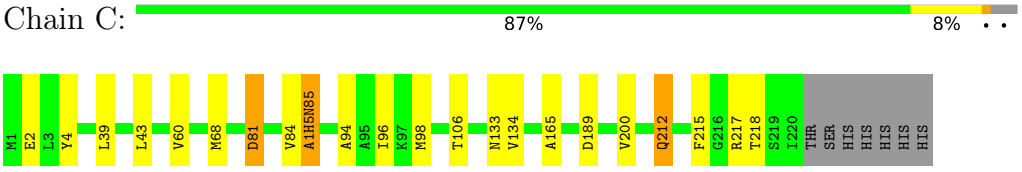
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain B:



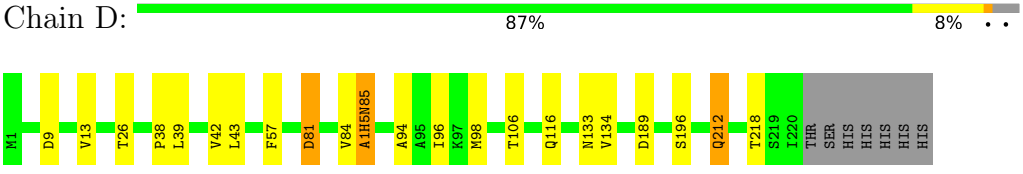
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain C:



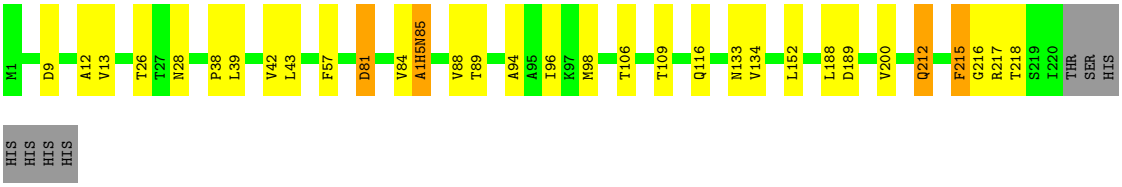
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain D:



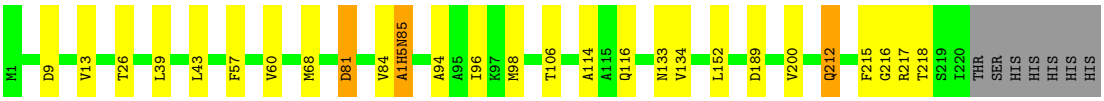
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain E:



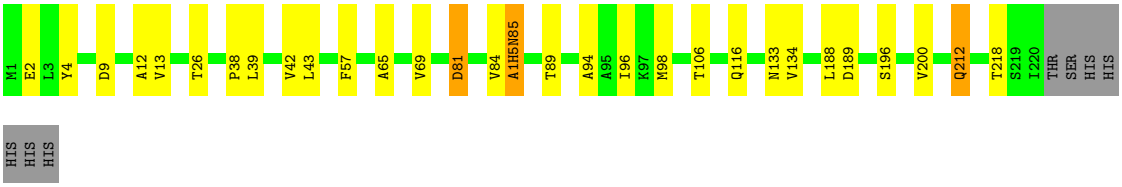
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain F:



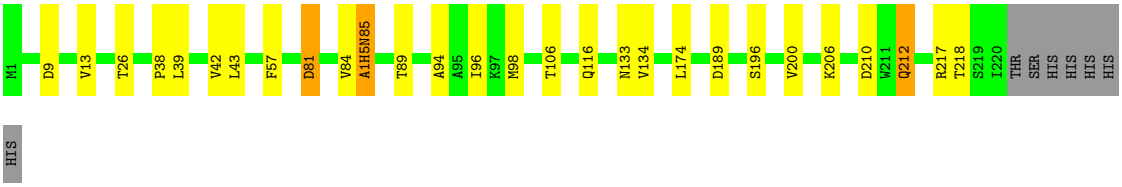
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain G:



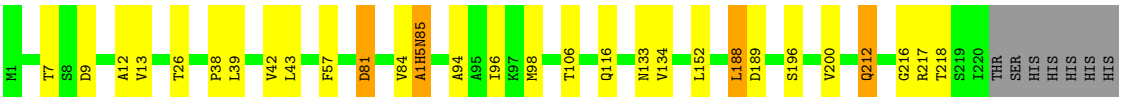
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain H:



• Molecule 1: Fructose-6-phosphate aldolase 1

Chain I:



• Molecule 1: Fructose-6-phosphate aldolase 1

Chain J:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D5	Depositor
Number of particles used	115055	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.04	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k 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: A1H5N

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	0/1616	0.46	0/2198
1	B	0.26	0/1616	0.46	0/2198
1	C	0.26	0/1616	0.46	0/2198
1	D	0.26	0/1616	0.46	0/2198
1	E	0.26	0/1616	0.46	0/2198
1	F	0.26	0/1616	0.47	0/2198
1	G	0.26	0/1616	0.46	0/2198
1	H	0.26	0/1616	0.46	0/2198
1	I	0.26	0/1616	0.46	0/2198
1	J	0.26	0/1616	0.46	0/2198
All	All	0.26	0/16160	0.46	0/21980

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	1610	1661	1643	23	0
1	B	1610	1661	1643	17	0
1	C	1610	1661	1643	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1610	1661	1643	15	0
1	E	1610	1661	1643	22	0
1	F	1610	1661	1643	19	0
1	G	1610	1661	1643	20	0
1	H	1610	1661	1643	17	0
1	I	1610	1661	1643	21	0
1	J	1610	1661	1643	14	0
2	A	35	0	0	1	0
2	B	26	0	0	0	0
2	C	17	0	0	0	0
2	D	28	0	0	0	0
2	E	26	0	0	0	0
2	F	28	0	0	0	0
2	G	33	0	0	0	0
2	H	26	0	0	0	0
2	I	30	0	0	0	0
2	J	23	0	0	0	0
All	All	16372	16610	16430	166	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 5.

All (166) 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:H:206:LYS:NZ	1:H:210:ASP:OD1	2.30	0.63
1:A:39:LEU:HD12	1:A:43:LEU:HD11	1.81	0.62
1:J:60:VAL:HG21	1:J:68:MET:HG2	1.83	0.61
1:E:39:LEU:HD12	1:E:43:LEU:HD11	1.83	0.60
1:I:7:THR:HG21	1:I:188:LEU:HD21	1.83	0.60
1:C:60:VAL:HG21	1:C:68:MET:HG2	1.84	0.60
1:E:38:PRO:O	1:E:42:VAL:HG23	2.02	0.59
1:G:38:PRO:O	1:G:42:VAL:HG23	2.02	0.59
1:G:212:GLN:OE1	1:G:218:THR:HG22	2.03	0.59
1:A:212:GLN:OE1	1:A:218:THR:HG22	2.02	0.59
1:C:212:GLN:OE1	1:C:218:THR:HG22	2.03	0.58
1:F:212:GLN:OE1	1:F:218:THR:HG22	2.02	0.58
1:G:39:LEU:HD12	1:G:43:LEU:HD11	1.86	0.58
1:G:2:GLU:OE1	1:G:4:TYR:OH	2.19	0.58
1:H:39:LEU:HD12	1:H:43:LEU:HD11	1.86	0.58
1:A:2:GLU:OE1	1:A:4:TYR:OH	2.21	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:ASN:OD1	1:G:134:VAL:N	2.37	0.58
1:F:60:VAL:HG21	1:F:68:MET:HG2	1.86	0.57
1:C:39:LEU:HD12	1:C:43:LEU:HD11	1.85	0.57
1:F:133:ASN:OD1	1:F:134:VAL:N	2.38	0.57
1:I:133:ASN:OD1	1:I:134:VAL:N	2.39	0.56
1:B:60:VAL:HG21	1:B:68:MET:HG2	1.88	0.55
1:A:133:ASN:OD1	1:A:134:VAL:N	2.39	0.55
1:A:151:GLN:O	1:A:155:MET:HG2	2.07	0.55
1:B:39:LEU:HD12	1:B:43:LEU:HD11	1.87	0.55
1:H:38:PRO:O	1:H:42:VAL:HG23	2.07	0.55
1:E:212:GLN:OE1	1:E:218:THR:HG22	2.06	0.55
1:D:38:PRO:O	1:D:42:VAL:HG23	2.06	0.54
1:J:39:LEU:HD12	1:J:43:LEU:HD11	1.90	0.54
1:B:133:ASN:OD1	1:B:134:VAL:HG23	2.08	0.54
1:E:133:ASN:OD1	1:E:134:VAL:HG23	2.07	0.54
1:E:133:ASN:OD1	1:E:134:VAL:N	2.40	0.54
1:D:26:THR:HG23	1:D:57:PHE:HB2	1.88	0.54
1:G:12:ALA:HB1	1:G:188:LEU:HD11	1.89	0.54
1:G:133:ASN:OD1	1:G:134:VAL:HG23	2.09	0.53
1:I:133:ASN:OD1	1:I:134:VAL:HG23	2.08	0.53
1:C:133:ASN:OD1	1:C:134:VAL:HG23	2.09	0.53
1:F:39:LEU:HD12	1:F:43:LEU:HD11	1.91	0.52
1:D:212:GLN:OE1	1:D:218:THR:HG22	2.10	0.52
1:C:84:VAL:HG12	1:C:85:A1H5N:N	2.25	0.52
1:I:38:PRO:O	1:I:42:VAL:HG23	2.09	0.52
1:C:85:A1H5N:CAD	1:C:165:ALA:HB2	2.40	0.51
1:D:39:LEU:HD12	1:D:43:LEU:HD11	1.92	0.51
1:H:212:GLN:OE1	1:H:218:THR:HG22	2.10	0.51
1:E:217:ARG:HH11	1:E:217:ARG:HG2	1.76	0.51
1:I:39:LEU:HD12	1:I:43:LEU:HD11	1.91	0.51
1:F:84:VAL:HG12	1:F:85:A1H5N:N	2.26	0.51
1:F:133:ASN:OD1	1:F:134:VAL:HG23	2.11	0.51
1:H:26:THR:HG23	1:H:57:PHE:HB2	1.93	0.51
1:B:9:ASP:O	1:B:13:VAL:HG23	2.12	0.50
1:E:9:ASP:O	1:E:13:VAL:HG23	2.11	0.50
1:G:84:VAL:HG12	1:G:85:A1H5N:N	2.27	0.50
1:A:9:ASP:O	1:A:13:VAL:HG23	2.11	0.50
1:B:26:THR:HG23	1:B:57:PHE:HB2	1.92	0.50
1:J:84:VAL:HG12	1:J:85:A1H5N:N	2.27	0.50
1:C:2:GLU:OE1	1:C:4:TYR:OH	2.22	0.50
1:E:26:THR:HG23	1:E:57:PHE:HB2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:ASP:O	1:F:13:VAL:HG23	2.12	0.50
1:B:116:GLN:HE22	1:C:200:VAL:HG21	1.77	0.50
1:F:217:ARG:HG2	1:F:218:THR:N	2.26	0.50
1:J:85:A1H5N:CAD	1:J:165:ALA:HB2	2.41	0.50
1:F:26:THR:HG23	1:F:57:PHE:HB2	1.94	0.49
1:H:84:VAL:HG12	1:H:85:A1H5N:N	2.27	0.49
1:C:94:ALA:O	1:C:98:MET:HG3	2.13	0.49
1:H:217:ARG:HG2	1:H:217:ARG:HH11	1.76	0.49
1:I:12:ALA:HB1	1:I:188:LEU:HD11	1.93	0.49
1:A:26:THR:HG23	1:A:57:PHE:HB2	1.93	0.49
1:D:133:ASN:OD1	1:D:134:VAL:N	2.46	0.49
1:B:133:ASN:OD1	1:B:134:VAL:N	2.45	0.49
1:I:9:ASP:O	1:I:13:VAL:HG23	2.13	0.49
1:I:212:GLN:O	1:I:216:GLY:N	2.44	0.49
1:G:200:VAL:HG21	1:H:116:GLN:HE22	1.77	0.48
1:D:9:ASP:O	1:D:13:VAL:HG23	2.13	0.48
1:D:133:ASN:OD1	1:D:134:VAL:HG23	2.14	0.48
1:D:84:VAL:HG12	1:D:85:A1H5N:N	2.29	0.48
1:J:94:ALA:O	1:J:98:MET:HG3	2.14	0.48
1:J:212:GLN:O	1:J:216:GLY:N	2.45	0.48
1:A:133:ASN:OD1	1:A:134:VAL:HG23	2.12	0.48
1:I:200:VAL:HG21	1:J:116:GLN:HE22	1.79	0.48
1:H:94:ALA:O	1:H:98:MET:HG3	2.14	0.48
1:E:94:ALA:O	1:E:98:MET:HG3	2.14	0.48
1:G:26:THR:HG23	1:G:57:PHE:HB2	1.95	0.47
1:F:81:ASP:C	1:F:81:ASP:OD2	2.53	0.47
1:D:94:ALA:O	1:D:98:MET:HG3	2.14	0.47
1:A:81:ASP:OD2	1:A:81:ASP:C	2.53	0.47
1:A:217:ARG:NH2	2:A:302:HOH:O	2.47	0.47
1:G:81:ASP:C	1:G:81:ASP:OD2	2.53	0.47
1:B:81:ASP:C	1:B:81:ASP:OD2	2.53	0.47
1:B:212:GLN:OE1	1:B:218:THR:HG22	2.15	0.47
1:C:96:ILE:HG12	1:C:106:THR:HG21	1.96	0.47
1:F:94:ALA:O	1:F:98:MET:HG3	2.15	0.47
1:H:9:ASP:O	1:H:13:VAL:HG23	2.14	0.47
1:I:81:ASP:OD2	1:I:81:ASP:C	2.53	0.47
1:J:81:ASP:C	1:J:81:ASP:OD2	2.53	0.47
1:D:81:ASP:OD2	1:D:81:ASP:C	2.53	0.47
1:H:174:LEU:CD1	1:I:152:LEU:HD11	2.45	0.47
1:E:12:ALA:HB1	1:E:188:LEU:HD11	1.97	0.46
1:I:212:GLN:OE1	1:I:218:THR:HG22	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:VAL:HG12	1:B:85:A1H5N:N	2.31	0.46
1:I:94:ALA:O	1:I:98:MET:HG3	2.15	0.46
1:B:25:VAL:HG23	1:B:50:MET:SD	2.56	0.46
1:B:94:ALA:O	1:B:98:MET:HG3	2.16	0.46
1:C:81:ASP:C	1:C:81:ASP:OD2	2.53	0.46
1:E:81:ASP:OD2	1:E:81:ASP:C	2.53	0.46
1:F:200:VAL:HG21	1:G:116:GLN:HE22	1.81	0.45
1:G:9:ASP:O	1:G:13:VAL:HG23	2.17	0.45
1:H:81:ASP:OD2	1:H:81:ASP:C	2.54	0.45
1:I:84:VAL:HG12	1:I:85:A1H5N:N	2.32	0.45
1:A:84:VAL:HG12	1:A:85:A1H5N:N	2.32	0.45
1:A:94:ALA:O	1:A:98:MET:HG3	2.16	0.45
1:C:133:ASN:OD1	1:C:134:VAL:N	2.50	0.45
1:I:26:THR:HG23	1:I:57:PHE:HB2	1.98	0.45
1:A:174:LEU:CD1	1:E:152:LEU:HD11	2.48	0.44
1:G:94:ALA:O	1:G:98:MET:HG3	2.16	0.44
1:J:217:ARG:HG2	1:J:218:THR:N	2.32	0.44
1:E:84:VAL:HG12	1:E:85:A1H5N:N	2.32	0.44
1:C:217:ARG:HG2	1:C:217:ARG:HH11	1.83	0.43
1:D:96:ILE:HG12	1:D:106:THR:HG21	2.01	0.43
1:B:189:ASP:N	1:B:189:ASP:OD1	2.50	0.43
1:E:96:ILE:HG12	1:E:106:THR:HG21	2.00	0.43
1:J:189:ASP:OD1	1:J:189:ASP:N	2.52	0.43
1:A:189:ASP:N	1:A:189:ASP:OD1	2.50	0.43
1:F:96:ILE:HG12	1:F:106:THR:HG21	2.01	0.43
1:G:189:ASP:N	1:G:189:ASP:OD1	2.50	0.43
1:G:200:VAL:HG11	1:H:89:THR:HG23	2.00	0.43
1:I:96:ILE:HG12	1:I:106:THR:HG21	2.01	0.43
1:A:12:ALA:HB1	1:A:188:LEU:HD11	2.00	0.42
1:A:200:VAL:HG21	1:E:116:GLN:HE22	1.84	0.42
1:B:96:ILE:HG12	1:B:106:THR:HG21	2.01	0.42
1:D:212:GLN:CD	1:D:218:THR:HG22	2.40	0.42
1:H:189:ASP:N	1:H:189:ASP:OD1	2.52	0.42
1:E:189:ASP:N	1:E:189:ASP:OD1	2.52	0.42
1:C:189:ASP:OD1	1:C:189:ASP:N	2.52	0.42
1:F:116:GLN:HE22	1:J:200:VAL:HG21	1.84	0.42
1:G:96:ILE:HG12	1:G:106:THR:HG21	2.01	0.42
1:D:189:ASP:N	1:D:189:ASP:OD1	2.53	0.42
1:H:96:ILE:HG12	1:H:106:THR:HG21	2.00	0.42
1:A:96:ILE:HG12	1:A:106:THR:HG21	2.01	0.42
1:F:114:ALA:HB1	1:F:152:LEU:HD12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:ALA:O	1:G:69:VAL:HG23	2.20	0.42
1:A:25:VAL:HG23	1:A:50:MET:SD	2.60	0.42
1:H:133:ASN:OD1	1:H:134:VAL:N	2.53	0.42
1:E:88:VAL:HG23	1:E:109:THR:O	2.20	0.41
1:F:189:ASP:N	1:F:189:ASP:OD1	2.52	0.41
1:I:189:ASP:N	1:I:189:ASP:OD1	2.53	0.41
1:A:89:THR:HG23	1:B:200:VAL:HG11	2.02	0.41
1:B:89:THR:HG23	1:C:200:VAL:HG11	2.03	0.41
1:F:152:LEU:HD11	1:J:174:LEU:CD1	2.50	0.41
1:F:200:VAL:HG11	1:G:89:THR:HG23	2.03	0.41
1:F:212:GLN:O	1:F:216:GLY:N	2.53	0.41
1:G:212:GLN:CD	1:G:218:THR:HG22	2.41	0.41
1:J:96:ILE:HG12	1:J:106:THR:HG21	2.02	0.41
1:D:26:THR:HG23	1:D:57:PHE:CB	2.49	0.41
1:A:60:VAL:HG13	1:A:84:VAL:CG1	2.50	0.41
1:A:190:VAL:O	1:A:194:MET:HG3	2.21	0.41
1:E:28:ASN:ND2	1:E:85:A1H5N:OAB	2.54	0.41
1:I:217:ARG:HG2	1:I:218:THR:N	2.36	0.41
1:B:204:VAL:O	1:B:208:GLU:OE2	2.40	0.40
1:A:200:VAL:HG11	1:E:89:THR:HG23	2.02	0.40
1:D:116:GLN:HE22	1:E:200:VAL:HG21	1.85	0.40
1:E:215:PHE:CD2	1:E:215:PHE:N	2.89	0.40
1:E:212:GLN:O	1:E:216:GLY:N	2.53	0.40
1:H:200:VAL:HG21	1:I:116:GLN:HE22	1.86	0.40
1:I:200:VAL:HG11	1:J:89:THR:HG23	2.03	0.40
1:I:217:ARG:HE	1:I:217:ARG:HB3	1.73	0.40
1:A:28:ASN:ND2	1:A:85:A1H5N:OAB	2.55	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	217/227 (96%)	214 (99%)	3 (1%)	0	100	100
1	B	217/227 (96%)	213 (98%)	4 (2%)	0	100	100
1	C	217/227 (96%)	211 (97%)	6 (3%)	0	100	100
1	D	217/227 (96%)	213 (98%)	4 (2%)	0	100	100
1	E	217/227 (96%)	214 (99%)	3 (1%)	0	100	100
1	F	217/227 (96%)	214 (99%)	3 (1%)	0	100	100
1	G	217/227 (96%)	214 (99%)	3 (1%)	0	100	100
1	H	217/227 (96%)	214 (99%)	3 (1%)	0	100	100
1	I	217/227 (96%)	213 (98%)	4 (2%)	0	100	100
1	J	217/227 (96%)	214 (99%)	3 (1%)	0	100	100
All	All	2170/2270 (96%)	2134 (98%)	36 (2%)	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	165/172 (96%)	162 (98%)	3 (2%)	54	77
1	B	165/172 (96%)	163 (99%)	2 (1%)	67	85
1	C	165/172 (96%)	162 (98%)	3 (2%)	54	77
1	D	165/172 (96%)	162 (98%)	3 (2%)	54	77
1	E	165/172 (96%)	162 (98%)	3 (2%)	54	77
1	F	165/172 (96%)	162 (98%)	3 (2%)	54	77
1	G	165/172 (96%)	162 (98%)	3 (2%)	54	77
1	H	165/172 (96%)	162 (98%)	3 (2%)	54	77
1	I	165/172 (96%)	161 (98%)	4 (2%)	44	71
1	J	165/172 (96%)	162 (98%)	3 (2%)	54	77
All	All	1650/1720 (96%)	1620 (98%)	30 (2%)	54	77

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ASP
1	A	196	SER
1	A	212	GLN
1	B	81	ASP
1	B	212	GLN
1	C	81	ASP
1	C	212	GLN
1	C	215	PHE
1	D	81	ASP
1	D	196	SER
1	D	212	GLN
1	E	81	ASP
1	E	212	GLN
1	E	215	PHE
1	F	81	ASP
1	F	212	GLN
1	F	215	PHE
1	G	81	ASP
1	G	196	SER
1	G	212	GLN
1	H	81	ASP
1	H	196	SER
1	H	212	GLN
1	I	81	ASP
1	I	188	LEU
1	I	196	SER
1	I	212	GLN
1	J	81	ASP
1	J	212	GLN
1	J	215	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	47	HIS
1	G	47	HIS
1	H	47	HIS
1	I	47	HIS
1	J	47	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	A1H5N	I	85	1	16,18,19	1.17	2 (12%)	14,21,23	1.73	3 (21%)
1	A1H5N	A	85	1	16,18,19	1.19	2 (12%)	14,21,23	1.67	2 (14%)
1	A1H5N	G	85	1	16,18,19	1.18	2 (12%)	14,21,23	1.70	2 (14%)
1	A1H5N	H	85	1	16,18,19	1.17	2 (12%)	14,21,23	1.70	2 (14%)
1	A1H5N	J	85	1	16,18,19	1.25	2 (12%)	14,21,23	1.54	2 (14%)
1	A1H5N	D	85	1	16,18,19	1.19	2 (12%)	14,21,23	1.68	3 (21%)
1	A1H5N	E	85	1	16,18,19	1.18	2 (12%)	14,21,23	1.67	2 (14%)
1	A1H5N	B	85	1	16,18,19	1.16	2 (12%)	14,21,23	1.72	3 (21%)
1	A1H5N	C	85	1	16,18,19	1.25	2 (12%)	14,21,23	1.53	2 (14%)
1	A1H5N	F	85	1	16,18,19	1.18	2 (12%)	14,21,23	1.74	3 (21%)

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
1	A1H5N	I	85	1	-	2/13/16/18	0/1/1/1
1	A1H5N	A	85	1	-	2/13/16/18	0/1/1/1
1	A1H5N	G	85	1	-	2/13/16/18	0/1/1/1
1	A1H5N	H	85	1	-	2/13/16/18	0/1/1/1
1	A1H5N	J	85	1	-	3/13/16/18	0/1/1/1
1	A1H5N	D	85	1	-	2/13/16/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A1H5N	E	85	1	-	2/13/16/18	0/1/1/1
1	A1H5N	B	85	1	-	2/13/16/18	0/1/1/1
1	A1H5N	C	85	1	-	3/13/16/18	0/1/1/1
1	A1H5N	F	85	1	-	2/13/16/18	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	85	A1H5N	CAJ-CAI	3.92	1.55	1.47
1	C	85	A1H5N	CAJ-CAI	3.90	1.55	1.47
1	D	85	A1H5N	CAJ-CAI	3.70	1.55	1.47
1	A	85	A1H5N	CAJ-CAI	3.68	1.55	1.47
1	E	85	A1H5N	CAJ-CAI	3.66	1.55	1.47
1	F	85	A1H5N	CAJ-CAI	3.64	1.55	1.47
1	G	85	A1H5N	CAJ-CAI	3.63	1.55	1.47
1	B	85	A1H5N	CAJ-CAI	3.60	1.55	1.47
1	H	85	A1H5N	CAJ-CAI	3.59	1.55	1.47
1	I	85	A1H5N	CAJ-CAI	3.58	1.55	1.47
1	F	85	A1H5N	CA-N	-2.23	1.41	1.48
1	C	85	A1H5N	CA-N	-2.18	1.41	1.48
1	J	85	A1H5N	CA-N	-2.18	1.41	1.48
1	A	85	A1H5N	CA-N	-2.15	1.41	1.48
1	G	85	A1H5N	CA-N	-2.14	1.41	1.48
1	E	85	A1H5N	CA-N	-2.14	1.41	1.48
1	I	85	A1H5N	CA-N	-2.13	1.41	1.48
1	B	85	A1H5N	CA-N	-2.12	1.41	1.48
1	H	85	A1H5N	CA-N	-2.12	1.41	1.48
1	D	85	A1H5N	CA-N	-2.10	1.41	1.48

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	85	A1H5N	CAG-CAJ-CAI	4.34	126.11	120.84
1	I	85	A1H5N	CAG-CAJ-CAI	4.31	126.08	120.84
1	B	85	A1H5N	CAG-CAJ-CAI	4.31	126.08	120.84
1	G	85	A1H5N	CAG-CAJ-CAI	4.31	126.08	120.84
1	H	85	A1H5N	CAG-CAJ-CAI	4.30	126.07	120.84
1	E	85	A1H5N	CAG-CAJ-CAI	4.24	126.00	120.84
1	A	85	A1H5N	CAG-CAJ-CAI	4.23	125.98	120.84
1	D	85	A1H5N	CAG-CAJ-CAI	4.07	125.78	120.84
1	F	85	A1H5N	CAF-CAJ-CAI	-3.70	116.33	120.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	85	A1H5N	CAF-CAJ-CAI	-3.67	116.37	120.84
1	I	85	A1H5N	CAF-CAJ-CAI	-3.66	116.39	120.84
1	J	85	A1H5N	CAG-CAJ-CAI	3.63	125.25	120.84
1	G	85	A1H5N	CAF-CAJ-CAI	-3.61	116.45	120.84
1	C	85	A1H5N	CAG-CAJ-CAI	3.58	125.19	120.84
1	H	85	A1H5N	CAF-CAJ-CAI	-3.56	116.50	120.84
1	E	85	A1H5N	CAF-CAJ-CAI	-3.54	116.53	120.84
1	A	85	A1H5N	CAF-CAJ-CAI	-3.50	116.58	120.84
1	D	85	A1H5N	CAF-CAJ-CAI	-3.47	116.61	120.84
1	J	85	A1H5N	CAF-CAJ-CAI	-2.50	117.80	120.84
1	C	85	A1H5N	CAF-CAJ-CAI	-2.37	117.96	120.84
1	D	85	A1H5N	CAH-CAI-CAJ	-2.21	116.16	119.46
1	I	85	A1H5N	CAH-CAI-CAJ	-2.18	116.20	119.46
1	F	85	A1H5N	CAH-CAI-CAJ	-2.09	116.33	119.46
1	B	85	A1H5N	CAH-CAI-CAJ	-2.07	116.37	119.46

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	85	A1H5N	CD-CE-NZ-CAI
1	B	85	A1H5N	CD-CE-NZ-CAI
1	C	85	A1H5N	CD-CE-NZ-CAI
1	D	85	A1H5N	CD-CE-NZ-CAI
1	E	85	A1H5N	CD-CE-NZ-CAI
1	F	85	A1H5N	CD-CE-NZ-CAI
1	G	85	A1H5N	CD-CE-NZ-CAI
1	H	85	A1H5N	CD-CE-NZ-CAI
1	I	85	A1H5N	CD-CE-NZ-CAI
1	J	85	A1H5N	CD-CE-NZ-CAI
1	A	85	A1H5N	CAJ-CAI-NZ-CE
1	B	85	A1H5N	CAJ-CAI-NZ-CE
1	C	85	A1H5N	CAJ-CAI-NZ-CE
1	D	85	A1H5N	CAJ-CAI-NZ-CE
1	E	85	A1H5N	CAJ-CAI-NZ-CE
1	F	85	A1H5N	CAJ-CAI-NZ-CE
1	G	85	A1H5N	CAJ-CAI-NZ-CE
1	H	85	A1H5N	CAJ-CAI-NZ-CE
1	I	85	A1H5N	CAJ-CAI-NZ-CE
1	J	85	A1H5N	CAJ-CAI-NZ-CE
1	C	85	A1H5N	OAB-CAH-CAI-CAJ
1	J	85	A1H5N	OAB-CAH-CAI-CAJ

There are no ring outliers.

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	85	A1H5N	1	0
1	A	85	A1H5N	2	0
1	G	85	A1H5N	1	0
1	H	85	A1H5N	1	0
1	J	85	A1H5N	2	0
1	D	85	A1H5N	1	0
1	E	85	A1H5N	2	0
1	B	85	A1H5N	1	0
1	C	85	A1H5N	2	0
1	F	85	A1H5N	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.