



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:32 PM UTC

PDB ID : 1OVW / pdb_00001ovw
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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

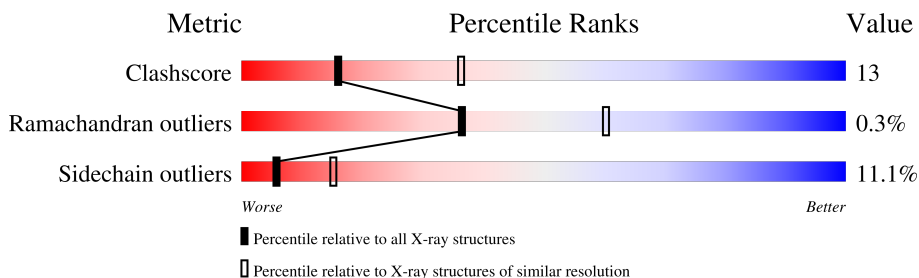
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	398	
1	B	398	
1	C	398	
1	D	398	
2	E	3	
2	F	3	
2	G	3	
2	H	3	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13412 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 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 an oligosaccharide called 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	S	0	0	0
			34	18	12	4			
2	F	3	Total	C	O	S	0	0	0
			34	18	12	4			
2	G	3	Total	C	O	S	0	0	0
			34	18	12	4			
2	H	3	Total	C	O	S	0	0	0
			34	18	12	4			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is water.

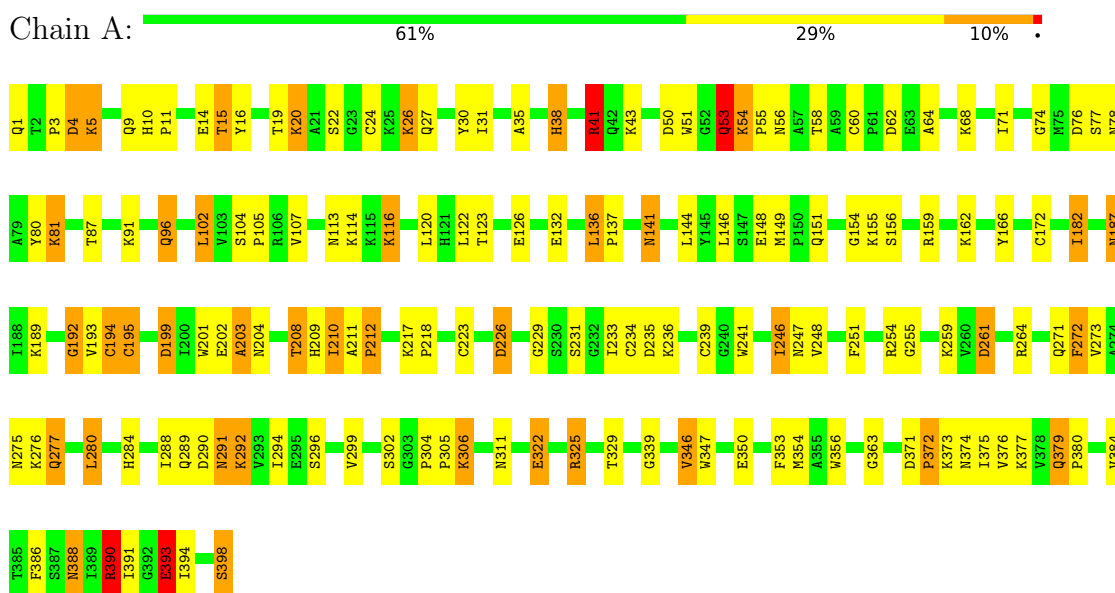
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	275	Total	O	0	0
			275	275		
4	B	267	Total	O	0	0
			267	267		
4	C	248	Total	O	0	0
			248	248		
4	D	282	Total	O	0	0
			282	282		

3 Residue-property plots

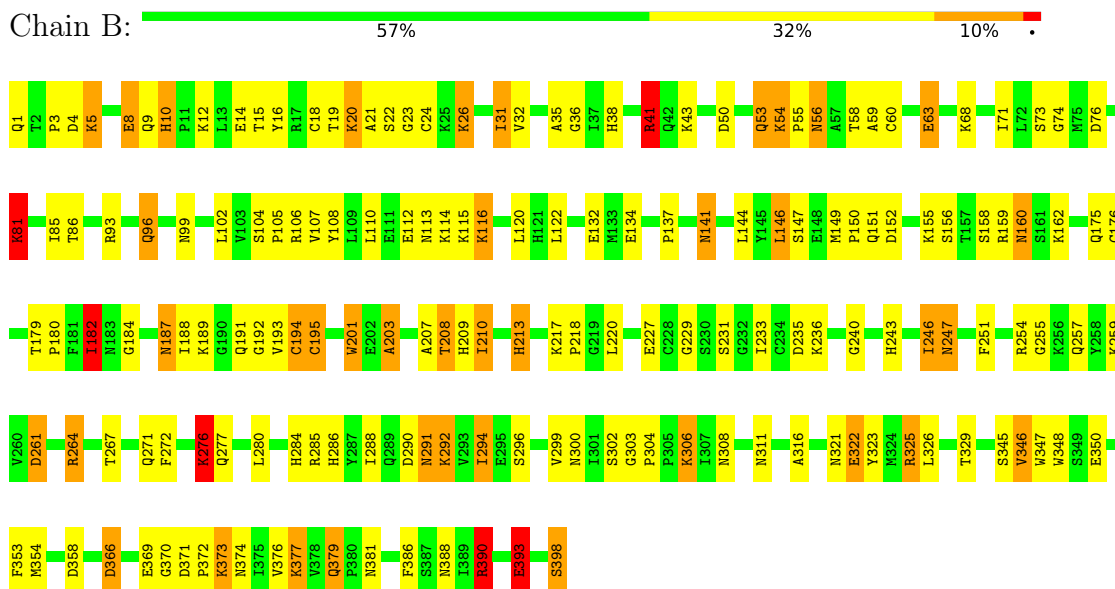
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

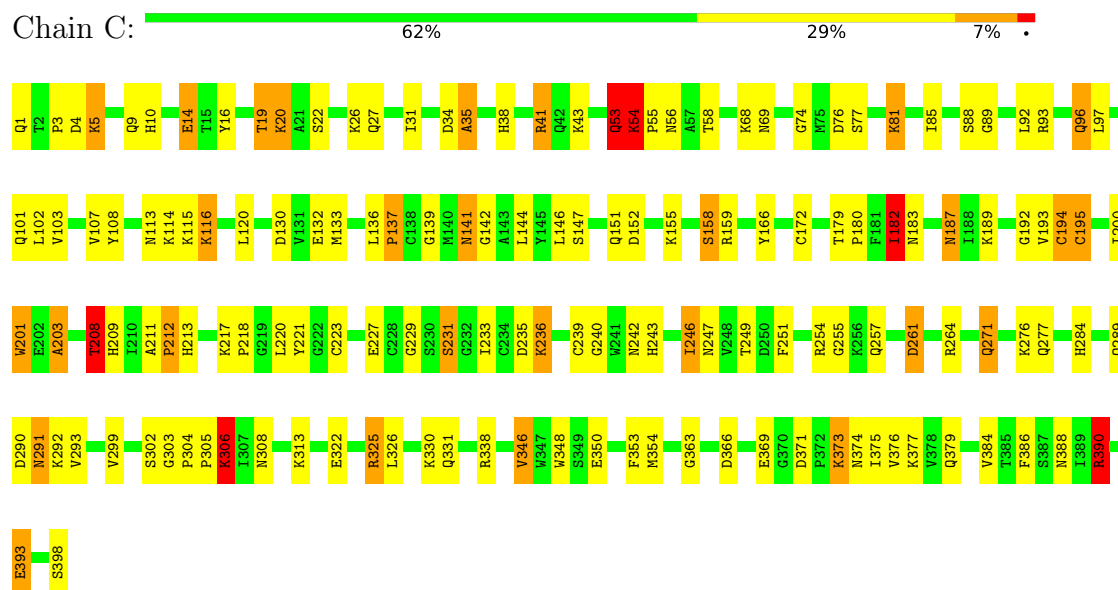
• Molecule 1: ENDOGLUCANASE I



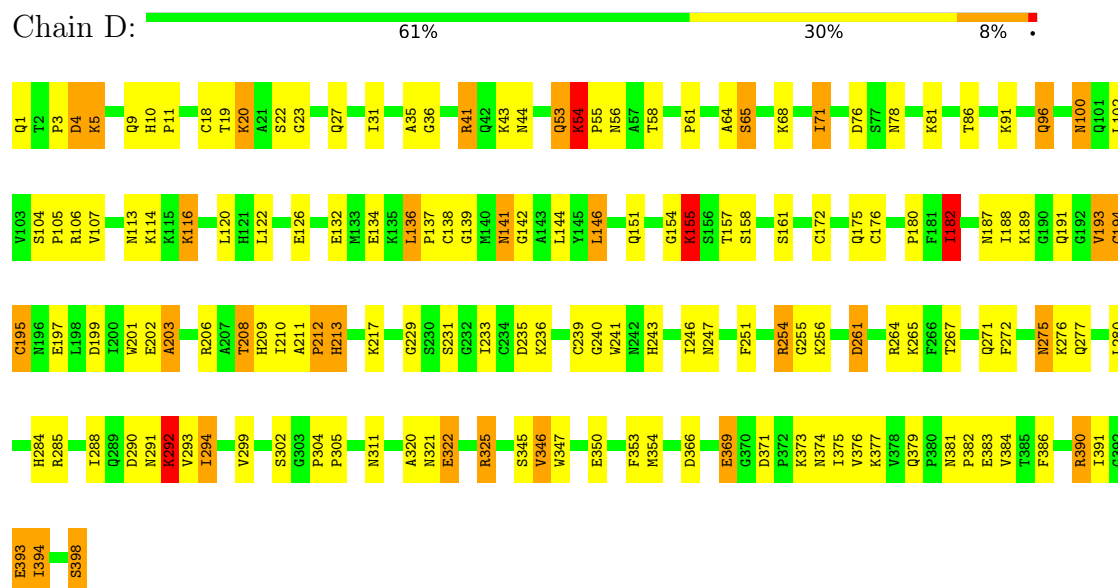
• Molecule 1: ENDOGLUCANASE I



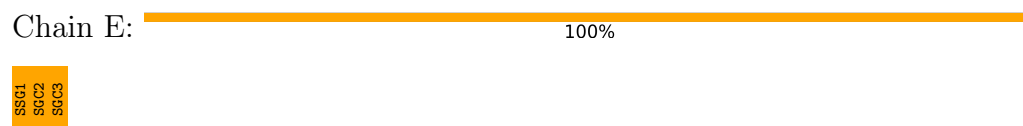
- Molecule 1: ENDOGLUCANASE I



- Molecule 1: ENDOGLUCANASE I



- Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose

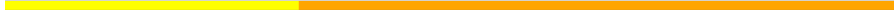


- Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose

Chain F:  100%

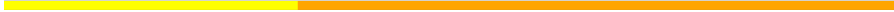
SS01
SCC2
SCC3

- Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose

Chain G:  33% 67%

SS01
SCC2
SCC3

- Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose

Chain H:  33% 67%

SS01
SCC2
SCC3

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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: SSG, PCA, NAG, SGC

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	0.79	0/3077	1.96	99/4155 (2.4%)
1	B	0.82	0/3077	1.98	102/4155 (2.5%)
1	C	0.83	0/3077	1.98	85/4155 (2.0%)
1	D	0.85	0/3077	1.99	91/4155 (2.2%)
All	All	0.82	0/12308	1.98	377/16620 (2.3%)

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 (377) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ARG	CD-NE-CZ	14.40	144.56	124.40
1	D	141	ASN	CA-CB-CG	12.87	125.47	112.60
1	B	4	ASP	CA-CB-CG	10.70	123.30	112.60
1	A	203	ALA	N-CA-C	9.81	122.93	108.60
1	B	346	VAL	CB-CA-C	-9.72	97.30	110.42
1	B	203	ALA	N-CA-C	9.71	123.42	108.96
1	B	390	ARG	NE-CZ-NH1	9.61	131.11	121.50
1	C	203	ALA	N-CA-C	9.61	122.63	108.60
1	D	353	PHE	CA-CB-CG	9.36	123.16	113.80
1	C	4	ASP	CA-CB-CG	9.33	121.93	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	VAL	N-CA-CB	9.30	124.47	111.82
1	B	10	HIS	CA-CB-CG	9.10	122.89	113.80
1	D	203	ALA	N-CA-C	9.02	121.77	108.60
1	A	192	GLY	CA-C-O	-8.96	113.39	121.64
1	A	346	VAL	N-CA-CB	8.89	124.50	111.52
1	A	353	PHE	CA-CB-CG	8.69	122.49	113.80
1	A	210	ILE	CA-C-O	-8.60	110.61	120.67
1	B	251	PHE	CA-CB-CG	-8.51	105.29	113.80
1	A	4	ASP	CA-CB-CG	8.49	121.09	112.60
1	D	390	ARG	NE-CZ-NH1	8.30	129.80	121.50
1	B	325	ARG	CD-NE-CZ	8.26	135.96	124.40
1	C	251	PHE	CA-CB-CG	-8.23	105.57	113.80
1	D	325	ARG	CD-NE-CZ	8.09	135.73	124.40
1	C	346	VAL	N-CA-CB	8.00	123.19	111.52
1	C	390	ARG	CA-CB-CG	8.00	130.09	114.10
1	B	36	GLY	O-C-N	-7.97	114.24	122.13
1	D	346	VAL	CB-CA-C	-7.91	98.78	110.33
1	B	235	ASP	CA-CB-CG	7.86	120.46	112.60
1	B	71	ILE	CB-CA-C	-7.85	99.91	110.98
1	D	261	ASP	CA-CB-CG	7.80	120.40	112.60
1	D	255	GLY	N-CA-C	7.73	121.64	111.52
1	A	390	ARG	CD-NE-CZ	7.67	135.14	124.40
1	D	158	SER	CA-C-O	7.63	129.39	121.23
1	C	325	ARG	NE-CZ-NH1	7.56	129.06	121.50
1	C	141	ASN	CA-CB-CG	7.54	120.14	112.60
1	A	154	GLY	CA-C-O	-7.52	110.66	119.01
1	C	255	GLY	N-CA-C	7.52	121.37	111.52
1	D	346	VAL	N-CA-CB	7.46	122.41	111.52
1	B	158	SER	CA-C-O	7.44	129.36	121.33
1	D	104	SER	CA-C-N	7.43	127.41	119.76
1	D	104	SER	C-N-CA	7.43	127.41	119.76
1	A	172	CYS	CA-C-O	-7.40	113.54	121.38
1	C	353	PHE	CA-CB-CG	7.37	121.17	113.80
1	D	203	ALA	N-CA-CB	-7.29	100.23	111.46
1	C	390	ARG	NE-CZ-NH1	7.27	128.77	121.50
1	C	261	ASP	CA-CB-CG	7.26	119.86	112.60
1	C	3	PRO	N-CA-CB	7.23	109.74	103.31
1	C	246	ILE	CA-C-N	7.20	132.34	122.19
1	C	246	ILE	C-N-CA	7.20	132.34	122.19
1	D	141	ASN	OD1-CG-ND2	-7.20	115.40	122.60
1	D	136	LEU	CA-C-O	7.19	128.27	120.08
1	A	390	ARG	CA-CB-CG	7.11	128.33	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	LYS	CA-C-N	7.11	127.10	119.78
1	A	217	LYS	C-N-CA	7.11	127.10	119.78
1	D	386	PHE	CA-C-O	-7.08	112.94	120.80
1	D	3	PRO	N-CA-CB	7.08	109.48	103.25
1	C	93	ARG	NE-CZ-NH2	-7.06	112.85	119.20
1	D	182	ILE	CB-CA-C	-7.04	100.21	110.63
1	C	85	ILE	CA-C-O	-7.02	113.02	120.39
1	D	10	HIS	CA-CB-CG	6.98	120.78	113.80
1	A	211	ALA	CA-C-N	6.93	127.18	119.90
1	A	211	ALA	C-N-CA	6.93	127.18	119.90
1	D	251	PHE	CA-CB-CG	-6.93	106.87	113.80
1	A	372	PRO	CA-C-N	6.91	130.23	120.28
1	A	372	PRO	C-N-CA	6.91	130.23	120.28
1	D	390	ARG	NH1-CZ-NH2	-6.91	110.31	119.30
1	C	27	GLN	OE1-CD-NE2	6.90	129.50	122.60
1	B	316	ALA	CA-C-O	6.90	128.06	120.82
1	A	241	TRP	CA-C-O	6.88	128.92	120.25
1	A	305	PRO	N-CA-CB	6.85	109.31	103.35
1	A	346	VAL	CB-CA-C	-6.85	100.33	110.33
1	C	74	GLY	N-CA-C	-6.85	102.79	112.37
1	C	289	GLN	OE1-CD-NE2	-6.83	115.77	122.60
1	C	211	ALA	CA-C-N	6.81	127.05	119.90
1	C	211	ALA	C-N-CA	6.81	127.05	119.90
1	C	182	ILE	N-CA-CB	6.80	120.79	111.41
1	C	212	PRO	N-CA-CB	6.80	109.34	103.36
1	D	100	ASN	OD1-CG-ND2	6.77	129.37	122.60
1	C	242	ASN	CA-CB-CG	6.76	119.36	112.60
1	A	102	LEU	CA-C-O	-6.75	112.58	120.62
1	A	166	TYR	CA-C-O	-6.70	112.69	120.20
1	A	289	GLN	OE1-CD-NE2	-6.69	115.91	122.60
1	C	346	VAL	CB-CA-C	-6.67	100.59	110.33
1	B	106	ARG	NE-CZ-NH2	6.65	125.19	119.20
1	D	243	HIS	CA-CB-CG	6.64	120.44	113.80
1	C	325	ARG	CD-NE-CZ	6.63	133.68	124.40
1	B	255	GLY	N-CA-C	6.62	121.22	111.76
1	D	4	ASP	CA-CB-CG	6.60	119.20	112.60
1	B	56	ASN	OD1-CG-ND2	6.58	129.18	122.60
1	D	294	ILE	CA-C-O	-6.58	113.11	120.74
1	B	390	ARG	CA-CB-CG	6.57	127.25	114.10
1	B	182	ILE	CB-CA-C	-6.56	100.85	110.62
1	B	296	SER	CA-C-O	-6.54	114.28	121.87
1	B	192	GLY	CA-C-N	-6.51	114.87	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	GLY	C-N-CA	-6.51	114.87	122.95
1	B	207	ALA	CA-C-O	-6.51	113.73	120.89
1	B	217	LYS	CA-C-N	6.49	126.41	119.85
1	B	217	LYS	C-N-CA	6.49	126.41	119.85
1	A	255	GLY	N-CA-C	6.48	120.00	111.70
1	C	217	LYS	CA-C-N	6.45	126.37	119.85
1	C	217	LYS	C-N-CA	6.45	126.37	119.85
1	D	188	ILE	CA-C-O	-6.45	114.34	121.05
1	D	71	ILE	CB-CA-C	-6.42	101.92	110.98
1	C	182	ILE	CB-CA-C	-6.42	101.13	110.63
1	C	203	ALA	N-CA-CB	-6.42	101.57	111.46
1	D	390	ARG	CA-CB-CG	6.41	126.92	114.10
1	B	141	ASN	CA-CB-CG	6.41	119.01	112.60
1	C	221	TYR	CA-C-O	-6.40	113.44	120.36
1	C	192	GLY	N-CA-C	-6.39	103.42	112.37
1	D	182	ILE	N-CA-CB	6.38	120.22	111.41
1	A	204	ASN	OD1-CG-ND2	6.38	128.98	122.60
1	B	203	ALA	N-CA-CB	-6.37	101.49	111.56
1	D	390	ARG	CD-NE-CZ	6.37	133.32	124.40
1	D	202	GLU	N-CA-CB	6.37	120.52	110.84
1	C	331	GLN	OE1-CD-NE2	6.33	128.93	122.60
1	A	104	SER	CA-C-N	6.33	126.28	119.76
1	A	104	SER	C-N-CA	6.33	126.28	119.76
1	D	146	LEU	CA-C-O	6.33	127.53	120.70
1	C	158	SER	CA-C-O	6.31	128.15	121.33
1	B	390	ARG	NH1-CZ-NH2	-6.31	111.10	119.30
1	A	10	HIS	CA-CB-CG	6.31	120.11	113.80
1	B	213	HIS	CA-CB-CG	6.28	120.08	113.80
1	A	212	PRO	N-CA-CB	6.26	108.86	103.36
1	D	382	PRO	N-CA-CB	6.26	108.90	103.27
1	D	213	HIS	CA-CB-CG	6.25	120.05	113.80
1	B	227	GLU	O-C-N	6.23	128.73	122.12
1	C	137	PRO	N-CA-CB	6.23	109.79	103.25
1	C	305	PRO	N-CA-CB	6.22	108.76	103.35
1	D	235	ASP	CA-CB-CG	6.22	118.82	112.60
1	C	235	ASP	CA-CB-CG	6.21	118.81	112.60
1	D	212	PRO	N-CA-CB	6.20	108.81	103.36
1	B	353	PHE	CA-CB-CG	6.19	119.99	113.80
1	C	10	HIS	CA-CB-CG	6.19	119.99	113.80
1	D	194	CYS	N-CA-C	6.18	119.55	110.59
1	A	261	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	390	ARG	NH1-CZ-NH2	-6.17	111.27	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	SER	CA-C-O	-6.17	114.71	121.87
1	B	311	ASN	CA-CB-CG	6.16	118.76	112.60
1	B	104	SER	CA-C-N	6.16	126.10	119.76
1	B	104	SER	C-N-CA	6.16	126.10	119.76
1	B	386	PHE	CA-C-O	-6.15	113.97	120.80
1	D	35	ALA	CA-C-N	6.15	126.92	120.03
1	D	35	ALA	C-N-CA	6.15	126.92	120.03
1	C	166	TYR	CA-C-O	-6.14	114.00	120.63
1	A	141	ASN	CA-C-O	6.11	128.51	120.15
1	D	311	ASN	CA-CB-CG	6.10	118.70	112.60
1	D	211	ALA	CA-C-N	6.09	126.30	119.90
1	D	211	ALA	C-N-CA	6.09	126.30	119.90
1	D	193	VAL	CA-C-O	-6.08	114.29	121.64
1	D	320	ALA	CA-C-N	6.04	128.29	120.44
1	D	320	ALA	C-N-CA	6.04	128.29	120.44
1	A	218	PRO	N-CA-CB	6.03	108.60	103.35
1	C	291	ASN	OD1-CG-ND2	6.03	128.63	122.60
1	C	308	ASN	CA-C-O	6.03	128.06	120.65
1	C	103	VAL	O-C-N	-6.00	116.35	122.23
1	A	60	CYS	CA-C-N	6.00	125.55	119.19
1	A	60	CYS	C-N-CA	6.00	125.55	119.19
1	A	15	THR	O-C-N	-5.98	114.75	122.94
1	A	149	MET	CA-C-N	5.98	126.29	119.83
1	A	149	MET	C-N-CA	5.98	126.29	119.83
1	D	381	ASN	CA-CB-CG	5.98	118.58	112.60
1	A	291	ASN	CA-CB-CG	-5.97	106.63	112.60
1	D	241	TRP	CA-C-O	5.96	127.77	120.25
1	A	379	GLN	OE1-CD-NE2	5.96	128.56	122.60
1	B	246	ILE	CA-C-O	5.95	128.21	120.78
1	A	41	ARG	N-CA-C	5.93	118.43	109.41
1	D	305	PRO	CA-C-O	-5.93	114.68	121.56
1	A	187	ASN	CA-CB-CG	5.92	118.52	112.60
1	B	229	GLY	O-C-N	-5.92	117.25	122.88
1	D	305	PRO	N-CA-CB	5.92	108.50	103.35
1	A	80	TYR	O-C-N	5.90	128.46	122.09
1	C	306	LYS	CA-CB-CG	5.89	125.89	114.10
1	B	56	ASN	CB-CG-OD1	-5.88	109.04	120.80
1	A	391	ILE	CA-C-O	-5.88	113.93	121.40
1	B	192	GLY	N-CA-C	-5.86	104.16	112.37
1	D	155	LYS	CA-C-O	5.86	126.96	120.63
1	A	393	GLU	N-CA-CB	5.85	118.57	109.97
1	D	302	SER	CB-CA-C	5.81	119.12	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	ASN	CA-CB-CG	5.81	118.41	112.60
1	A	390	ARG	NE-CZ-NH1	5.80	127.30	121.50
1	C	194	CYS	N-CA-C	5.79	119.03	110.46
1	C	35	ALA	CA-C-N	5.77	126.49	120.03
1	C	35	ALA	C-N-CA	5.77	126.49	120.03
1	A	64	ALA	CA-C-O	5.76	126.53	120.42
1	D	191	GLN	CA-C-N	-5.76	114.20	120.71
1	D	191	GLN	C-N-CA	-5.76	114.20	120.71
1	A	74	GLY	N-CA-C	-5.76	104.71	112.14
1	D	36	GLY	O-C-N	-5.75	116.59	122.17
1	B	182	ILE	N-CA-CB	5.73	121.36	111.39
1	C	142	GLY	N-CA-C	-5.73	99.60	113.18
1	A	192	GLY	N-CA-C	-5.73	102.65	111.64
1	B	229	GLY	CA-C-N	5.72	127.95	120.28
1	B	229	GLY	C-N-CA	5.72	127.95	120.28
1	D	213	HIS	CA-C-N	5.72	125.63	119.85
1	D	213	HIS	C-N-CA	5.72	125.63	119.85
1	A	30	TYR	CA-CB-CG	-5.72	103.61	113.90
1	B	74	GLY	N-CA-C	-5.71	104.78	112.14
1	B	60	CYS	CA-C-N	5.70	125.23	119.19
1	B	60	CYS	C-N-CA	5.70	125.23	119.19
1	C	56	ASN	OD1-CG-ND2	5.69	128.29	122.60
1	A	203	ALA	N-CA-CB	-5.68	102.71	111.46
1	B	321	ASN	CA-CB-CG	-5.68	106.92	112.60
1	B	3	PRO	N-CA-CB	5.67	108.24	103.25
1	B	243	HIS	CA-CB-CG	5.66	119.46	113.80
1	C	53	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	A	203	ALA	CB-CA-C	-5.64	100.11	111.17
1	C	386	PHE	CA-C-O	-5.64	114.54	120.80
1	C	229	GLY	O-C-N	-5.63	117.97	122.81
1	D	247	ASN	OD1-CG-ND2	5.61	128.21	122.60
1	B	194	CYS	N-CA-C	5.61	119.11	110.42
1	A	194	CYS	N-CA-C	5.60	118.75	110.46
1	D	105	PRO	N-CA-C	5.60	119.87	111.14
1	D	41	ARG	N-CA-C	5.59	117.68	109.24
1	A	247	ASN	OD1-CG-ND2	5.58	128.19	122.60
1	D	44	ASN	CA-C-O	5.58	126.45	119.59
1	D	345	SER	CA-C-N	5.57	130.74	122.99
1	D	345	SER	C-N-CA	5.57	130.74	122.99
1	D	56	ASN	CA-C-N	5.57	128.30	120.28
1	D	56	ASN	C-N-CA	5.57	128.30	120.28
1	A	199	ASP	CA-C-O	5.57	126.71	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	11	PRO	O-C-N	-5.56	116.61	123.01
1	B	306	LYS	CA-CB-CG	5.55	125.20	114.10
1	A	235	ASP	CA-CB-CG	5.53	118.13	112.60
1	B	93	ARG	NE-CZ-NH2	-5.53	114.22	119.20
1	A	302	SER	O-C-N	-5.53	116.72	122.96
1	B	321	ASN	OD1-CG-ND2	5.52	128.12	122.60
1	D	64	ALA	CA-C-O	5.52	126.37	120.24
1	A	154	GLY	O-C-N	5.52	129.01	122.50
1	B	146	LEU	CA-C-O	5.52	126.66	120.70
1	A	203	ALA	CA-C-O	5.51	127.22	121.38
1	C	308	ASN	O-C-N	-5.51	114.82	122.20
1	A	105	PRO	N-CA-C	5.50	119.72	111.14
1	D	142	GLY	N-CA-C	-5.49	100.16	113.18
1	C	69	ASN	N-CA-C	5.49	119.82	113.18
1	B	308	ASN	CA-C-O	5.49	126.59	119.95
1	C	179	THR	CA-C-N	5.49	125.84	119.47
1	C	179	THR	C-N-CA	5.49	125.84	119.47
1	D	134	GLU	N-CA-C	5.49	117.97	111.33
1	D	191	GLN	O-C-N	5.49	129.09	122.94
1	C	130	ASP	CA-C-O	-5.49	114.89	120.71
1	C	338	ARG	CD-NE-CZ	5.48	132.08	124.40
1	D	275	ASN	OD1-CG-ND2	5.48	128.08	122.60
1	D	391	ILE	CA-C-O	-5.48	114.47	120.72
1	B	210	ILE	CA-C-O	-5.48	114.26	120.67
1	D	292	LYS	CA-C-O	-5.47	114.24	120.32
1	B	152	ASP	O-C-N	-5.47	115.77	122.34
1	A	136	LEU	CA-C-O	5.47	126.32	120.08
1	A	56	ASN	CA-C-O	5.47	126.92	120.96
1	B	261	ASP	CA-C-O	5.46	126.60	120.92
1	C	236	LYS	O-C-N	-5.44	116.47	122.07
1	C	152	ASP	CA-CB-CG	5.43	118.03	112.60
1	C	200	ILE	O-C-N	5.43	127.54	121.90
1	A	226	ASP	CA-CB-CG	-5.42	107.17	112.60
1	C	346	VAL	CA-CB-CG2	5.41	119.60	110.40
1	A	273	VAL	N-CA-C	5.41	116.37	108.58
1	A	388	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	D	56	ASN	OD1-CG-ND2	5.40	128.00	122.60
1	A	388	ASN	CA-C-N	5.40	128.32	120.98
1	A	388	ASN	C-N-CA	5.40	128.32	120.98
1	B	191	GLN	CA-C-N	-5.40	115.15	120.60
1	B	191	GLN	C-N-CA	-5.40	115.15	120.60
1	B	86	THR	CA-C-N	-5.39	114.12	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	THR	C-N-CA	-5.39	114.12	122.59
1	C	208	THR	N-CA-CB	5.39	120.94	111.55
1	C	218	PRO	N-CA-CB	5.39	108.34	103.33
1	D	105	PRO	CB-CA-C	-5.38	104.52	111.46
1	B	104	SER	O-C-N	-5.38	115.13	121.32
1	D	293	VAL	CA-C-O	-5.37	113.93	120.69
1	C	54	LYS	N-CA-CB	5.36	117.18	109.78
1	C	243	HIS	CA-CB-CG	5.36	119.16	113.80
1	A	78	ASN	CA-CB-CG	-5.36	107.25	112.60
1	B	276	LYS	CA-CB-CG	5.36	124.81	114.10
1	C	249	THR	N-CA-C	5.35	119.56	113.19
1	A	27	GLN	OE1-CD-NE2	5.33	127.94	122.60
1	C	363	GLY	CA-C-N	5.33	126.51	119.84
1	C	363	GLY	C-N-CA	5.33	126.51	119.84
1	B	264	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	A	272	PHE	CA-CB-CG	-5.32	108.48	113.80
1	B	255	GLY	O-C-N	-5.32	117.52	123.10
1	B	108	TYR	CA-C-O	-5.32	115.22	121.44
1	A	311	ASN	CA-CB-CG	5.31	117.91	112.60
1	B	390	ARG	CD-NE-CZ	5.31	131.83	124.40
1	D	27	GLN	OE1-CD-NE2	5.30	127.90	122.60
1	A	148	GLU	CA-C-N	5.29	128.73	120.68
1	A	148	GLU	C-N-CA	5.29	128.73	120.68
1	B	358	ASP	N-CA-C	5.29	118.80	111.71
1	A	251	PHE	CA-CB-CG	-5.28	108.52	113.80
1	C	247	ASN	N-CA-C	5.28	118.86	111.74
1	D	217	LYS	CA-C-N	5.28	125.18	119.85
1	D	217	LYS	C-N-CA	5.28	125.18	119.85
1	B	180	PRO	N-CA-CB	5.27	108.75	103.48
1	B	345	SER	CA-C-N	5.26	130.46	122.98
1	B	345	SER	C-N-CA	5.26	130.46	122.98
1	C	271	GLN	CA-C-O	5.26	125.82	120.24
1	C	338	ARG	CA-C-O	-5.26	114.16	120.10
1	D	104	SER	N-CA-CB	-5.26	101.00	110.37
1	D	106	ARG	CD-NE-CZ	5.25	131.76	124.40
1	B	31	ILE	CA-C-O	-5.25	114.73	120.72
1	B	160	ASN	CA-CB-CG	-5.23	107.37	112.60
1	C	133	MET	N-CA-C	5.23	119.66	113.28
1	C	92	LEU	CA-C-O	-5.22	114.70	120.24
1	A	3	PRO	N-CA-CB	5.22	107.96	103.31
1	A	302	SER	CB-CA-C	5.22	119.06	109.46
1	D	122	LEU	CA-C-O	-5.21	113.64	119.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	54	LYS	CA-C-O	-5.20	113.78	121.27
1	B	291	ASN	CA-CB-CG	-5.20	107.40	112.60
1	C	187	ASN	CA-CB-CG	5.19	117.79	112.60
1	A	226	ASP	CB-CG-OD2	-5.18	106.48	118.40
1	B	149	MET	CA-C-N	5.18	125.42	119.83
1	B	149	MET	C-N-CA	5.18	125.42	119.83
1	C	56	ASN	CB-CG-OD1	-5.18	110.44	120.80
1	D	180	PRO	N-CA-CB	5.18	109.10	103.30
1	A	363	GLY	CA-C-N	5.17	126.30	119.84
1	A	363	GLY	C-N-CA	5.17	126.30	119.84
1	B	63	GLU	N-CA-C	5.17	117.58	111.33
1	A	87	THR	CA-C-O	-5.16	115.57	121.40
1	C	247	ASN	O-C-N	-5.16	115.50	122.41
1	A	11	PRO	N-CA-CB	5.16	107.91	103.27
1	A	122	LEU	CA-C-O	-5.15	113.24	119.27
1	D	138	CYS	CA-C-O	-5.15	115.88	121.44
1	A	386	PHE	CA-C-O	-5.15	115.08	120.80
1	B	81	LYS	CA-C-O	-5.15	115.07	120.63
1	B	73	SER	CA-C-O	5.14	126.55	120.69
1	C	180	PRO	N-CA-CB	5.14	109.06	103.30
1	B	21	ALA	N-CA-C	5.14	117.78	111.82
1	B	187	ASN	CA-CB-CG	5.13	117.73	112.60
1	B	302	SER	CB-CA-C	5.12	118.27	109.51
1	B	218	PRO	N-CA-CB	5.12	108.09	103.33
1	B	201	TRP	N-CA-C	5.11	116.65	107.80
1	C	348	TRP	CA-CB-CG	5.11	123.32	113.60
1	B	377	LYS	N-CA-C	-5.11	105.62	111.14
1	A	229	GLY	CA-C-N	5.11	127.08	120.44
1	A	229	GLY	C-N-CA	5.11	127.08	120.44
1	B	379	GLN	CA-C-N	5.10	124.60	119.19
1	B	379	GLN	C-N-CA	5.10	124.60	119.19
1	D	369	GLU	CA-C-O	5.10	125.87	120.10
1	C	201	TRP	N-CA-CB	-5.10	102.94	110.90
1	A	71	ILE	CB-CA-C	-5.10	104.23	111.21
1	A	280	LEU	CA-C-N	-5.10	112.80	121.97
1	A	280	LEU	C-N-CA	-5.10	112.80	121.97
1	A	123	THR	CA-C-O	5.09	126.51	120.96
1	B	112	GLU	CA-C-N	5.09	129.22	120.72
1	B	112	GLU	C-N-CA	5.09	129.22	120.72
1	D	321	ASN	N-CA-C	5.09	116.52	111.07
1	A	218	PRO	CB-CA-C	-5.08	104.72	111.23
1	B	150	PRO	N-CA-CB	5.08	107.84	103.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	GLY	N-CA-C	5.08	121.09	113.02
1	D	240	GLY	N-CA-C	5.07	121.09	113.02
1	C	302	SER	CB-CA-C	5.07	118.10	109.53
1	A	248	VAL	O-C-N	-5.07	116.24	122.57
1	B	247	ASN	OD1-CG-ND2	5.07	127.67	122.60
1	B	99	ASN	O-C-N	-5.07	116.24	122.57
1	B	105	PRO	CB-CA-C	-5.07	104.93	111.46
1	C	14	GLU	O-C-N	-5.07	116.71	122.89
1	B	122	LEU	CA-C-O	-5.06	113.35	119.27
1	A	272	PHE	CA-C-O	-5.06	115.66	120.92
1	B	8	GLU	CA-C-N	-5.05	115.30	123.23
1	B	8	GLU	C-N-CA	-5.05	115.30	123.23
1	B	366	ASP	O-C-N	5.05	128.29	121.83
1	A	388	ASN	O-C-N	-5.05	116.29	122.55
1	B	41	ARG	N-CA-C	5.05	117.34	109.52
1	A	62	ASP	CA-C-O	5.05	126.85	121.45
1	C	293	VAL	CA-C-O	-5.04	114.79	120.74
1	D	394	ILE	O-C-N	5.04	128.87	122.57
1	B	381	ASN	CA-CB-CG	5.04	117.64	112.60
1	D	229	GLY	CA-C-N	5.04	126.99	120.44
1	D	229	GLY	C-N-CA	5.04	126.99	120.44
1	A	38	HIS	CA-CB-CG	5.04	118.84	113.80
1	A	306	LYS	CA-CB-CG	5.03	124.17	114.10
1	A	30	TYR	O-C-N	5.02	129.84	123.11
1	D	65	SER	N-CA-C	-5.02	105.89	111.36
1	B	184	GLY	N-CA-C	-5.02	108.32	115.30
1	B	134	GLU	N-CA-C	5.01	116.74	111.28
1	B	366	ASP	CA-C-O	-5.01	115.24	121.50
1	B	393	GLU	N-CA-CB	5.00	117.33	109.97
1	A	53	GLN	N-CA-CB	-5.00	103.55	111.05
1	C	41	ARG	N-CA-C	5.00	117.27	109.52

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 Too-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 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	3023	0	2905	81	0
1	B	3023	0	2905	87	0
1	C	3023	0	2905	69	0
1	D	3023	0	2905	71	0
2	E	34	0	30	6	0
2	F	34	0	30	6	0
2	G	34	0	30	4	0
2	H	34	0	29	6	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	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	11843	319	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (319) 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: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
2:H:1:SSG:S4	2:H:2:SGC:H4	2.22	0.79
2:G:1:SSG:S4	2:G:2:SGC:H4	2.22	0.79
1:B:374:ASN:HA	1:B:377:LYS:HD2	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:THR:HA	1:A:393:GLU:HG3	1.64	0.78
2:E:1:SSG:S4	2:E:2:SGC:H4	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
2:F:1:SSG:S4	2:F:2:SGC:H4	2.25	0.76
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:HD3	1:C:5:LYS:H	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:HD3	1:A:5:LYS:H	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:H	1:D:5:LYS:HD3	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:H	1:B:5:LYS:HD3	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:A:116:LYS:HB3	1:A:151:GLN:HG2	1.77	0.66
1:C:182:ILE:HD11	1:C:187:ASN:HA	1.78	0.66
1:C:19:THR:HA	1:C:393:GLU:HG3	1.80	0.64
2:H:1:SSG:S4	2:H:2:SGC:C4	2.86	0.64
1:C:116:LYS:HB3	1:C:151:GLN:HG2	1.80	0.63
2:E:1:SSG:S4	2:E:2:SGC:C4	2.86	0.63
2:G:1:SSG:S4	2:G:2:SGC:C4	2.86	0.63
1:B:116:LYS:HB3	1:B:151:GLN:HG2	1.79	0.63
1:B:261:ASP:OD2	1:B:264:ARG:HD3	1.99	0.62
1:C:201:TRP:CZ3	1:C:208:THR:HG21	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:96:GLN:HA	1:B:96:GLN:HE21	1.65	0.61
1:C:195:CYS:HA	4:C:576:HOH:O	2.01	0.61
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
2:F:1:SSG:S4	2:F:2:SGC:C4	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
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:54:LYS:HB2	1:A:55:PRO:CD	2.32	0.59
1:A:201:TRP:CZ3	1:A:208:THR:HG21	2.37	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:H	1:D:5:LYS:CD	2.15	0.57
1:C:5:LYS:H	1:C:5:LYS:CD	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:A:113:ASN:O	1:A:114:LYS:HB2	2.06	0.55
1:D:54:LYS:HB2	1:D:55:PRO:CD	2.36	0.55
1:D:113:ASN:O	1:D:114:LYS:HB2	2.06	0.55
1:B:213:HIS:HE1	2:F:1:SSG:H2	1.70	0.55
1:D:182:ILE:HG23	1:D:193:VAL:HG22	1.88	0.54
1:B:299:VAL:HG11	1:B:304:PRO:HB2	1.89	0.54
1:C:20:LYS:N	1:C:393:GLU:OE2	2.35	0.54
1:D:194:CYS:O	1:D:195:CYS:HB3	2.07	0.54
1:D:256:LYS:HD3	4:D:796:HOH:O	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:PRO:HG3	1:A:379:GLN:HB3	1.90	0.53
1:B:288:ILE:CD1	1:B:398:SER:HB2	2.39	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
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:B:141:ASN:HB2	1:B:354:MET:HE3	1.90	0.53
1:C:144:LEU:C	1:C:144:LEU:HD23	2.34	0.53
1:B:179:THR:HB	4:B:592:HOH:O	2.09	0.53
1:C:159:ARG:NH2	4:C:616:HOH:O	2.35	0.53
1:D:208:THR:HG22	1:D:209:HIS:H	1.74	0.53
1:A:271:GLN:HB2	1:A:284:HIS:HB2	1.90	0.53
1:B:120:LEU:HD12	1:B:146:LEU:HD21	1.91	0.53
1:A:96:GLN:HE21	1:A:96:GLN:HA	1.73	0.52
1:C:388:ASN:OD1	1:C:390:ARG:NH1	2.39	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:D:137:PRO:HG2	1:D:375:ILE:HG23	1.92	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:A:14:GLU:OE1	1:A:26:LYS:HD2	2.10	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:HG2	4:A:569:HOH:O	2.10	0.51
1:D:144:LEU:HD23	1:D:144:LEU:C	2.35	0.51
1:A:50:ASP:O	1:A:51:TRP:C	2.54	0.51
1:C:194:CYS:O	1:C:195:CYS:HB3	2.10	0.51
1:C:141:ASN:HB2	1:C:354:MET:HE3	1.92	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:A:136:LEU:HD11	1:A:384:VAL:HB	1.92	0.50
1:B:208:THR:HG22	1:B:209:HIS:H	1.74	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:A:371:ASP:O	1:A:375:ILE:HG13	2.11	0.50
1:B:5:LYS:H	1:B:5:LYS:CD	2.19	0.50
1:B:194:CYS:O	1:B:195:CYS:HB3	2.10	0.50
1:B:115:LYS:HD2	4:B:614:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:141:ASN:HB2	1:A:354:MET:HE3	1.94	0.49
1:D:213:HIS:HE1	2:H:1:SSG:H2	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
1:C:137:PRO:HB2	4:C:524:HOH:O	2.12	0.49
1:A:202:GLU:OE2	2:E:1:SSG:S4	2.71	0.49
1:D:141:ASN:HB2	1:D:354:MET:HE3	1.95	0.49
1:B:32:VAL:HB	1:B:110:LEU:HD11	1.94	0.48
1:A:20:LYS:H	1:A:393:GLU:CD	2.21	0.48
1:B:195:CYS:HA	4:B:572:HOH:O	2.12	0.48
1:A:292:LYS:O	1:A:294:ILE:HD12	2.14	0.48
1:B:182:ILE:HG13	1:B:187:ASN:HB2	1.95	0.48
1:B:366:ASP:CG	1:B:369:GLU:HG2	2.39	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:376:VAL:HA	1:C:379:GLN:O	2.14	0.48
1:A:159:ARG:NH2	4:A:637:HOH:O	2.47	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:144:LEU:C	1:A:144:LEU:HD23	2.40	0.47
1:B:14:GLU:OE2	1:B:26:LYS:HB2	2.14	0.47
1:B:144:LEU:C	1:B:144:LEU:HD23	2.38	0.47
1:D:54:LYS:HG2	4:D:860:HOH:O	2.14	0.47
1:D:100:ASN:ND2	4:D:805:HOH:O	2.47	0.47
1:A:199:ASP:OD2	2:E:1:SSG:O3	2.33	0.47
1:A:31:ILE:HG23	1:A:107:VAL:HB	1.97	0.47
1:B:213:HIS:CE1	2:F:1:SSG:H2	2.49	0.47
1:D:210:ILE:HD11	1:D:285:ARG:NH1	2.30	0.47
1:B:16:TYR:HB2	1:B:390:ARG:HB3	1.95	0.47
1:B:54:LYS:CB	1:B:55:PRO:CD	2.92	0.47
1:B:280:LEU:HD23	1:B:329:THR:CG2	2.45	0.47
1:C:20:LYS:H	1:C:393:GLU:CD	2.22	0.47
1:A:288:ILE:CD1	1:A:398:SER:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:TRP:CE3	2:E:3:SGC:H5	2.50	0.47
1:C:303:GLY:HA3	4:C:611:HOH:O	2.14	0.47
1:C:366:ASP:CG	1:C:369:GLU:HG2	2.40	0.47
1:A:322:GLU:HG3	1:A:325:ARG:HH11	1.80	0.46
1:C:261:ASP:OD2	1:C:264:ARG:HD3	2.15	0.46
1:A:277:GLN:NE2	4:A:606:HOH:O	2.46	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:B:288:ILE:HD11	1:B:398:SER:HB2	1.98	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:20:LYS:H	1:B:393:GLU:CD	2.24	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
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
2:F:1:SSG:O3	2:F:2:SGC:C1	2.64	0.45
1:A:272:PHE:HB3	1:A:280:LEU:HD11	1.97	0.45
1:D:197:GLU:OE1	2:H:2:SGC:O2	2.32	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
2:H:1:SSG:O3	2:H:2:SGC:C1	2.65	0.45
1:A:322:GLU:HG3	1:A:325:ARG:NH1	2.32	0.45
1:D:374:ASN:O	1:D:375:ILE:C	2.59	0.45
1:A:120:LEU:HD12	1:A:146:LEU:HD21	1.99	0.45
1:D:206:ARG:HG3	1:D:206:ARG:HH11	1.82	0.45
1:A:91:LYS:HE2	4:A:511:HOH:O	2.17	0.45
1:A:116:LYS:HB3	1:A:151:GLN:CG	2.46	0.45
1:B:31:ILE:HG23	1:B:107:VAL:HB	1.98	0.45
1:D:31:ILE:HG23	1:D:107:VAL:HB	1.99	0.45
1:B:81:LYS:HE2	1:B:85:ILE:O	2.17	0.45
1:C:54:LYS:CB	1:C:55:PRO:HD2	2.46	0.45
1:D:53:GLN:NE2	1:D:54:LYS:O	2.50	0.45
1:C:9:GLN:OE1	1:C:76:ASP:HB2	2.17	0.44
1:B:20:LYS:N	1:B:393:GLU:OE2	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ARG:NH2	1:B:326:LEU:HD21	2.32	0.44
1:C:172:CYS:HB3	1:C:193:VAL:HG12	2.00	0.44
1:C:213:HIS:HE1	2:G:1:SSG:H2	1.82	0.44
1:D:208:THR:HG22	1:D:209:HIS:N	2.32	0.44
1:A:246:ILE:H	1:A:246:ILE:HG13	1.70	0.44
1:B:63:GLU:HG2	1:B:160:ASN:HD22	1.83	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:B:257:GLN:HG3	4:B:596:HOH:O	2.16	0.44
1:C:137:PRO:HG3	1:C:379:GLN:HB3	2.00	0.44
1:C:306:LYS:HE2	1:C:306:LYS:N	2.33	0.44
1:D:18:CYS:HA	1:D:23:GLY:O	2.16	0.44
1:D:203:ALA:CB	1:D:208:THR:HG23	2.37	0.44
1:A:16:TYR:HB3	1:A:24:CYS:HB3	1.99	0.44
1:B:193:VAL:HG13	1:B:220:LEU:HD21	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
1:D:383:GLU:HG3	4:D:770:HOH:O	2.17	0.44
1:A:96:GLN:HE21	1:A:96:GLN:CA	2.29	0.43
1:A:210:ILE:HG13	4:A:413:HOH:O	2.17	0.43
1:A:376:VAL:HA	1:A:379:GLN:O	2.18	0.43
1:C:19:THR:HA	1:C:393:GLU:CG	2.46	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:370:GLY:O	1:B:371:ASP:C	2.58	0.43
1:A:280:LEU:HD23	1:A:329:THR:HG22	2.01	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:D:267:THR:HB	1:D:288:ILE:HB	2.00	0.43
1:D:322:GLU:HG3	1:D:325:ARG:NH1	2.34	0.43
1:A:35:ALA:O	1:A:38:HIS:HB2	2.19	0.43
1:A:356:TRP:CZ2	2:E:1:SSG:H5	2.54	0.43
1:B:220:LEU:C	1:B:220:LEU:HD23	2.44	0.42
1:D:139:GLY:HA3	1:D:375:ILE:HD11	2.01	0.42
1:A:4:ASP:HB2	1:A:5:LYS:HD3	2.02	0.42
1:B:54:LYS:CB	1:B:55:PRO:HD2	2.42	0.42
1:B:50:ASP:H	1:B:53:GLN:HE21	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:THR:HG22	1:C:209:HIS:N	2.32	0.42
1:D:272:PHE:HB3	1:D:280:LEU:HD11	2.02	0.42
2:G:1:SSG:O3	2:G:2:SGC:C1	2.67	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:347:TRP:CE3	2:F:3:SGC:H5	2.54	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:A:374:ASN:O	1:A:375:ILE:C	2.63	0.42
1:B:56:ASN:HB3	1:B:59:ALA:HB3	2.00	0.42
1:C:16:TYR:HB2	1:C:390:ARG:HB3	2.01	0.42
1:C:34:ASP:OD1	1:C:108:TYR:OH	2.34	0.42
1:C:54:LYS:HB2	1:C:55:PRO:CD	2.48	0.42
1:C:88:SER:O	1:C:89:GLY:C	2.63	0.42
1:C:203:ALA:CB	1:C:208:THR:HG23	2.40	0.42
1:D:172:CYS:HB3	1:D:193:VAL:HG12	2.01	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
1:B:292:LYS:O	1:B:294:ILE:HD12	2.20	0.41
1:D:275:ASN:OD1	1:D:275:ASN:C	2.63	0.41
1:B:53:GLN:HE21	1:B:53:GLN:HB3	1.75	0.41
1:D:199:ASP:OD2	2:H:1:SSG:O3	2.38	0.41
1:D:347:TRP:CE3	1:D:354:MET:HE1	2.55	0.41
1:D:366:ASP:CG	1:D:369:GLU:HG2	2.44	0.41
1:A:194:CYS:HB3	1:A:234:CYS:SG	2.61	0.41
1:B:12:LYS:HE2	4:B:564:HOH:O	2.20	0.41
1:B:55:PRO:O	1:B:56:ASN:C	2.61	0.41
1:C:264:ARG:NH2	1:C:290:ASP:OD1	2.53	0.41
1:A:275:ASN:HB2	4:A:665:HOH:O	2.19	0.41
1:B:210:ILE:HD11	1:B:285:ARG:NH1	2.36	0.41
1:B:322:GLU:HG3	1:B:325:ARG:HH11	1.86	0.41
1:C:374:ASN:O	1:C:375:ILE:C	2.64	0.41
1:D:155:LYS:HA	1:D:161:SER:OG	2.20	0.41
1:B:16:TYR:HB3	1:B:24:CYS:HB3	2.02	0.41
1:B:53:GLN:NE2	1:B:54:LYS:O	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ASP:HA	1:A:372:PRO:HD3	1.82	0.41
1:B:267:THR:HB	1:B:288:ILE:HB	2.02	0.41
1:D:371:ASP:O	1:D:375:ILE:HG13	2.20	0.41
1:C:136:LEU:HD11	1:C:384:VAL:HB	2.03	0.41
1:B:188:ILE:H	1:B:188:ILE:HG12	1.70	0.41
1:D:20:LYS:H	1:D:393:GLU:CD	2.28	0.41
1:D:20:LYS:N	1:D:393:GLU:OE2	2.51	0.41
1:B:288:ILE:HD12	1:B:398:SER:HB2	2.01	0.40
1:D:154:GLY:O	1:D:157:THR:HG23	2.21	0.40
1:D:288:ILE:CD1	1:D:398:SER:HB2	2.51	0.40
1:B:8:GLU:HG2	1:B:10:HIS:CE1	2.56	0.40
1:C:330:LYS:HB2	4:C:591:HOH:O	2.21	0.40
1:D:54:LYS:CB	1:D:55:PRO:HD2	2.48	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:B:322:GLU:O	1:B:323:TYR:C	2.64	0.40
1:D:347:TRP:CZ3	1:D:354:MET:HE1	2.56	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:A:162:LYS:NZ	4:A:532:HOH:O	2.54	0.40
1:C:139:GLY:HA3	1:C:375:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	396/398 (100%)	377 (95%)	18 (4%)	1 (0%)	36	60
1	B	396/398 (100%)	379 (96%)	16 (4%)	1 (0%)	36	60
1	C	396/398 (100%)	378 (96%)	17 (4%)	1 (0%)	36	60
1	D	396/398 (100%)	381 (96%)	14 (4%)	1 (0%)	36	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1584/1592 (100%)	1515 (96%)	65 (4%)	4 (0%)	36	60

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%)	288 (89%)	35 (11%)	6	16
1	B	323/323 (100%)	284 (88%)	39 (12%)	5	12
1	C	323/323 (100%)	287 (89%)	36 (11%)	6	15
1	D	323/323 (100%)	289 (90%)	34 (10%)	6	17
All	All	1292/1292 (100%)	1148 (89%)	144 (11%)	6	15

All (144) 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	43	LYS
1	A	53	GLN
1	A	54	LYS
1	A	58	THR
1	A	68	LYS
1	A	81	LYS

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Mol	Chain	Res	Type
1	A	96	GLN
1	A	102	LEU
1	A	116	LYS
1	A	132	GLU
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	233	ILE
1	A	236	LYS
1	A	246	ILE
1	A	254	ARG
1	A	276	LYS
1	A	277	GLN
1	A	292	LYS
1	A	306	LYS
1	A	322	GLU
1	A	346	VAL
1	A	350	GLU
1	A	390	ARG
1	A	393	GLU
1	A	398	SER
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	68	LYS
1	B	81	LYS
1	B	96	GLN
1	B	102	LEU
1	B	116	LYS
1	B	132	GLU
1	B	147	SER
1	B	155	LYS
1	B	156	SER

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Mol	Chain	Res	Type
1	B	182	ILE
1	B	189	LYS
1	B	208	THR
1	B	231	SER
1	B	233	ILE
1	B	236	LYS
1	B	246	ILE
1	B	254	ARG
1	B	276	LYS
1	B	277	GLN
1	B	286	HIS
1	B	292	LYS
1	B	294	ILE
1	B	306	LYS
1	B	322	GLU
1	B	346	VAL
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	68	LYS
1	C	81	LYS
1	C	96	GLN
1	C	102	LEU
1	C	116	LYS
1	C	132	GLU
1	C	147	SER
1	C	155	LYS
1	C	182	ILE
1	C	189	LYS
1	C	208	THR
1	C	231	SER

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Mol	Chain	Res	Type
1	C	233	ILE
1	C	236	LYS
1	C	246	ILE
1	C	254	ARG
1	C	276	LYS
1	C	277	GLN
1	C	292	LYS
1	C	306	LYS
1	C	322	GLU
1	C	346	VAL
1	C	350	GLU
1	C	373	LYS
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	43	LYS
1	D	53	GLN
1	D	54	LYS
1	D	58	THR
1	D	68	LYS
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	155	LYS
1	D	182	ILE
1	D	189	LYS
1	D	208	THR
1	D	231	SER
1	D	233	ILE
1	D	236	LYS
1	D	246	ILE
1	D	254	ARG
1	D	265	LYS
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	350	GLU
1	D	390	ARG
1	D	393	GLU
1	D	398	SER

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

Mol	Chain	Res	Type
1	A	53	GLN
1	A	95	GLN
1	A	96	GLN
1	A	141	ASN
1	A	160	ASN
1	A	286	HIS
1	B	53	GLN
1	B	95	GLN
1	B	96	GLN
1	B	99	ASN
1	B	160	ASN
1	B	183	ASN
1	C	53	GLN
1	C	96	GLN
1	C	101	GLN
1	D	53	GLN
1	D	96	GLN
1	D	99	ASN
1	D	183	ASN
1	D	331	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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	C	1	1	7,8,9	1.45	1 (14%)	9,10,12	2.29	2 (22%)
1	PCA	A	1	1	7,8,9	1.26	1 (14%)	9,10,12	1.77	3 (33%)
1	PCA	D	1	1	7,8,9	1.22	0	9,10,12	1.84	3 (33%)
1	PCA	B	1	1	7,8,9	1.32	1 (14%)	9,10,12	1.90	2 (22%)

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	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	O-C	2.05	1.27	1.20
1	C	1	PCA	O-C	2.03	1.27	1.20
1	B	1	PCA	CG-CD	2.02	1.55	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	PCA	OE-CD-CG	-4.48	118.73	126.72
1	B	1	PCA	OE-CD-CG	-4.06	119.48	126.72
1	A	1	PCA	OE-CD-CG	-3.54	120.40	126.72
1	C	1	PCA	O-C-CA	-3.38	116.08	124.77
1	D	1	PCA	OE-CD-N	-2.92	118.65	124.96
1	D	1	PCA	OE-CD-CG	-2.90	121.54	126.72
1	B	1	PCA	OE-CD-N	-2.71	119.08	124.96
1	D	1	PCA	CB-CA-C	-2.39	109.38	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	CA-N-CD	-2.08	106.45	113.58
1	A	1	PCA	O-C-CA	-2.06	119.46	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

12 monosaccharides 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	SSG	E	1	2	10,12,12	1.94	3 (30%)	12,17,17	3.07	8 (66%)
2	SGC	E	2	2	10,11,12	1.94	2 (20%)	12,15,17	2.31	3 (25%)
2	SGC	E	3	2	10,11,12	0.87	0	12,15,17	1.57	2 (16%)
2	SSG	F	1	2	10,12,12	1.92	2 (20%)	12,17,17	3.02	6 (50%)
2	SGC	F	2	2	10,11,12	1.08	0	12,15,17	2.22	3 (25%)
2	SGC	F	3	2	10,11,12	0.81	0	12,15,17	1.33	2 (16%)
2	SSG	G	1	2	10,12,12	2.00	3 (30%)	12,17,17	3.01	6 (50%)
2	SGC	G	2	2	10,11,12	1.40	2 (20%)	12,15,17	2.26	3 (25%)
2	SGC	G	3	2	10,11,12	1.10	1 (10%)	12,15,17	1.49	2 (16%)
2	SSG	H	1	2	10,12,12	1.89	2 (20%)	12,17,17	2.84	6 (50%)
2	SGC	H	2	2	10,11,12	1.59	2 (20%)	12,15,17	2.36	3 (25%)
2	SGC	H	3	2	10,11,12	1.33	1 (10%)	12,15,17	1.43	2 (16%)

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	SSG	E	1	2	-	0/2/22/22	0/1/1/1
2	SGC	E	2	2	-	0/2/19/22	0/1/1/1
2	SGC	E	3	2	-	0/2/19/22	0/1/1/1
2	SSG	F	1	2	-	0/2/22/22	0/1/1/1
2	SGC	F	2	2	-	0/2/19/22	0/1/1/1
2	SGC	F	3	2	-	1/2/19/22	0/1/1/1
2	SSG	G	1	2	-	0/2/22/22	0/1/1/1
2	SGC	G	2	2	-	0/2/19/22	0/1/1/1
2	SGC	G	3	2	-	0/2/19/22	0/1/1/1
2	SSG	H	1	2	-	0/2/22/22	0/1/1/1
2	SGC	H	2	2	-	0/2/19/22	0/1/1/1
2	SGC	H	3	2	-	0/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	SSG	C1-C2	-4.51	1.46	1.53
2	E	2	SGC	C3-C4	4.45	1.57	1.53
2	G	1	SSG	C1-C2	-3.67	1.47	1.53
2	F	1	SSG	C1-C2	-3.63	1.47	1.53
2	E	1	SSG	C5-C4	-3.51	1.50	1.53
2	E	1	SSG	C1-C2	-3.45	1.47	1.53
2	G	1	SSG	C5-C4	-3.43	1.50	1.53
2	F	1	SSG	C5-C4	-3.36	1.50	1.53
2	H	3	SGC	C5-C4	-3.17	1.50	1.53
2	H	2	SGC	C5-C4	-3.05	1.50	1.53
2	G	2	SGC	C5-C4	-2.98	1.50	1.53
2	G	1	SSG	C3-C4	-2.89	1.51	1.53
2	E	2	SGC	C5-C4	-2.78	1.50	1.53
2	G	3	SGC	C5-C4	-2.75	1.50	1.53
2	H	2	SGC	O5-C1	-2.73	1.39	1.43
2	G	2	SGC	O3-C3	-2.21	1.37	1.43
2	E	1	SSG	C3-C4	-2.14	1.51	1.53
2	H	1	SSG	C5-C4	-2.04	1.51	1.53

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	SSG	O5-C5-C4	-7.61	102.03	109.50
2	E	1	SSG	O5-C5-C4	-5.93	103.68	109.50
2	G	1	SSG	O5-C5-C4	-5.83	103.77	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	SSG	O5-C5-C4	-5.55	104.05	109.50
2	E	2	SGC	C1-O5-C5	5.26	119.24	112.19
2	E	1	SSG	O3-C3-C4	5.14	119.67	109.17
2	H	2	SGC	C1-O5-C5	5.14	119.07	112.19
2	G	1	SSG	O3-C3-C4	4.97	119.33	109.17
2	G	2	SGC	C1-O5-C5	4.89	118.74	112.19
2	H	1	SSG	O3-C3-C4	4.44	118.25	109.17
2	F	2	SGC	O5-C1-C2	4.27	120.98	110.79
2	G	1	SSG	O5-C1-C2	4.17	116.06	110.32
2	F	2	SGC	C1-O5-C5	4.12	117.71	112.19
2	E	3	SGC	O3-C3-C4	4.02	117.39	109.17
2	H	2	SGC	O5-C1-C2	4.02	120.37	110.79
2	E	2	SGC	O5-C1-C2	3.97	120.26	110.79
2	H	1	SSG	O5-C1-C2	3.88	115.67	110.32
2	G	2	SGC	O5-C1-C2	3.84	119.95	110.79
2	G	3	SGC	O3-C3-C4	3.77	116.89	109.17
2	F	1	SSG	O3-C3-C4	3.76	116.86	109.17
2	E	1	SSG	O5-C1-C2	3.70	115.42	110.32
2	H	3	SGC	O3-C3-C4	3.69	116.72	109.17
2	F	2	SGC	C5-C4-S4	-3.58	101.45	110.16
2	E	2	SGC	C5-C4-S4	-3.53	101.58	110.16
2	H	2	SGC	C5-C4-S4	-3.46	101.75	110.16
2	G	2	SGC	C5-C4-S4	-3.41	101.87	110.16
2	H	1	SSG	C1-O5-C5	-3.24	106.75	112.55
2	E	1	SSG	C1-O5-C5	-3.10	107.00	112.55
2	F	3	SGC	O3-C3-C4	3.06	115.42	109.17
2	E	1	SSG	C6-C5-C4	3.03	119.10	112.76
2	F	1	SSG	C1-O5-C5	-3.00	107.18	112.55
2	G	1	SSG	C6-C5-C4	2.98	119.00	112.76
2	G	1	SSG	C1-O5-C5	-2.78	107.58	112.55
2	F	1	SSG	O5-C1-C2	2.61	113.92	110.32
2	H	3	SGC	C1-O5-C5	2.51	115.55	112.19
2	F	1	SSG	C6-C5-C4	2.47	117.92	112.76
2	G	3	SGC	O3-C3-C2	-2.40	105.16	110.05
2	E	1	SSG	O3-C3-C2	-2.36	104.82	110.38
2	E	1	SSG	O6-C6-C5	2.34	119.31	111.33
2	G	1	SSG	C1-C2-C3	-2.31	106.04	110.55
2	F	3	SGC	C1-O5-C5	2.28	115.24	112.19
2	H	1	SSG	O6-C6-C5	2.26	119.04	111.33
2	H	1	SSG	C6-C5-C4	2.20	117.36	112.76
2	F	1	SSG	C1-C2-C3	-2.16	106.32	110.55
2	E	3	SGC	C1-O5-C5	2.15	115.07	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	SSG	C1-C2-C3	-2.10	106.45	110.55

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	3	SGC	C4-C5-C6-O6

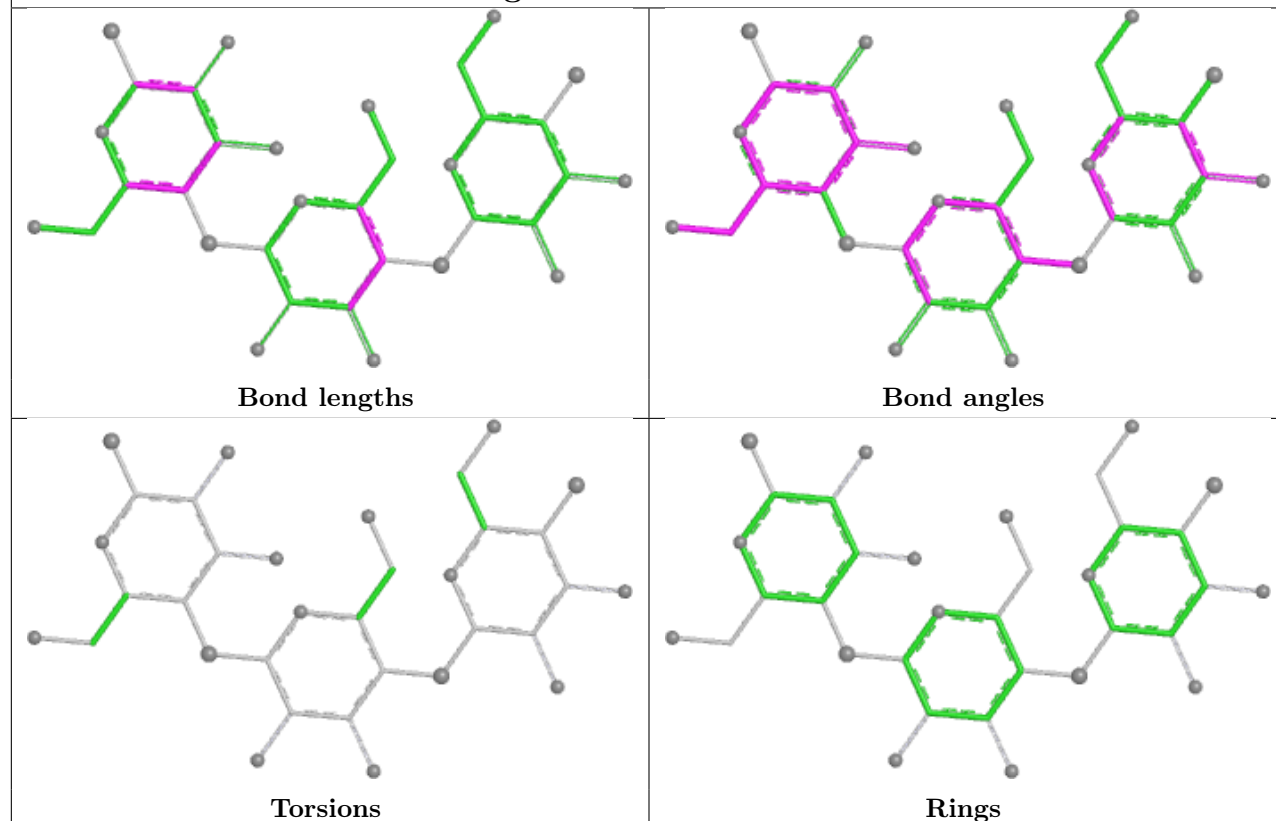
There are no ring outliers.

10 monomers are involved in 22 short contacts:

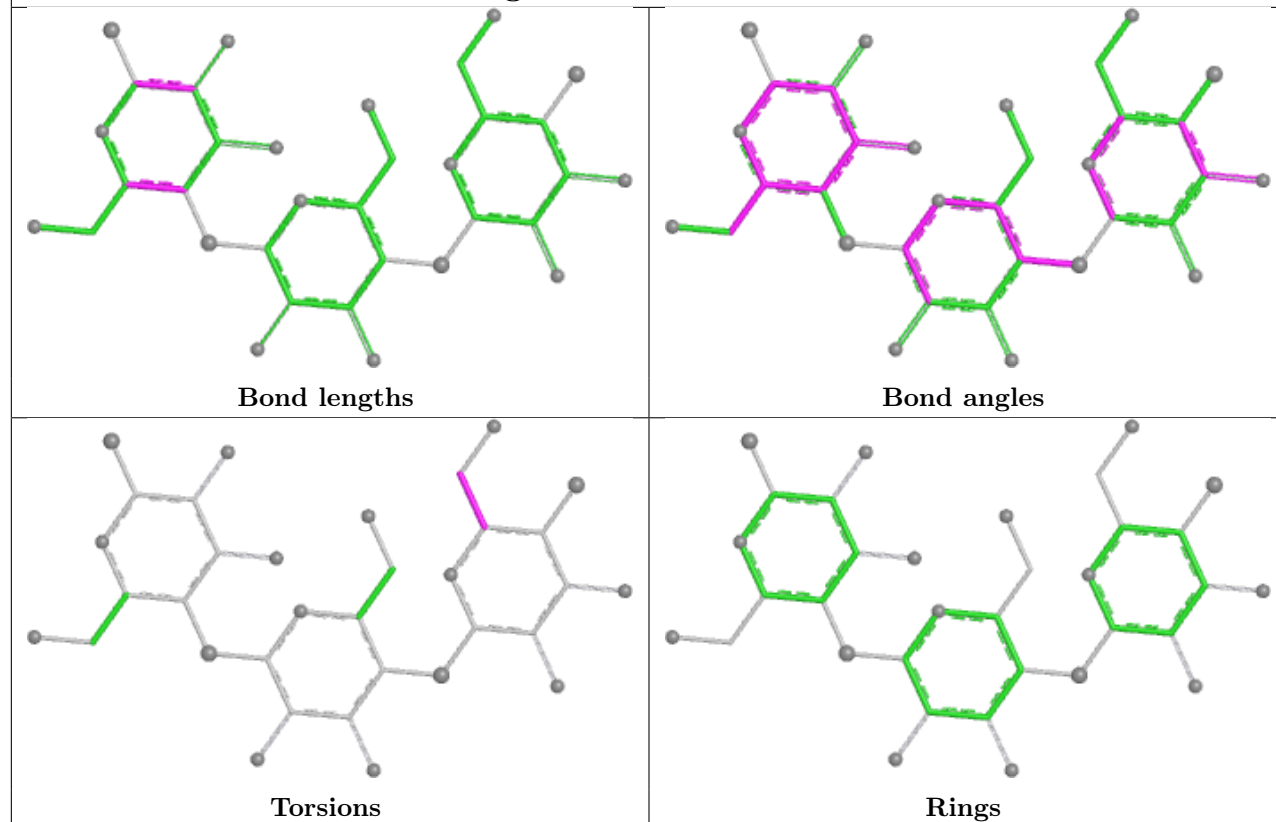
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3	SGC	1	0
2	E	2	SGC	2	0
2	F	2	SGC	3	0
2	G	2	SGC	3	0
2	H	1	SSG	5	0
2	E	3	SGC	1	0
2	E	1	SSG	5	0
2	H	2	SGC	4	0
2	G	1	SSG	4	0
2	F	1	SSG	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

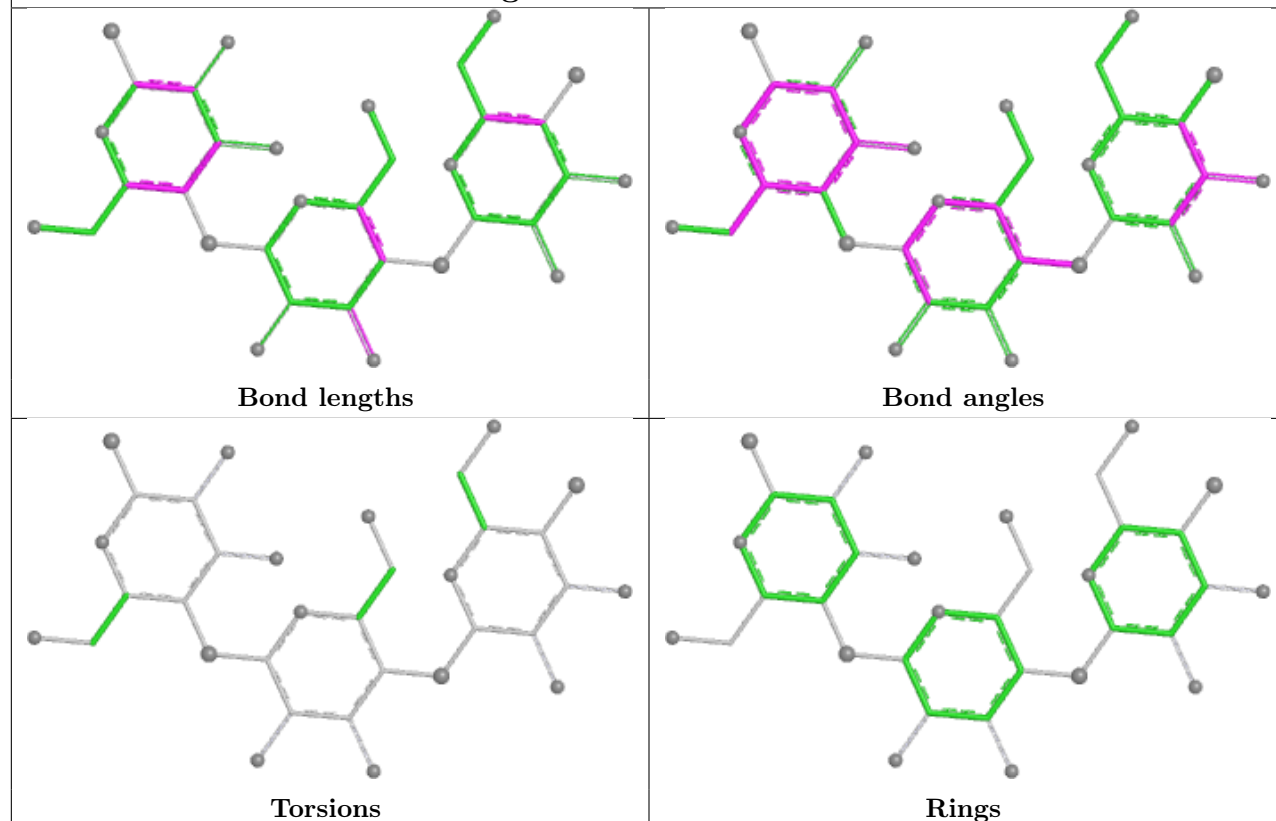
Oligosaccharide Chain E



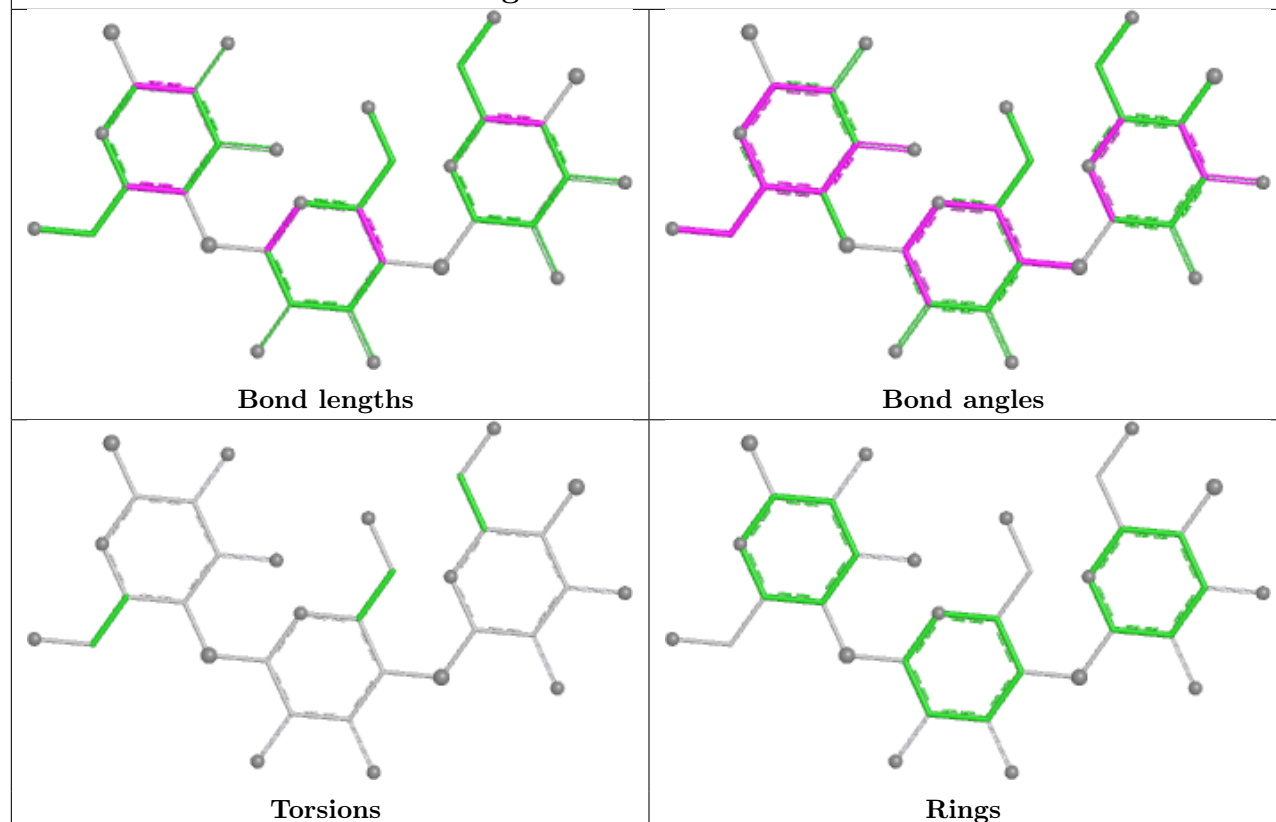
Oligosaccharide Chain F



Oligosaccharide Chain G



Oligosaccharide Chain H



5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	399	1	14,14,15	1.34	2 (14%)	17,19,21	1.20	1 (5%)
3	NAG	B	399	1	14,14,15	1.34	2 (14%)	17,19,21	1.82	3 (17%)
3	NAG	D	400	1	14,14,15	1.17	1 (7%)	17,19,21	1.23	3 (17%)
3	NAG	B	400	1	14,14,15	1.21	1 (7%)	17,19,21	1.55	4 (23%)
3	NAG	A	400	1	14,14,15	1.24	1 (7%)	17,19,21	1.50	3 (17%)
3	NAG	C	400	1	14,14,15	1.27	1 (7%)	17,19,21	1.49	3 (17%)
3	NAG	C	399	1	14,14,15	1.22	1 (7%)	17,19,21	2.13	5 (29%)
3	NAG	D	399	1	14,14,15	1.34	2 (14%)	17,19,21	2.25	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	399	1	-	0/6/23/26	0/1/1/1
3	NAG	B	399	1	-	0/6/23/26	0/1/1/1
3	NAG	D	400	1	-	2/6/23/26	0/1/1/1
3	NAG	B	400	1	-	2/6/23/26	0/1/1/1
3	NAG	A	400	1	-	2/6/23/26	0/1/1/1
3	NAG	C	400	1	-	2/6/23/26	0/1/1/1
3	NAG	C	399	1	-	0/6/23/26	0/1/1/1
3	NAG	D	399	1	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	400	NAG	O7-C7	-3.74	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	399	NAG	O7-C7	-3.72	1.14	1.23
3	A	400	NAG	O7-C7	-3.70	1.15	1.23
3	A	399	NAG	O7-C7	-3.70	1.15	1.23
3	C	399	NAG	O7-C7	-3.55	1.15	1.23
3	B	400	NAG	O7-C7	-3.42	1.15	1.23
3	D	399	NAG	O7-C7	-3.40	1.15	1.23
3	D	400	NAG	O7-C7	-3.29	1.15	1.23
3	D	399	NAG	O5-C1	2.12	1.47	1.43
3	B	399	NAG	O5-C1	2.10	1.47	1.43
3	A	399	NAG	O5-C1	2.02	1.47	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	399	NAG	O5-C1-C2	-5.40	102.94	111.29
3	D	399	NAG	C1-O5-C5	-5.06	105.41	112.19
3	B	399	NAG	C1-C2-N2	4.95	118.23	110.43
3	D	399	NAG	O5-C1-C2	-3.98	105.14	111.29
3	C	399	NAG	C1-O5-C5	-3.90	106.96	112.19
3	D	399	NAG	C2-N2-C7	-3.60	118.07	122.90
3	B	399	NAG	C1-O5-C5	-3.48	107.52	112.19
3	B	400	NAG	O5-C1-C2	-3.47	105.92	111.29
3	B	399	NAG	O5-C1-C2	-3.42	105.99	111.29
3	D	399	NAG	C8-C7-N2	-3.42	110.45	116.12
3	C	399	NAG	C8-C7-N2	-3.21	110.79	116.12
3	A	400	NAG	O5-C1-C2	-3.12	106.46	111.29
3	C	400	NAG	O5-C1-C2	-3.05	106.57	111.29
3	C	400	NAG	C4-C3-C2	-3.01	106.60	111.02
3	C	400	NAG	O6-C6-C5	2.78	120.81	111.33
3	A	400	NAG	O6-C6-C5	2.77	120.78	111.33
3	C	399	NAG	C1-C2-N2	2.74	114.75	110.43
3	D	399	NAG	O7-C7-C8	2.69	126.84	122.05
3	B	400	NAG	C4-C3-C2	-2.55	107.29	111.02
3	A	400	NAG	C4-C3-C2	-2.36	107.56	111.02
3	C	399	NAG	O7-C7-C8	2.31	126.16	122.05
3	B	400	NAG	C1-O5-C5	-2.25	109.17	112.19
3	D	400	NAG	O5-C1-C2	-2.23	107.84	111.29
3	D	400	NAG	O5-C5-C6	2.11	111.78	107.66
3	A	399	NAG	C1-O5-C5	-2.11	109.35	112.19
3	B	400	NAG	O4-C4-C5	-2.03	104.32	109.32
3	D	400	NAG	C1-C2-N2	2.00	113.59	110.43

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	400	NAG	O5-C5-C6-O6
3	A	400	NAG	O5-C5-C6-O6
3	B	400	NAG	O5-C5-C6-O6
3	C	400	NAG	O5-C5-C6-O6
3	D	400	NAG	C4-C5-C6-O6
3	B	400	NAG	C4-C5-C6-O6
3	C	400	NAG	C4-C5-C6-O6
3	A	400	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.