



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:34 AM GMT

PDB ID : 1NHC  
Title : Structural insights into the processivity of endopolygalacturonaseI from *Aspergillus niger*  
Authors : van Pouderoyen, G.; Snijder, H.J.; Benen, J.A.; Dijkstra, B.W.  
Deposited on : 2002-12-19  
Resolution : 1.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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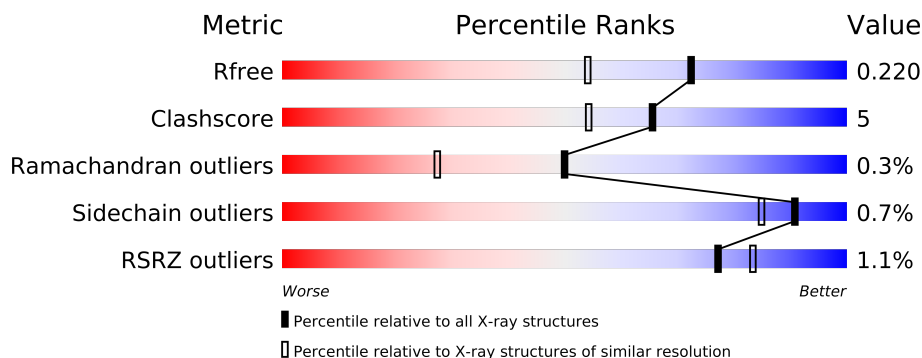
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.70 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))
$R_{free}$	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	336	
1	B	336	
1	C	336	
1	D	336	
1	E	336	
1	F	336	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MAN	A	401	-	X
2	MAN	A	402	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	MAN	B	401	-	X
2	MAN	C	401	-	X
2	MAN	D	401	-	X
2	MAN	E	401	-	X
3	NAG	A	403	-	X
3	NAG	A	404	-	X
3	NAG	C	403	-	X
3	NAG	D	403	-	X
3	NAG	E	403	-	X
3	NAG	F	403	-	X
6	SO4	E	2705	-	X
6	SO4	E	2717	-	X
6	SO4	F	2706	-	X
7	GOL	B	2001	-	X
7	GOL	E	2005	-	X
7	GOL	F	2004	-	X

## 2 Entry composition

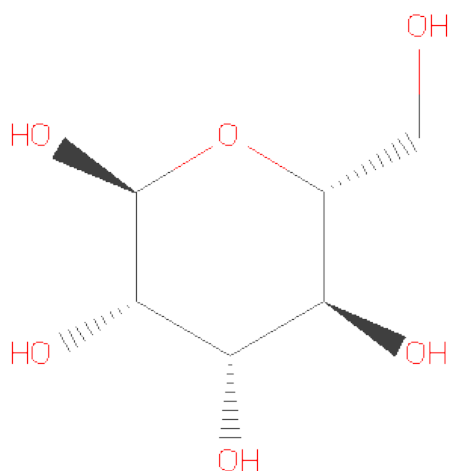
There are 8 unique types of molecules in this entry. The entry contains 16429 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Polygalacturonase I.

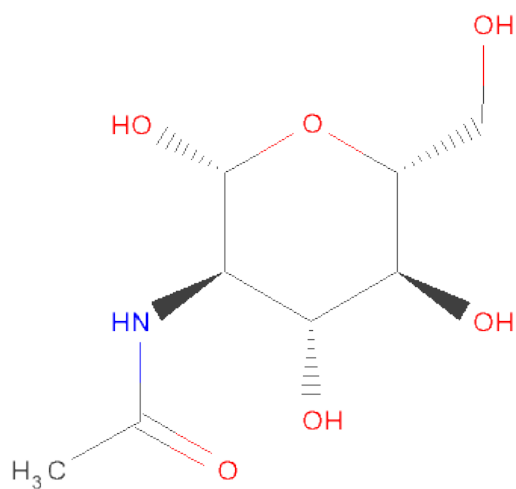
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	B	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	C	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	D	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	E	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	F	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			

- Molecule 2 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (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
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		
2	C	1	Total	C	O	0	0
			11	6	5		
2	C	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		
2	E	1	Total	C	O	0	0
			11	6	5		
2	E	1	Total	C	O	0	0
			11	6	5		
2	F	1	Total	C	O	0	0
			11	6	5		

- Molecule 3 is SUGAR (NAG-NAG) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	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	F	1	Total	C	N	O	0	0
			14	8	1	5		

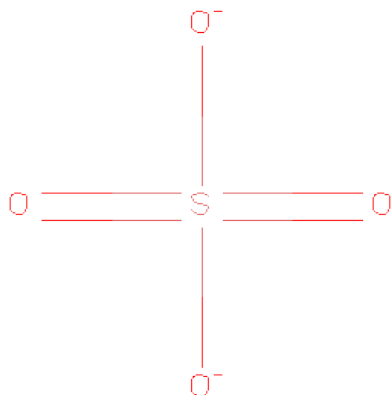
- Molecule 4 is a polymer of unknown type called SUGAR (NAG-NAG-MAN-MAN-MAN-MAN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

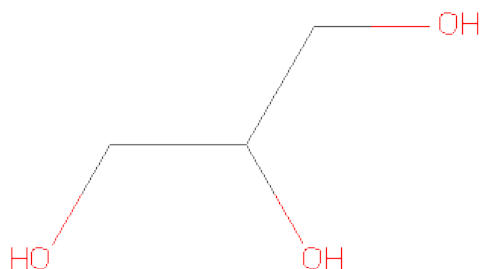
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	2	Total	C	N	O	0	0
			25	14	1	10		

- Molecule 6 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

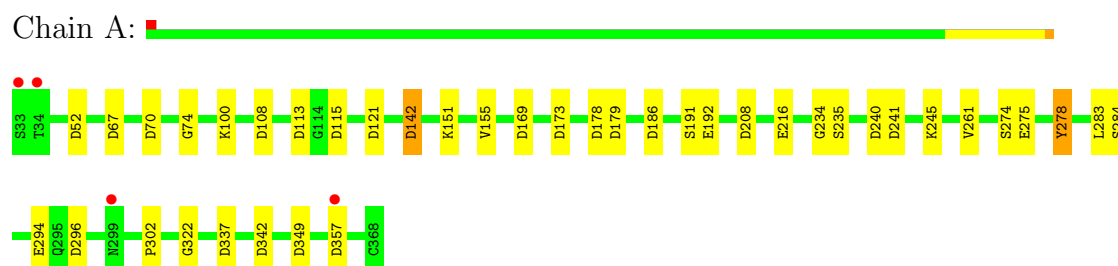
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	239	Total	O	0	0
			239	239		
8	B	166	Total	O	0	0
			166	166		
8	C	252	Total	O	0	0
			252	252		
8	D	211	Total	O	0	0
			211	211		
8	E	252	Total	O	0	0
			252	252		
8	F	233	Total	O	0	0
			233	233		



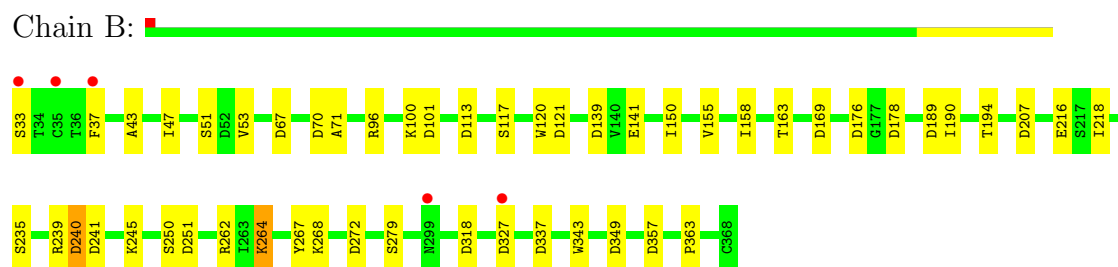
### 3 Residue-property plots

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.

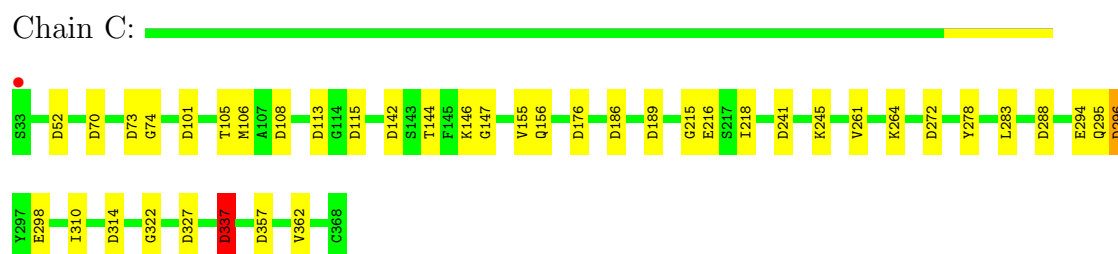
#### • Molecule 1: Polygalacturonase I



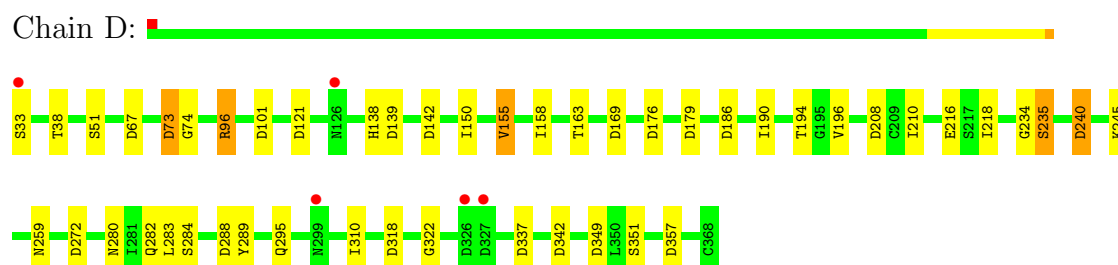
#### • Molecule 1: Polygalacturonase I



#### • Molecule 1: Polygalacturonase I

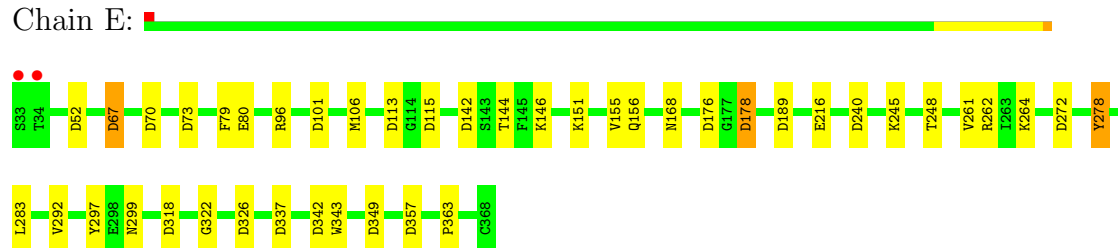


#### • Molecule 1: Polygalacturonase I



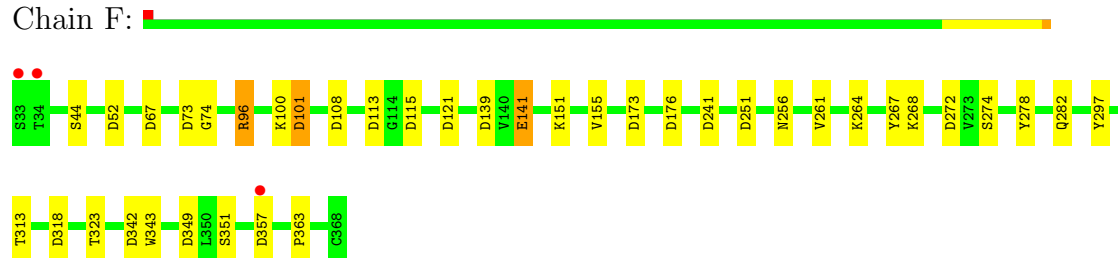
- Molecule 1: Polygalacturonase I

Chain E:



- Molecule 1: Polygalacturonase I

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.01Å 84.13Å 96.03Å 114.32° 98.00° 89.75°	Depositor
Resolution (Å)	35.81 – 1.70 35.79 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (35.81-1.70) 97.5 (35.79-1.70)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.175 , 0.209 0.187 , 0.220	Depositor DCC
$R_{free}$ test set	10409 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 36.8	EDS
Estimated twinning fraction	0.055 for -h,k,-k-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 205731 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16429	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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: MAN, GOL, BMA, NAG, SO4

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	0.74	1/2482 (0.0%)	1.02	17/3374 (0.5%)
1	B	0.68	0/2482	1.01	18/3374 (0.5%)
1	C	0.73	0/2482	1.03	17/3374 (0.5%)
1	D	0.71	0/2482	1.03	17/3374 (0.5%)
1	E	0.73	1/2482 (0.0%)	0.98	16/3374 (0.5%)
1	F	0.75	0/2482	1.00	19/3374 (0.6%)
All	All	0.72	2/14892 (0.0%)	1.01	104/20244 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	D	2	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	TYR	CZ-OH	5.50	1.47	1.37
1	E	278	TYR	CZ-OH	5.17	1.46	1.37

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	ASP	CB-CG-OD2	8.71	126.14	118.30
1	D	357	ASP	CB-CG-OD2	8.37	125.83	118.30
1	D	176	ASP	CB-CG-OD2	8.25	125.73	118.30
1	A	342	ASP	CB-CG-OD2	8.09	125.58	118.30
1	D	186	ASP	CB-CG-OD2	7.98	125.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	ASP	CB-CG-OD2	7.94	125.44	118.30
1	F	357	ASP	CB-CG-OD2	7.93	125.44	118.30
1	D	342	ASP	CB-CG-OD2	7.89	125.40	118.30
1	D	73	ASP	CB-CG-OD2	7.89	125.40	118.30
1	C	108	ASP	CB-CG-OD2	7.74	125.26	118.30
1	B	318	ASP	CB-CG-OD2	7.47	125.03	118.30
1	C	73	ASP	CB-CG-OD2	7.31	124.88	118.30
1	F	349	ASP	CB-CG-OD2	7.07	124.67	118.30
1	B	121	ASP	CB-CG-OD2	7.01	124.61	118.30
1	B	113	ASP	CB-CG-OD2	7.00	124.60	118.30
1	F	342	ASP	CB-CG-OD2	6.95	124.55	118.30
1	C	176	ASP	CB-CG-OD2	6.94	124.55	118.30
1	A	121	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	113	ASP	CB-CG-OD2	6.89	124.50	118.30
1	D	240	ASP	CB-CG-OD2	6.89	124.50	118.30
1	F	115	ASP	CB-CG-OD2	6.74	124.37	118.30
1	D	121	ASP	CB-CG-OD2	6.71	124.34	118.30
1	D	272	ASP	CB-CG-OD2	6.66	124.29	118.30
1	A	115	ASP	CB-CG-OD2	6.63	124.27	118.30
1	C	70	ASP	CB-CG-OD2	6.62	124.26	118.30
1	F	241	ASP	CB-CG-OD2	6.59	124.23	118.30
1	D	349	ASP	CB-CG-OD2	6.57	124.22	118.30
1	B	70	ASP	CB-CG-OD2	6.45	124.10	118.30
1	C	52	ASP	CB-CG-OD2	6.41	124.07	118.30
1	C	186	ASP	CB-CG-OD2	6.41	124.07	118.30
1	C	357	ASP	CB-CG-OD2	6.40	124.06	118.30
1	C	288	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	241	ASP	CB-CG-OD2	6.33	124.00	118.30
1	E	326	ASP	CB-CG-OD2	6.31	123.98	118.30
1	E	176	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	169	ASP	CB-CG-OD2	6.26	123.94	118.30
1	A	52	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	139	ASP	CB-CG-OD2	6.19	123.87	118.30
1	D	318	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	173	ASP	CB-CG-OD2	6.14	123.83	118.30
1	E	357	ASP	CB-CG-OD2	6.14	123.83	118.30
1	E	67	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	241	ASP	CB-CG-OD2	6.10	123.79	118.30
1	D	169	ASP	CB-CG-OD2	6.09	123.78	118.30
1	D	288	ASP	CB-CG-OD2	6.08	123.77	118.30
1	E	272	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	186	ASP	CB-CG-OD2	6.02	123.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	ASP	CB-CG-OD2	6.00	123.70	118.30
1	E	342	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	115	ASP	CB-CG-OD2	5.93	123.64	118.30
1	D	67	ASP	CB-CG-OD2	5.91	123.62	118.30
1	E	73	ASP	CB-CG-OD2	5.89	123.60	118.30
1	E	115	ASP	CB-CG-OD2	5.87	123.58	118.30
1	E	178	ASP	CB-CG-OD2	5.85	123.56	118.30
1	C	296	ASP	CB-CG-OD2	5.84	123.55	118.30
1	E	240	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	349	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	67	ASP	CB-CG-OD2	5.78	123.50	118.30
1	C	337	ASP	CB-CG-OD2	5.78	123.50	118.30
1	F	113	ASP	CB-CG-OD2	5.77	123.49	118.30
1	B	67	ASP	CB-CG-OD2	5.74	123.47	118.30
1	B	272	ASP	CB-CG-OD2	5.74	123.46	118.30
1	C	272	ASP	CB-CG-OD2	5.73	123.45	118.30
1	E	337	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	264	LYS	CD-CE-NZ	5.68	124.76	111.70
1	B	101	ASP	CB-CG-OD2	5.67	123.41	118.30
1	B	349	ASP	CB-CG-OD2	5.67	123.41	118.30
1	C	142	ASP	CB-CG-OD2	5.67	123.40	118.30
1	C	314	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	357	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	337	ASP	CB-CG-OD2	5.61	123.35	118.30
1	F	176	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	113	ASP	CB-CG-OD2	5.56	123.31	118.30
1	F	52	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	240	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	207	ASP	CB-CG-OD2	5.53	123.28	118.30
1	E	142	ASP	CB-CG-OD2	5.50	123.25	118.30
1	D	96	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	E	101	ASP	CB-CG-OD2	5.42	123.17	118.30
1	F	272	ASP	CB-CG-OD2	5.39	123.15	118.30
1	F	121	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	189	ASP	CB-CG-OD2	5.37	123.13	118.30
1	D	208	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	251	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	169	ASP	CB-CG-OD2	5.33	123.10	118.30
1	F	96	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	F	251	ASP	CB-CG-OD2	5.28	123.05	118.30
1	F	67	ASP	CB-CG-OD2	5.28	123.05	118.30
1	E	349	ASP	CB-CG-OD2	5.27	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	173	ASP	CB-CG-OD2	5.25	123.03	118.30
1	F	101	ASP	CB-CG-OD2	5.25	123.02	118.30
1	D	139	ASP	CB-CG-OD2	5.22	123.00	118.30
1	F	108	ASP	CB-CG-OD2	5.20	122.98	118.30
1	E	318	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	142	ASP	CB-CG-OD2	5.18	122.96	118.30
1	E	52	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	70	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	208	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	327	ASP	CB-CG-OD2	5.13	122.92	118.30
1	F	318	ASP	CB-CG-OD2	5.07	122.87	118.30
1	A	179	ASP	CB-CG-OD2	5.06	122.85	118.30
1	F	139	ASP	CB-CG-OD2	5.03	122.82	118.30
1	D	179	ASP	CB-CG-OD1	5.02	122.82	118.30
1	F	73	ASP	CB-CG-OD2	5.01	122.81	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	404	NAG	C1
5	D	405	MAN	C1

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2444	0	2273	18	2
1	B	2444	0	2273	32	2
1	C	2444	0	2273	15	2
1	D	2444	0	2273	30	1
1	E	2444	0	2273	26	1
1	F	2444	0	2274	25	0
2	A	22	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	22	0	20	0	0
2	C	22	0	20	0	0
2	D	33	0	30	0	0
2	E	22	0	20	0	0
2	F	11	0	10	0	0
3	A	28	0	25	2	0
3	C	14	0	13	0	0
3	D	14	0	12	0	0
3	E	14	0	13	0	0
3	F	14	0	13	4	0
4	B	61	0	51	1	0
5	D	25	0	22	0	0
6	A	10	0	0	0	0
6	B	10	0	0	0	0
6	C	20	0	0	0	0
6	D	10	0	0	0	0
6	E	20	0	0	0	0
6	F	10	0	0	0	0
7	A	6	0	8	1	0
7	B	6	0	8	4	0
7	D	6	0	8	5	0
7	E	6	0	8	8	0
7	F	6	0	8	5	0
8	A	239	0	0	9	1
8	B	166	0	0	3	0
8	C	252	0	0	4	0
8	D	211	0	0	6	0
8	E	252	0	0	5	1
8	F	233	0	0	4	0
All	All	16429	0	13948	149	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (149) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:96:ARG:NH2	7:B:2001:GOL:H12	1.23	1.46
1:F:100:LYS:HG2	1:F:141:GLU:OE2	1.50	1.12
1:D:284:SER:HB3	1:F:282:GLN:HE22	1.18	1.06
1:A:261:VAL:HG22	8:A:2905:HOH:O	1.55	1.04
1:D:240:ASP:HB2	8:D:2886:HOH:O	1.61	0.98
1:E:80:GLU:CD	8:E:2946:HOH:O	2.02	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:96:ARG:HH22	7:B:2001:GOL:C1	1.69	0.96
1:C:105:THR:OG1	8:C:2788:HOH:O	1.83	0.95
1:B:240:ASP:HB2	8:B:2810:HOH:O	1.69	0.93
1:A:261:VAL:HA	8:A:2905:HOH:O	1.70	0.91
1:F:44:SER:CB	8:F:2757:HOH:O	2.04	0.91
1:A:74:GLY:O	8:A:2937:HOH:O	1.89	0.91
1:C:264:LYS:CE	8:C:2947:HOH:O	2.20	0.89
3:F:403:NAG:H83	3:F:403:NAG:H3	1.56	0.88
1:B:96:ARG:HH21	7:B:2001:GOL:H12	0.82	0.83
1:D:138:HIS:ND1	7:D:2003:GOL:C1	2.43	0.82
1:D:138:HIS:ND1	7:D:2003:GOL:H11	1.95	0.82
1:F:100:LYS:CG	1:F:141:GLU:OE2	2.28	0.81
1:B:216:GLU:OE2	1:B:245:LYS:HB3	1.81	0.81
1:D:284:SER:HB3	1:F:282:GLN:NE2	1.94	0.80
1:D:73:ASP:HB3	8:D:2915:HOH:O	1.81	0.80
1:F:96:ARG:NH2	7:F:2004:GOL:H32	1.96	0.80
4:B:407:MAN:H2	1:E:299:ASN:HA	1.66	0.77
1:D:284:SER:CB	1:F:282:GLN:HE22	1.96	0.76
1:A:108:ASP:OD2	8:A:2940:HOH:O	2.04	0.74
1:A:261:VAL:CA	8:A:2905:HOH:O	2.32	0.73
1:F:44:SER:HB2	8:F:2757:HOH:O	1.75	0.73
1:B:262:ARG:CZ	1:B:264:LYS:HE2	2.19	0.72
1:E:80:GLU:CG	8:E:2946:HOH:O	2.36	0.71
1:E:96:ARG:HE	7:E:2005:GOL:C3	2.03	0.71
1:A:100:LYS:HE3	1:A:142:ASP:OD2	1.91	0.70
1:B:33:SER:HB2	1:B:51:SER:H	1.56	0.70
1:B:96:ARG:HH21	7:B:2001:GOL:C1	1.75	0.70
1:B:267:TYR:CE2	1:B:268:LYS:HD3	2.28	0.69
1:A:261:VAL:CG2	8:A:2905:HOH:O	2.25	0.69
1:E:113:ASP:OD1	1:E:151:LYS:HE2	1.93	0.68
1:C:264:LYS:HE3	8:C:2947:HOH:O	1.86	0.68
1:E:67:ASP:OD1	7:E:2005:GOL:H2	1.94	0.67
1:D:96:ARG:NH2	7:D:2003:GOL:O3	2.28	0.67
1:E:67:ASP:CG	7:E:2005:GOL:H2	2.15	0.67
1:D:190:ILE:HD12	1:D:210:ILE:HD11	1.78	0.66
7:A:2002:GOL:H12	8:A:2948:HOH:O	1.94	0.65
1:D:38:THR:OG1	8:D:2827:HOH:O	2.15	0.65
3:F:403:NAG:H82	3:F:403:NAG:C1	2.26	0.65
1:E:80:GLU:OE2	8:E:2950:HOH:O	2.14	0.64
1:D:282:GLN:NE2	1:F:323:THR:HG23	2.13	0.63
1:D:280:ASN:HB3	8:D:2884:HOH:O	1.99	0.62
1:D:33:SER:HB2	1:D:51:SER:OG	2.00	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:96:ARG:HE	7:E:2005:GOL:H32	1.65	0.61
1:A:151:LYS:HE3	8:A:2934:HOH:O	2.01	0.61
1:E:96:ARG:NE	7:E:2005:GOL:H32	2.17	0.60
1:D:196:VAL:HB	1:D:218:ILE:HD12	1.85	0.59
1:D:138:HIS:ND1	7:D:2003:GOL:H12	2.17	0.59
1:F:256:ASN:OD1	8:F:2939:HOH:O	2.16	0.59
1:D:73:ASP:OD2	8:D:2916:HOH:O	2.17	0.58
1:B:100:LYS:HG2	1:B:141:GLU:OE1	2.03	0.58
3:F:403:NAG:C8	3:F:403:NAG:C1	2.76	0.58
1:F:100:LYS:HG2	1:F:141:GLU:CD	2.22	0.58
3:A:403:NAG:H62	3:A:404:NAG:N2	2.20	0.57
1:E:80:GLU:HG3	8:E:2946:HOH:O	2.03	0.56
1:B:240:ASP:CB	8:B:2810:HOH:O	2.40	0.56
1:C:264:LYS:HE2	8:C:2947:HOH:O	1.97	0.56
1:D:190:ILE:CD1	1:D:210:ILE:HD11	2.36	0.56
3:A:403:NAG:H62	3:A:404:NAG:HN2	1.71	0.55
1:E:96:ARG:NE	7:E:2005:GOL:C3	2.70	0.54
1:D:196:VAL:HB	1:D:218:ILE:CD1	2.38	0.54
1:B:47:ILE:CD1	1:B:53:VAL:HG21	2.37	0.53
1:A:261:VAL:HG13	1:A:278:TYR:CE2	2.44	0.52
1:F:96:ARG:HH21	7:F:2004:GOL:H32	1.74	0.52
1:B:343:TRP:CD2	1:B:363:PRO:HG2	2.45	0.52
1:B:47:ILE:HD12	1:B:53:VAL:HG21	1.92	0.51
1:B:267:TYR:CZ	1:B:268:LYS:HD3	2.46	0.51
1:C:215:GLY:HA3	1:C:218:ILE:HD11	1.93	0.51
1:A:261:VAL:CB	8:A:2905:HOH:O	2.56	0.50
1:E:79:PHE:HB2	1:E:106:MET:HG2	1.93	0.50
1:B:267:TYR:CZ	1:B:268:LYS:NZ	2.80	0.49
7:F:2004:GOL:H12	8:F:2904:HOH:O	2.12	0.49
1:C:261:VAL:HG13	1:C:278:TYR:CZ	2.48	0.49
1:B:150:ILE:CD1	1:B:158:ILE:HD11	2.42	0.48
1:E:261:VAL:HG13	1:E:278:TYR:CZ	2.49	0.48
1:C:106:MET:HG3	1:C:147:GLY:O	2.12	0.48
1:D:282:GLN:NE2	1:F:323:THR:CG2	2.76	0.48
1:B:262:ARG:CZ	1:B:264:LYS:CE	2.90	0.48
1:E:216:GLU:HA	1:E:245:LYS:O	2.14	0.48
1:C:144:THR:HG22	1:C:146:LYS:HG2	1.96	0.48
1:D:245:LYS:NZ	8:D:2897:HOH:O	2.47	0.47
1:E:264:LYS:HD2	1:E:297:TYR:CZ	2.48	0.47
1:B:47:ILE:HG13	1:B:71:ALA:HA	1.96	0.47
1:C:295:GLN:NE2	1:C:310:ILE:O	2.47	0.47
1:F:100:LYS:HG2	1:F:141:GLU:CG	2.45	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:138:HIS:CE1	7:D:2003:GOL:H11	2.48	0.47
1:B:216:GLU:OE2	1:B:245:LYS:CB	2.59	0.47
1:B:267:TYR:CD2	1:B:268:LYS:HD3	2.50	0.47
1:D:101:ASP:HA	1:D:142:ASP:O	2.15	0.47
1:D:283:LEU:O	1:D:322:GLY:HA3	2.15	0.46
1:A:261:VAL:HG13	1:A:278:TYR:CZ	2.50	0.46
1:B:216:GLU:HA	1:B:245:LYS:O	2.15	0.46
1:B:194:THR:HA	1:B:216:GLU:O	2.15	0.46
1:E:146:LYS:NZ	1:E:168:ASN:HD22	2.13	0.46
1:B:262:ARG:NH1	1:B:264:LYS:HE2	2.31	0.46
1:D:74:GLY:HA2	1:D:101:ASP:O	2.16	0.46
1:A:245:LYS:NZ	1:A:275:GLU:OE1	2.42	0.46
3:F:403:NAG:C8	3:F:403:NAG:H3	2.35	0.46
1:F:100:LYS:HG2	1:F:141:GLU:HG2	1.98	0.45
1:C:283:LEU:O	1:C:322:GLY:HA3	2.15	0.45
1:B:37:PHE:CD1	1:B:43:ALA:HA	2.51	0.45
1:F:96:ARG:NH2	7:F:2004:GOL:C3	2.75	0.44
1:F:264:LYS:HD2	1:F:297:TYR:CZ	2.52	0.44
1:D:216:GLU:HA	1:D:245:LYS:O	2.17	0.44
1:C:74:GLY:HA2	1:C:101:ASP:O	2.18	0.44
1:C:156:GLN:HG2	1:C:189:ASP:OD2	2.18	0.44
1:B:163:THR:HA	1:B:194:THR:O	2.18	0.44
1:F:96:ARG:HH21	7:F:2004:GOL:H12	1.83	0.43
1:D:234:GLY:HA2	1:D:235:SER:C	2.39	0.43
1:D:150:ILE:CD1	1:D:158:ILE:HD11	2.48	0.43
1:A:283:LEU:O	1:A:322:GLY:HA3	2.19	0.43
1:B:190:ILE:HG21	1:B:218:ILE:HD13	2.00	0.43
1:C:294:GLU:OE1	1:C:296:ASP:OD2	2.37	0.42
1:E:343:TRP:CD2	1:E:363:PRO:HG2	2.54	0.42
1:A:234:GLY:HA2	1:A:235:SER:C	2.40	0.42
1:A:294:GLU:OE1	1:A:296:ASP:OD2	2.38	0.42
1:E:248:THR:HG22	8:E:2935:HOH:O	2.19	0.42
1:B:117:SER:HA	1:B:120:TRP:CE3	2.54	0.42
1:E:156:GLN:HG2	1:E:189:ASP:OD2	2.20	0.42
1:C:216:GLU:HA	1:C:245:LYS:O	2.18	0.42
1:A:245:LYS:HA	1:A:274:SER:O	2.19	0.42
1:E:283:LEU:O	1:E:322:GLY:HA3	2.19	0.42
1:B:96:ARG:HG3	1:B:96:ARG:NH1	2.35	0.42
1:E:261:VAL:HG13	1:E:278:TYR:CE1	2.55	0.42
1:D:259:ASN:HA	1:D:289:TYR:O	2.19	0.42
1:D:295:GLN:NE2	1:D:310:ILE:O	2.53	0.41
1:E:262:ARG:HA	1:E:292:VAL:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:343:TRP:CD2	1:F:363:PRO:HG2	2.54	0.41
1:F:74:GLY:HA2	1:F:101:ASP:O	2.20	0.41
1:F:274:SER:HA	1:F:313:THR:O	2.20	0.41
1:E:96:ARG:HD2	7:E:2005:GOL:H31	2.02	0.41
1:F:264:LYS:HB2	1:F:264:LYS:HE3	1.81	0.41
1:F:261:VAL:HG13	1:F:278:TYR:CZ	2.55	0.41
1:A:191:SER:O	1:A:192:GLU:C	2.57	0.41
1:E:67:ASP:OD1	7:E:2005:GOL:C2	2.65	0.41
1:C:261:VAL:HG13	1:C:278:TYR:CE2	2.56	0.41
1:E:144:THR:HG22	1:E:146:LYS:HG3	2.02	0.41
1:B:235:SER:O	1:B:239:ARG:NH2	2.48	0.41
1:D:163:THR:HA	1:D:194:THR:O	2.21	0.41
1:A:216:GLU:HA	1:A:245:LYS:O	2.21	0.41
1:F:267:TYR:CE2	1:F:268:LYS:HG3	2.55	0.41
1:B:250:SER:HA	1:B:279:SER:O	2.20	0.40
1:B:240:ASP:HB2	8:B:2751:HOH:O	2.21	0.40
1:F:264:LYS:HD2	1:F:297:TYR:CE1	2.56	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:178:ASP:OD2	1:C:337:ASP:OD2[1_646]	1.79	0.41
8:A:2872:HOH:O	8:E:2943:HOH:O[1_554]	1.94	0.26
1:A:337:ASP:OD2	1:E:178:ASP:OD2[1_554]	2.11	0.09
1:B:327:ASP:OD2	1:C:298:GLU:OE2[1_646]	2.17	0.03
1:A:178:ASP:OD2	1:D:337:ASP:OD2[1_454]	2.19	0.01

## 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	334/336 (99%)	313 (94%)	20 (6%)	1 (0%)	50	27
1	B	334/336 (99%)	315 (94%)	18 (5%)	1 (0%)	50	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	334/336 (99%)	315 (94%)	18 (5%)	1 (0%)	50	27
1	D	334/336 (99%)	315 (94%)	18 (5%)	1 (0%)	50	27
1	E	334/336 (99%)	313 (94%)	20 (6%)	1 (0%)	50	27
1	F	334/336 (99%)	315 (94%)	18 (5%)	1 (0%)	50	27
All	All	2004/2016 (99%)	1886 (94%)	112 (6%)	6 (0%)	50	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	155	VAL
1	A	155	VAL
1	B	155	VAL
1	D	155	VAL
1	C	155	VAL
1	E	155	VAL

### 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	278/278 (100%)	276 (99%)	2 (1%)	91	85
1	B	278/278 (100%)	277 (100%)	1 (0%)	95	92
1	C	278/278 (100%)	276 (99%)	2 (1%)	91	85
1	D	278/278 (100%)	275 (99%)	3 (1%)	84	72
1	E	278/278 (100%)	277 (100%)	1 (0%)	95	92
1	F	278/278 (100%)	275 (99%)	3 (1%)	84	72
All	All	1668/1668 (100%)	1656 (99%)	12 (1%)	91	85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	284	SER
1	A	302	PRO

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Mol	Chain	Res	Type
1	B	240	ASP
1	C	337	ASP
1	C	362	VAL
1	D	155	VAL
1	D	235	SER
1	D	351	SER
1	E	70	ASP
1	F	141	GLU
1	F	151	LYS
1	F	351	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	282	GLN
1	C	126	ASN
1	C	299	ASN
1	D	282	GLN
1	E	168	ASN
1	F	282	GLN
1	F	299	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

7 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	NAG	B	403	1,4	12,14,15	0.73	0	15,19,21	1.18	2 (13%)
4	NAG	B	404	4	12,14,15	0.71	0	15,19,21	1.36	1 (6%)
4	BMA	B	405	4	10,11,12	0.88	1 (10%)	11,15,17	1.57	1 (9%)
4	MAN	B	406	2,4	10,11,12	0.86	1 (10%)	11,15,17	1.38	2 (18%)
4	MAN	B	407	4	10,11,12	0.84	1 (10%)	11,15,17	0.54	0
5	NAG	D	404	3,5	12,14,15	0.75	0	15,19,21	1.67	5 (33%)
5	MAN	D	405	5	10,11,12	0.80	0	11,15,17	1.70	3 (27%)

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	NAG	B	403	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	404	4	-	0/6/23/26	0/1/1/1
4	BMA	B	405	4	-	0/2/19/22	0/1/1/1
4	MAN	B	406	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	407	4	-	0/2/19/22	0/1/1/1
5	NAG	D	404	3,5	1/1/5/7	0/6/23/26	0/1/1/1
5	MAN	D	405	5	1/1/4/5	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	405	BMA	O5-C5	-2.39	1.41	1.45
4	B	407	MAN	O5-C5	-2.21	1.41	1.45
4	B	406	MAN	O5-C5	-2.13	1.41	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	405	BMA	O5-C5-C6	-4.43	102.33	106.98
5	D	404	NAG	O4-C4-C3	-3.59	102.31	110.35
5	D	405	MAN	C4-C3-C2	-3.03	106.44	110.50
4	B	404	NAG	O5-C5-C4	2.66	114.03	110.65
5	D	405	MAN	O5-C5-C4	2.66	114.03	110.65
5	D	404	NAG	C3-C4-C5	2.56	114.77	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	NAG	O4-C4-C3	-2.54	104.67	110.35
5	D	405	MAN	O5-C5-C6	2.49	109.59	106.98
4	B	406	MAN	O3-C3-C4	-2.48	104.80	110.35
4	B	406	MAN	O3-C3-C2	2.38	114.30	109.94
5	D	404	NAG	C3-C2-N2	-2.37	108.15	111.76
5	D	404	NAG	O5-C5-C6	2.30	109.39	106.98
5	D	404	NAG	O5-C5-C4	2.29	113.56	110.65
4	B	403	NAG	C2-N2-C7	-2.14	119.50	123.09

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	405	MAN	C1
5	D	404	NAG	C1

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

39 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
7	GOL	A	2002	-	5,5,5	0.40	0	5,5,5	0.53	0
6	SO4	A	2701	-	4,4,4	0.57	0	6,6,6	0.65	0
6	SO4	A	2711	-	4,4,4	0.73	0	6,6,6	0.51	0
2	MAN	A	401	1	10,11,12	0.93	1 (10%)	11,15,17	1.20	1 (9%)
2	MAN	A	402	1	10,11,12	0.81	0	11,15,17	1.19	1 (9%)
3	NAG	A	403	1,3	12,14,15	0.61	0	15,19,21	2.86	5 (33%)
3	NAG	A	404	3	12,14,15	0.61	0	15,19,21	1.71	3 (20%)
7	GOL	B	2001	1	5,5,5	0.40	0	5,5,5	0.69	0
6	SO4	B	2702	-	4,4,4	0.31	0	6,6,6	0.31	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	B	2712	-	4,4,4	0.68	0	6,6,6	0.24	0
2	MAN	B	401	1	10,11,12	0.90	1 (10%)	11,15,17	0.87	0
2	MAN	B	402	1	10,11,12	0.81	0	11,15,17	1.39	1 (9%)
6	SO4	C	2703	-	4,4,4	0.08	0	6,6,6	0.75	0
6	SO4	C	2707	-	4,4,4	0.35	0	6,6,6	0.42	0
6	SO4	C	2713	-	4,4,4	0.96	0	6,6,6	0.65	0
6	SO4	C	2718	-	4,4,4	0.34	0	6,6,6	0.38	0
2	MAN	C	401	1	10,11,12	0.77	0	11,15,17	1.07	0
2	MAN	C	402	1	10,11,12	0.93	1 (10%)	11,15,17	1.20	1 (9%)
3	NAG	C	403	1	12,14,15	0.73	1 (8%)	15,19,21	0.71	0
7	GOL	D	2003	1	5,5,5	0.57	0	5,5,5	2.30	3 (60%)
6	SO4	D	2704	-	4,4,4	0.57	0	6,6,6	0.40	0
6	SO4	D	2714	-	4,4,4	0.56	0	6,6,6	0.41	0
2	MAN	D	401	1	10,11,12	0.75	0	11,15,17	0.72	0
2	MAN	D	402	1	10,11,12	0.92	1 (10%)	11,15,17	0.73	0
3	NAG	D	403	1,5	12,14,15	0.77	0	15,19,21	1.11	1 (6%)
2	MAN	D	408	4	10,11,12	0.81	0	11,15,17	0.65	0
7	GOL	E	2005	-	5,5,5	0.14	0	5,5,5	0.73	0
6	SO4	E	2705	-	4,4,4	0.44	0	6,6,6	0.34	0
6	SO4	E	2708	-	4,4,4	0.37	0	6,6,6	0.50	0
6	SO4	E	2715	-	4,4,4	1.00	0	6,6,6	0.51	0
6	SO4	E	2717	-	4,4,4	0.35	0	6,6,6	0.32	0
2	MAN	E	401	1	10,11,12	0.75	0	11,15,17	1.22	2 (18%)
2	MAN	E	402	1	10,11,12	0.68	0	11,15,17	2.08	3 (27%)
3	NAG	E	403	1	12,14,15	0.89	1 (8%)	15,19,21	1.06	1 (6%)
7	GOL	F	2004	-	5,5,5	0.50	0	5,5,5	0.32	0
6	SO4	F	2706	-	4,4,4	0.58	0	6,6,6	0.42	0
6	SO4	F	2716	-	4,4,4	1.01	0	6,6,6	0.72	0
2	MAN	F	402	1	10,11,12	0.87	1 (10%)	11,15,17	1.10	0
3	NAG	F	403	1	12,14,15	1.28	2 (16%)	15,19,21	2.78	7 (46%)

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
7	GOL	A	2002	-	-	0/4/4/4	0/0/0/0
6	SO4	A	2701	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2711	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	A	401	1	-	0/2/19/22	0/1/1/1
2	MAN	A	402	1	-	0/2/19/22	0/1/1/1
3	NAG	A	403	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	404	3	1/1/5/7	0/6/23/26	0/1/1/1
7	GOL	B	2001	1	-	0/4/4/4	0/0/0/0
6	SO4	B	2702	-	-	0/0/0/0	0/0/0/0
6	SO4	B	2712	-	-	0/0/0/0	0/0/0/0
2	MAN	B	401	1	-	0/2/19/22	0/1/1/1
2	MAN	B	402	1	-	0/2/19/22	0/1/1/1
6	SO4	C	2703	-	-	0/0/0/0	0/0/0/0
6	SO4	C	2707	-	-	0/0/0/0	0/0/0/0
6	SO4	C	2713	-	-	0/0/0/0	0/0/0/0
6	SO4	C	2718	-	-	0/0/0/0	0/0/0/0
2	MAN	C	401	1	-	0/2/19/22	0/1/1/1
2	MAN	C	402	1	-	0/2/19/22	0/1/1/1
3	NAG	C	403	1	-	0/6/23/26	0/1/1/1
7	GOL	D	2003	1	-	0/4/4/4	0/0/0/0
6	SO4	D	2704	-	-	0/0/0/0	0/0/0/0
6	SO4	D	2714	-	-	0/0/0/0	0/0/0/0
2	MAN	D	401	1	-	0/2/19/22	0/1/1/1
2	MAN	D	402	1	-	0/2/19/22	0/1/1/1
3	NAG	D	403	1,5	-	0/6/23/26	0/1/1/1
2	MAN	D	408	4	-	0/2/19/22	0/1/1/1
7	GOL	E	2005	-	-	0/4/4/4	0/0/0/0
6	SO4	E	2705	-	-	0/0/0/0	0/0/0/0
6	SO4	E	2708	-	-	0/0/0/0	0/0/0/0
6	SO4	E	2715	-	-	0/0/0/0	0/0/0/0
6	SO4	E	2717	-	-	0/0/0/0	0/0/0/0
2	MAN	E	401	1	-	0/2/19/22	0/1/1/1
2	MAN	E	402	1	-	0/2/19/22	0/1/1/1
3	NAG	E	403	1	-	0/6/23/26	0/1/1/1
7	GOL	F	2004	-	-	0/4/4/4	0/0/0/0
6	SO4	F	2706	-	-	0/0/0/0	0/0/0/0
6	SO4	F	2716	-	-	0/0/0/0	0/0/0/0
2	MAN	F	402	1	-	0/2/19/22	0/1/1/1
3	NAG	F	403	1	-	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	F	403	NAG	C2-N2	-2.96	1.42	1.46
3	E	403	NAG	O5-C5	-2.69	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	MAN	O5-C5	-2.40	1.41	1.45
2	B	401	MAN	O5-C5	-2.26	1.41	1.45
3	F	403	NAG	C3-C2	2.14	1.57	1.52
3	C	403	NAG	O5-C5	-2.14	1.41	1.45
2	D	402	MAN	O2-C2	-2.13	1.39	1.43
2	F	402	MAN	O5-C5	-2.12	1.41	1.45
2	C	402	MAN	O5-C5	-2.05	1.41	1.45

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	403	NAG	C3-C2-N2	7.18	122.69	111.76
3	A	403	NAG	O5-C5-C6	-5.85	100.84	106.98
2	E	402	MAN	O5-C5-C6	5.29	112.53	106.98
3	A	403	NAG	O4-C4-C3	-5.25	98.58	110.35
3	A	403	NAG	C3-C2-N2	-4.80	104.45	111.76
3	F	403	NAG	C2-N2-C7	-4.58	115.41	123.09
7	D	2003	GOL	C3-C2-C1	3.83	128.16	111.26
3	A	403	NAG	O5-C5-C4	3.82	115.50	110.65
3	A	404	NAG	O5-C5-C6	3.66	110.82	106.98
2	B	402	MAN	O5-C5-C6	3.38	110.53	106.98
3	A	403	NAG	O4-C4-C5	3.16	117.61	109.28
2	E	402	MAN	O5-C5-C4	-2.95	106.91	110.65
3	F	403	NAG	O5-C5-C6	2.86	109.98	106.98
3	F	403	NAG	C8-C7-N2	2.86	121.69	116.11
3	A	404	NAG	O5-C5-C4	2.78	114.18	110.65
3	A	404	NAG	C2-N2-C7	-2.75	118.47	123.09
2	A	402	MAN	C4-C3-C2	-2.72	106.86	110.50
3	F	403	NAG	O3-C3-C2	2.69	114.74	109.09
3	F	403	NAG	O7-C7-C8	-2.67	116.84	122.04
2	C	402	MAN	O5-C5-C4	-2.53	107.44	110.65
7	D	2003	GOL	O2-C2-C1	-2.34	97.57	108.22
3	D	403	NAG	O4-C4-C3	-2.32	105.15	110.35
2	E	401	MAN	O5-C5-C6	2.30	109.40	106.98
3	F	403	NAG	O3-C3-C4	-2.25	105.31	110.35
2	E	402	MAN	C4-C3-C2	-2.24	107.50	110.50
2	E	401	MAN	C4-C3-C2	-2.17	107.60	110.50
2	A	401	MAN	C4-C3-C2	-2.14	107.63	110.50
3	E	403	NAG	O5-C5-C4	-2.03	108.08	110.65
7	D	2003	GOL	O3-C3-C2	2.01	119.51	109.71

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	404	NAG	C1

There are no torsion outliers.

There are no ring outliers.

## 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	336/336 (100%)	-0.22	4 (1%) 75 82	14, 22, 34, 50	0
1	B	336/336 (100%)	-0.02	5 (1%) 70 76	15, 25, 42, 66	0
1	C	336/336 (100%)	-0.27	1 (0%) 91 95	13, 21, 33, 54	0
1	D	336/336 (100%)	-0.16	5 (1%) 70 76	15, 22, 34, 52	0
1	E	336/336 (100%)	-0.22	2 (0%) 86 91	13, 21, 33, 63	0
1	F	336/336 (100%)	-0.21	3 (0%) 81 86	14, 22, 35, 60	0
All	All	2016/2016 (100%)	-0.18	20 (0%) 77 85	13, 22, 35, 66	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	33	SER	9.5
1	F	33	SER	9.0
1	B	33	SER	8.5
1	F	34	THR	4.9
1	A	33	SER	4.5
1	D	33	SER	4.1
1	A	34	THR	3.7
1	E	34	THR	3.6
1	B	299	ASN	2.9
1	A	357	ASP	2.8
1	D	327	ASP	2.6
1	D	299	ASN	2.5
1	A	299	ASN	2.4
1	C	33	SER	2.4
1	D	126	ASN	2.3
1	B	35	CYS	2.1
1	B	327	ASP	2.1
1	F	357	ASP	2.1
1	D	326	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	37	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MAN	B	407	11/12	0.50	8.99	63,65,66,67	0
4	MAN	B	406	11/12	0.28	5.17	58,59,60,62	0
5	NAG	D	404	14/15	0.31	4.71	46,53,55,57	0
4	NAG	B	403	14/15	0.20	4.17	27,33,37,39	0
4	NAG	B	404	14/15	0.27	3.52	46,48,50,50	0
5	MAN	D	405	11/12	0.28	2.86	50,51,52,52	0
4	BMA	B	405	11/12	0.25	1.19	48,49,50,50	0

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	E	2005	6/6	0.48	47.97	53,54,54,55	0
3	NAG	A	404	14/15	0.32	6.05	65,65,68,69	0
3	NAG	E	403	14/15	0.21	5.04	47,49,53,55	0
3	NAG	A	403	14/15	0.21	5.01	40,46,50,50	0
3	NAG	D	403	14/15	0.18	4.59	30,37,40,42	0
2	MAN	D	401	11/12	0.18	4.57	43,45,47,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	E	2717	5/5	0.12	3.80	28,29,31,34	0
2	MAN	A	401	11/12	0.16	3.55	42,45,48,51	0
3	NAG	F	403	14/15	0.18	3.46	38,42,50,52	0
7	GOL	B	2001	6/6	0.21	3.46	44,45,48,48	0
3	NAG	C	403	14/15	0.19	3.30	44,46,49,50	0
2	MAN	A	402	11/12	0.15	3.26	33,36,39,40	0
7	GOL	F	2004	6/6	0.24	3.18	34,44,46,50	0
6	SO4	E	2705	5/5	0.11	2.86	22,24,26,28	0
6	SO4	F	2706	5/5	0.12	2.66	29,30,32,33	0
2	MAN	C	401	11/12	0.18	2.47	38,41,45,46	0
2	MAN	E	401	11/12	0.16	2.45	36,39,42,43	0
2	MAN	B	401	11/12	0.19	2.14	57,58,59,61	0
6	SO4	D	2714	5/5	0.13	1.78	36,37,39,40	0
6	SO4	C	2713	5/5	0.12	1.75	34,35,39,43	0
7	GOL	A	2002	6/6	0.18	1.73	41,44,44,46	0
6	SO4	E	2715	5/5	0.12	1.73	34,37,38,43	0
2	MAN	F	402	11/12	0.13	1.55	33,35,37,38	0
7	GOL	D	2003	6/6	0.21	1.41	37,39,44,46	0
6	SO4	C	2703	5/5	0.09	1.40	24,25,25,26	0
6	SO4	C	2718	5/5	0.09	1.37	26,29,32,32	0
2	MAN	E	402	11/12	0.12	1.01	36,40,43,47	0
2	MAN	C	402	11/12	0.13	0.96	32,37,40,42	0
2	MAN	B	402	11/12	0.30	0.57	50,51,52,52	0
6	SO4	A	2711	5/5	0.10	0.35	30,35,37,39	0
6	SO4	F	2716	5/5	0.12	0.32	30,30,36,37	0
6	SO4	B	2712	5/5	0.09	0.26	35,35,37,39	0
2	MAN	D	402	11/12	0.10	0.19	23,27,31,31	0
6	SO4	D	2704	5/5	0.11	0.11	28,30,31,33	0
6	SO4	A	2701	5/5	0.07	-0.31	26,26,27,32	0
6	SO4	B	2702	5/5	0.12	-0.47	48,51,52,52	0
6	SO4	C	2707	5/5	0.04	-2.44	15,16,17,18	0
6	SO4	E	2708	5/5	0.04	-2.51	16,16,17,17	0
2	MAN	D	408	11/12	0.36	-	69,70,71,71	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.