Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 09:07 PM GMT

PDB ID	:	1NHC
Title	:	Structural insights into the processivity of endopolygalacturonase I 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

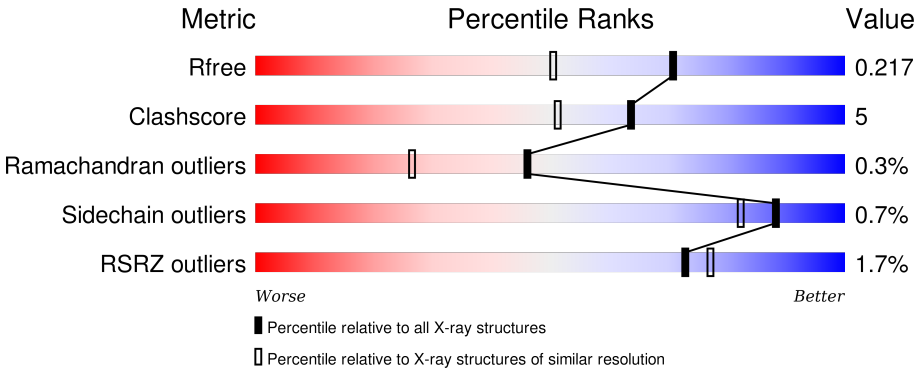
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (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 >=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 <=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	336	88% 11%
1	B	336	3% 85% 15%
1	C	336	88% 12%
1	D	336	2% 86% 13%
1	E	336	87% 12%

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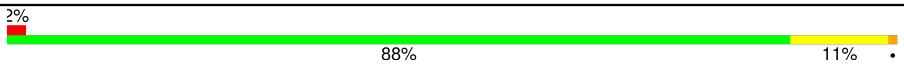
Mol	Chain	Length	Quality of chain
1	F	336	

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	MAN	A	402	-	-	-	X
2	MAN	F	402	-	-	-	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
4	NAG	B	403	-	-	-	X
5	NAG	D	404	X	-	-	-
5	MAN	D	405	X	-	-	-
6	SO4	C	2713	-	-	-	X
6	SO4	D	2714	-	-	-	X
6	SO4	E	2705	-	-	-	X
6	SO4	E	2715	-	-	-	X
6	SO4	F	2706	-	-	-	X
7	GOL	B	2001	-	-	X	X
7	GOL	D	2003	-	-	X	-
7	GOL	E	2005	-	-	X	-
7	GOL	F	2004	-	-	X	X

2 Entry composition

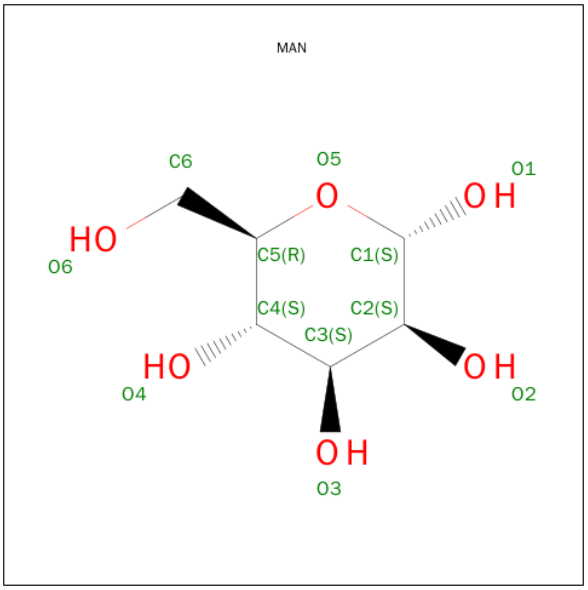
There are 8 unique types of molecules in this entry. The entry contains 16429 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Polygalacturonase I.

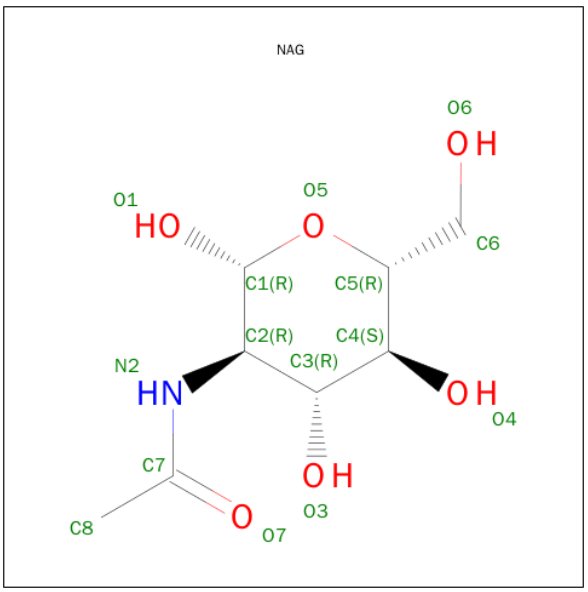
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	B	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	C	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	D	336	Total	C	N	O	S	0	0	0
			2444	1488	399	547	10			
1	E	336	Total	C	N	O	S	0	0	0
			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: $C_6H_{12}O_6$).



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

- 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		

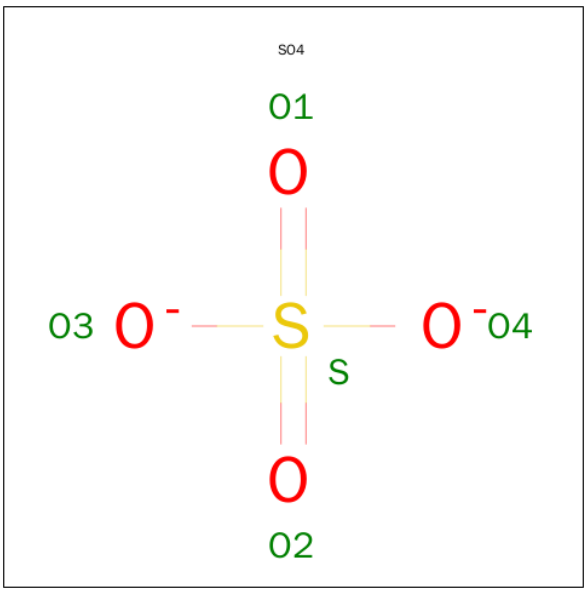
- Molecule 4 is a polymer of unknown type called SUGAR (NAG-NAG-MAN-MAN-MAN-MAN).

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).

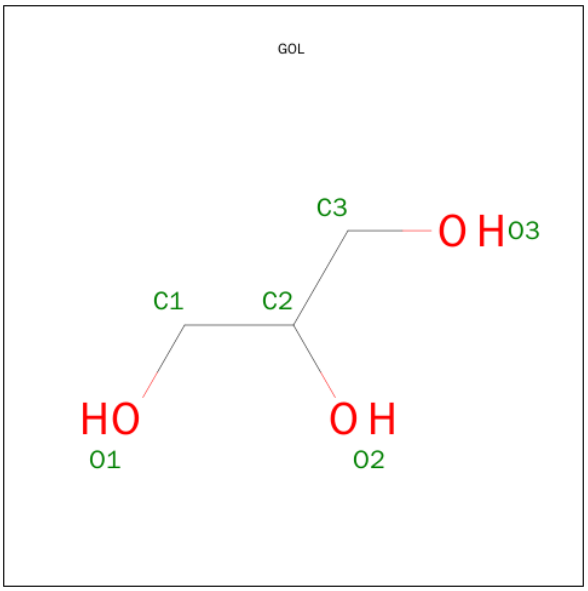
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	2	Total	C	N	O	0	0
			25	14	1	10		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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: $C_3H_8O_3$).



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

- Molecule 8 is water.

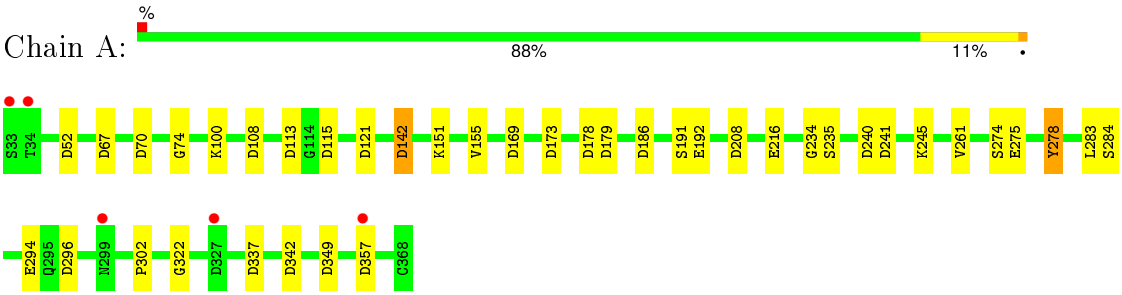
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	239	Total O 239 239	0	0
8	B	166	Total O 166 166	0	0
8	C	252	Total O 252 252	0	0
8	D	211	Total O 211 211	0	0
8	E	252	Total O 252 252	0	0
8	F	233	Total O 233 233	0	0

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.

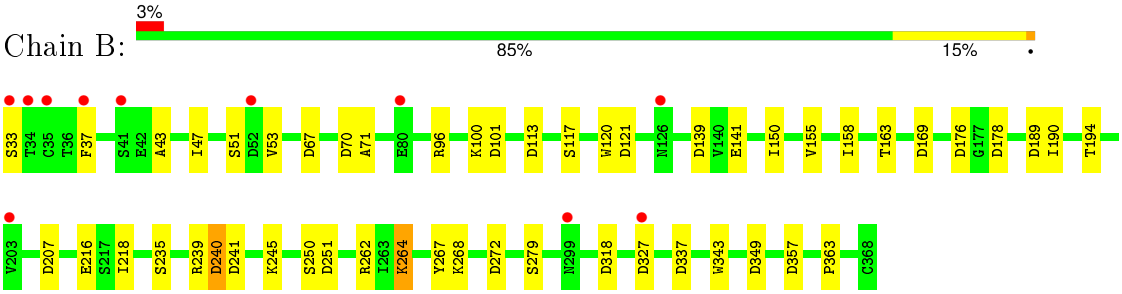
- Molecule 1: Polygalacturonase I

Chain A:



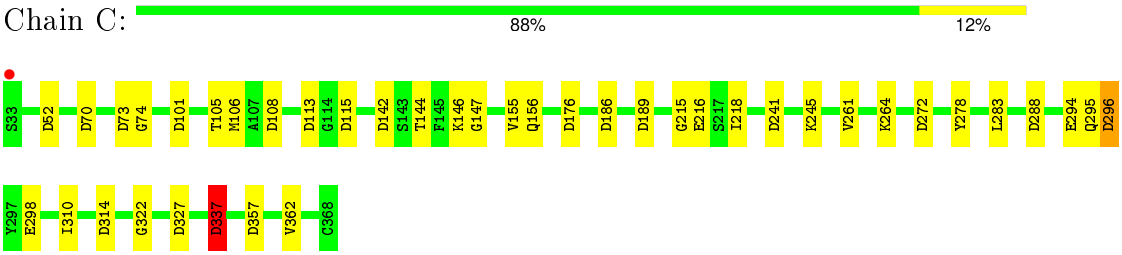
- Molecule 1: Polygalacturonase I

Chain B:



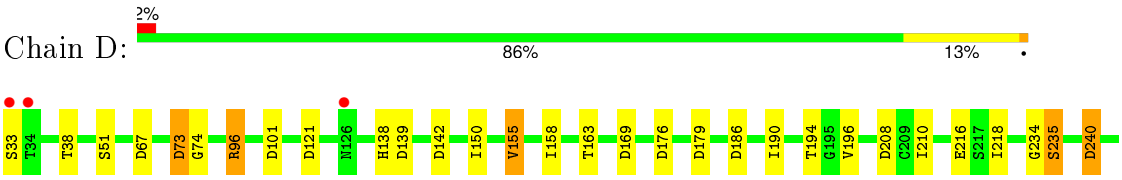
- Molecule 1: Polygalacturonase I

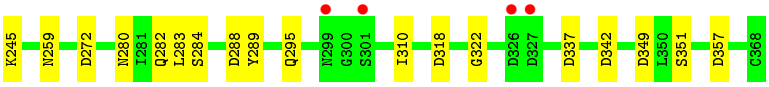
Chain C:



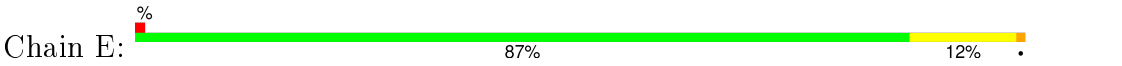
- Molecule 1: Polygalacturonase I

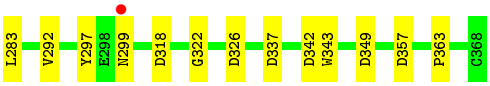
Chain D:



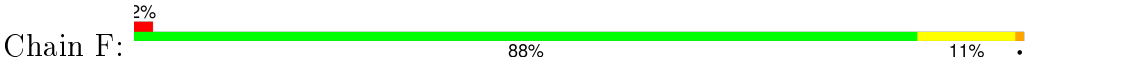


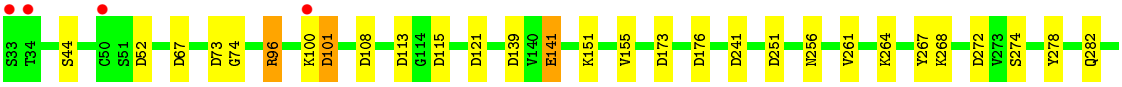
• Molecule 1: Polygalacturonase I

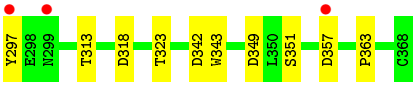




• Molecule 1: Polygalacturonase I







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	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) 84.0 (35.79-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.175 , 0.209 0.185 , 0.217	Depositor DCC
R_{free} test set	10409 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.9	EDS
Estimated twinning fraction	0.055 for -h,k,-k-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 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	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
2	B	22	0	20	0	0
2	C	22	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (149) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:SER:HB2	1:D:51:SER:OG	2.00	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	Interatomic distance (Å)	Clash overlap (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 (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	334/336 (99%)	313 (94%)	20 (6%)	1 (0%)	46	26
1	B	334/336 (99%)	315 (94%)	18 (5%)	1 (0%)	46	26
1	C	334/336 (99%)	315 (94%)	18 (5%)	1 (0%)	46	26
1	D	334/336 (99%)	315 (94%)	18 (5%)	1 (0%)	46	26
1	E	334/336 (99%)	313 (94%)	20 (6%)	1 (0%)	46	26
1	F	334/336 (99%)	315 (94%)	18 (5%)	1 (0%)	46	26
All	All	2004/2016 (99%)	1886 (94%)	112 (6%)	6 (0%)	46	26

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 (i)

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%)	88	82
1	B	278/278 (100%)	277 (100%)	1 (0%)	93	90
1	C	278/278 (100%)	276 (99%)	2 (1%)	88	82
1	D	278/278 (100%)	275 (99%)	3 (1%)	80	69
1	E	278/278 (100%)	277 (100%)	1 (0%)	93	90
1	F	278/278 (100%)	275 (99%)	3 (1%)	80	69
All	All	1668/1668 (100%)	1656 (99%)	12 (1%)	88	82

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

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

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	14,14,15	0.49	0	15,19,21	1.08	2 (13%)
4	NAG	B	404	4	14,14,15	0.56	0	15,19,21	2.23	2 (13%)
4	BMA	B	405	4	11,11,12	0.86	1 (9%)	14,15,17	2.13	4 (28%)
4	MAN	B	406	2,4	11,11,12	0.64	0	14,15,17	1.42	2 (14%)
4	MAN	B	407	4	11,11,12	0.65	0	14,15,17	1.04	1 (7%)
5	NAG	D	404	3,5	14,14,15	0.54	0	15,19,21	2.40	3 (20%)
5	MAN	D	405	5	11,11,12	0.66	0	14,15,17	2.96	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	405	BMA	O5-C1	-2.36	1.39	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	404	NAG	O4-C4-C3	-3.56	102.31	110.34
4	B	403	NAG	C2-N2-C7	-2.75	119.50	123.04
5	D	405	MAN	C2-C3-C4	-2.71	106.44	111.04
4	B	403	NAG	O4-C4-C3	-2.52	104.67	110.34
4	B	406	MAN	O3-C3-C4	-2.46	104.80	110.34
4	B	405	BMA	O5-C5-C6	-2.32	102.33	107.35
4	B	404	NAG	C3-C4-C5	2.01	113.70	110.20
4	B	406	MAN	O3-C3-C2	2.38	114.30	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	407	MAN	C1-C2-C3	2.40	112.38	109.54
5	D	404	NAG	C3-C4-C5	2.62	114.77	110.20
4	B	405	BMA	C1-C2-C3	3.40	113.56	109.54
4	B	405	BMA	O5-C1-C2	4.17	117.62	110.86
4	B	405	BMA	C1-O5-C5	4.64	118.14	112.25
5	D	405	MAN	O5-C1-C2	6.83	121.94	110.86
5	D	405	MAN	C1-O5-C5	7.39	121.62	112.25
4	B	404	NAG	C1-O5-C5	7.51	121.78	112.25
5	D	404	NAG	C1-O5-C5	7.58	121.87	112.25

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	407	MAN	1	0

5.6 Ligand geometry (i)

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	0.46	0
6	SO4	A	2701	-	4,4,4	0.54	0	6,6,6	0.66	0
6	SO4	A	2711	-	4,4,4	0.69	0	6,6,6	0.53	0
2	MAN	A	401	1	11,11,12	0.88	1 (9%)	14,15,17	1.41	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	A	402	1	11,11,12	0.62	0	14,15,17	1.04	2 (14%)
3	NAG	A	403	1,3	14,14,15	0.60	0	15,19,21	2.27	6 (40%)
3	NAG	A	404	3	14,14,15	0.55	0	15,19,21	2.33	3 (20%)
7	GOL	B	2001	1	5,5,5	0.41	0	5,5,5	0.69	0
6	SO4	B	2702	-	4,4,4	0.31	0	6,6,6	0.32	0
6	SO4	B	2712	-	4,4,4	0.62	0	6,6,6	0.24	0
2	MAN	B	401	1	11,11,12	0.83	1 (9%)	14,15,17	1.10	1 (7%)
2	MAN	B	402	1	11,11,12	0.68	0	14,15,17	1.24	1 (7%)
6	SO4	C	2703	-	4,4,4	0.10	0	6,6,6	0.77	0
6	SO4	C	2707	-	4,4,4	0.31	0	6,6,6	0.42	0
6	SO4	C	2713	-	4,4,4	0.91	0	6,6,6	0.68	0
6	SO4	C	2718	-	4,4,4	0.32	0	6,6,6	0.38	0
2	MAN	C	401	1	11,11,12	0.72	0	14,15,17	1.31	1 (7%)
2	MAN	C	402	1	11,11,12	0.91	1 (9%)	14,15,17	0.91	0
3	NAG	C	403	1	14,14,15	0.48	0	15,19,21	0.75	0
7	GOL	D	2003	1	5,5,5	0.58	0	5,5,5	2.48	2 (40%)
6	SO4	D	2704	-	4,4,4	0.55	0	6,6,6	0.39	0
6	SO4	D	2714	-	4,4,4	0.51	0	6,6,6	0.41	0
2	MAN	D	401	1	11,11,12	0.78	1 (9%)	14,15,17	1.02	1 (7%)
2	MAN	D	402	1	11,11,12	0.90	1 (9%)	14,15,17	0.89	0
3	NAG	D	403	1,5	14,14,15	0.63	0	15,19,21	1.05	2 (13%)
2	MAN	D	408	4	11,11,12	0.65	0	14,15,17	0.62	0
7	GOL	E	2005	-	5,5,5	0.15	0	5,5,5	0.72	0
6	SO4	E	2705	-	4,4,4	0.41	0	6,6,6	0.36	0
6	SO4	E	2708	-	4,4,4	0.33	0	6,6,6	0.50	0
6	SO4	E	2715	-	4,4,4	0.94	0	6,6,6	0.53	0
6	SO4	E	2717	-	4,4,4	0.35	0	6,6,6	0.32	0
2	MAN	E	401	1	11,11,12	0.57	0	14,15,17	1.04	1 (7%)
2	MAN	E	402	1	11,11,12	0.59	0	14,15,17	1.28	3 (21%)
3	NAG	E	403	1	14,14,15	0.64	0	15,19,21	0.93	0
7	GOL	F	2004	-	5,5,5	0.51	0	5,5,5	0.29	0
6	SO4	F	2706	-	4,4,4	0.55	0	6,6,6	0.43	0
6	SO4	F	2716	-	4,4,4	0.94	0	6,6,6	0.73	0
2	MAN	F	402	1	11,11,12	0.74	0	14,15,17	1.02	0
3	NAG	F	403	1	14,14,15	1.08	1 (7%)	15,19,21	2.56	6 (40%)

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
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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	MAN	O5-C1	-2.27	1.39	1.43
3	F	403	NAG	O5-C1	-2.26	1.39	1.43
2	D	401	MAN	O5-C1	-2.25	1.39	1.43
2	C	402	MAN	O5-C1	-2.19	1.40	1.43
2	B	401	MAN	O5-C1	-2.08	1.40	1.43
2	D	402	MAN	O5-C1	-2.06	1.40	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	403	NAG	C2-N2-C7	-5.94	115.41	123.04
3	A	403	NAG	O4-C4-C3	-5.22	98.58	110.34
3	A	404	NAG	C2-N2-C7	-3.55	118.47	123.04
3	A	403	NAG	O5-C5-C6	-3.01	100.84	107.35
2	B	401	MAN	O5-C1-C2	-2.86	106.22	110.86
3	F	403	NAG	O7-C7-C8	-2.85	116.84	122.06
3	A	403	NAG	C3-C2-N2	-2.55	104.45	110.56
3	A	404	NAG	C4-C3-C2	-2.49	107.36	111.23
2	D	401	MAN	O5-C1-C2	-2.47	106.85	110.86
2	A	402	MAN	C2-C3-C4	-2.46	106.86	111.04
7	D	2003	GOL	O2-C2-C1	-2.42	97.57	108.65
3	D	403	NAG	C2-N2-C7	-2.37	119.99	123.04
3	D	403	NAG	O4-C4-C3	-2.30	105.15	110.34
3	F	403	NAG	O3-C3-C4	-2.23	105.31	110.34
2	E	402	MAN	C2-C3-C4	-2.09	107.50	111.04
2	E	402	MAN	C1-O5-C5	-2.05	109.65	112.25
2	A	401	MAN	O2-C2-C3	-2.04	106.02	110.12
3	A	403	NAG	C3-C4-C5	-2.03	106.66	110.20
2	A	402	MAN	O2-C2-C1	-2.03	105.14	109.21
2	E	401	MAN	C2-C3-C4	-2.03	107.60	111.04
2	A	401	MAN	C2-C3-C4	-2.01	107.63	111.04
2	E	402	MAN	O5-C5-C6	2.39	112.53	107.35
3	F	403	NAG	O3-C3-C2	2.84	114.74	109.11
3	F	403	NAG	C8-C7-N2	2.92	121.69	116.11
2	B	402	MAN	C1-C2-C3	2.95	113.03	109.54
3	A	403	NAG	C1-O5-C5	2.97	116.02	112.25
3	A	403	NAG	O4-C4-C5	3.16	117.61	109.24
2	A	401	MAN	C1-C2-C3	3.50	113.68	109.54
2	C	401	MAN	C1-C2-C3	3.57	113.77	109.54
7	D	2003	GOL	C3-C2-C1	4.35	128.16	111.12
3	F	403	NAG	C3-C2-N2	5.06	122.69	110.56
3	A	404	NAG	C1-O5-C5	6.99	121.12	112.25

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.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2002	GOL	1	0
3	A	403	NAG	2	0
3	A	404	NAG	2	0
7	B	2001	GOL	4	0
7	D	2003	GOL	5	0
7	E	2005	GOL	8	0
7	F	2004	GOL	5	0
3	F	403	NAG	4	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^{th} 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^2)	Q<0.9
1	A	336/336 (100%)	-0.07	5 (1%) 76 80	14, 22, 34, 50	0
1	B	336/336 (100%)	0.16	11 (3%) 50 54	15, 25, 42, 66	0
1	C	336/336 (100%)	-0.10	1 (0%) 94 95	13, 21, 33, 54	0
1	D	336/336 (100%)	0.02	7 (2%) 67 71	15, 22, 34, 52	0
1	E	336/336 (100%)	-0.08	3 (0%) 85 88	13, 21, 33, 63	0
1	F	336/336 (100%)	-0.07	7 (2%) 67 71	14, 22, 35, 60	0
All	All	2016/2016 (100%)	-0.02	34 (1%) 73 77	13, 22, 35, 66	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	33	SER	9.2
1	F	33	SER	9.0
1	B	33	SER	8.4
1	A	33	SER	5.4
1	F	34	THR	4.9
1	E	34	THR	4.1
1	D	33	SER	4.1
1	A	34	THR	3.8
1	A	357	ASP	3.7
1	D	299	ASN	3.3
1	B	299	ASN	3.2
1	A	299	ASN	3.1
1	D	327	ASP	3.0
1	B	37	PHE	3.0
1	B	327	ASP	2.9
1	B	34	THR	2.7
1	F	297	TYR	2.6
1	B	35	CYS	2.6
1	B	126	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	126	ASN	2.5
1	F	100	LYS	2.5
1	B	52	ASP	2.4
1	D	34	THR	2.4
1	F	357	ASP	2.4
1	F	50	CYS	2.3
1	D	326	ASP	2.3
1	B	41	SER	2.1
1	C	33	SER	2.1
1	F	299	ASN	2.1
1	A	327	ASP	2.1
1	E	299	ASN	2.1
1	B	80	GLU	2.1
1	B	203	VAL	2.1
1	D	301	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^{th} 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^2)	Q<0.9
4	NAG	B	403	14/15	0.89	0.23	5.07	27,33,37,39	0
4	MAN	B	406	11/12	0.73	0.30	-	58,59,60,62	0
4	MAN	B	407	11/12	0.44	0.41	-	63,65,66,67	0
4	NAG	B	404	14/15	0.74	0.30	-	46,48,50,50	0
5	MAN	D	405	11/12	0.54	0.29	-	50,51,52,52	0
5	NAG	D	404	14/15	0.70	0.35	-	46,53,55,57	0
4	BMA	B	405	11/12	0.83	0.25	-	48,49,50,50	0

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^{th} 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^2)	Q<0.9
3	NAG	D	403	14/15	0.82	0.21	7.06	30,37,40,42	0
3	NAG	E	403	14/15	0.80	0.23	6.00	47,49,53,55	0
6	SO4	E	2705	5/5	0.98	0.14	5.48	22,24,26,28	0
3	NAG	F	403	14/15	0.81	0.20	4.68	38,42,50,52	0
3	NAG	C	403	14/15	0.74	0.22	4.47	44,46,49,50	0
6	SO4	C	2713	5/5	0.88	0.15	3.56	34,35,39,43	0
6	SO4	F	2706	5/5	0.98	0.14	3.51	29,30,32,33	0
6	SO4	D	2714	5/5	0.92	0.17	3.33	36,37,39,40	0
7	GOL	B	2001	6/6	0.82	0.22	3.19	44,45,48,48	0
7	GOL	F	2004	6/6	0.82	0.23	2.53	34,44,46,50	0
6	SO4	E	2715	5/5	0.86	0.14	2.50	34,37,38,43	0
2	MAN	A	402	11/12	0.81	0.17	2.38	33,36,39,40	0
2	MAN	F	402	11/12	0.92	0.17	2.08	33,35,37,38	0
7	GOL	A	2002	6/6	0.78	0.17	1.49	41,44,44,46	0
6	SO4	A	2711	5/5	0.94	0.13	1.44	30,35,37,39	0
2	MAN	E	402	11/12	0.90	0.14	1.38	36,40,43,47	0
6	SO4	C	2703	5/5	0.99	0.11	1.33	24,25,25,26	0
7	GOL	D	2003	6/6	0.73	0.21	1.18	37,39,44,46	0
6	SO4	B	2712	5/5	0.94	0.12	1.00	35,35,37,39	0
2	MAN	D	402	11/12	0.92	0.11	0.94	23,27,31,31	0
2	MAN	B	402	11/12	0.75	0.33	0.76	50,51,52,52	0
6	SO4	F	2716	5/5	0.94	0.14	0.50	30,30,36,37	0
6	SO4	D	2704	5/5	0.98	0.12	0.18	28,30,31,33	0
6	SO4	A	2701	5/5	0.98	0.09	0.09	26,26,27,32	0
6	SO4	B	2702	5/5	0.94	0.14	-0.43	48,51,52,52	0
6	SO4	E	2708	5/5	1.00	0.04	-3.05	16,16,17,17	0
6	SO4	C	2707	5/5	0.99	0.04	-3.16	15,16,17,18	0
2	MAN	A	401	11/12	0.83	0.15	-	42,45,48,51	0
6	SO4	E	2717	5/5	0.97	0.13	-	28,29,31,34	0
3	NAG	A	404	14/15	0.65	0.34	-	65,65,68,69	0
3	NAG	A	403	14/15	0.79	0.23	-	40,46,50,50	0
2	MAN	D	408	11/12	0.67	0.43	-	69,70,71,71	0
2	MAN	C	401	11/12	0.77	0.21	-	38,41,45,46	0
7	GOL	E	2005	6/6	0.17	0.46	-	53,54,54,55	0
6	SO4	C	2718	5/5	0.98	0.10	-	26,29,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MAN	C	402	11/12	0.92	0.17	-	32,37,40,42	0
2	MAN	B	401	11/12	0.82	0.21	-	57,58,59,61	0
2	MAN	D	401	11/12	0.70	0.20	-	43,45,47,48	0
2	MAN	E	401	11/12	0.83	0.17	-	36,39,42,43	0

6.5 Other polymers (i)

There are no such residues in this entry.