



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:05 PM GMT

PDB ID : 1NE7  
Title : HUMAN GLUCOSAMINE-6-PHOSPHATE DEAMINASE ISOMERASE AT  
1.75 Å RESOLUTION COMPLEXED WITH N-ACETYL-GLUCOSAMINE  
-6-PHOSPHATE AND 2-DEOXY-2-AMINO-GLUCITOL-6-PHOSPHATE  
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Deposited on : 2002-12-10  
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

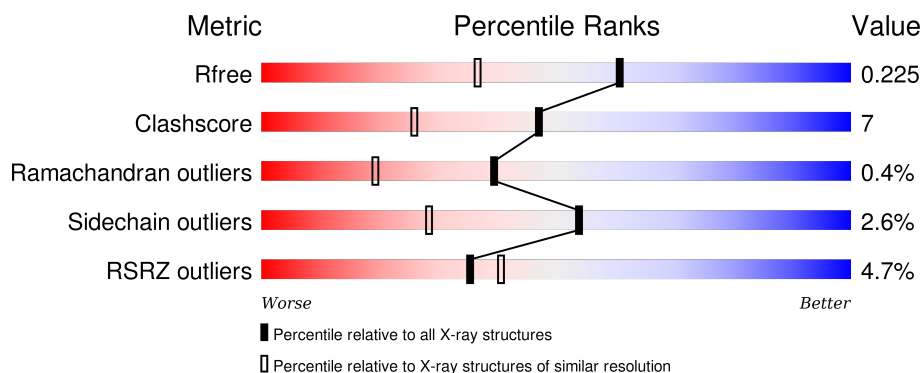
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	289	<div> <div>6%</div> <div>83% 12% . .</div> </div>
1	B	289	<div> <div>6%</div> <div>80% 13% . 5%</div> </div>
1	C	289	<div> <div>2%</div> <div>79% 14% . 5%</div> </div>
1	D	289	<div> <div>3%</div> <div>85% 9% . 5%</div> </div>
1	E	289	<div> <div>8%</div> <div>80% 13% . 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	289	 3% 82% 11% • 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	C	295	-	-	-	X
2	GLC	E	295	-	-	-	X
5	SO4	C	4297[B]	-	-	-	X
6	AGP	A	2298[A]	-	-	-	X
6	AGP	B	3298[A]	-	-	-	X
6	AGP	C	4298[A]	-	-	-	X
6	AGP	D	5298[A]	-	-	-	X
6	AGP	E	6298[A]	-	-	-	X
6	AGP	F	7298[A]	-	-	-	X

## 2 Entry composition [i](#)

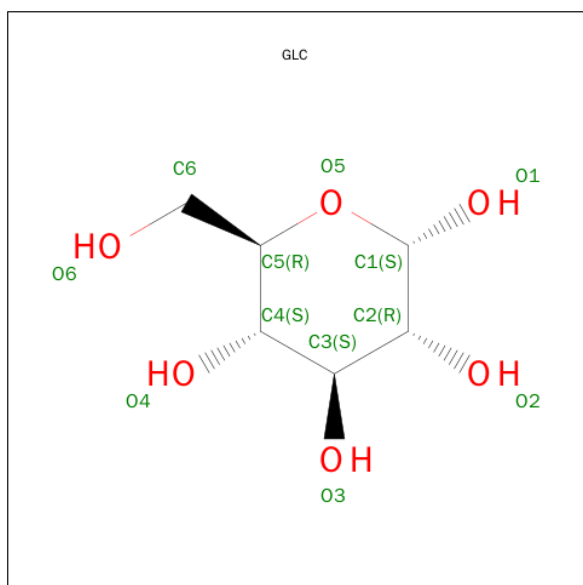
There are 7 unique types of molecules in this entry. The entry contains 16013 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glucosamine-6-phosphate isomerase.

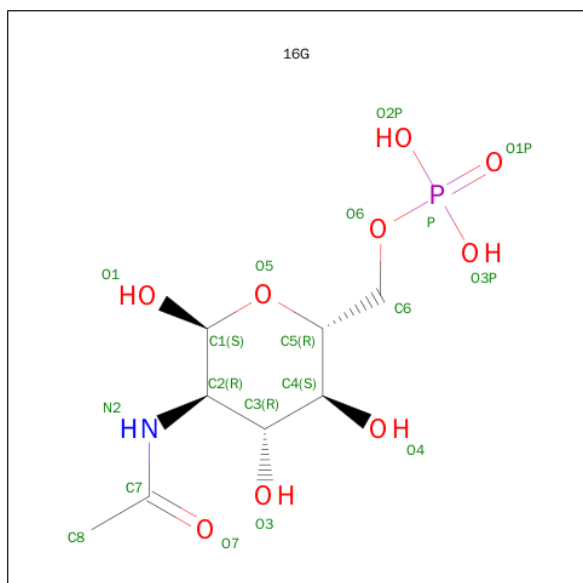
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	21	7	0
			2294	1480	382	419	13			
1	B	274	Total	C	N	O	S	5	3	0
			2203	1425	364	400	14			
1	C	274	Total	C	N	O	S	7	8	0
			2244	1451	372	406	15			
1	D	274	Total	C	N	O	S	4	7	0
			2231	1443	369	406	13			
1	E	274	Total	C	N	O	S	17	7	0
			2237	1446	372	405	14			
1	F	274	Total	C	N	O	S	9	6	0
			2227	1438	371	405	13			

- Molecule 2 is SUGAR (GLU-GLU) (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			11	6	5		
2	C	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			11	6	5		
2	E	1	Total	C	O	0	0
			12	6	6		
2	E	1	Total	C	O	0	0
			11	6	5		
2	F	1	Total	C	O	0	0
			12	6	6		
2	F	1	Total	C	O	0	0
			11	6	5		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE-6-PHOSPHATE) (three-letter code: 16G) (formula: C<sub>8</sub>H<sub>16</sub>NO<sub>9</sub>P).



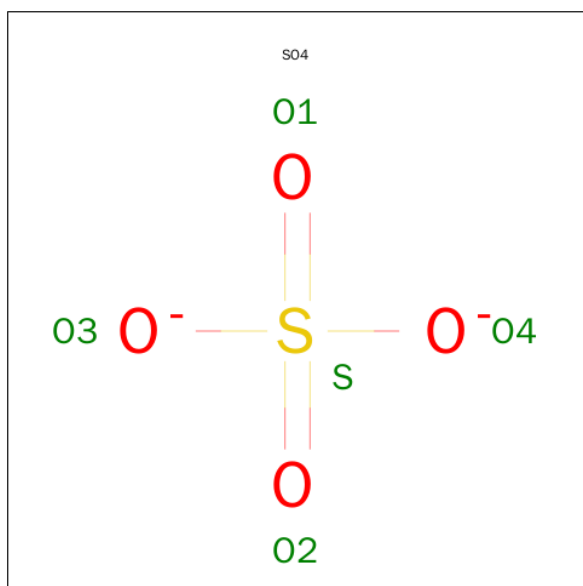
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			19	8	1	9	1		
3	A	1	Total	C	N	O	P	0	0
			19	8	1	9	1		
3	E	1	Total	C	N	O	P	0	0
			19	8	1	9	1		
3	F	1	Total	C	N	O	P	0	0
			19	8	1	9	1		
3	D	1	Total	C	N	O	P	0	0
			19	8	1	9	1		

- Molecule 4 is a polymer of unknown type called SUGAR (GLU-GLU).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	2	Total	C	O	0	0
			23	12	11		

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



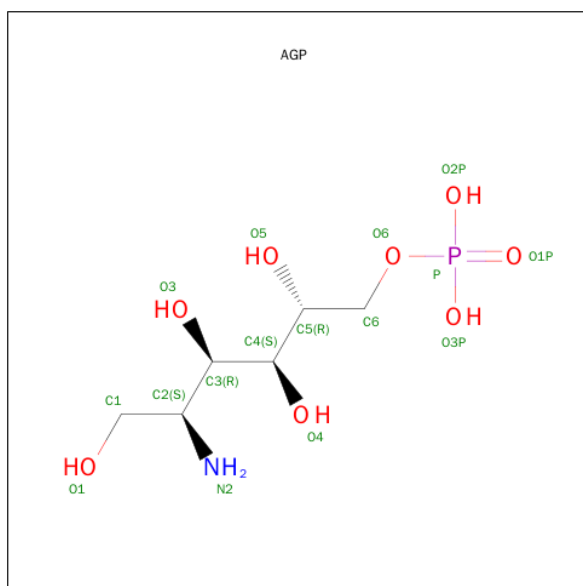
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	1
			5	4	1		
5	B	1	Total	O	S	0	1
			5	4	1		
5	C	1	Total	O	S	0	1
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	1
			5	4	1		
5	D	1	Total	O	S	0	1
			5	4	1		
5	E	1	Total	O	S	0	1
			5	4	1		
5	F	1	Total	O	S	0	1
			5	4	1		

- Molecule 6 is 2-DEOXY-2-AMINO GLUCITOL-6-PHOSPHATE (three-letter code: AGP) (formula: C<sub>6</sub>H<sub>16</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 16	C 6	N 1	O 8	P 1	3	1
6	B	1	Total 16	C 6	N 1	O 8	P 1	2	1
6	C	1	Total 16	C 6	N 1	O 8	P 1	2	1
6	D	1	Total 16	C 6	N 1	O 8	P 1	2	1
6	E	1	Total 16	C 6	N 1	O 8	P 1	2	1
6	F	1	Total 16	C 6	N 1	O 8	P 1	0	1

- Molecule 7 is water.

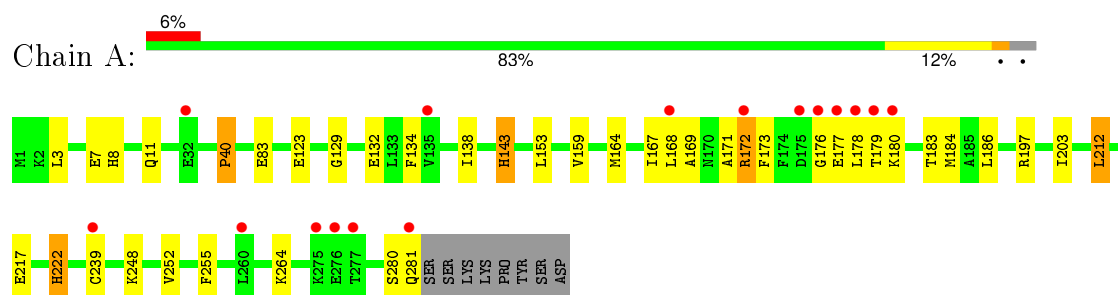
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	376	Total 376	O 376	0	0
7	B	364	Total 364	O 364	0	0
7	C	406	Total 406	O 406	0	0
7	D	366	Total 366	O 366	0	0
7	E	305	Total 305	O 305	0	0
7	F	377	Total 377	O 377	0	0



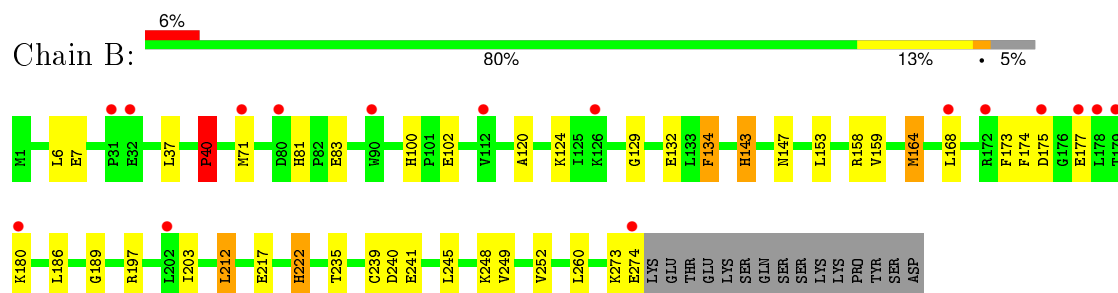
### 3 Residue-property plots [i](#)

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.

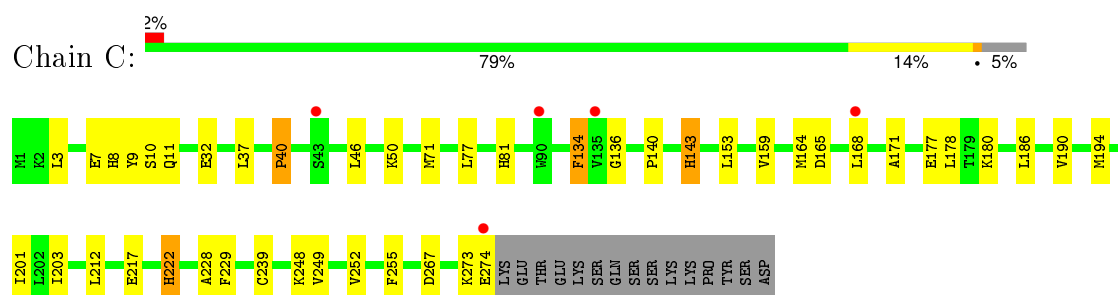
- Molecule 1: Glucosamine-6-phosphate isomerase



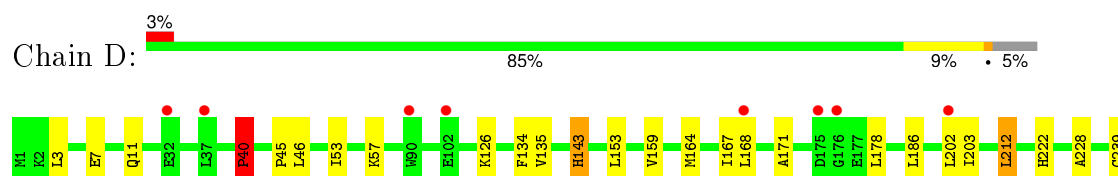
- Molecule 1: Glucosamine-6-phosphate isomerase

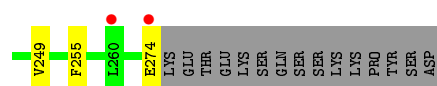


- Molecule 1: Glucosamine-6-phosphate isomerase

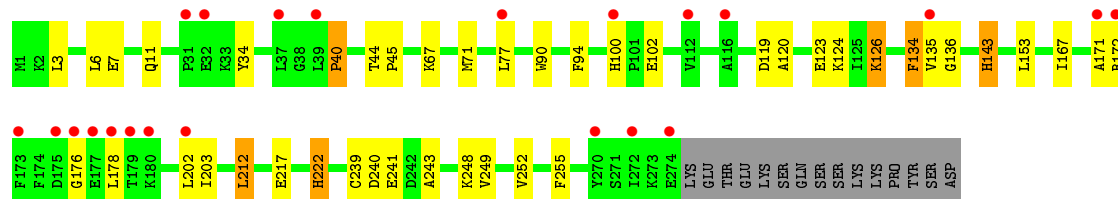
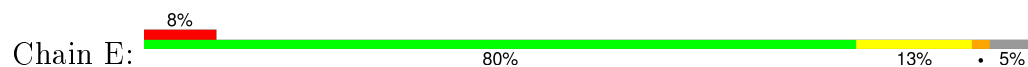


- Molecule 1: Glucosamine-6-phosphate isomerase

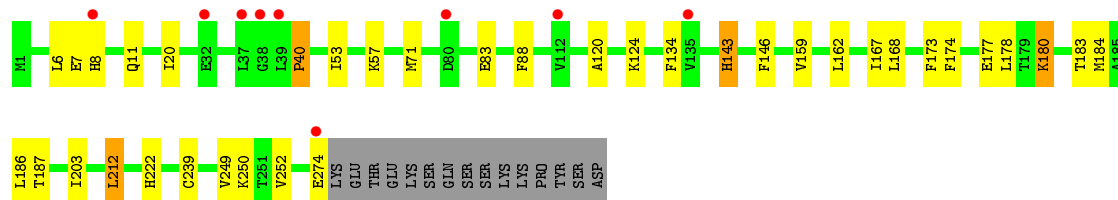
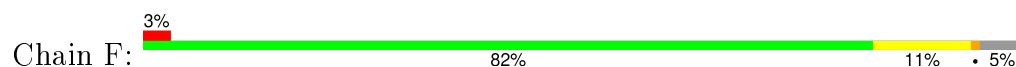




- Molecule 1: Glucosamine-6-phosphate isomerase



- Molecule 1: Glucosamine-6-phosphate isomerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.88Å 110.89Å 180.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 1.75 29.54 – 1.75	Depositor EDS
% Data completeness (in resolution range)	94.3 (19.97-1.75) 94.1 (29.54-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.86 (at 1.75Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.193 , 0.217 0.203 , 0.225	Depositor DCC
$R_{free}$ test set	20802 reflections (9.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 58.7	EDS
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 209834 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: GLC, 16G, SO4, AGP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.33	0/2351	0.66	4/3178 (0.1%)
1	B	0.30	0/2259	0.58	0/3057
1	C	0.32	0/2300	0.60	0/3111
1	D	0.31	0/2288	0.58	0/3096
1	E	0.30	0/2293	0.57	0/3101
1	F	0.30	0/2283	0.57	0/3088
All	All	0.31	0/13774	0.60	4/18631 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172[A]	ARG	NE-CZ-NH1	-8.57	116.01	120.30
1	A	172[B]	ARG	NE-CZ-NH1	-8.57	116.01	120.30
1	A	172[A]	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	A	172[B]	ARG	NE-CZ-NH2	6.42	123.51	120.30

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	2294	0	2284	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2203	0	2189	42	0
1	C	2244	0	2234	37	0
1	D	2231	0	2217	29	0
1	E	2237	0	2228	35	0
1	F	2227	0	2213	33	0
2	A	23	0	16	0	0
2	C	23	0	16	0	0
2	D	23	0	16	0	0
2	E	23	0	16	0	0
2	F	23	0	16	0	0
3	A	19	0	14	0	0
3	B	19	0	14	0	0
3	C	19	0	14	0	0
3	D	19	0	14	0	0
3	E	19	0	14	0	0
3	F	19	0	14	0	0
4	B	23	0	16	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	10	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	1	0
6	A	16	0	14	1	0
6	B	16	0	13	0	0
6	C	16	0	14	0	0
6	D	16	0	14	0	0
6	E	16	0	14	0	0
6	F	16	0	14	5	0
7	A	376	0	0	2	0
7	B	364	0	0	3	0
7	C	406	0	0	1	0
7	D	366	0	0	3	0
7	E	305	0	0	1	0
7	F	377	0	0	8	0
All	All	16013	0	13628	204	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 7.

All (204) 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)
6:F:7298[A]:AGP:H61	7:F:7673:HOH:O	1.47	1.12
6:A:2298[A]:AGP:O3	7:A:4587:HOH:O	1.68	1.10
1:A:7:GLU:HB3	1:A:11:GLN:HE22	1.25	1.00
1:E:7:GLU:HB3	1:E:11:GLN:HE22	1.36	0.90
1:A:7:GLU:HB3	1:A:11:GLN:NE2	1.90	0.85
1:B:235:THR:HB	7:B:3593:HOH:O	1.78	0.84
1:B:147:ASN:HD22	1:B:158:ARG:HH22	1.26	0.83
1:A:280:SER:O	1:A:281:GLN:HG2	1.79	0.82
1:D:135:VAL:HG13	1:D:202[B]:LEU:HD21	1.62	0.81
1:F:53:ILE:HG22	1:F:57:LYS:HE2	1.63	0.81
6:F:7298[A]:AGP:O3P	7:F:7673:HOH:O	2.00	0.80
1:C:8:HIS:CD2	1:C:10:SER:H	2.00	0.80
1:B:81:HIS:HD2	1:B:83:GLU:H	1.30	0.78
5:F:7296[B]:SO4:O3	7:F:7673:HOH:O	2.02	0.77
1:C:7:GLU:HB3	1:C:11:GLN:NE2	1.98	0.77
1:C:140:PRO:HG2	1:C:165:ASP:OD1	1.85	0.76
1:A:217:GLU:OE1	1:A:248:LYS:HG3	1.86	0.75
1:C:7:GLU:HB3	1:C:11:GLN:HE22	1.49	0.74
1:C:8:HIS:H	1:C:11:GLN:HE21	1.37	0.72
1:E:71[B]:MET:HG2	1:E:134:PHE:CE1	2.24	0.72
1:C:164:MET:O	1:C:168:LEU:HD13	1.89	0.72
1:F:180:LYS:HE2	1:F:180:LYS:O	1.91	0.71
1:B:100:HIS:HD2	1:B:102:GLU:H	1.38	0.70
1:D:202[B]:LEU:HD22	1:D:202[B]:LEU:N	2.07	0.69
1:B:81:HIS:CD2	1:B:83:GLU:H	2.10	0.69
1:A:177:GLU:HB2	1:A:180:LYS:HG3	1.73	0.69
1:B:71[B]:MET:HG2	1:B:134:PHE:CE1	2.27	0.69
1:A:132:GLU:HA	1:A:197:ARG:HD2	1.73	0.69
1:E:119:ASP:O	1:E:123:GLU:HG2	1.93	0.69
1:E:71[B]:MET:HG2	1:E:134:PHE:HE1	1.58	0.69
1:F:20:ILE:HD13	7:F:7675:HOH:O	1.92	0.68
1:C:190:VAL:O	1:C:194[B]:MET:HG3	1.94	0.67
1:E:135:VAL:HG13	1:E:202[B]:LEU:HD21	1.77	0.66
1:E:7:GLU:HA	1:E:241:GLU:HG2	1.77	0.66
1:B:132:GLU:HA	1:B:197:ARG:HH11	1.61	0.66
1:E:171:ALA:HB2	1:E:178:LEU:HD23	1.77	0.65
1:A:129:GLY:O	1:A:197:ARG:NH2	2.30	0.65
1:D:7:GLU:HB3	1:D:11:GLN:OE1	1.96	0.65
1:C:71[B]:MET:HG2	1:C:134:PHE:CE1	2.32	0.64
1:C:273:LYS:O	1:C:274:GLU:HB2	1.97	0.64
1:E:135:VAL:CG1	1:E:202[B]:LEU:HD21	2.28	0.64
1:E:217:GLU:OE1	1:E:248:LYS:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:MET:O	1:A:168:LEU:HD13	1.98	0.64
1:F:183:THR:HG22	1:F:184:MET:HG3	1.80	0.64
1:C:8:HIS:H	1:C:11:GLN:NE2	1.95	0.64
1:C:8:HIS:HD2	1:C:10:SER:HB3	1.63	0.64
1:F:203:ILE:HD13	1:F:212:LEU:HG	1.81	0.63
1:B:217:GLU:OE1	1:B:248:LYS:HG3	2.00	0.61
1:B:245:LEU:HB3	1:F:250:LYS:HZ1	1.65	0.61
1:B:177:GLU:HB2	1:B:180:LYS:CG	2.31	0.61
1:D:164:MET:O	1:D:168:LEU:HD13	2.01	0.61
1:D:135:VAL:CG1	1:D:202[B]:LEU:HD21	2.29	0.61
6:F:7298[A]:AGP:P	7:F:7673:HOH:O	2.59	0.60
1:D:171:ALA:HB2	1:D:178:LEU:HD23	1.83	0.60
1:E:71[A]:MET:HE1	1:E:136:GLY:HA2	1.83	0.59
1:D:167[A]:ILE:HG22	1:D:178:LEU:HD22	1.83	0.59
1:D:164:MET:HB3	7:D:7452:HOH:O	2.03	0.59
1:B:164:MET:O	1:B:168:LEU:HD13	2.03	0.58
1:A:169:ALA:O	1:A:172[B]:ARG:HD3	2.03	0.58
1:B:129:GLY:O	1:B:197:ARG:NH2	2.37	0.58
1:F:177:GLU:HB2	1:F:180:LYS:HB2	1.86	0.58
1:B:100:HIS:CD2	1:B:102:GLU:H	2.19	0.58
1:F:7:GLU:HG2	1:F:8:HIS:CE1	2.40	0.57
1:B:40:PRO:HB3	1:B:71[B]:MET:HE2	1.86	0.57
6:F:7298[A]:AGP:O3	7:F:7322:HOH:O	2.17	0.57
1:F:183:THR:HA	7:F:7592:HOH:O	2.05	0.57
1:B:71[B]:MET:HG2	1:B:134:PHE:HE1	1.70	0.56
1:F:120:ALA:O	1:F:124[B]:LYS:HG3	2.06	0.56
1:D:153:LEU:HD22	1:D:228:ALA:HB2	1.88	0.55
1:F:274:GLU:CD	1:F:274:GLU:H	2.10	0.55
1:F:250:LYS:NZ	1:F:250:LYS:HB2	2.23	0.54
1:B:175:ASP:OD2	1:B:180:LYS:HE2	2.08	0.54
1:D:168:LEU:HA	1:D:178:LEU:HD21	1.88	0.54
1:C:71[A]:MET:HE1	1:C:136:GLY:HA2	1.89	0.54
1:E:203[A]:ILE:O	1:E:239[A]:CYS:HA	2.08	0.54
1:A:197:ARG:HH11	1:A:197:ARG:HG3	1.73	0.53
1:C:71[B]:MET:HG2	1:C:134:PHE:HE1	1.71	0.53
1:A:171:ALA:O	1:A:176:GLY:HA2	2.09	0.52
1:A:83:GLU:HG3	1:A:173:PHE:O	2.09	0.52
1:A:138:ILE:HG22	1:A:203[A]:ILE:HG12	1.92	0.52
1:D:168:LEU:HA	1:D:178:LEU:CD2	2.40	0.51
1:C:203[A]:ILE:O	1:C:239[A]:CYS:HA	2.11	0.51
1:E:7:GLU:HB3	1:E:11:GLN:NE2	2.15	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:HIS:O	1:A:143:HIS:HD2	1.93	0.51
1:F:120:ALA:O	1:F:124[A]:LYS:HG3	2.10	0.51
1:B:147:ASN:ND2	1:B:158:ARG:HH22	2.01	0.51
1:B:71[B]:MET:CG	1:B:134:PHE:HE1	2.24	0.51
1:A:7:GLU:CB	1:A:11:GLN:HE22	2.11	0.51
1:B:260:LEU:HG	7:B:3651:HOH:O	2.12	0.50
1:D:202[B]:LEU:H	1:D:202[B]:LEU:HD22	1.77	0.50
1:F:162:LEU:HB2	1:F:167[A]:ILE:HD11	1.93	0.50
1:E:143:HIS:O	1:E:143:HIS:HD2	1.94	0.50
1:B:249:VAL:HG21	1:F:252:VAL:HG21	1.93	0.50
1:E:202[B]:LEU:HD22	1:E:202[B]:LEU:N	2.27	0.49
1:B:132:GLU:OE1	1:B:197:ARG:HD2	2.12	0.49
1:C:249:VAL:HG21	1:E:252:VAL:HG21	1.94	0.49
1:F:143:HIS:O	1:F:143:HIS:HD2	1.95	0.49
1:A:197:ARG:HG3	1:A:197:ARG:NH1	2.26	0.49
1:B:177:GLU:HB2	1:B:180:LYS:HG3	1.94	0.49
1:B:252:VAL:HG21	1:F:249:VAL:HG21	1.94	0.49
1:D:203:ILE:CD1	1:D:212:LEU:HG	2.43	0.49
1:C:194[B]:MET:HE3	1:C:229:PHE:HA	1.93	0.48
1:E:34:TYR:CG	1:E:67:LYS:HE3	2.48	0.48
1:A:169:ALA:O	1:A:172[B]:ARG:NH1	2.46	0.48
1:C:203[B]:ILE:O	1:C:239[B]:CYS:HA	2.14	0.48
1:B:147:ASN:HD21	1:B:158:ARG:HH12	1.61	0.48
1:F:6:LEU:HD22	1:F:6:LEU:N	2.29	0.48
1:D:203:ILE:HD13	1:D:212:LEU:HG	1.95	0.48
1:C:159:VAL:HG22	1:C:186:LEU:CD2	2.44	0.48
1:C:267:ASP:HB3	7:C:4692:HOH:O	2.13	0.48
1:A:252:VAL:HG21	1:D:249:VAL:HG21	1.96	0.47
1:B:174:PHE:HB3	1:B:180:LYS:HB3	1.97	0.47
1:E:120:ALA:O	1:E:124:LYS:HG3	2.14	0.47
1:D:203:ILE:O	1:D:239[B]:CYS:HB3	2.15	0.47
1:A:203[A]:ILE:HD13	1:A:212:LEU:HG	1.96	0.47
1:D:167[B]:ILE:HG22	1:D:178:LEU:HD22	1.96	0.47
1:B:273:LYS:O	1:B:274:GLU:HG2	2.15	0.47
1:D:202[B]:LEU:CD2	1:D:202[B]:LEU:N	2.78	0.46
1:B:143:HIS:HD2	1:B:143:HIS:O	1.97	0.46
1:E:126:LYS:HG2	7:E:6598:HOH:O	2.15	0.46
1:E:153:LEU:HD21	1:E:222:HIS:HA	1.96	0.46
1:C:203[B]:ILE:HD12	1:C:203[B]:ILE:N	2.31	0.46
1:A:167:ILE:HG22	1:A:178:LEU:HD22	1.97	0.46
1:C:7:GLU:CB	1:C:11:GLN:HE22	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:VAL:HG21	1:E:249:VAL:HG21	1.98	0.46
1:F:53:ILE:HG22	1:F:57:LYS:CE	2.39	0.46
1:C:8:HIS:CG	1:C:9:TYR:N	2.83	0.46
1:C:8:HIS:HD2	1:C:10:SER:CB	2.29	0.46
1:D:53:ILE:CG2	1:D:57:LYS:HE2	2.46	0.45
1:C:153:LEU:HD22	1:C:228:ALA:HB2	1.96	0.45
1:E:171:ALA:CB	1:E:178:LEU:HD23	2.45	0.45
1:B:6:LEU:HD22	1:B:6:LEU:N	2.31	0.45
1:F:71:MET:SD	6:F:7298[A]:AGP:H12	2.57	0.45
1:F:203:ILE:CD1	1:F:212:LEU:HG	2.45	0.45
1:D:45:PRO:HD3	7:D:7586:HOH:O	2.16	0.45
1:D:126:LYS:HA	7:D:7444:HOH:O	2.16	0.45
1:C:177:GLU:HB2	1:C:180:LYS:HG3	1.98	0.45
1:E:167:ILE:HG22	1:E:178:LEU:HD22	1.99	0.44
1:C:46:LEU:HG	1:C:50:LYS:HE3	1.99	0.44
1:C:143:HIS:HD2	1:C:143:HIS:O	1.99	0.44
1:F:250:LYS:HZ2	1:F:250:LYS:HB2	1.81	0.44
1:F:159:VAL:HG22	1:F:186:LEU:CD2	2.46	0.44
1:D:203:ILE:O	1:D:239[A]:CYS:HA	2.17	0.44
1:A:183:THR:HG22	1:A:184:MET:HG3	2.00	0.44
1:B:6:LEU:O	1:B:240:ASP:HA	2.18	0.43
1:C:217:GLU:OE1	1:C:248:LYS:HG3	2.19	0.43
1:D:40:PRO:HD3	1:D:135:VAL:O	2.19	0.43
1:F:174:PHE:HB3	1:F:180:LYS:HB3	1.99	0.43
1:B:203:ILE:HD13	1:B:212:LEU:HG	2.00	0.43
1:D:159:VAL:HG22	1:D:186:LEU:CD2	2.48	0.43
1:D:143:HIS:O	1:D:143:HIS:HD2	2.01	0.43
1:E:90:TRP:HA	1:E:94:PHE:HB2	1.99	0.43
1:B:159:VAL:HG22	1:B:186:LEU:CD2	2.49	0.43
1:F:180:LYS:HE2	1:F:180:LYS:CA	2.48	0.43
1:E:3:LEU:HB3	1:E:255:PHE:CG	2.54	0.43
1:A:203[A]:ILE:O	1:A:239[A]:CYS:HA	2.18	0.43
1:B:260:LEU:HB3	7:B:3373:HOH:O	2.19	0.42
1:E:100:HIS:HB3	1:E:102:GLU:CD	2.39	0.42
1:B:147:ASN:HD21	1:B:189:GLY:HA2	1.84	0.42
1:B:7:GLU:HA	1:B:241:GLU:HG2	2.00	0.42
1:C:171:ALA:HB2	1:C:178:LEU:HD23	2.01	0.42
1:E:203[B]:ILE:O	1:E:239[B]:CYS:HA	2.19	0.42
1:E:143:HIS:C	1:E:143:HIS:CD2	2.93	0.42
1:E:203[B]:ILE:HD12	1:E:203[B]:ILE:N	2.34	0.42
1:C:11:GLN:HB2	1:C:11:GLN:HE21	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239[A]:CYS:HB2	1:E:243:ALA:HB3	2.02	0.42
1:A:203[B]:ILE:O	1:A:239[B]:CYS:HA	2.20	0.42
1:B:143:HIS:CD2	1:B:143:HIS:C	2.92	0.42
1:A:153:LEU:HD21	1:A:222:HIS:HA	2.02	0.41
1:F:168:LEU:HD12	1:F:178:LEU:HD21	2.01	0.41
1:B:153:LEU:HD21	1:B:222:HIS:HA	2.01	0.41
1:A:159:VAL:HG22	1:A:186:LEU:CD2	2.50	0.41
1:D:203:ILE:O	1:D:239[B]:CYS:HA	2.18	0.41
1:B:71[B]:MET:HG2	1:B:134:PHE:CZ	2.54	0.41
1:E:77:LEU:HA	1:E:77:LEU:HD23	1.95	0.41
1:B:120:ALA:O	1:B:124:LYS:HG3	2.20	0.41
1:F:250:LYS:HZ2	1:F:250:LYS:CB	2.33	0.41
1:C:77:LEU:HD22	1:C:81:HIS:CD2	2.55	0.41
1:A:3:LEU:HB3	1:A:255:PHE:CG	2.55	0.41
1:E:6:LEU:N	1:E:6:LEU:HD22	2.35	0.41
1:A:264:LYS:HE3	7:A:4535:HOH:O	2.21	0.41
1:C:201:ILE:HG22	1:C:203[B]:ILE:HD11	2.03	0.41
1:F:143:HIS:CD2	1:F:143:HIS:C	2.93	0.41
1:F:83:GLU:HG3	1:F:173:PHE:O	2.21	0.41
1:D:46:LEU:HA	1:D:46:LEU:HD12	1.94	0.41
1:E:203[A]:ILE:HD13	1:E:212:LEU:HG	2.03	0.41
1:C:153:LEU:HD21	1:C:222:HIS:HA	2.03	0.41
1:E:6:LEU:O	1:E:240:ASP:HA	2.21	0.41
1:F:88:PHE:CD1	1:F:88:PHE:C	2.94	0.41
1:D:3:LEU:HB3	1:D:255:PHE:CG	2.56	0.41
1:F:203:ILE:O	1:F:239[B]:CYS:HB3	2.20	0.41
1:B:203:ILE:O	1:B:239[B]:CYS:HA	2.21	0.41
1:E:44:THR:HB	1:E:45:PRO:HD3	2.02	0.41
1:F:146:PHE:HB2	1:F:187:THR:HB	2.02	0.41
1:D:164:MET:SD	1:D:168:LEU:HD11	2.60	0.40
1:C:32:GLU:HA	1:C:32:GLU:OE1	2.21	0.40
1:C:143:HIS:C	1:C:143:HIS:CD2	2.94	0.40
1:F:11:GLN:HG3	7:F:7603:HOH:O	2.21	0.40
1:A:7:GLU:HG3	1:A:8:HIS:CD2	2.55	0.40
1:B:83:GLU:HG3	1:B:173:PHE:O	2.22	0.40
1:B:203:ILE:O	1:B:239[A]:CYS:HA	2.21	0.40
1:E:172[B]:ARG:HA	1:E:176:GLY:HA2	2.04	0.40
1:B:147:ASN:ND2	1:B:158:ARG:HH12	2.19	0.40
1:C:3:LEU:HB3	1:C:255:PHE:CG	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	286/289 (99%)	276 (96%)	8 (3%)	2 (1%)	26	10
1	B	275/289 (95%)	266 (97%)	8 (3%)	1 (0%)	39	19
1	C	280/289 (97%)	273 (98%)	6 (2%)	1 (0%)	39	19
1	D	279/289 (96%)	272 (98%)	6 (2%)	1 (0%)	39	19
1	E	279/289 (96%)	269 (96%)	9 (3%)	1 (0%)	39	19
1	F	278/289 (96%)	270 (97%)	7 (2%)	1 (0%)	39	19
All	All	1677/1734 (97%)	1626 (97%)	44 (3%)	7 (0%)	39	19

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	THR
1	F	40	PRO
1	A	40	PRO
1	D	40	PRO
1	E	40	PRO
1	C	40	PRO
1	B	40	PRO

### 5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/249 (100%)	242 (98%)	6 (2%)	57	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	237/249 (95%)	230 (97%)	7 (3%)	48	22
1	C	242/249 (97%)	236 (98%)	6 (2%)	55	30
1	D	241/249 (97%)	235 (98%)	6 (2%)	55	30
1	E	241/249 (97%)	235 (98%)	6 (2%)	55	30
1	F	240/249 (96%)	234 (98%)	6 (2%)	55	30
All	All	1449/1494 (97%)	1412 (97%)	37 (3%)	54	28

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	A	123	GLU
1	A	134	PHE
1	A	143	HIS
1	A	212	LEU
1	A	222	HIS
1	B	37	LEU
1	B	40	PRO
1	B	134	PHE
1	B	143	HIS
1	B	164	MET
1	B	212	LEU
1	B	222	HIS
1	C	37	LEU
1	C	40	PRO
1	C	134	PHE
1	C	143	HIS
1	C	212	LEU
1	C	222	HIS
1	D	40	PRO
1	D	134	PHE
1	D	143	HIS
1	D	212	LEU
1	D	222	HIS
1	D	274	GLU
1	E	40	PRO
1	E	126	LYS
1	E	134	PHE
1	E	143	HIS
1	E	212	LEU

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Mol	Chain	Res	Type
1	E	222	HIS
1	F	40	PRO
1	F	134	PHE
1	F	143	HIS
1	F	180	LYS
1	F	212	LEU
1	F	222	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	58	ASN
1	B	58	ASN
1	B	81	HIS
1	B	100	HIS
1	B	147	ASN
1	B	170	ASN
1	C	8	HIS
1	C	11	GLN
1	C	58	ASN
1	C	100	HIS
1	C	170	ASN
1	D	58	ASN
1	E	11	GLN
1	E	28	ASN
1	E	58	ASN
1	F	11	GLN
1	F	28	ASN
1	F	58	ASN
1	F	86	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

2 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	GLC	B	294	4	12,12,12	3.08	5 (41%)	17,17,17	3.36	6 (35%)
4	GLC	B	295	4	11,11,12	3.14	4 (36%)	14,15,17	1.66	2 (14%)

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
4	GLC	B	294	4	-	0/2/22/22	0/1/1/1
4	GLC	B	295	4	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	295	GLC	O2-C2	-8.18	1.25	1.43
4	B	294	GLC	O3-C3	-7.77	1.24	1.43
4	B	295	GLC	O6-C6	-4.21	1.24	1.42
4	B	294	GLC	O6-C6	-4.16	1.24	1.42
4	B	295	GLC	C4-C5	2.32	1.58	1.53
4	B	294	GLC	C4-C3	2.46	1.58	1.52
4	B	294	GLC	C4-C5	2.59	1.58	1.53
4	B	295	GLC	C2-C3	2.95	1.56	1.52
4	B	294	GLC	O1-C1	4.02	1.53	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	294	GLC	O2-C2-C1	-6.39	95.73	109.82
4	B	294	GLC	O1-C1-O5	-4.23	98.67	110.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	294	GLC	C1-C2-C3	-2.98	105.99	110.43
4	B	294	GLC	O6-C6-C5	2.41	119.30	111.33
4	B	295	GLC	O6-C6-C5	2.47	119.50	111.33
4	B	295	GLC	C1-O5-C5	4.38	117.80	112.25
4	B	294	GLC	O2-C2-C3	7.26	126.68	110.34
4	B	294	GLC	O1-C1-C2	7.74	129.96	109.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

29 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
5	SO4	A	2296[B]	-	4,4,4	0.64	0	6,6,6	0.29	0
6	AGP	A	2298[A]	-	15,15,15	0.98	0	14,21,21	1.39	3 (21%)
2	GLC	A	294	2	12,12,12	3.09	5 (41%)	17,17,17	3.36	6 (35%)
2	GLC	A	295	2	11,11,12	3.20	5 (45%)	14,15,17	1.71	2 (14%)
3	16G	A	4299	-	19,19,19	2.06	6 (31%)	23,28,28	1.69	4 (17%)
3	16G	B	2299	-	19,19,19	2.10	7 (36%)	23,28,28	1.63	3 (13%)
5	SO4	B	3296[B]	-	4,4,4	0.64	0	6,6,6	0.29	0
6	AGP	B	3298[A]	-	15,15,15	1.12	0	14,21,21	1.86	3 (21%)
2	GLC	C	294	2	12,12,12	3.08	6 (50%)	17,17,17	3.39	6 (35%)
2	GLC	C	295	2	11,11,12	3.15	4 (36%)	14,15,17	1.67	2 (14%)
3	16G	C	3299	-	19,19,19	2.06	7 (36%)	23,28,28	1.65	3 (13%)
5	SO4	C	4296[B]	-	4,4,4	0.64	0	6,6,6	0.28	0
5	SO4	C	4297[B]	-	4,4,4	0.70	0	6,6,6	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	AGP	C	4298[A]	-	15,15,15	1.16	1 (6%)	14,21,21	3.02	3 (21%)
2	GLC	D	294	2	12,12,12	3.09	6 (50%)	17,17,17	3.40	6 (35%)
2	GLC	D	295	2	11,11,12	3.18	4 (36%)	14,15,17	1.72	3 (21%)
5	SO4	D	5296[B]	-	4,4,4	0.65	0	6,6,6	0.29	0
6	AGP	D	5298[A]	-	15,15,15	1.03	0	14,21,21	1.86	2 (14%)
3	16G	D	7299	-	19,19,19	2.09	7 (36%)	23,28,28	1.62	4 (17%)
2	GLC	E	294	2	12,12,12	3.07	6 (50%)	17,17,17	3.39	6 (35%)
2	GLC	E	295	2	11,11,12	3.20	5 (45%)	14,15,17	1.74	3 (21%)
3	16G	E	5299	-	19,19,19	2.11	6 (31%)	23,28,28	1.67	4 (17%)
5	SO4	E	6296[B]	-	4,4,4	0.63	0	6,6,6	0.29	0
6	AGP	E	6298[A]	-	15,15,15	1.13	1 (6%)	14,21,21	4.45	3 (21%)
2	GLC	F	294	2	12,12,12	3.12	6 (50%)	17,17,17	3.39	6 (35%)
2	GLC	F	295	2	11,11,12	3.17	5 (45%)	14,15,17	1.68	2 (14%)
3	16G	F	6299	-	19,19,19	2.06	6 (31%)	23,28,28	1.66	4 (17%)
5	SO4	F	7296[B]	-	4,4,4	0.55	0	6,6,6	0.28	0
6	AGP	F	7298[A]	-	15,15,15	1.17	0	14,21,21	4.61	4 (28%)

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
5	SO4	A	2296[B]	-	-	0/0/0/0	0/0/0/0
6	AGP	A	2298[A]	-	-	0/20/20/20	0/0/0/0
2	GLC	A	294	2	-	0/2/22/22	0/1/1/1
2	GLC	A	295	2	-	0/2/19/22	0/1/1/1
3	16G	A	4299	-	-	0/10/30/30	0/1/1/1
3	16G	B	2299	-	-	0/10/30/30	0/1/1/1
5	SO4	B	3296[B]	-	-	0/0/0/0	0/0/0/0
6	AGP	B	3298[A]	-	-	0/20/20/20	0/0/0/0
2	GLC	C	294	2	-	0/2/22/22	0/1/1/1
2	GLC	C	295	2	-	0/2/19/22	0/1/1/1
3	16G	C	3299	-	-	0/10/30/30	0/1/1/1
5	SO4	C	4296[B]	-	-	0/0/0/0	0/0/0/0
5	SO4	C	4297[B]	-	-	0/0/0/0	0/0/0/0
6	AGP	C	4298[A]	-	-	0/20/20/20	0/0/0/0
2	GLC	D	294	2	-	0/2/22/22	0/1/1/1
2	GLC	D	295	2	-	0/2/19/22	0/1/1/1
5	SO4	D	5296[B]	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AGP	D	5298[A]	-	-	0/20/20/20	0/0/0/0
3	16G	D	7299	-	-	0/10/30/30	0/1/1/1
2	GLC	E	294	2	-	0/2/22/22	0/1/1/1
2	GLC	E	295	2	-	0/2/19/22	0/1/1/1
3	16G	E	5299	-	-	0/10/30/30	0/1/1/1
5	SO4	E	6296[B]	-	-	0/0/0/0	0/0/0/0
6	AGP	E	6298[A]	-	-	0/20/20/20	0/0/0/0
2	GLC	F	294	2	-	0/2/22/22	0/1/1/1
2	GLC	F	295	2	-	0/2/19/22	0/1/1/1
3	16G	F	6299	-	-	0/10/30/30	0/1/1/1
5	SO4	F	7296[B]	-	-	0/0/0/0	0/0/0/0
6	AGP	F	7298[A]	-	-	0/20/20/20	0/0/0/0

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	295	GLC	O2-C2	-8.40	1.24	1.43
2	E	295	GLC	O2-C2	-8.38	1.24	1.43
2	D	295	GLC	O2-C2	-8.33	1.24	1.43
2	F	295	GLC	O2-C2	-8.32	1.24	1.43
2	C	295	GLC	O2-C2	-8.28	1.24	1.43
2	F	294	GLC	O3-C3	-7.86	1.24	1.43
2	A	294	GLC	O3-C3	-7.74	1.24	1.43
2	E	294	GLC	O3-C3	-7.70	1.24	1.43
2	D	294	GLC	O3-C3	-7.66	1.24	1.43
2	C	294	GLC	O3-C3	-7.61	1.24	1.43
3	E	5299	16G	O6-C6	-5.03	1.24	1.44
3	B	2299	16G	O6-C6	-4.99	1.24	1.44
3	C	3299	16G	O6-C6	-4.95	1.24	1.44
3	A	4299	16G	O6-C6	-4.95	1.24	1.44
3	D	7299	16G	O6-C6	-4.87	1.24	1.44
3	F	6299	16G	O6-C6	-4.83	1.25	1.44
2	C	295	GLC	O6-C6	-4.23	1.24	1.42
2	A	295	GLC	O6-C6	-4.21	1.24	1.42
2	D	295	GLC	O6-C6	-4.21	1.24	1.42
2	E	295	GLC	O6-C6	-4.20	1.24	1.42
2	F	294	GLC	O6-C6	-4.19	1.24	1.42
2	C	294	GLC	O6-C6	-4.15	1.24	1.42
2	E	294	GLC	O6-C6	-4.15	1.24	1.42
2	F	295	GLC	O6-C6	-4.14	1.24	1.42
2	D	294	GLC	O6-C6	-4.14	1.24	1.42
2	A	294	GLC	O6-C6	-4.06	1.24	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	7299	16G	P-O2P	-2.40	1.46	1.54
3	B	2299	16G	P-O2P	-2.19	1.46	1.54
3	E	5299	16G	P-O2P	-2.19	1.46	1.54
3	C	3299	16G	P-O2P	-2.16	1.46	1.54
3	F	6299	16G	P-O2P	-2.13	1.47	1.54
3	A	4299	16G	P-O2P	-2.06	1.47	1.54
3	B	2299	16G	P-O3P	-2.02	1.47	1.54
3	C	3299	16G	P-O3P	-2.01	1.47	1.54
2	E	294	GLC	C3-C2	2.01	1.57	1.52
3	E	5299	16G	P-O6	2.02	1.67	1.60
3	F	6299	16G	O5-C1	2.02	1.46	1.43
2	C	294	GLC	C3-C2	2.03	1.57	1.52
3	D	7299	16G	O5-C1	2.04	1.46	1.43
3	B	2299	16G	C4-C3	2.05	1.57	1.52
2	A	295	GLC	O5-C1	2.05	1.47	1.43
2	F	294	GLC	C3-C2	2.06	1.57	1.52
3	C	3299	16G	O5-C1	2.09	1.47	1.43
2	D	294	GLC	C3-C2	2.11	1.57	1.52
3	A	4299	16G	O5-C1	2.12	1.47	1.43
6	E	6298[A]	AGP	C6-C5	2.16	1.55	1.51
2	E	295	GLC	C4-C3	2.20	1.58	1.52
2	D	295	GLC	C4-C5	2.22	1.57	1.53
2	A	295	GLC	C4-C5	2.22	1.57	1.53
2	F	295	GLC	O5-C1	2.27	1.47	1.43
3	D	7299	16G	C4-C3	2.29	1.58	1.52
2	E	295	GLC	C4-C5	2.30	1.58	1.53
2	C	295	GLC	C4-C5	2.33	1.58	1.53
6	C	4298[A]	AGP	C6-C5	2.34	1.55	1.51
2	F	295	GLC	C4-C5	2.39	1.58	1.53
2	F	295	GLC	C2-C3	2.41	1.55	1.52
2	E	294	GLC	C4-C3	2.49	1.58	1.52
2	A	294	GLC	C4-C3	2.55	1.59	1.52
2	F	294	GLC	C4-C3	2.56	1.59	1.52
2	F	294	GLC	C4-C5	2.58	1.58	1.53
2	D	294	GLC	C4-C3	2.60	1.59	1.52
3	F	6299	16G	C4-C5	2.61	1.58	1.53
2	C	294	GLC	C4-C5	2.63	1.58	1.53
2	C	295	GLC	C2-C3	2.63	1.56	1.52
2	E	294	GLC	C4-C5	2.65	1.58	1.53
2	C	294	GLC	C4-C3	2.66	1.59	1.52
3	C	3299	16G	C4-C5	2.67	1.58	1.53
3	E	5299	16G	C4-C5	2.70	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2299	16G	C4-C5	2.70	1.58	1.53
3	D	7299	16G	C4-C5	2.71	1.58	1.53
2	D	294	GLC	C4-C5	2.74	1.58	1.53
3	A	4299	16G	C4-C5	2.79	1.59	1.53
2	A	294	GLC	C4-C5	2.80	1.59	1.53
2	D	295	GLC	C2-C3	2.81	1.56	1.52
2	A	295	GLC	C2-C3	2.91	1.56	1.52
2	E	295	GLC	C2-C3	2.99	1.56	1.52
3	C	3299	16G	C8-C7	3.31	1.57	1.50
3	F	6299	16G	C8-C7	3.41	1.57	1.50
3	A	4299	16G	C8-C7	3.44	1.57	1.50
3	E	5299	16G	C8-C7	3.45	1.57	1.50
3	D	7299	16G	C8-C7	3.54	1.57	1.50
3	B	2299	16G	C8-C7	3.55	1.57	1.50
3	D	7299	16G	O1-C1	3.56	1.52	1.39
3	C	3299	16G	O1-C1	3.58	1.52	1.39
3	A	4299	16G	O1-C1	3.61	1.52	1.39
3	B	2299	16G	O1-C1	3.73	1.52	1.39
3	F	6299	16G	O1-C1	3.83	1.53	1.39
3	E	5299	16G	O1-C1	3.90	1.53	1.39
2	E	294	GLC	O1-C1	4.12	1.54	1.39
2	A	294	GLC	O1-C1	4.14	1.54	1.39
2	C	294	GLC	O1-C1	4.16	1.54	1.39
2	F	294	GLC	O1-C1	4.16	1.54	1.39
2	D	294	GLC	O1-C1	4.22	1.54	1.39

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	6298[A]	AGP	O3-C3-C2	-15.76	81.34	110.22
6	F	7298[A]	AGP	O3-C3-C2	-13.51	85.47	110.22
6	C	4298[A]	AGP	O3-C3-C4	-7.16	92.27	109.45
6	C	4298[A]	AGP	O3-C3-C2	-7.15	97.12	110.22
2	C	294	GLC	O2-C2-C1	-6.62	95.23	109.82
2	E	294	GLC	O2-C2-C1	-6.61	95.26	109.82
2	D	294	GLC	O2-C2-C1	-6.43	95.65	109.82
2	F	294	GLC	O2-C2-C1	-6.42	95.68	109.82
2	A	294	GLC	O2-C2-C1	-6.34	95.86	109.82
3	A	4299	16G	O7-C7-C8	-5.38	112.19	122.06
3	E	5299	16G	O7-C7-C8	-5.29	112.35	122.06
3	C	3299	16G	O7-C7-C8	-5.24	112.44	122.06
3	F	6299	16G	O7-C7-C8	-5.20	112.51	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	7299	16G	O7-C7-C8	-5.13	112.65	122.06
3	B	2299	16G	O7-C7-C8	-5.11	112.69	122.06
6	D	5298[A]	AGP	O3-C3-C2	-4.93	101.18	110.22
6	B	3298[A]	AGP	O3-C3-C2	-4.50	101.97	110.22
2	D	294	GLC	O1-C1-O5	-4.11	99.02	110.25
2	A	294	GLC	O1-C1-O5	-4.10	99.02	110.25
2	E	294	GLC	O1-C1-O5	-4.09	99.06	110.25
2	C	294	GLC	O1-C1-O5	-4.07	99.12	110.25
2	F	294	GLC	O1-C1-O5	-4.02	99.25	110.25
6	F	7298[A]	AGP	O3-C3-C4	-3.98	99.91	109.45
6	B	3298[A]	AGP	O6-P-O1P	-3.25	98.86	107.14
6	F	7298[A]	AGP	O6-P-O1P	-3.25	98.86	107.14
6	A	2298[A]	AGP	O6-P-O1P	-3.14	99.14	107.14
2	F	294	GLC	C1-C2-C3	-3.12	105.79	110.43
6	D	5298[A]	AGP	O6-P-O1P	-3.02	99.45	107.14
6	C	4298[A]	AGP	O6-P-O1P	-3.01	99.48	107.14
6	E	6298[A]	AGP	O6-P-O1P	-2.99	99.54	107.14
2	C	294	GLC	C1-C2-C3	-2.98	105.99	110.43
2	A	294	GLC	C1-C2-C3	-2.98	106.00	110.43
2	D	294	GLC	C1-C2-C3	-2.79	106.27	110.43
2	E	294	GLC	C1-C2-C3	-2.72	106.38	110.43
6	E	6298[A]	AGP	O3-C3-C4	-2.36	103.78	109.45
2	E	295	GLC	O5-C1-C2	-2.20	107.29	110.86
6	B	3298[A]	AGP	O1-C1-C2	-2.03	107.25	111.53
6	A	2298[A]	AGP	C5-C4-C3	-2.03	109.18	112.47
2	D	295	GLC	O5-C1-C2	-2.01	107.59	110.86
3	F	6299	16G	O7-C7-N2	2.05	126.04	121.86
3	D	7299	16G	O6-C6-C5	2.05	116.68	109.12
3	E	5299	16G	O6-C6-C5	2.07	116.75	109.12
3	D	7299	16G	O7-C7-N2	2.07	126.08	121.86
3	A	4299	16G	O6-C6-C5	2.10	116.84	109.12
3	C	3299	16G	O7-C7-N2	2.10	126.16	121.86
3	E	5299	16G	O7-C7-N2	2.11	126.16	121.86
3	B	2299	16G	O7-C7-N2	2.11	126.17	121.86
3	A	4299	16G	O7-C7-N2	2.15	126.25	121.86
6	A	2298[A]	AGP	O2P-P-O1P	2.27	117.89	110.58
3	F	6299	16G	O6-C6-C5	2.30	117.60	109.12
2	C	294	GLC	O6-C6-C5	2.32	119.01	111.33
2	D	294	GLC	O6-C6-C5	2.37	119.15	111.33
2	C	295	GLC	O6-C6-C5	2.39	119.23	111.33
2	E	294	GLC	O6-C6-C5	2.42	119.34	111.33
2	F	294	GLC	O6-C6-C5	2.43	119.37	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	295	GLC	O6-C6-C5	2.44	119.39	111.33
2	D	295	GLC	O6-C6-C5	2.49	119.57	111.33
2	E	295	GLC	O6-C6-C5	2.51	119.62	111.33
2	A	294	GLC	O6-C6-C5	2.52	119.65	111.33
3	B	2299	16G	C8-C7-N2	2.64	121.15	116.11
3	D	7299	16G	C8-C7-N2	2.70	121.26	116.11
3	C	3299	16G	C8-C7-N2	2.77	121.40	116.11
2	F	295	GLC	O6-C6-C5	2.77	120.47	111.33
3	F	6299	16G	C8-C7-N2	2.79	121.44	116.11
3	E	5299	16G	C8-C7-N2	2.81	121.49	116.11
3	A	4299	16G	C8-C7-N2	2.85	121.56	116.11
2	C	295	GLC	C1-O5-C5	4.35	117.77	112.25
2	F	295	GLC	C1-O5-C5	4.40	117.83	112.25
2	E	295	GLC	C1-O5-C5	4.41	117.85	112.25
2	A	295	GLC	C1-O5-C5	4.55	118.02	112.25
2	D	295	GLC	C1-O5-C5	4.58	118.06	112.25
2	E	294	GLC	O2-C2-C3	7.22	126.59	110.34
2	A	294	GLC	O2-C2-C3	7.26	126.68	110.34
2	D	294	GLC	O2-C2-C3	7.30	126.77	110.34
2	C	294	GLC	O2-C2-C3	7.31	126.81	110.34
2	F	294	GLC	O2-C2-C3	7.36	126.91	110.34
2	C	294	GLC	O1-C1-C2	7.75	129.98	109.21
2	A	294	GLC	O1-C1-C2	7.75	129.99	109.21
2	F	294	GLC	O1-C1-C2	7.83	130.20	109.21
2	E	294	GLC	O1-C1-C2	7.89	130.34	109.21
2	D	294	GLC	O1-C1-C2	7.92	130.44	109.21
6	F	7298[A]	AGP	O1-C1-C2	8.66	129.75	111.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2298[A]	AGP	1	0
5	F	7296[B]	SO4	1	0
6	F	7298[A]	AGP	5	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	281/289 (97%)	0.12	16 (5%)	27 32	13, 21, 40, 53	7 (2%)
1	B	274/289 (94%)	0.20	16 (5%)	26 31	13, 22, 38, 51	2 (0%)
1	C	274/289 (94%)	-0.06	5 (1%)	71 78	13, 18, 30, 50	3 (1%)
1	D	274/289 (94%)	0.12	10 (3%)	46 52	14, 21, 33, 52	3 (1%)
1	E	274/289 (94%)	0.27	22 (8%)	15 19	14, 24, 43, 53	5 (1%)
1	F	274/289 (94%)	0.20	9 (3%)	50 56	14, 22, 34, 51	3 (1%)
All	All	1651/1734 (95%)	0.14	78 (4%)	35 40	13, 21, 37, 53	23 (1%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	274	GLU	7.5
1	B	178	LEU	7.5
1	F	274	GLU	7.2
1	D	274	GLU	6.9
1	E	274	GLU	6.5
1	B	90	TRP	6.3
1	E	176	GLY	6.1
1	B	274	GLU	6.0
1	F	112	VAL	5.2
1	E	112	VAL	4.9
1	A	239[A]	CYS	4.8
1	B	112	VAL	4.8
1	E	175	ASP	4.8
1	A	178	LEU	4.6
1	A	177	GLU	4.6
1	B	175	ASP	4.5
1	A	172[A]	ARG	4.4
1	A	281	GLN	4.2
1	E	179	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	178	LEU	4.2
1	B	177	GLU	4.1
1	A	175	ASP	4.1
1	A	275	LYS	3.9
1	F	39	LEU	3.6
1	F	37	LEU	3.5
1	E	180	LYS	3.5
1	A	168	LEU	3.5
1	C	135	VAL	3.3
1	B	179	THR	3.3
1	F	32	GLU	3.3
1	A	179	THR	3.2
1	A	176	GLY	3.2
1	B	168	LEU	3.0
1	C	168	LEU	3.0
1	D	175	ASP	3.0
1	F	80	ASP	2.9
1	B	172	ARG	2.9
1	F	135	VAL	2.9
1	E	32	GLU	2.8
1	A	180	LYS	2.8
1	E	173	PHE	2.8
1	D	90	TRP	2.7
1	A	277	THR	2.7
1	D	168	LEU	2.7
1	C	90	TRP	2.7
1	D	260	LEU	2.7
1	E	171	ALA	2.6
1	E	31	PRO	2.6
1	A	32	GLU	2.5
1	B	80	ASP	2.5
1	F	8	HIS	2.5
1	B	32	GLU	2.5
1	E	37	LEU	2.5
1	D	102	GLU	2.4
1	E	135	VAL	2.4
1	E	116	ALA	2.4
1	E	100	HIS	2.4
1	A	260	LEU	2.3
1	E	77	LEU	2.3
1	D	32	GLU	2.3
1	B	71[A]	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	176	GLY	2.2
1	E	39	LEU	2.2
1	B	202[A]	LEU	2.2
1	D	37	LEU	2.2
1	A	276	GLU	2.2
1	E	272	ILE	2.2
1	E	270	TYR	2.2
1	B	180	LYS	2.1
1	E	177	GLU	2.1
1	A	135	VAL	2.1
1	E	202[A]	LEU	2.1
1	B	31	PRO	2.1
1	D	202[A]	LEU	2.1
1	B	126	LYS	2.0
1	F	38	GLY	2.0
1	E	172[A]	ARG	2.0
1	C	43	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GLC	B	295	11/12	0.91	0.10	0.89	22,23,25,26	11
4	GLC	B	294	12/12	0.84	0.14	-	23,26,28,28	12

## 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
6	AGP	C	4298[A]	16/16	0.78	0.28	4.99	41,44,46,47	16
2	GLC	E	295	11/12	0.82	0.14	3.44	28,30,32,33	11
6	AGP	D	5298[A]	16/16	0.90	0.20	3.28	33,38,40,40	16
6	AGP	A	2298[A]	16/16	0.73	0.38	3.01	13,24,32,32	16
6	AGP	E	6298[A]	16/16	0.90	0.21	2.70	37,38,41,42	16
2	GLC	C	295	11/12	0.90	0.12	2.59	21,22,23,26	11
6	AGP	F	7298[A]	16/16	0.89	0.23	2.53	36,37,38,39	16
6	AGP	B	3298[A]	16/16	0.85	0.25	2.36	36,39,42,43	16
5	SO4	C	4297[B]	5/5	0.95	0.11	2.28	34,36,37,38	0
2	GLC	F	295	11/12	0.83	0.15	1.78	23,25,27,32	11
2	GLC	D	295	11/12	0.86	0.13	1.78	26,28,29,31	11
5	SO4	A	2296[B]	5/5	0.88	0.31	1.49	52,52,53,53	5
5	SO4	C	4296[B]	5/5	0.92	0.15	0.91	61,61,61,62	5
2	GLC	A	295	11/12	0.90	0.10	0.15	22,23,24,27	11
5	SO4	B	3296[B]	5/5	0.90	0.13	0.12	55,56,56,56	5
3	16G	D	7299	19/19	0.97	0.08	0.04	16,17,18,19	0
3	16G	E	5299	19/19	0.97	0.08	0.01	19,21,27,27	0
3	16G	B	2299	19/19	0.97	0.08	-0.06	16,18,21,22	0
5	SO4	D	5296[B]	5/5	0.95	0.10	-0.09	44,44,45,45	5
5	SO4	F	7296[B]	5/5	0.96	0.11	-0.16	44,44,44,44	5
3	16G	F	6299	19/19	0.97	0.08	-0.17	18,20,22,24	0
3	16G	A	4299	19/19	0.97	0.07	-0.48	15,18,19,19	0
3	16G	C	3299	19/19	0.98	0.07	-0.51	14,16,18,19	0
5	SO4	E	6296[B]	5/5	0.96	0.07	-0.69	48,49,49,49	5
2	GLC	A	294	12/12	0.83	0.15	-	24,25,28,29	12
2	GLC	D	294	12/12	0.74	0.22	-	27,30,34,34	12
2	GLC	C	294	12/12	0.83	0.12	-	20,24,27,27	12
2	GLC	F	294	12/12	0.86	0.13	-	26,28,28,29	12
2	GLC	E	294	12/12	0.79	0.18	-	30,32,34,34	12

## 6.5 Other polymers ⓘ

There are no such residues in this entry.