



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:49 PM GMT

PDB ID : 5E2Y  
Title : Crystal structure of H5 hemagglutinin Q226L mutant from the influenza virus  
A/duck/Egypt/10185SS/2010 (H5N1)  
Authors : Zhu, X.; Wilson, I.A.  
Deposited on : 2015-10-01  
Resolution : 2.60 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

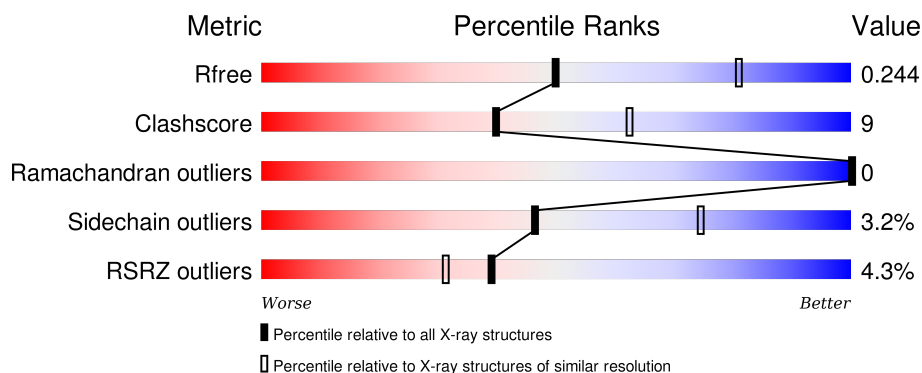
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	333	<div> <div>2%</div> <div>76%</div> <div>19%</div> <div>..</div> </div>
1	C	333	<div> <div>%</div> <div>77%</div> <div>18%</div> <div>..</div> </div>
1	E	333	<div> <div>%</div> <div>80%</div> <div>15%</div> <div>..</div> </div>
2	B	180	<div> <div>16%</div> <div>70%</div> <div>26%</div> <div>..</div> </div>
2	D	180	<div> <div>6%</div> <div>67%</div> <div>30%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	180	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	E	1002	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12273 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2558	1611	443	490	14			
1	C	323	Total	C	N	O	S	0	0	0
			2558	1611	443	490	14			
1	E	323	Total	C	N	O	S	0	0	0
			2558	1611	443	490	14			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP G8IPF0
A	8	ASP	-	expression tag	UNP G8IPF0
A	9	PRO	-	expression tag	UNP G8IPF0
A	10	GLY	-	expression tag	UNP G8IPF0
A	226	LEU	GLN	engineered mutation	UNP G8IPF0
C	7	ALA	-	expression tag	UNP G8IPF0
C	8	ASP	-	expression tag	UNP G8IPF0
C	9	PRO	-	expression tag	UNP G8IPF0
C	10	GLY	-	expression tag	UNP G8IPF0
C	226	LEU	GLN	engineered mutation	UNP G8IPF0
E	7	ALA	-	expression tag	UNP G8IPF0
E	8	ASP	-	expression tag	UNP G8IPF0
E	9	PRO	-	expression tag	UNP G8IPF0
E	10	GLY	-	expression tag	UNP G8IPF0
E	226	LEU	GLN	engineered mutation	UNP G8IPF0

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1418	880	248	282	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	175	Total	C	N	O	S	0	0	0
			1418	880	248	282	8			
2	F	175	Total	C	N	O	S	0	0	0
			1418	880	248	282	8			

There are 18 discrepancies between the modelled and reference sequences:

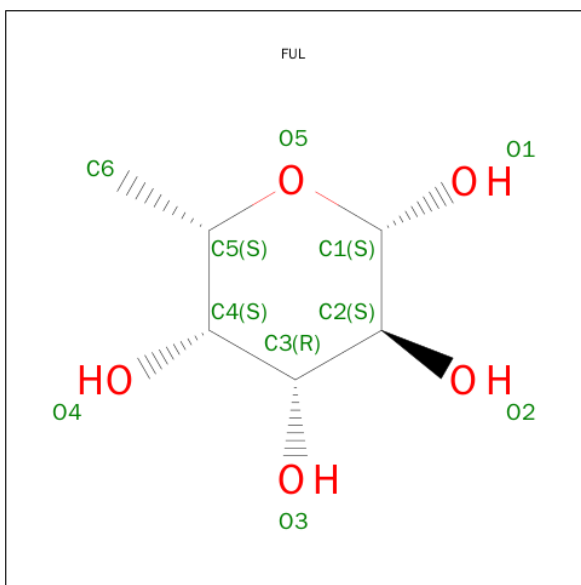
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP G8IPF0
B	176	ARG	-	expression tag	UNP G8IPF0
B	177	LEU	-	expression tag	UNP G8IPF0
B	178	VAL	-	expression tag	UNP G8IPF0
B	179	PRO	-	expression tag	UNP G8IPF0
B	180	ARG	-	expression tag	UNP G8IPF0
D	1	GLY	-	expression tag	UNP G8IPF0
D	176	ARG	-	expression tag	UNP G8IPF0
D	177	LEU	-	expression tag	UNP G8IPF0
D	178	VAL	-	expression tag	UNP G8IPF0
D	179	PRO	-	expression tag	UNP G8IPF0
D	180	ARG	-	expression tag	UNP G8IPF0
F	1	GLY	-	expression tag	UNP G8IPF0
F	176	ARG	-	expression tag	UNP G8IPF0
F	177	LEU	-	expression tag	UNP G8IPF0
F	178	VAL	-	expression tag	UNP G8IPF0
F	179	PRO	-	expression tag	UNP G8IPF0
F	180	ARG	-	expression tag	UNP G8IPF0

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



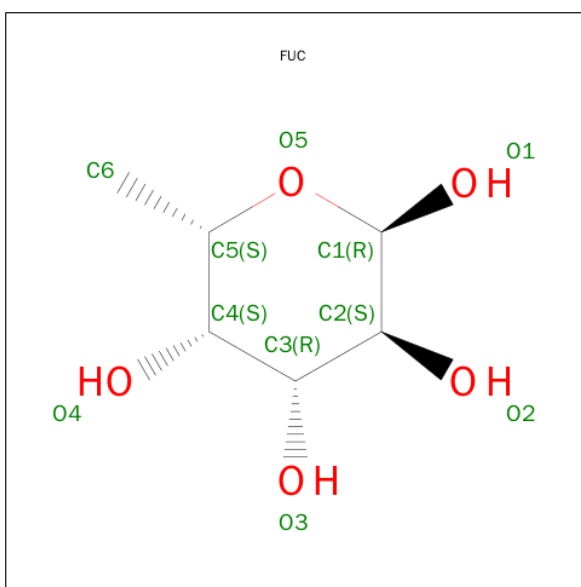
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1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

- Molecule 4 is BETA-L-FUCOSE (three-letter code: FUL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is water.

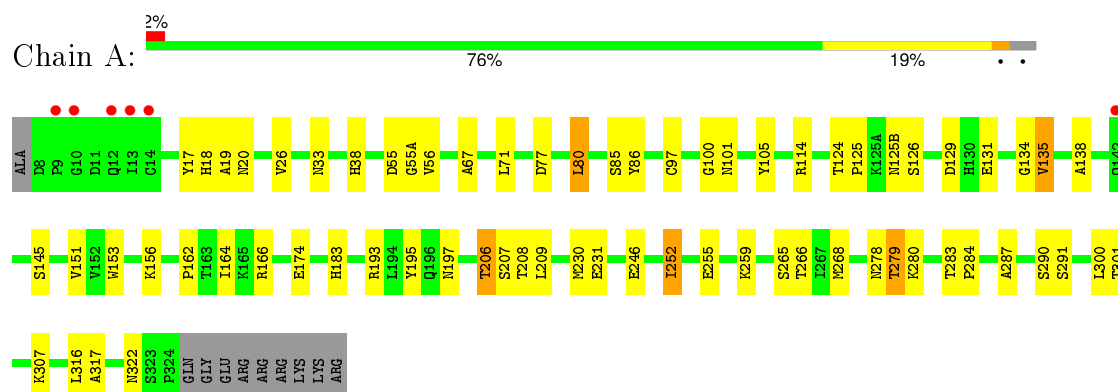
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total 47	O 47	0	0
6	B	5	Total 5	O 5	0	0
6	C	56	Total 56	O 56	0	0
6	D	9	Total 9	O 9	0	0
6	E	52	Total 52	O 52	0	0
6	F	10	Total 10	O 10	0	0



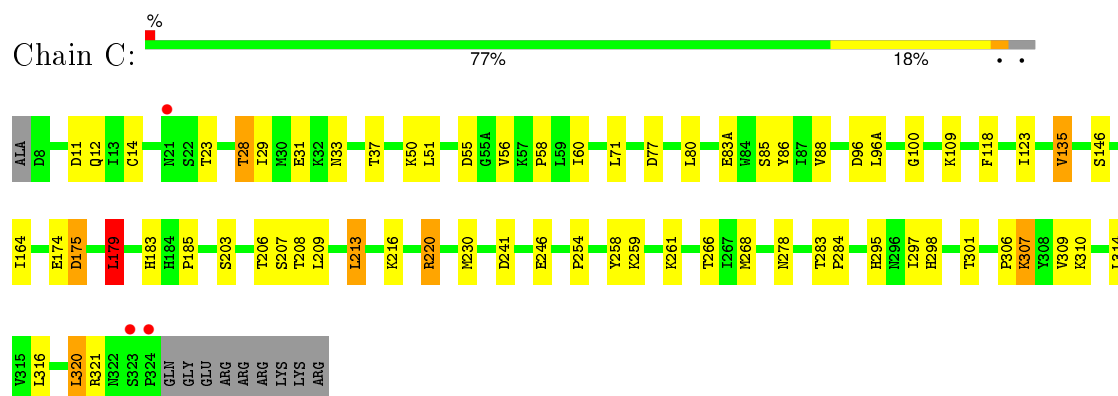
### 3 Residue-property plots [i](#)

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

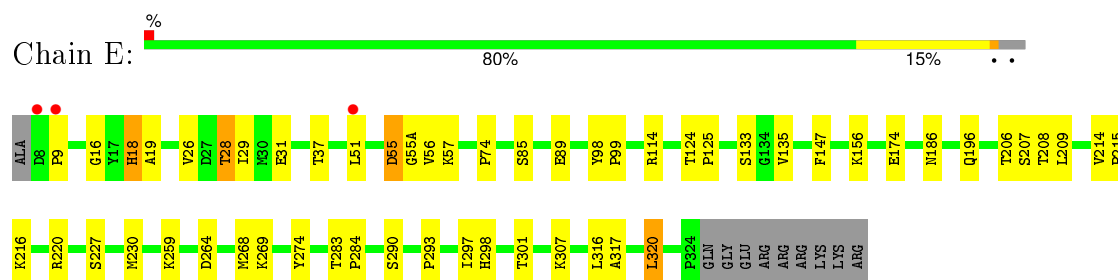
#### • Molecule 1: Hemagglutinin



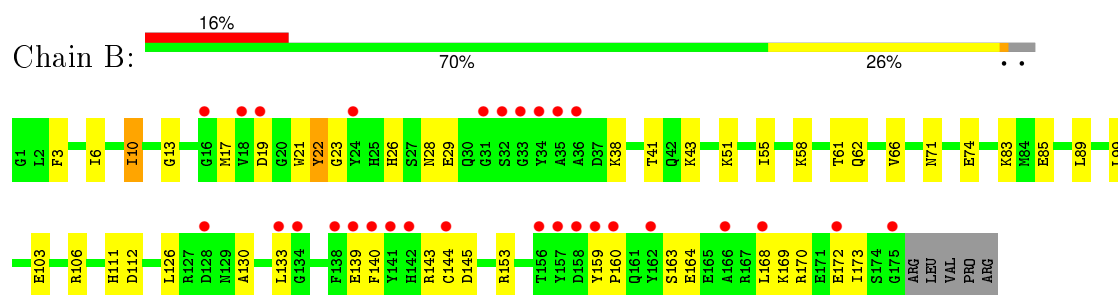
#### • Molecule 1: Hemagglutinin



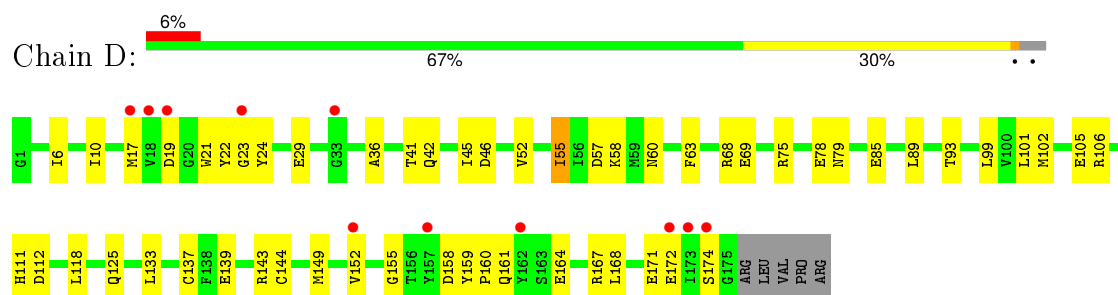
#### • Molecule 1: Hemagglutinin



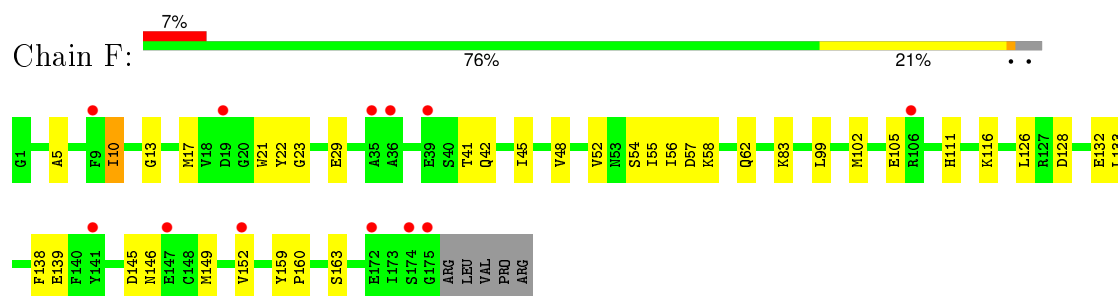
#### • Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.80Å 235.77Å 71.52Å 90.00° 114.37° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 49.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.9 (50.00-2.60) 86.9 (49.85-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.196 , 0.236 0.211 , 0.244	Depositor DCC
$R_{free}$ test set	2916 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.4	EDS
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 57121 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12273	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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 [i](#)

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

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

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	0.56	0/2619	0.66	1/3559 (0.0%)
1	C	0.54	0/2619	0.67	2/3559 (0.1%)
1	E	0.53	0/2619	0.65	0/3559
2	B	0.43	0/1445	0.57	0/1942
2	D	0.42	0/1445	0.55	0/1942
2	F	0.43	0/1445	0.55	0/1942
All	All	0.50	0/12192	0.63	3/16503 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	179	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	252	ILE	CG1-CB-CG2	-5.28	99.79	111.40
1	C	213	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2558	0	2493	45	0
1	C	2558	0	2493	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2558	0	2493	38	0
2	B	1418	0	1322	41	0
2	D	1418	0	1322	40	0
2	F	1418	0	1322	27	0
3	A	42	0	37	1	0
3	C	42	0	36	2	0
3	E	42	0	37	0	0
4	A	10	0	10	0	0
4	C	10	0	10	1	0
4	E	10	0	10	0	0
5	C	10	0	10	0	0
6	A	47	0	0	1	0
6	B	5	0	0	0	0
6	C	56	0	0	1	0
6	D	9	0	0	0	0
6	E	52	0	0	0	0
6	F	10	0	0	0	0
All	All	12273	0	11595	208	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 9.

All (208) 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:206:THR:HG22	1:A:208:THR:H	1.33	0.94
1:E:174:GLU:HG3	1:E:259:LYS:HB3	1.58	0.85
2:B:168:LEU:O	2:B:172:GLU:HG3	1.79	0.83
1:E:307:LYS:HE2	2:F:62:GLN:HB3	1.59	0.82
1:E:55:ASP:OD1	1:E:55(A):GLY:N	2.15	0.79
1:E:206:THR:HG22	1:E:208:THR:H	1.49	0.78
1:A:307:LYS:HE2	2:B:62:GLN:HB3	1.65	0.76
1:A:174:GLU:HG3	1:A:259:LYS:HB3	1.68	0.75
1:C:55:ASP:O	1:C:278:ASN:ND2	2.21	0.73
1:C:310:LYS:HE3	2:D:89:LEU:HD21	1.70	0.73
1:E:28:THR:HG22	1:E:31:GLU:H	1.55	0.72
2:B:169:LYS:HD2	2:B:172:GLU:OE1	1.89	0.71
1:C:206:THR:HG22	1:C:208:THR:H	1.54	0.71
1:C:310:LYS:HG3	2:D:89:LEU:HD11	1.71	0.71
2:D:75:ARG:NH1	2:D:78:GLU:OE1	2.23	0.71
2:B:133:LEU:HD11	2:B:139:GLU:HG2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:THR:HG22	1:A:301:THR:HG22	1.76	0.67
2:D:171:GLU:HA	2:D:174:SER:HB2	1.76	0.67
1:E:89:GLU:OE1	1:E:269:LYS:NZ	2.27	0.66
2:F:5:ALA:HB2	2:F:116:LYS:HB2	1.77	0.66
1:A:206:THR:HB	1:A:209:LEU:HB3	1.77	0.66
2:D:168:LEU:O	2:D:172:GLU:HG3	1.95	0.66
2:B:17:MET:HE3	2:B:23:GLY:HA3	1.77	0.66
1:C:206:THR:HB	1:C:209:LEU:HB3	1.78	0.65
1:C:11:ASP:OD2	2:D:144:CYS:N	2.24	0.65
2:B:169:LYS:CD	2:B:172:GLU:OE1	2.45	0.63
2:D:106:ARG:NH2	2:F:105:GLU:HG2	2.13	0.63
2:F:17:MET:HE1	2:F:23:GLY:HA3	1.79	0.63
1:C:295:HIS:CD2	1:C:306:PRO:HG2	2.34	0.62
1:E:293:PRO:HG3	2:F:56:ILE:HG12	1.80	0.62
1:A:77:ASP:HA	1:A:80:LEU:HD13	1.82	0.61
1:C:123:ILE:HD11	1:C:254:PRO:HB2	1.81	0.61
1:A:135:VAL:HG13	1:A:145:SER:HB3	1.84	0.60
2:B:106:ARG:NH2	2:D:105:GLU:HG2	2.17	0.60
1:C:175:ASP:OD1	1:C:175:ASP:N	2.34	0.60
2:F:133:LEU:HD11	2:F:139:GLU:HB2	1.84	0.59
1:C:283:THR:HG22	1:C:301:THR:HG22	1.85	0.59
1:C:28:THR:HG22	1:C:31:GLU:H	1.70	0.57
2:B:29:GLU:OE2	2:B:143:ARG:NH1	2.38	0.57
1:E:283:THR:HG22	1:E:301:THR:HG22	1.87	0.57
1:E:56:VAL:HB	1:E:85:SER:HB3	1.87	0.57
1:A:166:ARG:NH2	6:A:1102:HOH:O	2.28	0.57
2:B:170:ARG:O	2:B:173:ILE:HG13	2.05	0.56
2:B:26:HIS:HD2	2:B:153:ARG:NH2	2.04	0.56
1:E:206:THR:HB	1:E:209:LEU:HB3	1.86	0.56
2:D:55:ILE:HD11	2:D:99:LEU:HG	1.87	0.56
1:A:156:LYS:NZ	1:A:193:ARG:O	2.39	0.56
1:A:26:VAL:HG11	1:A:317:ALA:HB2	1.88	0.55
1:E:29:ILE:HD11	2:F:102:MET:HA	1.87	0.55
1:E:98:TYR:CD1	1:E:99:PRO:HD2	2.42	0.55
1:C:58:PRO:HG2	1:C:60:ILE:HD11	1.88	0.54
2:F:145:ASP:CG	2:F:146:ASN:H	2.11	0.54
1:A:268:MET:HE3	1:A:284:PRO:HA	1.90	0.54
1:E:283:THR:HG21	1:E:297:ILE:HD11	1.90	0.54
2:D:6:ILE:HD13	2:D:112:ASP:HA	1.88	0.54
1:A:100:GLY:HA3	1:A:230:MET:O	2.08	0.54
2:B:21:TRP:H	2:B:41:THR:HG21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:MET:HE1	2:D:23:GLY:HA3	1.89	0.53
2:D:159:TYR:HB3	2:D:160:PRO:HD3	1.90	0.52
2:D:63:PHE:HZ	2:D:85:GLU:HG2	1.75	0.52
1:C:297:ILE:HG13	1:C:298:HIS:N	2.25	0.52
2:B:130:ALA:HA	2:B:140:PHE:HA	1.91	0.52
1:C:316:LEU:HD23	2:D:52:VAL:HG22	1.92	0.52
1:A:279:THR:HG21	1:A:287:ALA:HB1	1.91	0.52
2:B:28:ASN:ND2	2:B:144:CYS:O	2.37	0.52
1:E:186:ASN:HD21	1:E:227:SER:C	2.13	0.52
1:C:109:LYS:NZ	2:D:69:GLU:OE2	2.36	0.52
2:D:57:ASP:O	2:D:60:ASN:ND2	2.42	0.52
1:A:284:PRO:HD3	1:A:300:LEU:O	2.10	0.52
2:B:26:HIS:HD2	2:B:153:ARG:HH22	1.57	0.51
2:D:19:ASP:HB3	2:D:36:ALA:HB2	1.91	0.51
1:E:320:LEU:HB3	2:F:111:HIS:CG	2.45	0.51
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.92	0.50
2:D:63:PHE:CZ	2:D:85:GLU:HG2	2.46	0.50
1:C:71:LEU:HD23	1:C:179:LEU:HD23	1.93	0.50
1:A:38:HIS:CD2	2:B:21:TRP:HE1	2.29	0.50
2:D:29:GLU:OE2	2:D:143:ARG:NH1	2.44	0.50
1:E:9:PRO:HA	2:F:139:GLU:OE2	2.11	0.49
2:F:160:PRO:HA	2:F:163:SER:HB2	1.94	0.49
1:A:164:ILE:O	1:A:246:GLU:HA	2.11	0.49
1:C:295:HIS:HD2	1:C:306:PRO:HG2	1.77	0.49
2:B:55:ILE:HG13	2:B:99:LEU:HD23	1.93	0.49
2:D:58:LYS:HD3	2:D:58:LYS:HA	1.61	0.49
1:E:316:LEU:HD13	2:F:52:VAL:HG22	1.95	0.49
1:A:56:VAL:HB	1:A:85:SER:HB3	1.95	0.49
1:E:268:MET:HE3	1:E:284:PRO:HA	1.95	0.49
1:C:174:GLU:HG3	1:C:259:LYS:HB3	1.95	0.48
2:D:164:GLU:OE1	2:D:167:ARG:NH2	2.42	0.48
1:A:124:THR:HG22	1:A:255:GLU:HA	1.95	0.48
1:E:297:ILE:HG13	1:E:298:HIS:N	2.28	0.48
1:E:18:HIS:ND1	1:E:19:ALA:N	2.61	0.48
2:D:42:GLN:NE2	2:D:46:ASP:OD1	2.47	0.48
1:A:151:VAL:HB	1:A:252:ILE:HG22	1.94	0.48
1:C:309:VAL:HG13	2:D:93:THR:HA	1.95	0.48
1:A:97:CYS:HB2	1:A:138:ALA:O	2.13	0.48
2:F:132:GLU:HG2	2:F:138:PHE:HE1	1.79	0.47
1:A:20:ASN:H	1:A:322:ASN:HD21	1.62	0.47
1:E:114:ARG:NH1	1:E:264:ASP:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:GLU:O	2:B:89:LEU:HG	2.15	0.47
2:F:55:ILE:HG23	2:F:99:LEU:HD23	1.96	0.47
1:A:195:TYR:O	1:A:197:ASN:N	2.46	0.47
1:C:310:LYS:HE3	2:D:89:LEU:CD2	2.44	0.47
1:E:19:ALA:HB2	2:F:13:GLY:HA3	1.97	0.47
2:D:21:TRP:CZ3	2:D:111:HIS:HE1	2.32	0.47
2:B:51:LYS:O	2:B:55:ILE:HG22	2.14	0.47
1:C:216:LYS:O	1:C:220:ARG:NH2	2.47	0.46
2:B:106:ARG:HH22	2:D:105:GLU:HG2	1.79	0.46
1:C:283:THR:HG21	1:C:297:ILE:HD11	1.97	0.46
2:B:140:PHE:CE2	2:B:144:CYS:HB2	2.50	0.46
1:C:58:PRO:HB3	1:C:86:TYR:CE1	2.50	0.46
1:A:125:PRO:HG2	1:A:126:SER:HB3	1.97	0.46
2:B:51:LYS:HD3	2:B:103:GLU:HB3	1.98	0.46
1:A:101:ASN:OD1	1:A:231:GLU:HG3	2.16	0.46
1:A:33:ASN:HD21	3:A:1001:NAG:C1	2.28	0.46
1:E:26:VAL:HG11	1:E:317:ALA:HB2	1.98	0.46
1:E:55:ASP:CG	1:E:55(A):GLY:H	2.11	0.46
1:C:56:VAL:HB	1:C:85:SER:HB3	1.97	0.45
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.99	0.45
1:E:156:LYS:HE3	1:E:196:GLN:OE1	2.17	0.45
2:F:42:GLN:OE1	2:F:45:ILE:HD11	2.17	0.45
2:B:19:ASP:OD2	2:B:38:LYS:NZ	2.44	0.45
2:F:128:ASP:OD1	2:F:159:TYR:OH	2.30	0.45
1:A:17:TYR:CZ	2:B:6:ILE:HG23	2.52	0.45
2:B:38:LYS:HA	2:B:41:THR:OG1	2.17	0.45
1:E:216:LYS:O	1:E:220:ARG:NH2	2.48	0.45
1:A:18:HIS:N	2:B:21:TRP:O	2.45	0.44
1:A:55:ASP:HB3	1:A:55(A):GLY:H	1.63	0.44
2:D:125:GLN:OE1	2:D:155:GLY:HA2	2.17	0.44
1:E:16:GLY:HA2	2:F:10:ILE:HD11	1.98	0.44
1:C:83(A):GLU:OE2	1:C:261:LYS:NZ	2.37	0.44
2:B:168:LEU:O	2:B:172:GLU:N	2.50	0.44
2:D:41:THR:O	2:D:45:ILE:HG12	2.18	0.44
2:F:54:SER:HA	2:F:57:ASP:OD2	2.17	0.44
1:A:67:ALA:HB2	1:A:105:TYR:CE1	2.53	0.44
1:A:114:ARG:HH22	2:D:79:ASN:ND2	2.14	0.44
2:B:22:TYR:OH	2:B:111:HIS:ND1	2.37	0.44
1:E:16:GLY:HA2	2:F:10:ILE:CD1	2.48	0.44
2:F:21:TRP:HB2	2:F:41:THR:HG22	2.00	0.44
2:D:118:LEU:HA	2:D:118:LEU:HD12	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:PRO:HG3	1:E:147:PHE:O	2.17	0.44
1:E:133:SER:O	1:E:135:VAL:HG13	2.18	0.43
2:B:160:PRO:HA	2:B:163:SER:HB3	2.00	0.43
2:B:159:TYR:HB3	2:B:160:PRO:HD3	2.00	0.43
2:D:17:MET:HE1	2:D:36:ALA:HA	2.00	0.43
1:C:29:ILE:HD11	2:D:102:MET:HA	2.00	0.43
1:C:164:ILE:O	1:C:246:GLU:HA	2.18	0.43
1:E:37:THR:HG23	1:E:320:LEU:O	2.18	0.43
1:C:51:LEU:HD13	1:C:88:VAL:HG21	1.99	0.43
1:A:279:THR:HG22	1:A:280:LYS:H	1.84	0.43
1:A:125:PRO:HB2	1:A:125(B):ASN:OD1	2.18	0.43
2:D:149:MET:O	2:D:152:VAL:HG12	2.19	0.43
2:D:29:GLU:N	2:D:29:GLU:OE1	2.51	0.43
2:B:10:ILE:O	2:B:10:ILE:HG12	2.17	0.43
1:E:114:ARG:HB3	1:E:114:ARG:HE	1.60	0.42
1:C:50:LYS:HE2	1:C:50:LYS:HB3	1.56	0.42
1:C:100:GLY:HA3	1:C:230:MET:O	2.18	0.42
1:A:20:ASN:OD1	1:A:322:ASN:ND2	2.53	0.42
1:C:37:THR:HG23	1:C:320:LEU:O	2.19	0.42
1:A:252:ILE:N	1:A:252:ILE:HD12	2.35	0.42
1:C:206:THR:HG21	6:C:1113:HOH:O	2.19	0.42
2:B:26:HIS:CD2	2:B:153:ARG:HH22	2.36	0.42
1:A:85:SER:HG	1:A:86:TYR:HD1	1.64	0.42
1:C:268:MET:HE3	1:C:284:PRO:HA	2.02	0.42
1:A:135:VAL:HG13	1:A:145:SER:CB	2.50	0.42
2:F:21:TRP:H	2:F:41:THR:HG21	1.84	0.42
2:F:29:GLU:N	2:F:29:GLU:OE1	2.51	0.42
1:C:96:ASP:CG	1:C:96(A):LEU:H	2.22	0.42
1:C:206:THR:HG23	1:C:241:ASP:OD2	2.20	0.42
2:D:158:ASP:OD1	2:D:160:PRO:HD2	2.19	0.42
1:A:290:SER:OG	1:A:291:SER:N	2.53	0.42
1:C:14:CYS:O	2:D:24:TYR:HA	2.19	0.42
1:C:183:HIS:O	1:C:185:PRO:HD3	2.19	0.42
1:C:307:LYS:HD2	1:C:307:LYS:N	2.34	0.42
1:A:206:THR:CG2	1:A:207:SER:N	2.82	0.41
2:B:83:LYS:HA	2:B:83:LYS:HD3	1.89	0.41
1:C:206:THR:CG2	1:C:207:SER:N	2.83	0.41
4:C:1004:FUL:H61	3:C:1005:NAG:H2	2.03	0.41
2:B:71:ASN:N	2:B:74:GLU:OE1	2.42	0.41
1:E:206:THR:CG2	1:E:207:SER:N	2.83	0.41
1:E:57:LYS:HE3	1:E:274:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:LYS:HD3	2:B:172:GLU:OE1	2.20	0.41
1:E:156:LYS:CD	1:E:196:GLN:HB2	2.51	0.41
1:E:98:TYR:CD1	1:E:230:MET:HG2	2.54	0.41
2:D:158:ASP:HB3	2:D:161:GLN:OE1	2.20	0.41
2:D:68:ARG:HH22	2:F:83:LYS:HG3	1.84	0.41
1:C:31:GLU:OE2	1:C:321:ARG:NH1	2.39	0.41
2:F:145:ASP:O	2:F:149:MET:HG2	2.21	0.41
2:F:149:MET:O	2:F:152:VAL:HG12	2.21	0.41
1:A:55:ASP:O	1:A:278:ASN:OD1	2.38	0.41
1:C:33:ASN:HD21	3:C:1001:NAG:C1	2.34	0.41
2:B:3:PHE:HB2	2:B:112:ASP:OD2	2.21	0.41
1:C:118:PHE:CD1	1:C:258:TYR:HB3	2.56	0.41
1:A:129:ASP:HB3	1:A:162:PRO:HG2	2.03	0.41
1:C:135:VAL:HG22	1:C:146:SER:HA	2.01	0.41
1:E:124:THR:HA	1:E:125:PRO:HD2	1.87	0.41
2:B:145:ASP:N	2:B:145:ASP:OD1	2.53	0.41
2:B:43:LYS:HE2	2:B:43:LYS:HB3	1.90	0.41
1:C:77:ASP:HA	1:C:80:LEU:HG	2.03	0.41
2:B:21:TRP:H	2:B:41:THR:CG2	2.34	0.41
2:B:38:LYS:HA	2:B:41:THR:HG1	1.85	0.40
1:E:214:VAL:HA	1:E:215:PRO:HD3	1.95	0.40
2:B:21:TRP:HB2	2:B:41:THR:HG22	2.03	0.40
1:A:86:TYR:HA	1:A:265:SER:HB2	2.04	0.40
1:A:71:LEU:HA	1:A:71:LEU:HD23	1.81	0.40
2:D:133:LEU:HD11	2:D:139:GLU:HB2	2.03	0.40
2:D:143:ARG:HD3	2:D:143:ARG:HA	1.90	0.40
1:A:19:ALA:HB2	2:B:13:GLY:HA3	2.03	0.40
2:F:58:LYS:HD3	2:F:58:LYS:HA	1.79	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	321/333 (96%)	303 (94%)	18 (6%)	0	100	100
1	C	321/333 (96%)	305 (95%)	16 (5%)	0	100	100
1	E	321/333 (96%)	303 (94%)	18 (6%)	0	100	100
2	B	173/180 (96%)	162 (94%)	11 (6%)	0	100	100
2	D	173/180 (96%)	161 (93%)	12 (7%)	0	100	100
2	F	173/180 (96%)	162 (94%)	11 (6%)	0	100	100
All	All	1482/1539 (96%)	1396 (94%)	86 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	290/298 (97%)	283 (98%)	7 (2%)	57	82
1	C	290/298 (97%)	277 (96%)	13 (4%)	34	62
1	E	290/298 (97%)	284 (98%)	6 (2%)	61	85
2	B	149/154 (97%)	142 (95%)	7 (5%)	32	59
2	D	149/154 (97%)	144 (97%)	5 (3%)	44	72
2	F	149/154 (97%)	145 (97%)	4 (3%)	52	79
All	All	1317/1356 (97%)	1275 (97%)	42 (3%)	46	74

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LEU
1	A	131	GLU
1	A	135	VAL
1	A	206	THR
1	A	266	THR
1	A	279	THR
1	A	316	LEU

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Mol	Chain	Res	Type
2	B	10	ILE
2	B	22	TYR
2	B	58	LYS
2	B	61	THR
2	B	66	VAL
2	B	126	LEU
2	B	164	GLU
1	C	12	GLN
1	C	23	THR
1	C	28	THR
1	C	135	VAL
1	C	175	ASP
1	C	179	LEU
1	C	203	SER
1	C	213	LEU
1	C	220	ARG
1	C	266	THR
1	C	307	LYS
1	C	314	LEU
1	C	320	LEU
2	D	10	ILE
2	D	22	TYR
2	D	55	ILE
2	D	101	LEU
2	D	137	CYS
1	E	18	HIS
1	E	28	THR
1	E	51	LEU
1	E	55	ASP
1	E	290	SER
1	E	320	LEU
2	F	10	ILE
2	F	22	TYR
2	F	48	VAL
2	F	126	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	322	ASN
2	B	15	GLN

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Mol	Chain	Res	Type
2	B	26	HIS
2	B	142	HIS
1	C	33	ASN
1	C	197	ASN
1	C	278	ASN
1	E	186	ASN
1	E	240	ASN
2	F	15	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

13 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	$\# Z  > 2$
3	NAG	A	1001	-	14,14,15	0.34	0	15,19,21	0.41	0
3	NAG	A	1002	1,3,4	14,14,15	0.79	1 (7%)	15,19,21	0.95	1 (6%)
4	FUL	A	1003	3	10,10,11	1.21	1 (10%)	13,14,16	0.74	0
3	NAG	A	1004	3	14,14,15	0.31	0	15,19,21	0.32	0
3	NAG	C	1001	-	14,14,15	0.27	0	15,19,21	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	1002	1,3,5,4	14,14,15	0.77	1 (7%)	15,19,21	1.05	0
5	FUC	C	1003	3	10,10,11	1.58	2 (20%)	13,14,16	1.69	4 (30%)
4	FUL	C	1004	3	10,10,11	1.21	1 (10%)	13,14,16	0.96	1 (7%)
3	NAG	C	1005	3	14,14,15	0.50	0	15,19,21	0.58	0
3	NAG	E	1001	-	14,14,15	0.26	0	15,19,21	0.45	0
3	NAG	E	1002	1,3,4	14,14,15	0.89	1 (7%)	15,19,21	1.00	1 (6%)
4	FUL	E	1003	3	10,10,11	1.37	2 (20%)	13,14,16	0.90	0
3	NAG	E	1004	3	14,14,15	0.26	0	15,19,21	0.25	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
3	NAG	A	1001	-	-	0/6/23/26	0/1/1/1
3	NAG	A	1002	1,3,4	-	0/6/23/26	0/1/1/1
4	FUL	A	1003	3	-	0/0/17/20	0/1/1/1
3	NAG	A	1004	3	-	0/6/23/26	0/1/1/1
3	NAG	C	1001	-	-	0/6/23/26	0/1/1/1
3	NAG	C	1002	1,3,5,4	-	0/6/23/26	0/1/1/1
5	FUC	C	1003	3	-	0/0/17/20	0/1/1/1
4	FUL	C	1004	3	-	0/0/17/20	0/1/1/1
3	NAG	C	1005	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1001	-	-	0/6/23/26	0/1/1/1
3	NAG	E	1002	1,3,4	-	0/6/23/26	0/1/1/1
4	FUL	E	1003	3	-	0/0/17/20	0/1/1/1
3	NAG	E	1004	3	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1002	NAG	O5-C1	-3.26	1.38	1.43
3	A	1002	NAG	O5-C1	-2.82	1.39	1.43
3	C	1002	NAG	O5-C1	-2.62	1.39	1.43
4	E	1003	FUL	O5-C1	-2.06	1.40	1.43
4	A	1003	FUL	C4-C3	2.03	1.57	1.52
4	C	1004	FUL	C4-C3	2.12	1.58	1.52
5	C	1003	FUC	C6-C5	2.41	1.57	1.51
4	E	1003	FUL	C4-C3	2.98	1.60	1.52
5	C	1003	FUC	C4-C5	3.17	1.59	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1003	FUC	C2-C3-C4	-2.95	105.91	111.05
5	C	1003	FUC	C1-C2-C3	-2.14	106.95	109.55
3	E	1002	NAG	C3-C4-C5	2.12	114.01	110.23
3	A	1002	NAG	C3-C4-C5	2.16	114.08	110.23
4	C	1004	FUL	O5-C1-C2	2.43	114.79	110.89
5	C	1003	FUC	C6-C5-C4	2.75	118.35	113.02
5	C	1003	FUC	O2-C2-C1	3.24	115.72	109.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	NAG	1	0
3	C	1001	NAG	1	0
4	C	1004	FUL	1	0
3	C	1005	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	323/333 (96%)	-0.24	6 (1%)	70 64	19, 41, 84, 147	0
1	C	323/333 (96%)	-0.17	3 (0%)	85 83	22, 43, 79, 117	0
1	E	323/333 (96%)	-0.23	3 (0%)	85 83	22, 43, 81, 124	0
2	B	175/180 (97%)	0.82	29 (16%)	2 1	23, 92, 137, 142	0
2	D	175/180 (97%)	0.52	11 (6%)	23 17	24, 81, 109, 127	0
2	F	175/180 (97%)	0.57	12 (6%)	20 14	25, 82, 108, 129	0
All	All	1494/1539 (97%)	0.09	64 (4%)	39 31	19, 51, 112, 147	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	174	SER	6.3
2	B	168	LEU	5.9
2	B	139	GLU	5.6
2	B	140	PHE	5.3
2	B	157	TYR	4.9
1	A	12	GLN	4.7
1	C	324	PRO	4.2
2	B	175	GLY	4.1
2	D	18	VAL	4.0
2	B	158	ASP	4.0
1	E	9	PRO	3.8
2	B	35	ALA	3.7
2	B	16	GLY	3.7
2	F	175	GLY	3.7
1	A	9	PRO	3.6
1	C	21	ASN	3.5
2	B	172	GLU	3.4
2	D	157	TYR	3.4
2	B	156	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	8	ASP	3.4
2	D	33	GLY	3.2
2	D	152	VAL	3.2
2	B	141	TYR	3.1
2	F	147	GLU	3.1
2	F	172	GLU	3.1
1	A	10	GLY	3.0
2	B	134	GLY	3.0
2	B	160	PRO	3.0
1	A	13	ILE	2.9
2	B	138	PHE	2.9
2	D	162	TYR	2.7
2	B	19	ASP	2.7
2	D	17	MET	2.6
1	A	142	GLN	2.6
2	B	34	TYR	2.6
2	B	133	LEU	2.5
2	F	9	PHE	2.5
2	B	36	ALA	2.5
2	B	18	VAL	2.5
2	D	172	GLU	2.5
2	B	144	CYS	2.5
2	B	162	TYR	2.4
2	F	35	ALA	2.4
1	C	323	SER	2.4
2	F	36	ALA	2.4
1	A	14	CYS	2.3
2	B	128	ASP	2.3
2	B	33	GLY	2.3
2	D	19	ASP	2.3
2	F	39	GLU	2.3
2	F	141	TYR	2.3
2	F	152	VAL	2.3
2	B	142	HIS	2.3
2	B	32	SER	2.2
2	D	23	GLY	2.2
1	E	51	LEU	2.2
2	D	173	ILE	2.1
2	B	166	ALA	2.1
2	B	24	TYR	2.1
2	D	174	SER	2.1
2	B	159	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	31	GLY	2.1
2	F	19	ASP	2.1
2	F	106	ARG	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](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	E	1002	14/15	0.91	0.17	2.37	51,61,79,81	0
3	NAG	C	1002	14/15	0.89	0.14	0.28	51,67,79,83	0
3	NAG	A	1002	14/15	0.93	0.14	-0.24	38,56,75,77	0
3	NAG	A	1001	14/15	0.82	0.18	-	91,98,101,101	0
4	FUL	E	1003	10/11	0.76	0.24	-	70,81,89,96	0
3	NAG	E	1004	14/15	0.89	0.19	-	74,91,100,101	0
4	FUL	C	1004	10/11	0.82	0.28	-	75,81,92,92	0
3	NAG	A	1004	14/15	0.89	0.27	-	70,78,86,86	0
5	FUC	C	1003	10/11	0.71	0.25	-	58,74,84,90	0
3	NAG	E	1001	14/15	0.77	0.20	-	99,109,116,120	0
4	FUL	A	1003	10/11	0.81	0.31	-	68,82,93,93	0
3	NAG	C	1001	14/15	0.69	0.15	-	92,101,107,115	0
3	NAG	C	1005	14/15	0.86	0.26	-	74,85,93,102	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.