



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:11 PM GMT

PDB ID : 1OVW
Title : ENDOGLUCANASE I COMPLEXED WITH NON-HYDROLYSABLE SUB-
STRATE ANALOGUE
Authors : Sulzenbacher, G.; Davies, G.J.; Schulein, M.
Deposited on : 1996-10-17
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

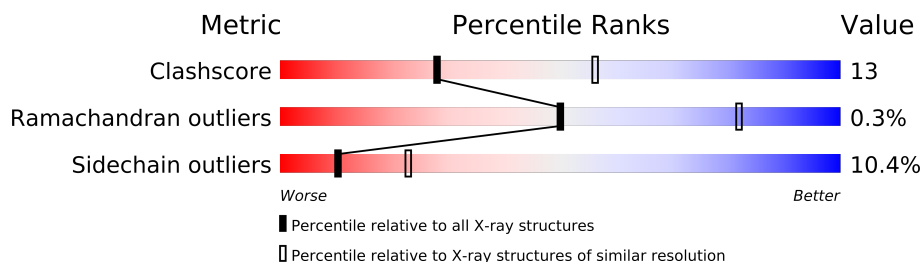
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 2.70 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))
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	398	
1	B	398	
1	C	398	
1	D	398	

2 Entry composition i

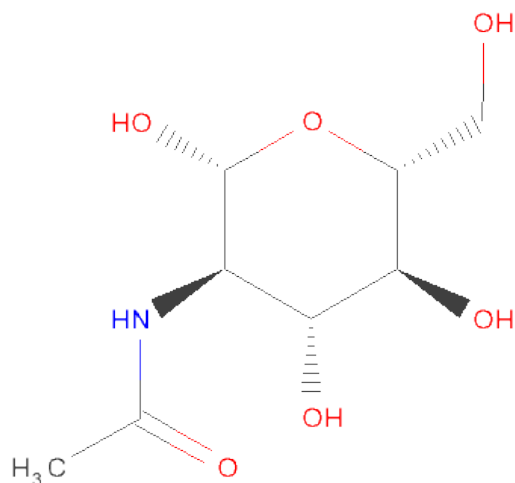
There are 4 unique types of molecules in this entry. The entry contains 13412 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ENDOGLUCANASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3023	1870	534	590	29			
1	B	398	Total	C	N	O	S	0	0	0
			3023	1870	534	590	29			
1	C	398	Total	C	N	O	S	0	0	0
			3023	1870	534	590	29			
1	D	398	Total	C	N	O	S	0	0	0
			3023	1870	534	590	29			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



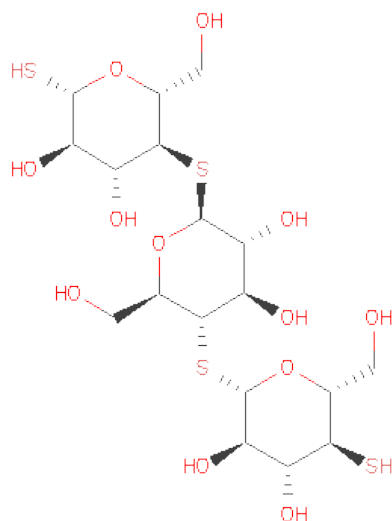
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 1,4-DIMERCAPTO-ALPHA-D-GLUCOPYRANOSYL-(1-4)-S-1,4-DIMERCAPTO-BETA-D-GLUCOPYRANOSYL-(1-4)-S-1,4-DIMERCAPTO-BETA-D-GLUCOPYRANOSE (three-letter code: DP5) (formula: $C_{18}H_{32}O_{12}S_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			34	18	12	4		
3	B	1	Total	C	O	S	0	0
			34	18	12	4		
3	C	1	Total	C	O	S	0	0
			34	18	12	4		
3	D	1	Total	C	O	S	0	0
			34	18	12	4		

- Molecule 4 is water.

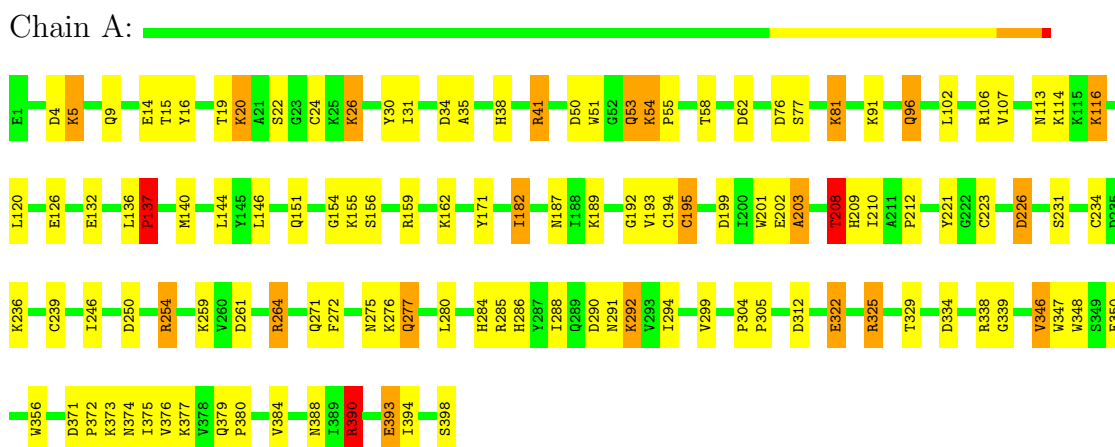
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	275	Total 275	O 275	0	0
4	B	267	Total 267	O 267	0	0
4	C	248	Total 248	O 248	0	0
4	D	282	Total 282	O 282	0	0

3 Residue-property plots

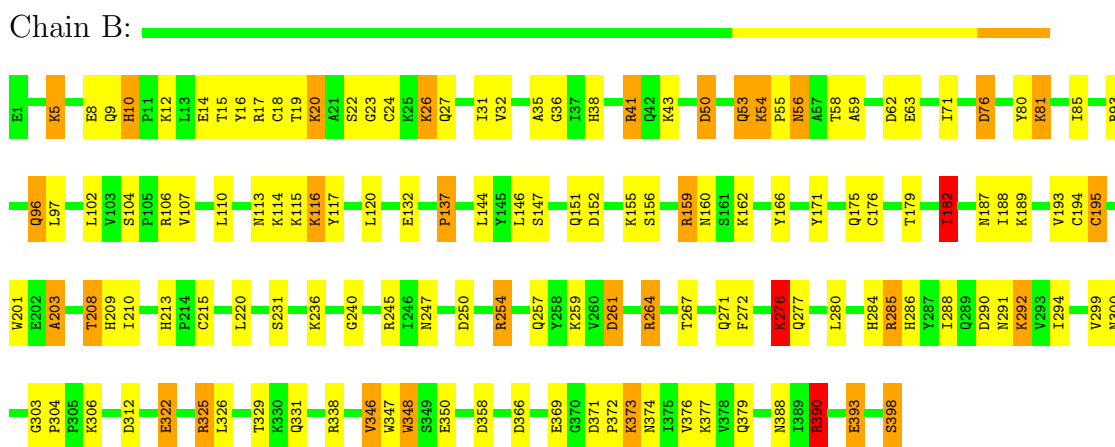
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

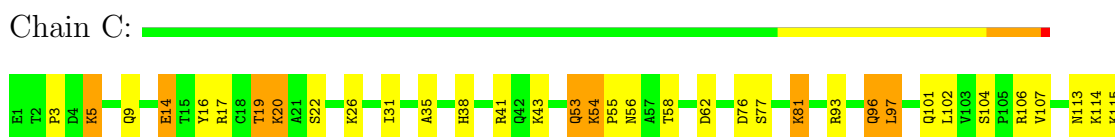
• Molecule 1: ENDOGLUCANASE I

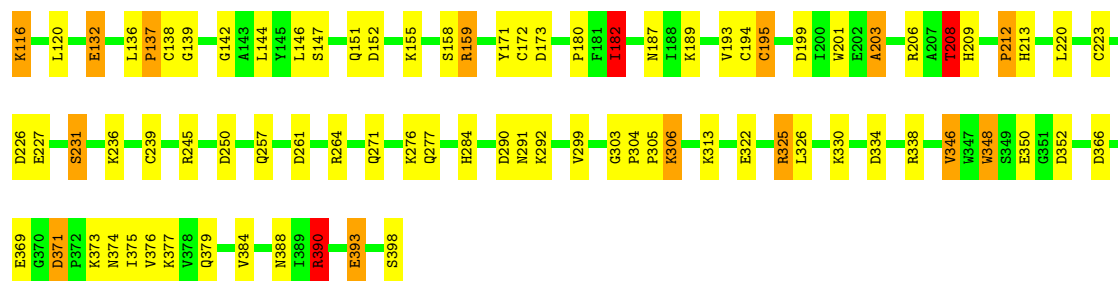


• Molecule 1: ENDOGLUCANASE I



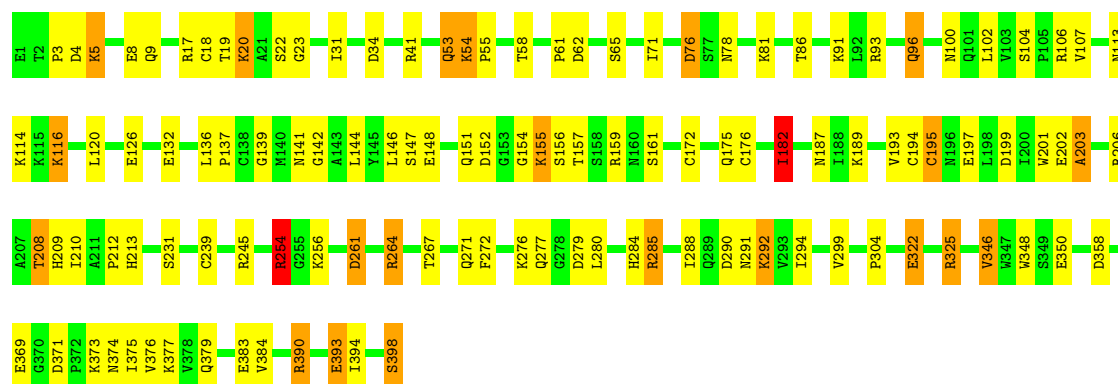
• Molecule 1: ENDOGLUCANASE I





• Molecule 1: ENDOGLUCANASE I

Chain D:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.16Å 78.28Å 142.46Å 90.00° 96.89° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70	Depositor
% Data completeness (in resolution range)	89.5 (15.00-2.70)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13412	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DP5, PCA, NAG

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	0.64	0/3077	1.54	31/4155 (0.7%)
1	B	0.67	0/3077	1.62	45/4155 (1.1%)
1	C	0.66	0/3077	1.61	49/4155 (1.2%)
1	D	0.67	0/3077	1.57	38/4155 (0.9%)
All	All	0.66	0/12308	1.58	163/16620 (1.0%)

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
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	390	ARG	NE-CZ-NH1	21.63	131.11	120.30
1	D	390	ARG	NE-CZ-NH1	18.99	129.80	120.30
1	C	325	ARG	NE-CZ-NH1	17.52	129.06	120.30
1	C	390	ARG	NE-CZ-NH1	16.93	128.77	120.30
1	A	325	ARG	CD-NE-CZ	14.97	144.56	123.60
1	C	93	ARG	NE-CZ-NH2	-14.90	112.85	120.30
1	A	390	ARG	NE-CZ-NH1	14.01	127.30	120.30
1	A	226	ASP	CB-CG-OD2	-13.14	106.48	118.30
1	B	93	ARG	NE-CZ-NH2	-12.16	114.22	120.30
1	B	264	ARG	NE-CZ-NH2	-11.79	114.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	325	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	B	325	ARG	NE-CZ-NH1	10.79	125.70	120.30
1	A	338	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	C	152	ASP	CB-CG-OD1	10.29	127.56	118.30
1	C	352	ASP	CB-CG-OD1	10.24	127.51	118.30
1	A	334	ASP	CB-CG-OD2	-9.82	109.46	118.30
1	B	325	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	B	106	ARG	NE-CZ-NH2	9.78	125.19	120.30
1	B	358	ASP	CB-CG-OD2	9.50	126.85	118.30
1	A	325	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	D	325	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	C	62	ASP	CB-CG-OD2	-8.83	110.35	118.30
1	B	325	ARG	CD-NE-CZ	8.83	135.96	123.60
1	B	17	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	D	285	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	D	325	ARG	CD-NE-CZ	8.66	135.73	123.60
1	D	325	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	D	264	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	C	250	ASP	CB-CG-OD1	8.59	126.03	118.30
1	A	325	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	D	285	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	D	390	ARG	NH1-CZ-NH2	-8.26	110.31	119.40
1	A	390	ARG	CD-NE-CZ	8.24	135.14	123.60
1	C	159	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	C	17	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	D	93	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	A	250	ASP	CB-CG-OD1	7.68	125.21	118.30
1	C	390	ARG	CA-CB-CG	7.59	130.09	113.40
1	B	390	ARG	NH1-CZ-NH2	-7.55	111.10	119.40
1	C	390	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	D	152	ASP	CB-CG-OD1	7.44	125.00	118.30
1	B	346	VAL	CB-CA-C	-7.42	97.30	111.40
1	A	390	ARG	NH1-CZ-NH2	-7.39	111.27	119.40
1	D	261	ASP	CB-CG-OD1	7.33	124.90	118.30
1	B	117	TYR	CB-CG-CD2	7.25	125.35	121.00
1	D	358	ASP	CB-CG-OD1	7.23	124.81	118.30
1	D	261	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	C	325	ARG	CD-NE-CZ	7.20	133.68	123.60
1	D	34	ASP	CB-CG-OD2	7.09	124.68	118.30
1	D	203	ALA	N-CA-CB	-7.05	100.23	110.10
1	D	390	ARG	CD-NE-CZ	6.94	133.32	123.60
1	A	312	ASP	CB-CG-OD1	6.90	124.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	ARG	CA-CB-CG	6.79	128.33	113.40
1	C	17	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	203	ALA	CB-CA-C	-6.66	100.11	110.10
1	C	371	ASP	CB-CG-OD1	6.66	124.29	118.30
1	D	346	VAL	CB-CA-C	-6.64	98.78	111.40
1	B	254	ARG	NE-CZ-NH2	6.61	123.61	120.30
1	C	245	ARG	NE-CZ-NH2	6.53	123.56	120.30
1	B	245	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	159	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	C	106	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	C	173	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	D	76	ASP	CB-CG-OD1	6.42	124.08	118.30
1	D	62	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	338	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	B	254	ARG	NE-CZ-NH1	-6.33	117.13	120.30
1	D	104	SER	N-CA-CB	-6.33	101.00	110.50
1	C	226	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	D	159	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	B	171	TYR	CB-CG-CD2	-6.31	117.22	121.00
1	B	390	ARG	CA-CB-CG	6.29	127.25	113.40
1	B	56	ASN	CB-CG-OD1	-6.28	109.04	121.60
1	B	261	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	D	254	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	B	203	ALA	N-CA-CB	-6.15	101.49	110.10
1	D	390	ARG	CA-CB-CG	6.14	126.92	113.40
1	C	203	ALA	N-CA-CB	-6.09	101.57	110.10
1	C	338	ARG	CD-NE-CZ	6.05	132.08	123.60
1	D	245	ARG	NE-CZ-NH1	-5.95	117.32	120.30
1	A	264	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	346	VAL	N-CA-CB	5.91	124.50	111.50
1	B	346	VAL	N-CA-CB	5.89	124.47	111.50
1	B	390	ARG	CD-NE-CZ	5.88	131.83	123.60
1	A	62	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	71	ILE	CB-CA-C	-5.85	99.91	111.60
1	A	221	TYR	CB-CG-CD1	5.84	124.51	121.00
1	C	132	GLU	OE1-CD-OE2	-5.84	116.29	123.30
1	D	106	ARG	CD-NE-CZ	5.83	131.76	123.60
1	A	346	VAL	CB-CA-C	-5.83	100.33	111.40
1	D	254	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	C	346	VAL	CA-CB-CG2	5.80	119.60	110.90
1	B	152	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	62	ASP	CB-CG-OD1	5.78	123.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	334	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	A	30	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	B	80	TYR	CB-CG-CD1	-5.71	117.58	121.00
1	D	182	ILE	CB-CA-C	-5.69	100.21	111.60
1	C	346	VAL	CB-CA-C	-5.69	100.59	111.40
1	C	306	LYS	CA-CB-CG	5.68	125.89	113.40
1	C	152	ASP	OD1-CG-OD2	-5.63	112.60	123.30
1	D	17	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	C	208	THR	N-CA-CB	5.60	120.94	110.30
1	A	254	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	C	56	ASN	CB-CG-OD1	-5.58	110.44	121.60
1	D	369	GLU	OE1-CD-OE2	-5.56	116.62	123.30
1	A	154	GLY	CA-C-O	-5.52	110.66	120.60
1	D	202	GLU	N-CA-CB	5.51	120.52	110.60
1	D	141	ASN	CA-CB-CG	5.49	125.47	113.40
1	C	206	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	285	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	10	HIS	CA-CB-CG	5.47	122.89	113.60
1	B	312	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	93	ARG	NH1-CZ-NH2	5.46	125.41	119.40
1	C	171	TYR	CB-CG-CD2	-5.46	117.73	121.00
1	C	245	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	B	76	ASP	CB-CG-OD1	5.43	123.19	118.30
1	B	104	SER	N-CA-CB	-5.42	102.37	110.50
1	C	137	PRO	N-CA-CB	5.41	109.79	103.30
1	C	142	GLY	N-CA-C	-5.40	99.60	113.10
1	B	215	CYS	CA-CB-SG	5.40	123.71	114.00
1	C	334	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	62	ASP	CB-CG-OD1	5.39	123.15	118.30
1	D	8	GLU	OE1-CD-OE2	-5.38	116.85	123.30
1	B	182	ILE	CB-CA-C	-5.38	100.85	111.60
1	C	3	PRO	N-CA-CB	5.37	109.74	103.30
1	B	306	LYS	CA-CB-CG	5.37	125.20	113.40
1	A	106	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	C	199	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	D	279	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	B	245	ARG	NH1-CZ-NH2	5.34	125.28	119.40
1	C	346	VAL	N-CA-CB	5.32	123.19	111.50
1	A	34	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	B	36	GLY	O-C-N	-5.29	114.24	122.70
1	A	203	ALA	N-CA-CB	-5.28	102.71	110.10
1	A	137	PRO	N-CA-CB	5.28	109.63	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	MET	CA-CB-CG	5.27	122.26	113.30
1	B	245	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	D	17	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	C	14	GLU	CG-CD-OE2	5.25	128.80	118.30
1	C	182	ILE	CB-CA-C	-5.24	101.13	111.60
1	B	250	ASP	CB-CG-OD1	5.23	123.00	118.30
1	B	50	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	C	208	THR	CA-CB-CG2	-5.20	105.12	112.40
1	A	285	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	C	138	CYS	CA-CB-SG	5.19	123.35	114.00
1	B	276	LYS	CA-CB-CG	5.19	124.81	113.40
1	D	93	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	D	142	GLY	N-CA-C	-5.17	100.16	113.10
1	C	203	ALA	CB-CA-C	-5.16	102.36	110.10
1	A	30	TYR	CA-CB-CG	-5.16	103.61	113.40
1	D	3	PRO	N-CA-CB	5.15	109.48	103.30
1	A	208	THR	CA-CB-CG2	-5.12	105.24	112.40
1	B	166	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	B	338	ARG	CD-NE-CZ	5.08	130.71	123.60
1	D	148	GLU	CG-CD-OE1	5.07	128.44	118.30
1	C	348	TRP	CA-CB-CG	5.06	123.32	113.70
1	A	171	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	C	104	SER	N-CA-CB	-5.04	102.94	110.50
1	C	212	PRO	N-CA-CB	5.04	109.34	103.30
1	B	390	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	B	27	GLN	CB-CA-C	-5.03	100.35	110.40
1	A	305	PRO	N-CA-CB	5.01	109.31	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	THR	Mainchain
1	B	15	THR	Mainchain

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	3023	0	2905	79	0
1	B	3023	0	2905	82	0
1	C	3023	0	2905	65	0
1	D	3023	0	2905	66	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0
2	C	28	0	26	0	0
2	D	28	0	26	0	0
3	A	34	0	32	7	0
3	B	34	0	32	7	0
3	C	34	0	32	5	0
3	D	34	0	31	8	0
4	A	275	0	0	13	0
4	B	267	0	0	13	0
4	C	248	0	0	12	0
4	D	282	0	0	9	0
All	All	13412	0	11851	307	0

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 13.

All (307) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:182:ILE:HG21	4:D:940:HOH:O	1.64	0.95
1:A:203:ALA:HB2	1:A:208:THR:HG23	1.50	0.93
1:D:78:ASN:HB3	4:D:858:HOH:O	1.67	0.93
1:B:203:ALA:HB2	1:B:208:THR:HG23	1.52	0.88
1:D:203:ALA:HB2	1:D:208:THR:HG23	1.55	0.88
1:B:41:ARG:HD3	4:B:584:HOH:O	1.75	0.86
1:C:203:ALA:HB2	1:C:208:THR:HG23	1.56	0.86
1:A:226:ASP:HB2	4:A:632:HOH:O	1.78	0.84
3:D:401:DP5:S4C	3:D:401:DP5:H4B	2.22	0.79
3:C:401:DP5:S4C	3:C:401:DP5:H4B	2.22	0.79
1:B:374:ASN:HA	1:B:377:LYS:HD2	1.62	0.79
1:A:19:THR:HA	1:A:393:GLU:HG3	1.64	0.78
3:A:401:DP5:H4B	3:A:401:DP5:S4C	2.24	0.78
1:A:374:ASN:HA	1:A:377:LYS:HD2	1.65	0.78
1:B:303:GLY:HA3	4:B:627:HOH:O	1.84	0.77
1:A:54:LYS:HB2	1:A:55:PRO:HD2	1.67	0.77
3:B:401:DP5:S4C	3:B:401:DP5:H4B	2.25	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:182:ILE:HD11	1:A:187:ASN:HA	1.68	0.76
1:B:54:LYS:HB2	1:B:55:PRO:HD2	1.68	0.75
1:D:374:ASN:HA	1:D:377:LYS:HD2	1.69	0.75
1:C:374:ASN:HA	1:C:377:LYS:HD2	1.69	0.73
1:A:259:LYS:NZ	4:A:653:HOH:O	2.18	0.72
1:C:5:LYS:H	1:C:5:LYS:HD3	1.54	0.71
1:D:182:ILE:HD11	1:D:187:ASN:HA	1.72	0.70
1:D:54:LYS:HB2	1:D:55:PRO:HD2	1.73	0.70
1:D:19:THR:HA	1:D:393:GLU:HG3	1.74	0.70
1:C:14:GLU:HG2	4:C:566:HOH:O	1.90	0.70
1:D:201:TRP:CZ3	1:D:208:THR:HG21	2.27	0.69
1:C:182:ILE:HG23	1:C:193:VAL:HG22	1.75	0.69
1:A:5:LYS:H	1:A:5:LYS:HD3	1.58	0.68
1:B:201:TRP:CZ3	1:B:208:THR:HG21	2.29	0.68
1:B:113:ASN:O	1:B:114:LYS:HB2	1.92	0.68
1:D:5:LYS:HD3	1:D:5:LYS:H	1.59	0.67
1:D:116:LYS:HB3	1:D:151:GLN:HG2	1.77	0.67
1:B:19:THR:HA	1:B:393:GLU:HG3	1.74	0.67
1:B:5:LYS:HD3	1:B:5:LYS:H	1.59	0.67
1:D:261:ASP:OD2	1:D:264:ARG:HD3	1.94	0.66
1:B:276:LYS:HB2	4:B:657:HOH:O	1.96	0.66
1:C:182:ILE:HD11	1:C:187:ASN:HA	1.78	0.66
1:A:116:LYS:HB3	1:A:151:GLN:HG2	1.77	0.66
3:D:401:DP5:O3C	3:D:401:DP5:H1B	1.97	0.64
1:C:19:THR:HA	1:C:393:GLU:HG3	1.80	0.64
3:B:401:DP5:O3C	3:B:401:DP5:H1B	1.97	0.64
3:D:401:DP5:S4C	3:D:401:DP5:C4B	2.86	0.64
3:A:401:DP5:S4C	3:A:401:DP5:C4B	2.86	0.63
1:C:116:LYS:HB3	1:C:151:GLN:HG2	1.80	0.63
3:C:401:DP5:C4B	3:C:401:DP5:S4C	2.86	0.63
1:B:116:LYS:HB3	1:B:151:GLN:HG2	1.79	0.63
1:C:201:TRP:CZ3	1:C:208:THR:HG21	2.34	0.62
1:B:261:ASP:OD2	1:B:264:ARG:HD3	1.99	0.62
1:C:113:ASN:O	1:C:114:LYS:HB2	1.99	0.62
1:C:120:LEU:HD12	1:C:146:LEU:HD21	1.81	0.62
1:C:54:LYS:HB2	1:C:55:PRO:HD2	1.82	0.62
1:C:299:VAL:HG11	1:C:304:PRO:HB2	1.80	0.62
1:B:182:ILE:HD11	1:B:187:ASN:HA	1.83	0.61
1:B:182:ILE:HG23	1:B:193:VAL:HG22	1.83	0.61
3:C:401:DP5:H1B	3:C:401:DP5:O3C	1.99	0.61
1:C:195:CYS:HA	4:C:576:HOH:O	2.01	0.61
1:B:96:GLN:HE21	1:B:96:GLN:HA	1.65	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:151:GLN:HB3	4:B:647:HOH:O	2.00	0.60
1:A:261:ASP:OD2	1:A:264:ARG:HD3	2.00	0.60
3:B:401:DP5:S4C	3:B:401:DP5:C4B	2.88	0.60
1:D:182:ILE:HG13	1:D:187:ASN:HB2	1.83	0.60
1:A:290:ASP:O	1:A:291:ASN:HB2	2.00	0.60
3:A:401:DP5:O3C	3:A:401:DP5:H1B	2.02	0.60
1:A:194:CYS:O	1:A:195:CYS:HB3	2.02	0.59
1:C:182:ILE:HG13	1:C:187:ASN:HB2	1.83	0.59
1:B:54:LYS:HB2	1:B:55:PRO:CD	2.32	0.59
1:A:201:TRP:CZ3	1:A:208:THR:HG21	2.37	0.59
1:A:54:LYS:HB2	1:A:55:PRO:CD	2.32	0.59
1:C:231:SER:HB3	4:C:487:HOH:O	2.02	0.58
1:C:96:GLN:HA	1:C:96:GLN:HE21	1.69	0.58
1:D:5:LYS:CD	1:D:5:LYS:H	2.15	0.57
1:C:5:LYS:CD	1:C:5:LYS:H	2.15	0.57
1:B:376:VAL:HA	1:B:379:GLN:O	2.05	0.57
1:B:137:PRO:HB2	4:B:524:HOH:O	2.04	0.57
1:A:5:LYS:H	1:A:5:LYS:CD	2.14	0.57
1:D:96:GLN:HA	1:D:96:GLN:HE21	1.70	0.57
1:C:208:THR:HG22	1:C:209:HIS:H	1.69	0.56
1:A:182:ILE:HG13	1:A:187:ASN:HB2	1.87	0.56
1:C:14:GLU:OE1	1:C:26:LYS:HD2	2.06	0.56
1:C:290:ASP:O	1:C:291:ASN:HB2	2.05	0.56
1:D:376:VAL:HA	1:D:379:GLN:O	2.05	0.56
1:A:151:GLN:HB3	4:A:611:HOH:O	2.06	0.55
1:D:120:LEU:HD12	1:D:146:LEU:HD21	1.87	0.55
1:C:271:GLN:HB2	1:C:284:HIS:HB2	1.89	0.55
1:D:54:LYS:HB2	1:D:55:PRO:CD	2.36	0.55
1:A:113:ASN:O	1:A:114:LYS:HB2	2.06	0.55
1:D:113:ASN:O	1:D:114:LYS:HB2	2.06	0.55
1:B:213:HIS:HE1	3:B:401:DP5:H2C	1.70	0.55
1:D:182:ILE:HG23	1:D:193:VAL:HG22	1.88	0.54
1:C:20:LYS:N	1:C:393:GLU:OE2	2.35	0.54
1:B:299:VAL:HG11	1:B:304:PRO:HB2	1.89	0.54
1:D:256:LYS:HD3	4:D:796:HOH:O	2.06	0.54
1:D:194:CYS:O	1:D:195:CYS:HB3	2.07	0.54
1:B:290:ASP:O	1:B:291:ASN:HB2	2.06	0.54
1:A:212:PRO:HD2	1:A:239:CYS:O	2.08	0.54
1:B:288:ILE:CD1	1:B:398:SER:HB2	2.39	0.53
1:A:137:PRO:HG3	1:A:379:GLN:HB3	1.90	0.53
1:B:371:ASP:OD1	1:B:373:LYS:HB3	2.08	0.53
1:D:9:GLN:OE1	1:D:76:ASP:HB2	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:299:VAL:HG11	1:A:304:PRO:HB2	1.89	0.53
1:A:208:THR:HG22	1:A:209:HIS:H	1.73	0.53
1:D:208:THR:HG22	1:D:209:HIS:H	1.74	0.53
1:C:159:ARG:NH2	4:C:616:HOH:O	2.35	0.53
1:B:179:THR:HB	4:B:592:HOH:O	2.09	0.53
1:B:120:LEU:HD12	1:B:146:LEU:HD21	1.91	0.53
1:A:271:GLN:HB2	1:A:284:HIS:HB2	1.90	0.53
1:A:96:GLN:HA	1:A:96:GLN:HE21	1.73	0.52
1:C:388:ASN:OD1	1:C:390:ARG:NH1	2.39	0.52
1:D:137:PRO:HG2	1:D:375:ILE:HG23	1.92	0.52
1:A:388:ASN:OD1	1:A:390:ARG:NH1	2.32	0.52
1:B:388:ASN:OD1	1:B:390:ARG:NH1	2.41	0.52
1:B:159:ARG:HB3	4:B:621:HOH:O	2.09	0.52
1:D:212:PRO:HD2	1:D:239:CYS:O	2.10	0.52
1:C:115:LYS:HE3	4:C:613:HOH:O	2.09	0.52
1:D:137:PRO:HB2	4:D:600:HOH:O	2.10	0.52
1:D:299:VAL:HG11	1:D:304:PRO:HB2	1.92	0.52
1:A:14:GLU:OE1	1:A:26:LYS:HD2	2.10	0.52
1:A:14:GLU:HG2	4:A:569:HOH:O	2.10	0.51
1:B:194:CYS:O	1:B:195:CYS:HB3	2.10	0.51
1:C:194:CYS:O	1:C:195:CYS:HB3	2.10	0.51
1:C:193:VAL:HG13	1:C:220:LEU:HD21	1.93	0.51
1:A:182:ILE:HG23	1:A:193:VAL:HG22	1.93	0.51
1:C:53:GLN:NE2	1:C:54:LYS:O	2.44	0.51
1:B:208:THR:HG22	1:B:209:HIS:H	1.74	0.50
1:A:136:LEU:HD11	1:A:384:VAL:HB	1.92	0.50
1:C:35:ALA:O	1:C:38:HIS:HB2	2.11	0.50
1:D:371:ASP:OD1	1:D:373:LYS:HB3	2.11	0.50
1:A:53:GLN:NE2	1:A:54:LYS:O	2.44	0.50
1:B:5:LYS:CD	1:B:5:LYS:H	2.19	0.50
1:A:371:ASP:O	1:A:375:ILE:HG13	2.11	0.50
1:B:115:LYS:HD2	4:B:614:HOH:O	2.12	0.50
1:A:9:GLN:OE1	1:A:76:ASP:HB2	2.11	0.50
1:A:41:ARG:HD3	4:A:585:HOH:O	2.11	0.50
1:D:290:ASP:O	1:D:291:ASN:HB2	2.11	0.50
1:C:212:PRO:HD2	1:C:239:CYS:O	2.12	0.49
1:C:223:CYS:HB2	1:C:227:GLU:HB2	1.95	0.49
1:D:213:HIS:HE1	3:D:401:DP5:H2C	1.76	0.49
1:B:259:LYS:HE3	4:B:634:HOH:O	2.11	0.49
1:B:35:ALA:O	1:B:38:HIS:HB2	2.13	0.49
1:A:16:TYR:CE2	1:A:26:LYS:HG3	2.48	0.49
1:A:380:PRO:HG2	4:A:672:HOH:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:137:PRO:HB2	4:C:524:HOH:O	2.12	0.49
1:A:202:GLU:OE2	3:A:401:DP5:S4C	2.71	0.49
1:B:32:VAL:HB	1:B:110:LEU:HD11	1.94	0.48
1:B:195:CYS:HA	4:B:572:HOH:O	2.12	0.48
1:B:182:ILE:HG13	1:B:187:ASN:HB2	1.95	0.48
1:A:292:LYS:O	1:A:294:ILE:HD12	2.14	0.48
1:D:91:LYS:HE2	4:D:587:HOH:O	2.14	0.48
1:D:254:ARG:HG3	4:D:500:HOH:O	2.14	0.48
1:C:144:LEU:C	1:C:144:LEU:HD23	2.34	0.48
1:C:376:VAL:HA	1:C:379:GLN:O	2.14	0.48
1:A:203:ALA:CB	1:A:208:THR:HG23	2.35	0.48
1:B:137:PRO:HG3	1:B:379:GLN:HB3	1.96	0.48
1:C:257:GLN:HB3	4:C:610:HOH:O	2.13	0.48
1:A:159:ARG:NH2	4:A:637:HOH:O	2.47	0.48
1:D:54:LYS:HG2	4:D:860:HOH:O	2.14	0.47
1:B:14:GLU:OE2	1:B:26:LYS:HB2	2.14	0.47
1:D:100:ASN:ND2	4:D:805:HOH:O	2.47	0.47
1:A:199:ASP:OD2	3:A:401:DP5:O3C	2.33	0.47
1:A:31:ILE:HG23	1:A:107:VAL:HB	1.97	0.47
1:B:213:HIS:CE1	3:B:401:DP5:H2C	2.49	0.47
1:D:210:ILE:HD11	1:D:285:ARG:NH1	2.30	0.47
1:B:54:LYS:CB	1:B:55:PRO:CD	2.92	0.47
1:B:16:TYR:HB2	1:B:390:ARG:HB3	1.95	0.47
1:B:280:LEU:HD23	1:B:329:THR:CG2	2.45	0.47
1:A:347:TRP:CE3	3:A:401:DP5:H5A	2.50	0.47
1:A:288:ILE:CD1	1:A:398:SER:HB2	2.44	0.47
1:D:144:LEU:HD23	1:D:144:LEU:C	2.35	0.47
1:C:303:GLY:HA3	4:C:611:HOH:O	2.14	0.47
1:A:50:ASP:O	1:A:51:TRP:C	2.54	0.47
1:C:261:ASP:OD2	1:C:264:ARG:HD3	2.15	0.46
1:A:322:GLU:HG3	1:A:325:ARG:HH11	1.80	0.46
1:B:288:ILE:HD11	1:B:398:SER:HB2	1.98	0.46
1:B:175:GLN:O	1:B:176:CYS:HB2	2.15	0.46
1:B:247:ASN:HB3	1:B:300:ASN:HB3	1.97	0.46
1:A:277:GLN:NE2	4:A:606:HOH:O	2.46	0.46
1:A:77:SER:O	1:A:81:LYS:HD2	2.16	0.46
1:A:54:LYS:CB	1:A:55:PRO:CD	2.92	0.46
1:B:9:GLN:OE1	1:B:76:ASP:HB2	2.16	0.46
1:C:313:LYS:HD3	4:C:522:HOH:O	2.15	0.46
1:B:18:CYS:HA	1:B:23:GLY:O	2.15	0.46
1:D:136:LEU:HD11	1:D:384:VAL:HB	1.98	0.46
1:D:175:GLN:O	1:D:176:CYS:HB2	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:20:LYS:N	1:A:393:GLU:OE2	2.46	0.45
1:C:371:ASP:O	1:C:375:ILE:HG13	2.16	0.45
1:D:126:GLU:HB2	1:D:394:ILE:HA	1.99	0.45
1:D:197:GLU:OE1	3:D:401:DP5:O2B	2.32	0.45
1:A:272:PHE:HB3	1:A:280:LEU:HD11	1.97	0.45
1:A:54:LYS:CB	1:A:55:PRO:HD2	2.42	0.45
1:A:137:PRO:HG2	1:A:375:ILE:HG23	1.99	0.45
1:A:371:ASP:OD1	1:A:373:LYS:HB3	2.16	0.45
1:B:280:LEU:HD23	1:B:329:THR:HG22	1.98	0.45
1:A:322:GLU:HG3	1:A:325:ARG:NH1	2.32	0.45
1:A:120:LEU:HD12	1:A:146:LEU:HD21	1.99	0.45
1:D:206:ARG:HH11	1:D:206:ARG:HG3	1.82	0.45
1:A:116:LYS:HB3	1:A:151:GLN:CG	2.46	0.45
1:A:91:LYS:HE2	4:A:511:HOH:O	2.17	0.45
1:D:31:ILE:HG23	1:D:107:VAL:HB	1.99	0.45
1:B:31:ILE:HG23	1:B:107:VAL:HB	1.98	0.45
1:D:53:GLN:NE2	1:D:54:LYS:O	2.50	0.45
1:C:54:LYS:CB	1:C:55:PRO:HD2	2.46	0.45
1:B:81:LYS:HE2	1:B:85:ILE:O	2.17	0.45
1:C:9:GLN:OE1	1:C:76:ASP:HB2	2.17	0.44
1:D:208:THR:HG22	1:D:209:HIS:N	2.32	0.44
1:C:213:HIS:HE1	3:C:401:DP5:H2C	1.82	0.44
1:C:172:CYS:HB3	1:C:193:VAL:HG12	2.00	0.44
1:B:20:LYS:N	1:B:393:GLU:OE2	2.44	0.44
1:B:325:ARG:NH2	1:B:326:LEU:HD21	2.32	0.44
1:C:158:SER:OG	1:C:159:ARG:N	2.51	0.44
1:C:371:ASP:OD1	1:C:373:LYS:HB3	2.18	0.44
1:A:246:ILE:HG13	1:A:246:ILE:H	1.70	0.44
1:B:63:GLU:HG2	1:B:160:ASN:HD22	1.83	0.44
1:D:203:ALA:CB	1:D:208:THR:HG23	2.37	0.44
1:C:137:PRO:HG3	1:C:379:GLN:HB3	2.00	0.44
1:C:306:LYS:N	1:C:306:LYS:HE2	2.33	0.44
1:D:18:CYS:HA	1:D:23:GLY:O	2.16	0.44
1:B:257:GLN:HG3	4:B:596:HOH:O	2.16	0.44
1:B:193:VAL:HG13	1:B:220:LEU:HD21	1.99	0.44
1:A:16:TYR:HB3	1:A:24:CYS:HB3	1.99	0.44
1:B:208:THR:HG22	1:B:209:HIS:N	2.32	0.44
1:C:81:LYS:HD3	4:C:638:HOH:O	2.18	0.44
1:A:19:THR:HA	1:A:393:GLU:CG	2.41	0.44
1:A:126:GLU:HB2	1:A:394:ILE:HA	1.99	0.44
1:B:50:ASP:H	1:B:53:GLN:NE2	2.15	0.44
1:D:271:GLN:HB2	1:D:284:HIS:HB2	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:383:GLU:HG3	4:D:770:HOH:O	2.17	0.44
1:A:20:LYS:H	1:A:393:GLU:CD	2.21	0.43
1:C:19:THR:HA	1:C:393:GLU:CG	2.46	0.43
1:A:376:VAL:HA	1:A:379:GLN:O	2.18	0.43
1:A:96:GLN:CA	1:A:96:GLN:HE21	2.29	0.43
1:A:210:ILE:HG13	4:A:413:HOH:O	2.17	0.43
1:B:366:ASP:CG	1:B:369:GLU:HG2	2.39	0.43
3:B:401:DP5:O3C	3:B:401:DP5:C1B	2.64	0.43
1:C:137:PRO:HG2	1:C:375:ILE:HG23	2.01	0.43
1:D:61:PRO:HD2	1:D:65:SER:HB2	2.00	0.43
1:B:203:ALA:CB	1:B:208:THR:HG23	2.38	0.43
1:D:54:LYS:CB	1:D:55:PRO:CD	2.97	0.43
1:A:280:LEU:HD23	1:A:329:THR:HG22	2.01	0.43
1:D:322:GLU:HG3	1:D:325:ARG:NH1	2.34	0.43
1:D:267:THR:HB	1:D:288:ILE:HB	2.00	0.43
1:B:144:LEU:HD23	1:B:144:LEU:C	2.38	0.43
1:A:356:TRP:CZ2	3:A:401:DP5:H5C	2.54	0.43
1:A:144:LEU:C	1:A:144:LEU:HD23	2.40	0.43
1:A:35:ALA:O	1:A:38:HIS:HB2	2.19	0.43
1:D:139:GLY:HA3	1:D:375:ILE:HD11	2.01	0.42
1:B:54:LYS:CB	1:B:55:PRO:HD2	2.42	0.42
1:A:4:ASP:HB2	1:A:5:LYS:HD3	2.02	0.42
1:C:208:THR:HG22	1:C:209:HIS:N	2.32	0.42
3:D:401:DP5:O3C	3:D:401:DP5:C1B	2.65	0.42
1:B:50:ASP:H	1:B:53:GLN:HE21	1.67	0.42
1:C:366:ASP:CG	1:C:369:GLU:HG2	2.40	0.42
1:D:272:PHE:HB3	1:D:280:LEU:HD11	2.02	0.42
1:D:199:ASP:OD2	3:D:401:DP5:H1B	2.19	0.42
1:B:347:TRP:CE3	3:B:401:DP5:H5A	2.54	0.42
1:C:20:LYS:H	1:C:393:GLU:CD	2.22	0.42
1:A:120:LEU:O	1:A:339:GLY:HA2	2.19	0.42
1:A:192:GLY:HA3	1:A:223:CYS:SG	2.59	0.42
1:B:162:LYS:NZ	4:B:532:HOH:O	2.52	0.42
1:B:348:TRP:CE2	1:B:372:PRO:HB3	2.54	0.42
1:C:31:ILE:HG23	1:C:107:VAL:HB	2.01	0.42
1:C:325:ARG:NH2	1:C:326:LEU:HD21	2.33	0.42
1:C:77:SER:HB3	4:C:638:HOH:O	2.19	0.42
1:D:4:ASP:HB3	1:D:71:ILE:CG2	2.49	0.42
1:C:16:TYR:HB2	1:C:390:ARG:HB3	2.01	0.42
1:B:56:ASN:HB3	1:B:59:ALA:HB3	2.00	0.42
1:D:172:CYS:HB3	1:D:193:VAL:HG12	2.01	0.42
1:C:203:ALA:CB	1:C:208:THR:HG23	2.40	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:54:LYS:HB2	1:C:55:PRO:CD	2.48	0.42
1:D:292:LYS:O	1:D:294:ILE:HD12	2.19	0.42
1:A:116:LYS:HB3	1:A:116:LYS:HE3	1.88	0.41
3:C:401:DP5:C1B	3:C:401:DP5:O3C	2.67	0.41
1:B:292:LYS:O	1:B:294:ILE:HD12	2.20	0.41
1:D:199:ASP:OD2	3:D:401:DP5:O3C	2.38	0.41
1:B:53:GLN:HE21	1:B:53:GLN:HB3	1.75	0.41
1:A:194:CYS:HB3	1:A:234:CYS:SG	2.61	0.41
1:B:20:LYS:H	1:B:393:GLU:CD	2.24	0.41
1:C:264:ARG:NH2	1:C:290:ASP:OD1	2.53	0.41
1:B:12:LYS:HE2	4:B:564:HOH:O	2.20	0.41
1:B:322:GLU:HG3	1:B:325:ARG:HH11	1.86	0.41
1:D:155:LYS:HA	1:D:161:SER:OG	2.20	0.41
1:B:210:ILE:HD11	1:B:285:ARG:NH1	2.36	0.41
1:A:275:ASN:HB2	4:A:665:HOH:O	2.19	0.41
1:B:53:GLN:NE2	1:B:54:LYS:O	2.54	0.41
1:B:16:TYR:HB3	1:B:24:CYS:HB3	2.02	0.41
1:B:210:ILE:O	1:B:240:GLY:HA2	2.21	0.41
1:B:271:GLN:HB2	1:B:284:HIS:HB2	2.01	0.41
1:D:374:ASN:O	1:D:375:ILE:C	2.59	0.41
1:D:371:ASP:O	1:D:375:ILE:HG13	2.20	0.41
1:B:267:THR:HB	1:B:288:ILE:HB	2.02	0.41
1:A:371:ASP:HA	1:A:372:PRO:HD3	1.82	0.41
1:C:136:LEU:HD11	1:C:384:VAL:HB	2.03	0.41
1:D:20:LYS:N	1:D:393:GLU:OE2	2.51	0.41
1:B:188:ILE:HG12	1:B:188:ILE:H	1.70	0.41
1:B:288:ILE:HD12	1:B:398:SER:HB2	2.01	0.40
1:D:288:ILE:CD1	1:D:398:SER:HB2	2.51	0.40
1:D:154:GLY:O	1:D:157:THR:HG23	2.21	0.40
1:D:54:LYS:CB	1:D:55:PRO:HD2	2.48	0.40
1:C:330:LYS:HB2	4:C:591:HOH:O	2.21	0.40
1:B:8:GLU:HG2	1:B:10:HIS:CE1	2.56	0.40
1:A:113:ASN:HB3	4:A:577:HOH:O	2.21	0.40
1:B:272:PHE:HB3	1:B:280:LEU:HD11	2.04	0.40
1:A:41:ARG:HD3	1:A:41:ARG:HH11	1.75	0.40
1:C:97:LEU:HA	1:C:101:GLN:O	2.21	0.40
1:C:139:GLY:HA3	1:C:375:ILE:HD11	2.04	0.40
1:A:162:LYS:NZ	4:A:532:HOH:O	2.54	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	396/398 (100%)	377 (95%)	18 (4%)	1 (0%)	50	82
1	B	396/398 (100%)	379 (96%)	16 (4%)	1 (0%)	50	82
1	C	396/398 (100%)	378 (96%)	17 (4%)	1 (0%)	50	82
1	D	396/398 (100%)	381 (96%)	14 (4%)	1 (0%)	50	82
All	All	1584/1592 (100%)	1515 (96%)	65 (4%)	4 (0%)	50	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	195	CYS
1	A	195	CYS
1	B	195	CYS
1	C	195	CYS

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	323/323 (100%)	291 (90%)	32 (10%)	11	26
1	B	323/323 (100%)	285 (88%)	38 (12%)	8	18
1	C	323/323 (100%)	289 (90%)	34 (10%)	10	22
1	D	323/323 (100%)	292 (90%)	31 (10%)	12	27
All	All	1292/1292 (100%)	1157 (90%)	135 (10%)	10	23

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	20	LYS
1	A	22	SER
1	A	26	LYS
1	A	41	ARG
1	A	53	GLN
1	A	54	LYS
1	A	58	THR
1	A	81	LYS
1	A	96	GLN
1	A	102	LEU
1	A	116	LYS
1	A	132	GLU
1	A	137	PRO
1	A	155	LYS
1	A	156	SER
1	A	182	ILE
1	A	189	LYS
1	A	208	THR
1	A	231	SER
1	A	236	LYS
1	A	254	ARG
1	A	276	LYS
1	A	277	GLN
1	A	286	HIS
1	A	292	LYS
1	A	322	GLU
1	A	346	VAL
1	A	348	TRP
1	A	350	GLU
1	A	390	ARG
1	A	393	GLU
1	B	5	LYS
1	B	20	LYS
1	B	22	SER
1	B	26	LYS
1	B	41	ARG
1	B	43	LYS
1	B	53	GLN
1	B	54	LYS
1	B	58	THR
1	B	81	LYS
1	B	96	GLN

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Mol	Chain	Res	Type
1	B	97	LEU
1	B	102	LEU
1	B	116	LYS
1	B	132	GLU
1	B	137	PRO
1	B	147	SER
1	B	155	LYS
1	B	156	SER
1	B	182	ILE
1	B	189	LYS
1	B	208	THR
1	B	231	SER
1	B	236	LYS
1	B	254	ARG
1	B	276	LYS
1	B	277	GLN
1	B	286	HIS
1	B	292	LYS
1	B	322	GLU
1	B	331	GLN
1	B	346	VAL
1	B	348	TRP
1	B	350	GLU
1	B	373	LYS
1	B	390	ARG
1	B	393	GLU
1	B	398	SER
1	C	5	LYS
1	C	19	THR
1	C	20	LYS
1	C	22	SER
1	C	41	ARG
1	C	43	LYS
1	C	53	GLN
1	C	54	LYS
1	C	58	THR
1	C	81	LYS
1	C	96	GLN
1	C	97	LEU
1	C	102	LEU
1	C	116	LYS
1	C	132	GLU

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Mol	Chain	Res	Type
1	C	147	SER
1	C	155	LYS
1	C	180	PRO
1	C	182	ILE
1	C	189	LYS
1	C	208	THR
1	C	231	SER
1	C	236	LYS
1	C	276	LYS
1	C	277	GLN
1	C	292	LYS
1	C	305	PRO
1	C	322	GLU
1	C	346	VAL
1	C	348	TRP
1	C	350	GLU
1	C	390	ARG
1	C	393	GLU
1	C	398	SER
1	D	5	LYS
1	D	20	LYS
1	D	22	SER
1	D	41	ARG
1	D	53	GLN
1	D	54	LYS
1	D	58	THR
1	D	81	LYS
1	D	86	THR
1	D	96	GLN
1	D	102	LEU
1	D	116	LYS
1	D	132	GLU
1	D	147	SER
1	D	155	LYS
1	D	156	SER
1	D	182	ILE
1	D	189	LYS
1	D	208	THR
1	D	231	SER
1	D	254	ARG
1	D	276	LYS
1	D	277	GLN

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Mol	Chain	Res	Type
1	D	292	LYS
1	D	322	GLU
1	D	346	VAL
1	D	348	TRP
1	D	350	GLU
1	D	390	ARG
1	D	393	GLU
1	D	398	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	96	GLN
1	A	286	HIS
1	A	331	GLN
1	B	53	GLN
1	B	95	GLN
1	B	96	GLN
1	C	53	GLN
1	C	96	GLN
1	C	286	HIS
1	D	53	GLN
1	D	96	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PCA	A	1	1	8,8,9	8.54	2 (25%)	8,10,12	4.86	3 (37%)
1	PCA	B	1	1	8,8,9	7.80	2 (25%)	8,10,12	10.81	4 (50%)
1	PCA	C	1	1	8,8,9	8.50	2 (25%)	8,10,12	4.05	3 (37%)
1	PCA	D	1	1	8,8,9	8.33	2 (25%)	8,10,12	9.50	4 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	O-C	23.64	1.27	1.11
1	C	1	PCA	O-C	23.55	1.27	1.11
1	D	1	PCA	O-C	23.17	1.27	1.11
1	B	1	PCA	O-C	21.50	1.26	1.11
1	A	1	PCA	CA-C	4.29	1.56	1.48
1	B	1	PCA	CA-C	3.98	1.55	1.48
1	C	1	PCA	CA-C	3.71	1.55	1.48
1	D	1	PCA	CA-C	3.42	1.54	1.48

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	PCA	C-CA-N	-28.60	104.25	110.71
1	D	1	PCA	C-CA-N	-24.80	105.11	110.71
1	A	1	PCA	CA-N-CD	-10.14	106.45	114.37
1	C	1	PCA	CA-N-CD	-9.26	107.14	114.37
1	B	1	PCA	CA-N-CD	-8.15	108.00	114.37
1	D	1	PCA	CA-N-CD	-8.05	108.08	114.37
1	A	1	PCA	C-CA-N	-8.04	108.90	110.71
1	D	1	PCA	OE-CD-N	-5.37	118.65	125.11
1	C	1	PCA	OE-CD-CG	-5.08	118.73	126.70
1	B	1	PCA	OE-CD-N	-5.01	119.08	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	PCA	OE-CD-CG	-4.60	119.48	126.70
1	A	1	PCA	OE-CD-CG	-4.01	120.40	126.70
1	C	1	PCA	OE-CD-N	-3.46	120.95	125.11
1	D	1	PCA	OE-CD-CG	-3.29	121.54	126.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 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
2	NAG	A	399	1	12,14,15	1.46	3 (25%)	15,19,21	1.18	2 (13%)
2	NAG	A	400	1	12,14,15	1.42	2 (16%)	15,19,21	1.39	3 (20%)
3	DP5	A	401	-	36,36,36	1.68	7 (19%)	53,53,53	2.84	20 (37%)
2	NAG	B	399	1	12,14,15	1.45	1 (8%)	15,19,21	1.43	2 (13%)
2	NAG	B	400	1	12,14,15	1.36	2 (16%)	15,19,21	1.35	1 (6%)
3	DP5	B	401	-	36,36,36	1.42	5 (13%)	53,53,53	2.73	16 (30%)
2	NAG	C	399	1	12,14,15	1.34	1 (8%)	15,19,21	1.74	5 (33%)
2	NAG	C	400	1	12,14,15	1.42	1 (8%)	15,19,21	1.55	3 (20%)
3	DP5	C	401	-	36,36,36	1.36	7 (19%)	53,53,53	2.77	17 (32%)
2	NAG	D	399	1	12,14,15	1.43	2 (16%)	15,19,21	1.80	5 (33%)
2	NAG	D	400	1	12,14,15	1.39	2 (16%)	15,19,21	1.42	1 (6%)
3	DP5	D	401	-	36,36,36	1.57	7 (19%)	53,53,53	2.80	15 (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
2	NAG	A	399	1	-	0/6/23/26	0/1/1/1
2	NAG	A	400	1	-	0/6/23/26	0/1/1/1
3	DP5	A	401	-	-	0/14/74/74	0/3/3/3
2	NAG	B	399	1	-	0/6/23/26	0/1/1/1
2	NAG	B	400	1	-	0/6/23/26	0/1/1/1
3	DP5	B	401	-	-	0/14/74/74	0/3/3/3
2	NAG	C	399	1	-	0/6/23/26	0/1/1/1
2	NAG	C	400	1	-	0/6/23/26	0/1/1/1
3	DP5	C	401	-	-	0/14/74/74	0/3/3/3
2	NAG	D	399	1	-	0/6/23/26	0/1/1/1
2	NAG	D	400	1	-	0/6/23/26	0/1/1/1
3	DP5	D	401	-	-	0/14/74/74	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	DP5	C1B-S4C	4.05	1.87	1.81
3	A	401	DP5	C3B-C4B	3.92	1.57	1.53
3	D	401	DP5	C1C-C2C	-3.87	1.46	1.53
2	C	400	NAG	O7-C7	-3.76	1.14	1.23
2	B	399	NAG	O7-C7	-3.74	1.14	1.23
2	A	400	NAG	O7-C7	-3.72	1.15	1.23
2	A	399	NAG	O7-C7	-3.72	1.15	1.23
3	D	401	DP5	C1B-S4C	3.71	1.87	1.81
2	C	399	NAG	O7-C7	-3.57	1.15	1.23
3	B	401	DP5	C1B-S4C	3.49	1.86	1.81
2	B	400	NAG	O7-C7	-3.44	1.15	1.23
2	D	399	NAG	O7-C7	-3.42	1.15	1.23
2	D	400	NAG	O7-C7	-3.30	1.15	1.23
3	A	401	DP5	C1C-S1C	-3.29	1.78	1.82
3	C	401	DP5	C1C-C2C	-3.15	1.47	1.53
3	B	401	DP5	C1C-C2C	-3.11	1.47	1.53
2	D	400	NAG	O5-C5	-2.99	1.39	1.45
3	A	401	DP5	C5C-C4C	-2.97	1.50	1.53
3	A	401	DP5	C1C-C2C	-2.97	1.47	1.53
3	C	401	DP5	C5C-C4C	-2.91	1.50	1.53
3	C	401	DP5	C1B-S4C	2.87	1.85	1.81
3	B	401	DP5	C5C-C4C	-2.86	1.50	1.53
3	D	401	DP5	C1C-S1C	-2.82	1.79	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	DP5	C5A-C4A	-2.71	1.50	1.53
3	B	401	DP5	C1C-S1C	-2.62	1.79	1.82
3	D	401	DP5	C5B-C4B	-2.62	1.50	1.53
3	C	401	DP5	C5B-C4B	-2.56	1.50	1.53
3	A	401	DP5	C5B-C4B	-2.41	1.50	1.53
3	C	401	DP5	C5A-C4A	-2.39	1.50	1.53
2	D	399	NAG	C2-N2	2.31	1.49	1.46
3	C	401	DP5	O3B-C3B	-2.27	1.37	1.43
2	A	400	NAG	O5-C5	-2.22	1.41	1.45
3	D	401	DP5	O5B-C1B	-2.20	1.39	1.42
3	A	401	DP5	O5A-C1A	2.15	1.45	1.42
3	C	401	DP5	C3C-C4C	-2.13	1.51	1.53
2	B	400	NAG	O5-C5	-2.12	1.41	1.45
3	B	401	DP5	O5A-C1A	2.12	1.45	1.42
3	D	401	DP5	C4A-S4A	2.10	1.85	1.82
2	A	399	NAG	C2-N2	2.03	1.48	1.46
2	A	399	NAG	O5-C5	-2.01	1.41	1.45

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	DP5	C2B-C1B-S4C	-10.56	98.25	110.97
3	C	401	DP5	C2B-C1B-S4C	-10.13	98.77	110.97
3	B	401	DP5	C2B-C1B-S4C	-10.02	98.91	110.97
3	A	401	DP5	C2B-C1B-S4C	-9.80	99.17	110.97
3	B	401	DP5	O5B-C1B-C2B	8.20	120.98	110.42
3	D	401	DP5	O5B-C1B-C2B	7.73	120.37	110.42
3	A	401	DP5	O5B-C1B-C2B	7.64	120.26	110.42
3	C	401	DP5	O5B-C1B-C2B	7.40	119.95	110.42
3	D	401	DP5	C2A-C1A-S4B	-6.79	102.79	110.97
3	C	401	DP5	C2A-C1A-S4B	-6.73	102.86	110.97
3	B	401	DP5	C2A-C1A-S4B	-6.60	103.02	110.97
3	A	401	DP5	C2A-C1A-S4B	-6.59	103.04	110.97
3	B	401	DP5	C5B-C4B-S4B	-5.32	101.45	111.09
3	A	401	DP5	C5B-C4B-S4B	-5.25	101.58	111.09
3	A	401	DP5	O3C-C3C-C4C	5.21	119.67	108.95
3	D	401	DP5	C5B-C4B-S4B	-5.16	101.75	111.09
3	C	401	DP5	C5B-C4B-S4B	-5.09	101.87	111.09
3	C	401	DP5	O3C-C3C-C4C	5.05	119.33	108.95
3	A	401	DP5	C3B-C4B-S4B	-4.61	102.00	111.30
2	D	400	NAG	O5-C5-C6	4.57	111.78	106.98
3	D	401	DP5	C3B-C4B-S4B	-4.56	102.12	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	DP5	O3C-C3C-C4C	4.52	118.25	108.95
3	C	401	DP5	O5C-C1C-C2C	4.38	116.06	110.42
2	B	399	NAG	C3-C2-N2	-4.25	105.28	111.76
3	C	401	DP5	C3B-C4B-S4B	-4.13	102.98	111.30
3	A	401	DP5	O3A-C3A-C4A	4.10	117.39	108.95
3	D	401	DP5	O5C-C1C-C2C	4.08	115.67	110.42
3	A	401	DP5	O5C-C1C-C2C	3.88	115.42	110.42
3	C	401	DP5	O3A-C3A-C4A	3.86	116.89	108.95
3	B	401	DP5	O3C-C3C-C4C	3.84	116.86	108.95
3	B	401	DP5	C3B-C4B-S4B	-3.83	103.58	111.30
3	D	401	DP5	O3A-C3A-C4A	3.77	116.72	108.95
2	C	399	NAG	C3-C2-N2	-3.72	106.09	111.76
2	C	400	NAG	O5-C5-C4	-3.42	106.31	110.65
3	A	401	DP5	C1B-O5B-C5B	3.31	119.24	112.70
3	D	401	DP5	C1B-O5B-C5B	3.23	119.07	112.70
3	A	401	DP5	C2C-C3C-C4C	-3.19	105.19	110.87
2	D	399	NAG	C3-C2-N2	-3.15	106.96	111.76
3	B	401	DP5	O3A-C3A-C4A	3.14	115.42	108.95
3	B	401	DP5	O5C-C5C-C4C	-3.11	102.03	109.14
2	D	399	NAG	O5-C5-C4	-3.10	106.72	110.65
2	B	400	NAG	O5-C5-C4	-3.10	106.72	110.65
3	C	401	DP5	C1B-O5B-C5B	3.06	118.74	112.70
3	D	401	DP5	C1C-O5C-C5C	-3.02	106.75	112.68
3	B	401	DP5	C2C-C3C-C4C	-3.01	105.51	110.87
2	D	399	NAG	C2-N2-C7	-2.99	118.07	123.09
2	C	399	NAG	O5-C5-C4	-2.95	106.91	110.65
2	C	400	NAG	O5-C5-C6	2.93	110.06	106.98
2	D	399	NAG	C8-C7-N2	-2.89	110.45	116.11
3	A	401	DP5	C1C-O5C-C5C	-2.89	107.00	112.68
3	C	401	DP5	C2C-C3C-C4C	-2.87	105.76	110.87
3	A	401	DP5	C3B-C4B-C5B	-2.85	104.77	110.18
3	B	401	DP5	C1C-O5C-C5C	-2.80	107.18	112.68
2	C	400	NAG	O6-C6-C5	2.75	120.81	111.36
2	A	400	NAG	O6-C6-C5	2.74	120.78	111.36
3	B	401	DP5	O5C-C1C-C2C	2.72	113.92	110.42
2	C	399	NAG	C8-C7-N2	-2.72	110.79	116.11
3	C	401	DP5	C1C-O5C-C5C	-2.59	107.58	112.68
2	C	399	NAG	O5-C5-C6	2.59	109.70	106.98
3	B	401	DP5	C1B-O5B-C5B	2.54	117.71	112.70
3	A	401	DP5	O5C-C1C-S1C	2.53	111.43	107.98
3	D	401	DP5	C2C-C3C-C4C	-2.50	106.42	110.87
3	A	401	DP5	O3C-C3C-C2C	-2.47	104.82	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	399	NAG	O7-C7-C8	2.46	126.84	122.04
2	A	399	NAG	O5-C5-C4	-2.41	107.60	110.65
3	A	401	DP5	O5C-C5C-C4C	-2.39	103.68	109.14
2	A	399	NAG	C3-C2-N2	-2.38	108.14	111.76
3	D	401	DP5	C3B-C4B-C5B	-2.37	105.69	110.18
3	C	401	DP5	O5C-C5C-C4C	-2.35	103.77	109.14
3	C	401	DP5	O3A-C3A-C2A	-2.32	105.16	110.35
2	A	400	NAG	O5-C5-C4	-2.31	107.72	110.65
3	A	401	DP5	O6C-C6C-C5C	2.31	119.31	111.36
3	B	401	DP5	O5C-C1C-S1C	2.31	111.13	107.98
3	B	401	DP5	C3C-C4C-S4C	-2.28	106.70	111.30
3	C	401	DP5	C1C-C2C-C3C	-2.28	106.04	110.77
2	A	400	NAG	O5-C5-C6	2.25	109.34	106.98
3	D	401	DP5	O6C-C6C-C5C	2.23	119.04	111.36
3	D	401	DP5	O5C-C5C-C4C	-2.23	104.05	109.14
3	C	401	DP5	O5A-C1A-S4B	-2.23	105.78	110.69
2	B	399	NAG	O5-C5-C4	-2.20	107.86	110.65
3	D	401	DP5	C3A-C4A-S4A	2.19	116.12	111.26
3	C	401	DP5	C3A-C4A-S4A	2.17	116.08	111.26
3	B	401	DP5	C1C-C2C-C3C	-2.15	106.32	110.77
3	A	401	DP5	O5A-C1A-S4B	-2.12	106.02	110.69
2	C	399	NAG	O7-C7-C8	2.11	126.16	122.04
3	A	401	DP5	C1C-C2C-C3C	-2.08	106.45	110.77
3	A	401	DP5	C6C-C5C-C4C	2.08	119.10	113.25
3	C	401	DP5	C6C-C5C-C4C	2.05	119.00	113.25
3	B	401	DP5	C3B-C4B-C5B	-2.01	106.36	110.18
3	A	401	DP5	O2A-C2A-C1A	-2.00	106.82	110.12

There are no chirality outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.