



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:22 AM UTC

PDB ID : 1L3W / pdb_00001l3w
Title : C-cadherin Ectodomain
Authors : Boggon, T.J.; Murray, J.; Chappuis-Flament, S.; Wong, E.; Gumbiner, B.M.; Shapiro, L.
Deposited on : 2002-03-01
Resolution : 3.08 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

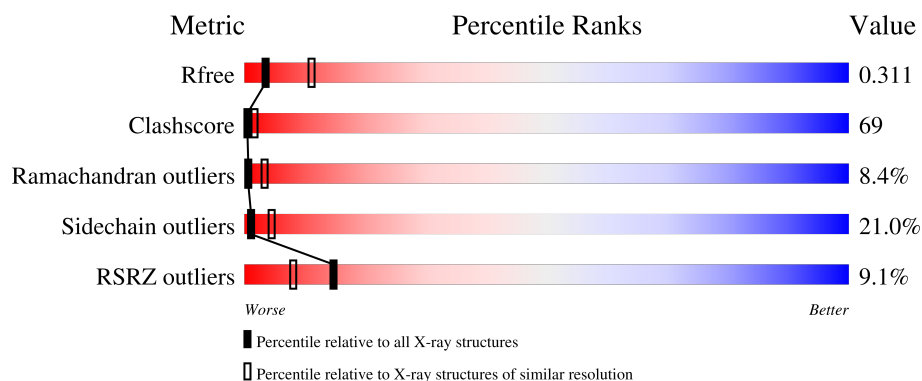
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	546	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	801	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	805	X	-	X	-
2	NAG	A	806	X	-	X	-
2	NAG	A	807	-	-	X	-
2	NAG	A	809	-	-	X	-
2	NAG	A	810	-	-	X	-
2	NAG	A	902	X	-	X	-
2	NAG	A	903	X	-	-	-
3	NDG	A	811	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4292 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.

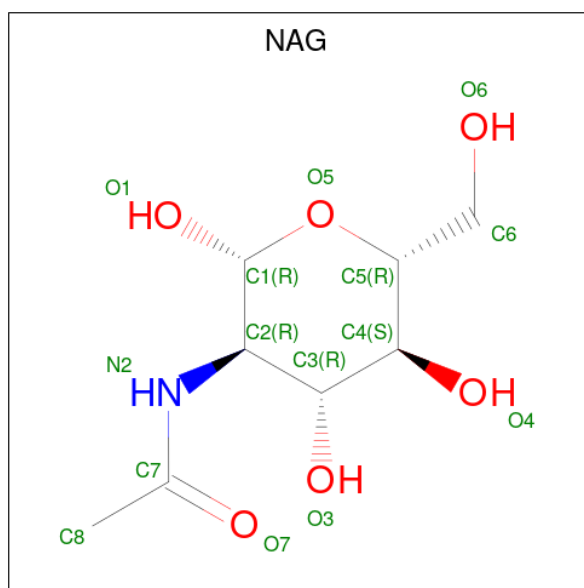
- Molecule 1 is a protein called EP-cadherin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	540	4032	2537	657	827	11	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

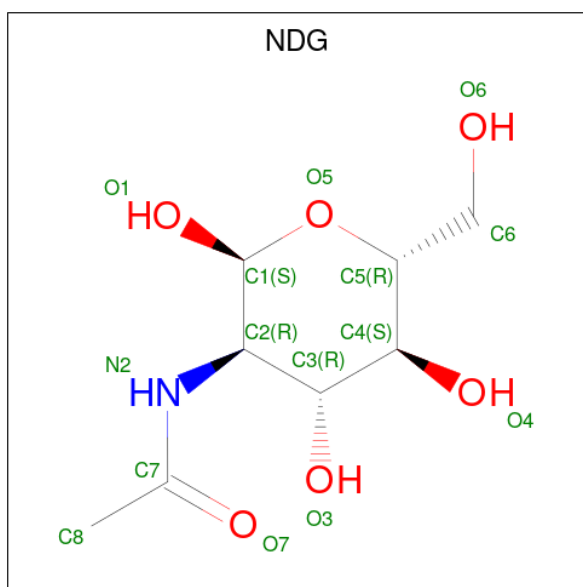
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P33148
A	-4	HIS	-	expression tag	UNP P33148
A	-3	HIS	-	expression tag	UNP P33148
A	-2	HIS	-	expression tag	UNP P33148
A	-1	HIS	-	expression tag	UNP P33148
A	0	HIS	-	expression tag	UNP P33148

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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		
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		
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		
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		
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		

- Molecule 3 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (CCD ID: NDG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	Ca	0	0
			12	12		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	0
			38	38		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.17Å 75.14Å 129.81Å 90.00° 105.50° 90.00°	Depositor
Resolution (Å)	20.00 – 3.08 20.00 – 3.08	Depositor EDS
% Data completeness (in resolution range)	69.8 (20.00-3.08) 88.0 (20.00-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.71 (at 2.98Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.243 , 0.276 0.280 , 0.311	Depositor DCC
R_{free} test set	1052 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 79.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4292	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.00	24/4115 (0.6%)	2.03	199/5651 (3.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	522	LEU	N-CA	-18.87	1.34	1.46
1	A	465	PRO	CA-C	11.97	1.58	1.51
1	A	335	ALA	CA-CB	-11.04	1.34	1.52
1	A	521	GLN	CA-C	-9.87	1.40	1.52
1	A	523	THR	N-CA	-9.55	1.33	1.46
1	A	522	LEU	CA-C	-9.34	1.40	1.52
1	A	499	THR	CA-CB	7.69	1.66	1.53
1	A	223	PRO	CG-CD	6.77	1.73	1.50
1	A	524	VAL	N-CA	-6.56	1.38	1.46
1	A	423	THR	CA-CB	-6.55	1.44	1.53
1	A	523	THR	CA-C	-6.52	1.44	1.52
1	A	290	PHE	CA-C	-6.18	1.45	1.52
1	A	399	GLU	CA-C	-6.07	1.46	1.52
1	A	482	THR	CA-CB	-6.06	1.43	1.53
1	A	464	ILE	C-N	6.05	1.38	1.33
1	A	481	LEU	N-CA	6.00	1.51	1.46
1	A	18	PRO	N-CD	5.93	1.56	1.47
1	A	17	PHE	CA-C	5.82	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	521	GLN	N-CA	-5.61	1.39	1.46
1	A	481	LEU	CA-C	-5.61	1.46	1.52
1	A	18	PRO	CA-CB	-5.51	1.43	1.53
1	A	320	THR	CA-CB	-5.39	1.46	1.53
1	A	483	TRP	N-CA	-5.36	1.40	1.46
1	A	17	PHE	C-O	-5.20	1.16	1.24

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	PHE	N-CA-C	25.18	145.36	108.60
1	A	516	ALA	N-CA-C	-20.88	88.44	114.75
1	A	376	ALA	N-CA-C	19.03	137.07	110.24
1	A	235	ILE	N-CA-C	17.32	145.36	109.34
1	A	374	ASP	CA-C-N	-17.30	98.21	119.84
1	A	374	ASP	C-N-CA	-17.30	98.21	119.84
1	A	481	LEU	N-CA-C	-16.70	85.94	113.50
1	A	520	PRO	N-CA-C	15.90	136.27	111.15
1	A	336	VAL	N-CA-C	15.90	132.07	108.54
1	A	519	ASN	CA-C-N	-15.49	104.10	119.90
1	A	519	ASN	C-N-CA	-15.49	104.10	119.90
1	A	277	SER	N-CA-C	-15.24	91.56	110.61
1	A	492	THR	N-CA-C	14.85	129.30	111.33
1	A	374	ASP	N-CA-C	14.72	142.34	109.81
1	A	398	SER	N-CA-C	14.50	141.69	110.80
1	A	521	GLN	CA-C-N	-13.08	103.27	121.84
1	A	521	GLN	C-N-CA	-13.08	103.27	121.84
1	A	289	ASP	CA-C-N	-12.37	100.64	121.80
1	A	289	ASP	C-N-CA	-12.37	100.64	121.80
1	A	233	ASN	N-CA-C	12.01	132.23	107.37
1	A	223	PRO	N-CA-C	-11.92	87.92	112.47
1	A	17	PHE	C-N-CD	-11.54	95.22	120.60
1	A	465	PRO	C-N-CD	-11.03	96.34	120.60
1	A	471	TYR	N-CA-C	10.80	126.48	110.17
1	A	222	ASP	CA-C-N	-10.77	106.37	119.84
1	A	222	ASP	C-N-CA	-10.77	106.37	119.84
1	A	236	GLY	N-CA-C	-10.56	88.14	113.18
1	A	234	GLU	CA-C-N	10.14	140.22	121.97
1	A	234	GLU	C-N-CA	10.14	140.22	121.97
1	A	522	LEU	CA-C-N	-10.12	102.22	121.54
1	A	522	LEU	C-N-CA	-10.12	102.22	121.54
1	A	230	VAL	CA-C-N	10.07	132.43	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	VAL	C-N-CA	10.07	132.43	119.84
1	A	332	PHE	N-CA-C	-9.94	97.41	110.53
1	A	221	PHE	N-CA-C	9.78	124.53	109.96
1	A	362	GLN	N-CA-C	-9.69	90.17	110.80
1	A	405	THR	N-CA-C	9.68	125.37	110.36
1	A	221	PHE	CA-C-N	-9.57	98.45	121.80
1	A	221	PHE	C-N-CA	-9.57	98.45	121.80
1	A	249	MET	CA-C-N	9.55	131.78	119.84
1	A	249	MET	C-N-CA	9.55	131.78	119.84
1	A	398	SER	CA-C-N	-9.54	105.28	122.46
1	A	398	SER	C-N-CA	-9.54	105.28	122.46
1	A	234	GLU	N-CA-C	-9.52	90.53	110.80
1	A	319	VAL	N-CA-C	9.41	122.48	108.46
1	A	479	SER	N-CA-C	-9.20	101.75	113.16
1	A	337	SER	N-CA-C	-9.18	91.63	108.24
1	A	503	LYS	N-CA-C	8.98	129.92	110.80
1	A	403	ASN	N-CA-C	-8.97	95.80	109.79
1	A	382	ASN	N-CA-C	-8.61	95.26	108.96
1	A	521	GLN	N-CA-C	-8.48	96.94	109.15
1	A	476	SER	N-CA-C	8.42	128.74	110.80
1	A	397	GLU	N-CA-C	8.38	123.24	112.34
1	A	520	PRO	CA-C-N	8.29	134.59	121.66
1	A	520	PRO	C-N-CA	8.29	134.59	121.66
1	A	291	GLU	N-CA-C	-8.26	101.30	112.94
1	A	532	CYS	N-CA-C	8.08	128.02	110.80
1	A	254	ALA	N-CA-C	-8.08	102.46	112.88
1	A	31	PHE	N-CA-C	8.06	121.23	111.40
1	A	222	ASP	N-CA-C	8.06	127.62	109.81
1	A	46	PRO	C-N-CD	-8.03	102.93	120.60
1	A	397	GLU	CA-C-N	-7.94	106.37	121.54
1	A	397	GLU	C-N-CA	-7.94	106.37	121.54
1	A	290	PHE	CA-C-O	7.94	129.80	121.38
1	A	523	THR	N-CA-CB	-7.92	97.11	110.49
1	A	222	ASP	CA-CB-CG	-7.85	104.75	112.60
1	A	381	VAL	N-CA-C	7.80	119.84	108.53
1	A	502	LEU	N-CA-C	7.76	127.34	110.80
1	A	432	ASP	N-CA-C	7.72	122.42	109.76
1	A	246	ASP	N-CA-C	-7.69	99.14	110.52
1	A	315	SER	N-CA-C	7.65	120.88	108.41
1	A	525	VAL	N-CA-C	-7.64	93.44	109.34
1	A	17	PHE	CA-C-O	-7.63	113.73	120.60
1	A	522	LEU	N-CA-C	-7.58	97.20	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	THR	N-CA-C	7.55	120.83	108.52
1	A	290	PHE	CA-C-N	7.54	133.98	122.37
1	A	290	PHE	C-N-CA	7.54	133.98	122.37
1	A	522	LEU	N-CA-CB	7.43	118.50	111.59
1	A	339	VAL	N-CA-C	7.43	124.79	109.34
1	A	217	ASN	N-CA-C	7.38	121.69	109.95
1	A	290	PHE	O-C-N	7.37	131.00	123.26
1	A	252	THR	CA-C-N	7.35	129.03	119.84
1	A	252	THR	C-N-CA	7.35	129.03	119.84
1	A	62	VAL	N-CA-C	-7.34	97.86	108.36
1	A	379	LEU	N-CA-C	7.19	119.58	110.24
1	A	266	GLY	N-CA-C	-7.17	103.32	115.80
1	A	90	GLU	N-CA-C	-7.12	99.23	109.48
1	A	519	ASN	N-CA-C	7.07	125.43	109.81
1	A	358	ASP	CA-C-N	7.06	128.67	119.84
1	A	358	ASP	C-N-CA	7.06	128.67	119.84
1	A	485	ALA	N-CA-C	7.04	120.42	110.50
1	A	399	GLU	N-CA-C	7.00	121.68	112.72
1	A	194	THR	N-CA-C	6.99	120.54	109.50
1	A	439	VAL	CA-C-N	6.97	126.73	119.76
1	A	439	VAL	C-N-CA	6.97	126.73	119.76
1	A	104	ASN	N-CA-C	6.93	120.23	109.07
1	A	481	LEU	CA-C-O	6.90	126.03	118.65
1	A	364	ILE	N-CA-C	-6.88	95.03	109.34
1	A	252	THR	N-CA-C	6.86	119.31	110.39
1	A	491	GLY	N-CA-C	6.85	129.42	113.18
1	A	221	PHE	CA-C-O	-6.83	112.85	120.70
1	A	520	PRO	CA-C-O	6.83	129.07	121.36
1	A	119	GLU	N-CA-C	6.80	118.69	111.28
1	A	484	LYS	CA-C-N	6.70	131.46	120.94
1	A	484	LYS	C-N-CA	6.70	131.46	120.94
1	A	2	TRP	N-CA-C	-6.62	94.73	107.57
1	A	46	PRO	CA-C-N	6.55	142.72	127.00
1	A	46	PRO	C-N-CA	6.55	142.72	127.00
1	A	486	GLU	N-CA-C	6.53	118.44	108.52
1	A	232	GLU	N-CA-C	6.51	118.97	111.02
1	A	437	GLY	CA-C-N	6.50	127.97	119.84
1	A	437	GLY	C-N-CA	6.50	127.97	119.84
1	A	335	ALA	N-CA-C	-6.50	93.92	107.37
1	A	539	CYS	N-CA-C	6.45	124.53	110.80
1	A	522	LEU	CA-CB-CG	-6.44	93.75	116.30
1	A	121	VAL	N-CA-C	6.42	117.46	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	VAL	C-N-CD	-6.41	98.72	125.00
1	A	400	TYR	N-CA-C	-6.40	103.59	111.40
1	A	531	SER	N-CA-C	6.38	124.39	110.80
1	A	42	GLY	N-CA-C	-6.34	107.54	115.08
1	A	328	GLU	N-CA-C	6.32	120.22	110.42
1	A	26	SER	N-CA-C	-6.32	99.40	109.76
1	A	431	LEU	N-CA-C	6.31	119.01	109.41
1	A	380	THR	N-CA-C	6.25	118.67	108.55
1	A	304	ASN	N-CA-C	-6.24	100.97	110.14
1	A	122	GLN	N-CA-C	6.23	118.89	110.29
1	A	233	ASN	CB-CA-C	-6.20	103.26	111.82
1	A	413	THR	N-CA-C	6.20	119.00	108.90
1	A	186	GLU	N-CA-C	6.18	118.37	107.61
1	A	222	ASP	N-CA-CB	6.15	121.32	110.37
1	A	470	PRO	N-CA-C	6.15	125.14	112.47
1	A	163	PHE	N-CA-C	6.14	118.29	109.14
1	A	39	THR	N-CA-C	6.13	119.02	109.52
1	A	234	GLU	O-C-N	6.10	130.70	122.59
1	A	18	PRO	CA-N-CD	-6.08	102.99	111.50
1	A	481	LEU	CA-CB-CG	-6.04	95.16	116.30
1	A	157	GLU	CA-C-N	6.04	141.48	127.00
1	A	157	GLU	C-N-CA	6.04	141.48	127.00
1	A	488	ASP	N-CA-C	-6.03	102.00	110.50
1	A	376	ALA	CA-C-N	6.02	133.04	121.54
1	A	376	ALA	C-N-CA	6.02	133.04	121.54
1	A	504	LYS	N-CA-C	5.92	119.36	108.58
1	A	245	THR	N-CA-C	5.88	117.06	107.23
1	A	314	THR	CA-C-N	-5.83	114.78	123.00
1	A	314	THR	C-N-CA	-5.83	114.78	123.00
1	A	505	GLY	N-CA-C	5.83	126.99	113.18
1	A	469	TYR	CA-C-N	5.74	127.02	119.84
1	A	469	TYR	C-N-CA	5.74	127.02	119.84
1	A	465	PRO	CA-C-N	5.74	140.77	127.00
1	A	465	PRO	C-N-CA	5.74	140.77	127.00
1	A	481	LEU	O-C-N	5.74	128.61	121.84
1	A	326	VAL	N-CA-C	-5.73	100.02	108.85
1	A	520	PRO	O-C-N	5.68	130.10	122.89
1	A	353	SER	N-CA-C	-5.65	99.91	108.67
1	A	376	ALA	CA-C-O	5.63	127.35	121.15
1	A	235	ILE	N-CA-CB	-5.63	101.94	111.23
1	A	365	GLN	CA-C-N	-5.58	112.94	123.27
1	A	365	GLN	C-N-CA	-5.58	112.94	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	THR	N-CA-C	5.57	117.53	109.07
1	A	237	PHE	N-CA-C	5.57	117.56	108.76
1	A	418	SER	N-CA-C	5.56	122.65	110.80
1	A	538	LYS	N-CA-C	-5.49	102.15	110.28
1	A	222	ASP	C-N-CD	-5.47	102.55	125.00
1	A	157	GLU	C-N-CD	-5.47	108.57	120.60
1	A	224	LYS	N-CA-C	-5.46	107.16	113.88
1	A	235	ILE	CA-C-N	5.43	132.05	121.41
1	A	235	ILE	C-N-CA	5.43	132.05	121.41
1	A	480	ASP	CA-C-N	5.43	128.53	120.17
1	A	480	ASP	C-N-CA	5.43	128.53	120.17
1	A	532	CYS	N-CA-CB	-5.43	101.32	110.49
1	A	392	GLY	N-CA-C	5.43	122.06	112.83
1	A	4	ILE	CA-C-N	5.41	125.95	120.38
1	A	4	ILE	C-N-CA	5.41	125.95	120.38
1	A	448	CYS	CA-CB-SG	-5.41	101.96	114.40
1	A	209	ILE	N-CA-C	5.35	115.67	108.17
1	A	527	ALA	N-CA-C	5.32	117.00	107.80
1	A	142	LEU	N-CA-C	-5.30	106.04	112.88
1	A	250	PRO	N-CA-C	5.27	123.32	112.47
1	A	295	GLN	N-CA-C	5.26	118.39	109.76
1	A	465	PRO	N-CA-C	5.25	115.52	110.47
1	A	423	THR	N-CA-C	5.25	116.86	108.41
1	A	520	PRO	CA-CB-CG	-5.24	94.55	104.50
1	A	316	THR	N-CA-C	5.23	117.61	110.55
1	A	506	ASP	N-CA-C	5.21	121.91	110.80
1	A	467	ASN	N-CA-C	5.21	121.90	110.80
1	A	537	ILE	N-CA-C	5.21	117.28	109.20
1	A	221	PHE	CB-CA-C	-5.20	102.67	110.16
1	A	235	ILE	CA-C-O	5.20	127.28	120.78
1	A	502	LEU	CA-C-N	5.20	131.46	121.54
1	A	502	LEU	C-N-CA	5.20	131.46	121.54
1	A	465	PRO	CA-C-O	5.18	124.63	120.90
1	A	336	VAL	N-CA-CB	-5.16	105.17	110.95
1	A	294	LYS	N-CA-C	-5.13	107.68	114.04
1	A	249	MET	N-CA-C	5.13	121.14	109.81
1	A	18	PRO	CA-CB-CG	-5.12	94.27	104.00
1	A	154	ASP	CA-C-N	-5.11	113.45	119.84
1	A	154	ASP	C-N-CA	-5.11	113.45	119.84
1	A	508	SER	N-CA-C	5.06	118.21	110.36
1	A	419	VAL	N-CA-C	5.03	114.90	107.75

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	PHE	Sidechain
1	A	18	PRO	Mainchain
1	A	222	ASP	Mainchain
1	A	520	PRO	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	4032	0	3772	558	0
2	A	182	0	169	86	0
3	A	28	0	24	9	0
4	A	12	0	0	0	0
5	A	38	0	0	3	0
All	All	4292	0	3965	568	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 69.

All (568) 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:A:482:THR:HG23	1:A:499:THR:CG2	1.75	1.17
1:A:234:GLU:H	1:A:235:ILE:HG23	1.08	1.15
1:A:154:ASP:C	2:A:801:NAG:H82	1.70	1.15
1:A:423:THR:HB	2:A:810:NAG:C7	1.76	1.15
1:A:8:LYS:H	1:A:8:LYS:HD2	1.04	1.14
1:A:474:SER:HB2	1:A:512:LEU:HG	1.25	1.12
1:A:227:THR:HG21	2:A:807:NAG:C8	1.82	1.08
1:A:222:ASP:OD1	1:A:222:ASP:O	1.69	1.08
1:A:301:THR:HG21	2:A:805:NAG:H82	1.29	1.07
1:A:335:ALA:HB1	3:A:811:NDG:O6	1.54	1.07
1:A:403:ASN:HB2	2:A:902:NAG:H83	1.30	1.07
1:A:482:THR:HG23	1:A:499:THR:HG22	1.09	1.07
1:A:290:PHE:HB2	1:A:292:LEU:N	1.69	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:SER:HA	1:A:427:ILE:HG23	1.38	1.05
1:A:482:THR:CG2	1:A:499:THR:N	2.22	1.02
1:A:290:PHE:HB2	1:A:292:LEU:H	0.88	1.02
1:A:482:THR:HG21	1:A:499:THR:H	1.23	1.01
1:A:403:ASN:HB2	2:A:902:NAG:C8	1.90	1.00
1:A:522:LEU:HD22	1:A:523:THR:HB	1.39	1.00
1:A:274:ASP:O	1:A:278:ASN:HA	1.61	1.00
1:A:188:THR:HG23	1:A:208:ILE:HG12	1.43	1.00
1:A:523:THR:HG23	1:A:524:VAL:H	1.27	0.99
1:A:320:THR:HG21	2:A:807:NAG:N2	1.78	0.98
1:A:366:LYS:HG3	1:A:367:LEU:H	1.28	0.97
1:A:482:THR:CG2	1:A:499:THR:H	1.76	0.96
1:A:235:ILE:CG1	1:A:287:GLY:HA2	1.96	0.96
1:A:320:THR:HG21	2:A:807:NAG:HN2	1.31	0.95
1:A:290:PHE:CB	1:A:292:LEU:H	1.79	0.95
1:A:374:ASP:O	1:A:375:PRO:C	2.06	0.95
1:A:27:ASN:HD22	1:A:28:LYS:N	1.66	0.94
1:A:227:THR:HG21	2:A:807:NAG:H83	1.48	0.94
1:A:195:ASP:HB2	1:A:201:LEU:H	1.34	0.93
1:A:352:ILE:HG13	1:A:388:VAL:HB	1.51	0.93
1:A:227:THR:HG21	2:A:807:NAG:C7	1.99	0.93
1:A:403:ASN:HB2	2:A:902:NAG:C7	2.00	0.92
1:A:366:LYS:CG	1:A:367:LEU:H	1.80	0.92
1:A:446:THR:HG23	1:A:539:CYS:SG	2.10	0.92
1:A:482:THR:HG21	1:A:499:THR:N	1.81	0.92
2:A:805:NAG:H62	2:A:806:NAG:C7	2.00	0.92
1:A:289:ASP:O	1:A:290:PHE:HB3	1.67	0.92
1:A:335:ALA:CB	3:A:811:NDG:O6	2.18	0.91
2:A:805:NAG:O5	2:A:806:NAG:H83	1.71	0.91
1:A:234:GLU:N	1:A:235:ILE:HG23	1.86	0.91
1:A:517:GLN:O	1:A:519:ASN:N	2.03	0.90
1:A:340:ASP:HA	1:A:429:HIS:HB3	1.53	0.90
1:A:378:TRP:HB2	1:A:379:LEU:HD23	1.53	0.90
1:A:154:ASP:HB3	1:A:155:PRO:HD2	1.54	0.90
1:A:518:ASN:O	1:A:520:PRO:HD3	1.72	0.90
1:A:8:LYS:HD2	1:A:8:LYS:N	1.87	0.89
1:A:318:THR:HG21	2:A:806:NAG:H5	1.56	0.88
1:A:371:ILE:CD1	1:A:381:VAL:HG11	2.03	0.88
1:A:483:TRP:CZ3	1:A:498:PRO:HG3	2.09	0.88
1:A:523:THR:HG23	1:A:524:VAL:CG2	2.03	0.88
1:A:343:GLU:HB3	1:A:433:VAL:HG21	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PRO:CD	1:A:522:LEU:HD12	2.05	0.87
1:A:8:LYS:H	1:A:8:LYS:CD	1.74	0.86
1:A:221:PHE:HE1	1:A:315:SER:O	1.56	0.86
1:A:441:SER:OG	1:A:442:PRO:HD3	1.75	0.86
1:A:449:ASP:H	1:A:532:CYS:HB3	1.37	0.86
1:A:257:ALA:O	1:A:273:THR:HG21	1.74	0.86
1:A:423:THR:CB	2:A:810:NAG:C7	2.54	0.86
1:A:333:VAL:HB	1:A:334:PRO:HD3	1.56	0.86
1:A:320:THR:HG21	2:A:807:NAG:C2	2.05	0.85
1:A:277:SER:C	1:A:278:ASN:HD22	1.83	0.85
1:A:438:PRO:HB3	1:A:471:TYR:HE2	1.41	0.85
1:A:483:TRP:HZ2	1:A:507:TYR:CE1	1.95	0.85
1:A:517:GLN:C	1:A:519:ASN:H	1.84	0.85
1:A:523:THR:HG23	1:A:524:VAL:N	1.90	0.85
1:A:235:ILE:HG13	1:A:287:GLY:HA2	1.58	0.85
1:A:222:ASP:OD1	1:A:222:ASP:C	2.20	0.84
1:A:375:PRO:HB3	1:A:400:TYR:CE2	2.12	0.84
1:A:155:PRO:HB2	2:A:801:NAG:H81	1.59	0.84
1:A:483:TRP:HZ2	1:A:507:TYR:HE1	1.24	0.83
1:A:451:ASN:N	1:A:533:GLU:O	2.10	0.83
1:A:423:THR:HB	2:A:810:NAG:N2	1.93	0.83
1:A:155:PRO:C	1:A:157:GLU:H	1.86	0.83
1:A:230:VAL:O	1:A:324:GLU:N	2.11	0.83
1:A:28:LYS:HD3	1:A:88:VAL:HG12	1.61	0.83
1:A:423:THR:CB	2:A:810:NAG:N2	2.42	0.82
1:A:154:ASP:HB3	2:A:801:NAG:N2	1.95	0.82
1:A:482:THR:HG21	1:A:500:GLN:N	1.95	0.82
1:A:440:PRO:HD2	1:A:522:LEU:HD12	1.59	0.82
1:A:448:CYS:O	1:A:452:PRO:HG3	1.78	0.82
1:A:234:GLU:H	1:A:235:ILE:CG2	1.92	0.82
1:A:154:ASP:HB3	2:A:801:NAG:HN2	1.45	0.81
1:A:289:ASP:O	1:A:289:ASP:OD2	1.97	0.81
1:A:446:THR:HG21	1:A:537:ILE:O	1.79	0.81
1:A:486:GLU:O	1:A:494:MET:HA	1.81	0.81
1:A:299:GLN:HG2	1:A:318:THR:HG23	1.62	0.81
1:A:127:VAL:HG13	1:A:128:MET:H	1.46	0.80
1:A:290:PHE:CE2	1:A:293:ARG:HB2	2.16	0.80
1:A:371:ILE:HD11	1:A:381:VAL:HG11	1.64	0.80
1:A:290:PHE:HD2	1:A:293:ARG:H	1.28	0.80
1:A:265:GLU:HB3	1:A:268:PHE:HE2	1.46	0.79
1:A:496:LEU:HD21	1:A:509:ILE:HD13	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TYR:CD1	2:A:808:NAG:H83	2.17	0.79
1:A:232:GLU:HG3	1:A:290:PHE:N	1.98	0.79
1:A:449:ASP:HB3	1:A:532:CYS:H	1.47	0.79
1:A:301:THR:HG21	2:A:805:NAG:C8	2.12	0.78
1:A:27:ASN:HD22	1:A:27:ASN:C	1.85	0.78
2:A:809:NAG:H61	2:A:810:NAG:H62	1.65	0.78
1:A:154:ASP:CB	1:A:155:PRO:HD2	2.13	0.78
1:A:194:THR:HB	1:A:198:GLY:HA2	1.67	0.77
1:A:524:VAL:CG2	2:A:904:NAG:H81	2.14	0.77
1:A:365:GLN:HG3	1:A:365:GLN:O	1.82	0.77
1:A:290:PHE:HZ	1:A:296:TYR:HH	1.33	0.77
1:A:523:THR:HG23	1:A:524:VAL:HG22	1.67	0.77
1:A:156:GLU:HG3	1:A:160:PRO:HB3	1.66	0.77
1:A:195:ASP:HB3	1:A:200:GLY:HA3	1.65	0.77
1:A:501:GLN:O	1:A:501:GLN:HG2	1.84	0.76
1:A:186:GLU:O	2:A:801:NAG:O7	2.03	0.76
1:A:440:PRO:HB3	1:A:457:LEU:HD21	1.67	0.76
1:A:238:GLU:HA	1:A:283:THR:HG22	1.66	0.76
1:A:223:PRO:HD2	1:A:226:TYR:OH	1.85	0.76
1:A:366:LYS:CG	1:A:367:LEU:N	2.48	0.76
1:A:196:LEU:HB2	1:A:199:ALA:HB3	1.67	0.75
1:A:272:THR:HG22	1:A:273:THR:H	1.51	0.75
1:A:523:THR:CG2	1:A:524:VAL:N	2.46	0.75
1:A:448:CYS:SG	1:A:537:ILE:HG22	2.27	0.75
1:A:241:ARG:HE	1:A:281:ILE:HD12	1.51	0.75
1:A:449:ASP:HB3	1:A:532:CYS:N	2.02	0.75
1:A:290:PHE:CD2	1:A:293:ARG:N	2.55	0.74
1:A:188:THR:HG23	1:A:208:ILE:CG1	2.16	0.74
1:A:371:ILE:HD12	1:A:410:MET:HB3	1.68	0.74
1:A:451:ASN:O	1:A:534:GLY:HA2	1.88	0.74
1:A:290:PHE:HE2	1:A:293:ARG:HB2	1.52	0.74
1:A:333:VAL:CB	1:A:334:PRO:HD3	2.18	0.73
1:A:223:PRO:HB2	1:A:226:TYR:CE2	2.23	0.73
1:A:27:ASN:C	1:A:27:ASN:ND2	2.46	0.73
1:A:373:ASN:ND2	1:A:374:ASP:H	1.87	0.73
1:A:276:GLU:HG3	1:A:277:SER:H	1.54	0.73
1:A:511:VAL:HG23	1:A:523:THR:O	1.89	0.73
1:A:1:ASP:CG	1:A:2:TRP:H	1.96	0.72
1:A:298:LEU:N	1:A:298:LEU:HD23	2.03	0.72
1:A:289:ASP:O	1:A:289:ASP:CG	2.30	0.72
1:A:273:THR:O	2:A:803:NAG:H82	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:THR:CG2	2:A:807:NAG:N2	2.52	0.72
1:A:320:THR:CG2	2:A:807:NAG:HN2	2.01	0.72
1:A:366:LYS:HG3	1:A:367:LEU:N	2.04	0.72
1:A:394:LEU:N	1:A:394:LEU:HD12	2.05	0.71
1:A:342:SER:HA	1:A:431:LEU:HB2	1.71	0.71
1:A:482:THR:CG2	1:A:499:THR:CG2	2.62	0.71
1:A:227:THR:O	2:A:812:NAG:O5	2.09	0.71
1:A:229:LEU:HD23	1:A:322:THR:HB	1.73	0.71
1:A:276:GLU:CG	1:A:277:SER:H	2.03	0.71
1:A:403:ASN:CB	2:A:902:NAG:N2	2.54	0.71
1:A:434:ASN:OD1	1:A:467:ASN:HB3	1.90	0.70
1:A:438:PRO:HB3	1:A:471:TYR:CE2	2.26	0.70
1:A:523:THR:HG23	1:A:524:VAL:HG23	1.74	0.70
1:A:316:THR:O	2:A:806:NAG:H82	1.91	0.69
1:A:187:TYR:HA	2:A:801:NAG:C7	2.21	0.69
1:A:414:ASP:HB3	1:A:420:GLY:HA3	1.73	0.69
1:A:53:ILE:HG13	1:A:59:TRP:O	1.93	0.69
1:A:128:MET:HE1	1:A:207:ALA:HB1	1.74	0.69
1:A:222:ASP:O	1:A:222:ASP:CG	2.32	0.68
1:A:282:LEU:HD23	1:A:283:THR:H	1.58	0.68
1:A:242:LEU:HD12	1:A:280:GLY:O	1.93	0.68
1:A:290:PHE:HZ	1:A:296:TYR:OH	1.77	0.68
1:A:155:PRO:HB2	2:A:801:NAG:C8	2.24	0.68
1:A:320:THR:HG21	2:A:807:NAG:H2	1.76	0.68
1:A:482:THR:HG21	1:A:500:GLN:H	1.58	0.68
1:A:337:SER:CA	1:A:427:ILE:HG23	2.20	0.68
1:A:483:TRP:CZ2	1:A:507:TYR:HE1	2.09	0.68
1:A:221:PHE:CE1	1:A:315:SER:O	2.45	0.68
1:A:137:ASP:OD2	1:A:139:ILE:HG22	1.94	0.68
1:A:272:THR:HG22	1:A:273:THR:N	2.09	0.68
1:A:371:ILE:CG2	1:A:372:GLY:N	2.57	0.68
1:A:423:THR:HB	2:A:810:NAG:C8	2.24	0.67
1:A:440:PRO:HA	1:A:458:THR:O	1.94	0.67
1:A:186:GLU:OE1	2:A:801:NAG:H62	1.93	0.67
1:A:195:ASP:HB2	1:A:201:LEU:N	2.08	0.67
1:A:347:ARG:CD	1:A:392:GLY:H	2.07	0.67
1:A:282:LEU:HD23	1:A:283:THR:N	2.08	0.67
1:A:289:ASP:O	1:A:290:PHE:CB	2.25	0.67
1:A:347:ARG:CG	1:A:392:GLY:H	2.08	0.67
1:A:524:VAL:HG21	2:A:904:NAG:H81	1.76	0.67
1:A:154:ASP:O	1:A:155:PRO:C	2.36	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:SER:HB2	1:A:512:LEU:CG	2.15	0.66
1:A:333:VAL:HB	1:A:334:PRO:CD	2.24	0.66
1:A:373:ASN:ND2	1:A:374:ASP:N	2.43	0.66
1:A:446:THR:CG2	1:A:537:ILE:O	2.44	0.66
1:A:464:ILE:O	1:A:467:ASN:HB2	1.96	0.66
1:A:366:LYS:HG3	1:A:367:LEU:HG	1.77	0.66
1:A:440:PRO:HD2	1:A:522:LEU:CD1	2.26	0.66
2:A:805:NAG:C6	2:A:806:NAG:C7	2.74	0.66
1:A:232:GLU:HG3	1:A:290:PHE:H	1.61	0.66
1:A:524:VAL:HG23	2:A:904:NAG:H81	1.78	0.66
1:A:265:GLU:HB3	1:A:268:PHE:CE2	2.31	0.65
1:A:401:VAL:HG13	1:A:405:THR:O	1.95	0.65
2:A:809:NAG:C6	2:A:810:NAG:H62	2.26	0.65
1:A:187:TYR:HA	2:A:801:NAG:C8	2.25	0.65
1:A:232:GLU:HG2	1:A:289:ASP:HA	1.77	0.65
1:A:405:THR:OG1	1:A:406:TYR:N	2.22	0.65
1:A:403:ASN:HB2	2:A:902:NAG:N2	2.10	0.65
1:A:406:TYR:CE1	2:A:808:NAG:H83	2.32	0.65
1:A:347:ARG:HD2	1:A:392:GLY:H	1.60	0.64
1:A:474:SER:CB	1:A:512:LEU:HG	2.14	0.64
1:A:327:ASN:HA	1:A:360:ASP:OD2	1.97	0.64
1:A:346:SER:OG	1:A:349:GLU:HG3	1.97	0.64
1:A:409:ILE:HG12	1:A:425:THR:HG23	1.80	0.64
1:A:517:GLN:C	1:A:519:ASN:N	2.47	0.64
1:A:341:VAL:HG21	1:A:345:LEU:HD12	1.79	0.64
1:A:142:LEU:HB3	1:A:196:LEU:HA	1.81	0.63
1:A:482:THR:HG21	1:A:499:THR:CA	2.27	0.63
1:A:127:VAL:HG22	1:A:128:MET:N	2.14	0.63
1:A:343:GLU:HB3	1:A:433:VAL:CG2	2.28	0.63
1:A:486:GLU:O	1:A:494:MET:CA	2.46	0.63
1:A:212:THR:HG22	1:A:213:ASP:H	1.62	0.63
1:A:227:THR:CG2	2:A:807:NAG:C7	2.76	0.63
1:A:22:VAL:HG22	1:A:23:GLN:N	2.14	0.63
1:A:440:PRO:HD3	1:A:522:LEU:HD12	1.78	0.63
1:A:154:ASP:CA	2:A:801:NAG:H82	2.29	0.63
1:A:446:THR:CG2	1:A:539:CYS:SG	2.86	0.63
1:A:524:VAL:HG23	2:A:904:NAG:C8	2.29	0.63
1:A:154:ASP:C	2:A:801:NAG:C8	2.62	0.62
1:A:299:GLN:C	1:A:300:ILE:HD12	2.24	0.62
1:A:347:ARG:HG3	1:A:392:GLY:H	1.62	0.62
1:A:411:LEU:HD22	1:A:421:THR:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:PRO:HB3	1:A:400:TYR:CD2	2.33	0.62
1:A:403:ASN:CB	2:A:902:NAG:C7	2.76	0.62
1:A:419:VAL:HG13	2:A:809:NAG:O7	1.98	0.62
1:A:3:VAL:O	5:A:1001:HOH:O	2.16	0.62
1:A:403:ASN:O	1:A:405:THR:N	2.33	0.62
1:A:68:ARG:HD3	1:A:100:ASP:HA	1.82	0.62
1:A:508:SER:HB3	1:A:526:ASN:OD1	2.00	0.62
1:A:524:VAL:CG2	2:A:904:NAG:C8	2.78	0.62
1:A:486:GLU:O	1:A:495:LEU:N	2.31	0.61
1:A:235:ILE:HG12	1:A:287:GLY:HA2	1.82	0.61
1:A:374:ASP:O	1:A:375:PRO:O	2.17	0.61
1:A:154:ASP:O	2:A:801:NAG:H82	1.98	0.61
1:A:212:THR:HG22	1:A:213:ASP:N	2.15	0.61
1:A:518:ASN:O	1:A:520:PRO:CD	2.46	0.61
1:A:393:ASN:C	1:A:394:LEU:HD12	2.25	0.61
1:A:449:ASP:H	1:A:532:CYS:CB	2.12	0.61
1:A:371:ILE:CG2	1:A:372:GLY:H	2.13	0.61
1:A:379:LEU:HD23	1:A:379:LEU:H	1.66	0.61
1:A:181:ARG:NE	1:A:213:ASP:OD1	2.34	0.60
1:A:232:GLU:CG	1:A:290:PHE:N	2.64	0.60
1:A:189:LEU:N	1:A:189:LEU:HD23	2.17	0.60
1:A:371:ILE:HG22	1:A:372:GLY:N	2.14	0.60
1:A:482:THR:HG21	1:A:499:THR:C	2.27	0.60
1:A:482:THR:HG22	1:A:499:THR:N	2.13	0.60
1:A:49:GLY:O	1:A:63:THR:HG21	2.02	0.59
1:A:336:VAL:HB	1:A:426:LEU:HD23	1.84	0.59
1:A:154:ASP:CG	1:A:155:PRO:CD	2.75	0.59
1:A:239:VAL:HG13	1:A:240:GLN:H	1.67	0.59
1:A:443:ARG:HG3	1:A:443:ARG:HH11	1.67	0.59
1:A:508:SER:HA	1:A:526:ASN:HA	1.84	0.59
1:A:195:ASP:CB	1:A:200:GLY:HA3	2.33	0.59
1:A:458:THR:HG22	1:A:493:SER:CB	2.32	0.59
1:A:268:PHE:HA	1:A:285:ALA:HB3	1.85	0.59
1:A:473:VAL:HA	1:A:513:LEU:HD23	1.85	0.59
1:A:514:SER:HA	1:A:517:GLN:O	2.02	0.58
1:A:367:LEU:CB	1:A:413:THR:O	2.51	0.58
1:A:38:ILE:HG22	1:A:53:ILE:HG22	1.85	0.58
1:A:443:ARG:HA	1:A:525:VAL:HG13	1.85	0.58
1:A:116:SER:HA	1:A:210:GLN:O	2.02	0.58
1:A:296:TYR:HB2	1:A:321:VAL:HB	1.86	0.58
1:A:367:LEU:C	1:A:367:LEU:HD12	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:MET:HB2	1:A:529:VAL:HG22	1.84	0.58
1:A:286:LYS:O	1:A:287:GLY:O	2.21	0.58
1:A:335:ALA:HB1	3:A:811:NDG:H6	1.65	0.58
1:A:406:TYR:HB3	1:A:428:LEU:CD2	2.33	0.58
1:A:335:ALA:HB1	3:A:811:NDG:C6	2.33	0.58
1:A:146:LEU:HA	1:A:194:THR:O	2.02	0.58
1:A:221:PHE:HA	1:A:244:VAL:HG12	1.85	0.58
1:A:232:GLU:HG2	1:A:289:ASP:CA	2.33	0.58
1:A:309:SER:O	1:A:310:VAL:HG23	2.03	0.58
1:A:154:ASP:CB	2:A:801:NAG:HN2	2.16	0.57
1:A:332:PHE:CD2	1:A:424:GLY:HA3	2.39	0.57
1:A:154:ASP:CB	1:A:155:PRO:CD	2.82	0.57
1:A:330:PRO:HD3	1:A:414:ASP:HB2	1.86	0.57
1:A:403:ASN:CB	2:A:902:NAG:H83	2.21	0.57
1:A:42:GLY:HA2	1:A:47:PRO:O	2.04	0.57
1:A:108:PHE:CE1	1:A:203:VAL:HG23	2.40	0.57
1:A:226:TYR:CE2	1:A:242:LEU:HD23	2.39	0.57
1:A:268:PHE:C	1:A:285:ALA:HB3	2.30	0.57
1:A:406:TYR:HB3	1:A:428:LEU:HD21	1.87	0.57
1:A:523:THR:CG2	1:A:524:VAL:H	1.94	0.56
1:A:189:LEU:HD21	1:A:209:ILE:HD12	1.87	0.56
1:A:240:GLN:HG3	1:A:241:ARG:N	2.19	0.56
1:A:68:ARG:HG3	1:A:69:GLU:N	2.19	0.56
1:A:369:TYR:HD1	1:A:383:LYS:O	1.88	0.56
1:A:537:ILE:HG12	1:A:538:LYS:N	2.19	0.56
1:A:222:ASP:N	1:A:243:SER:O	2.38	0.56
1:A:118:ARG:HA	1:A:212:THR:HB	1.87	0.56
1:A:162:LEU:O	1:A:174:LEU:HD12	2.06	0.56
1:A:272:THR:CG2	1:A:273:THR:H	2.19	0.56
1:A:403:ASN:C	1:A:405:THR:H	2.12	0.56
1:A:259:TYR:O	1:A:260:LYS:HB3	2.05	0.56
1:A:505:GLY:HA2	1:A:529:VAL:H	1.69	0.56
1:A:439:VAL:HG13	1:A:522:LEU:HD11	1.88	0.56
1:A:378:TRP:O	1:A:391:ASN:HB2	2.06	0.55
1:A:394:LEU:N	1:A:394:LEU:CD1	2.69	0.55
1:A:155:PRO:N	2:A:801:NAG:H82	2.20	0.55
1:A:450:GLN:CB	1:A:533:GLU:HA	2.37	0.55
1:A:482:THR:HG22	1:A:499:THR:H	1.70	0.55
1:A:339:VAL:HG21	1:A:351:ILE:CG2	2.36	0.55
1:A:333:VAL:CG2	1:A:334:PRO:HD3	2.36	0.55
1:A:278:ASN:HD22	1:A:278:ASN:N	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:PHE:CD2	1:A:268:PHE:N	2.75	0.55
1:A:138:ASN:C	1:A:138:ASN:HD22	2.13	0.55
1:A:75:VAL:O	1:A:76:LEU:HD23	2.07	0.54
1:A:419:VAL:CG1	1:A:420:GLY:N	2.70	0.54
1:A:27:ASN:C	1:A:29:ASP:H	2.15	0.54
1:A:117:VAL:O	1:A:211:ILE:HA	2.07	0.54
1:A:320:THR:CG2	2:A:807:NAG:C2	2.76	0.54
1:A:155:PRO:HG2	2:A:801:NAG:O7	2.07	0.54
1:A:371:ILE:HG23	1:A:372:GLY:H	1.73	0.54
1:A:438:PRO:HB2	1:A:513:LEU:HD12	1.89	0.54
1:A:169:THR:OG1	1:A:171:VAL:HG23	2.08	0.54
1:A:226:TYR:HB2	1:A:319:VAL:HG22	1.89	0.53
1:A:226:TYR:O	1:A:227:THR:CG2	2.55	0.53
1:A:249:MET:O	1:A:252:THR:HB	2.09	0.53
1:A:155:PRO:C	1:A:157:GLU:N	2.56	0.53
1:A:459:ILE:HG21	1:A:471:TYR:CE2	2.42	0.53
1:A:28:LYS:HB3	1:A:88:VAL:HG11	1.89	0.53
1:A:332:PHE:HD2	1:A:424:GLY:HA3	1.73	0.53
1:A:22:VAL:HG22	1:A:23:GLN:H	1.73	0.53
1:A:217:ASN:N	1:A:217:ASN:ND2	2.56	0.53
1:A:241:ARG:NE	1:A:281:ILE:HD12	2.22	0.53
1:A:154:ASP:CG	1:A:155:PRO:HD2	2.33	0.53
1:A:276:GLU:CG	1:A:277:SER:N	2.71	0.53
1:A:330:PRO:HB3	1:A:358:ASP:HB2	1.89	0.53
1:A:522:LEU:CD2	1:A:523:THR:HB	2.26	0.53
1:A:466:PRO:O	1:A:468:THR:N	2.40	0.53
1:A:226:TYR:C	1:A:227:THR:HG23	2.33	0.53
1:A:373:ASN:HB3	1:A:409:ILE:H	1.74	0.53
1:A:252:THR:HG23	1:A:253:PRO:HD2	1.90	0.53
1:A:347:ARG:HG3	1:A:391:ASN:HA	1.91	0.53
1:A:242:LEU:O	1:A:279:GLN:HB3	2.09	0.53
1:A:482:THR:CG2	1:A:499:THR:CA	2.87	0.52
1:A:312:LEU:O	3:A:804:NDG:C8	2.57	0.52
1:A:426:LEU:HD13	1:A:426:LEU:O	2.10	0.52
1:A:272:THR:CG2	2:A:803:NAG:HN2	2.23	0.52
1:A:352:ILE:HG13	1:A:388:VAL:CB	2.33	0.52
1:A:379:LEU:H	1:A:379:LEU:CD2	2.22	0.52
1:A:443:ARG:HG3	1:A:443:ARG:NH1	2.23	0.52
1:A:227:THR:CG2	2:A:807:NAG:H83	2.32	0.52
1:A:367:LEU:HD13	1:A:412:VAL:HG23	1.91	0.52
1:A:28:LYS:CD	1:A:88:VAL:HG12	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:GLU:HA	1:A:533:GLU:OE2	2.09	0.52
1:A:336:VAL:O	1:A:426:LEU:HD22	2.10	0.52
1:A:373:ASN:CG	1:A:374:ASP:H	2.18	0.52
1:A:450:GLN:CB	1:A:532:CYS:O	2.58	0.52
1:A:221:PHE:HB3	1:A:223:PRO:O	2.10	0.52
1:A:514:SER:HB3	1:A:517:GLN:O	2.10	0.52
1:A:105:ARG:HG3	1:A:106:PRO:HD2	1.91	0.51
1:A:482:THR:HG22	1:A:482:THR:O	2.09	0.51
1:A:471:TYR:CD1	1:A:471:TYR:N	2.79	0.51
1:A:458:THR:HA	1:A:493:SER:HA	1.93	0.51
1:A:155:PRO:CD	2:A:801:NAG:H82	2.40	0.51
1:A:347:ARG:HD2	1:A:392:GLY:N	2.25	0.51
1:A:80:ALA:O	1:A:88:VAL:HG23	2.11	0.51
1:A:194:THR:HG22	1:A:195:ASP:N	2.25	0.51
1:A:142:LEU:O	1:A:196:LEU:HD23	2.11	0.50
1:A:246:ASP:C	1:A:247:LEU:HD12	2.35	0.50
1:A:368:SER:OG	1:A:370:PHE:HE1	1.94	0.50
1:A:374:ASP:C	1:A:375:PRO:O	2.54	0.50
1:A:423:THR:HB	2:A:810:NAG:H83	1.94	0.50
1:A:327:ASN:OD1	1:A:360:ASP:OD1	2.30	0.50
1:A:402:LYS:C	1:A:403:ASN:O	2.46	0.50
1:A:419:VAL:HG22	2:A:809:NAG:H81	1.93	0.50
1:A:428:LEU:HD23	1:A:428:LEU:O	2.11	0.50
1:A:151:LEU:HD12	1:A:190:THR:O	2.11	0.50
1:A:217:ASN:N	1:A:217:ASN:HD22	2.09	0.50
1:A:234:GLU:HB2	1:A:235:ILE:HG22	1.93	0.50
1:A:297:VAL:CG2	2:A:807:NAG:H62	2.41	0.50
1:A:72:ASP:OD2	5:A:1016:HOH:O	2.19	0.50
1:A:109:THR:HG22	1:A:110:GLN:CG	2.42	0.49
1:A:457:LEU:HD23	1:A:494:MET:SD	2.52	0.49
1:A:496:LEU:HD21	1:A:509:ILE:CD1	2.38	0.49
1:A:68:ARG:HD3	1:A:100:ASP:CA	2.43	0.49
1:A:382:ASN:OD1	1:A:385:ASN:N	2.45	0.49
1:A:109:THR:HG22	1:A:110:GLN:HG3	1.94	0.49
1:A:155:PRO:HG2	2:A:801:NAG:C7	2.42	0.49
1:A:216:ASP:HB2	1:A:217:ASN:ND2	2.27	0.49
1:A:252:THR:CG2	1:A:253:PRO:HD2	2.43	0.49
1:A:397:GLU:OE1	1:A:397:GLU:N	2.45	0.49
1:A:449:ASP:CB	1:A:532:CYS:N	2.74	0.49
1:A:11:GLU:OE2	1:A:69:GLU:OE1	2.30	0.49
1:A:273:THR:H	2:A:803:NAG:HN2	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ASP:CG	5:A:1000:HOH:O	2.55	0.49
1:A:426:LEU:HD13	1:A:426:LEU:C	2.37	0.49
1:A:76:LEU:O	1:A:94:ILE:N	2.44	0.49
1:A:154:ASP:O	2:A:801:NAG:C8	2.60	0.48
1:A:367:LEU:HD13	1:A:412:VAL:CG2	2.43	0.48
2:A:809:NAG:H61	2:A:810:NAG:C6	2.39	0.48
2:A:809:NAG:H62	2:A:810:NAG:O6	2.13	0.48
1:A:67:ASP:OD2	1:A:69:GLU:HB2	2.13	0.48
1:A:119:GLU:OE2	1:A:216:ASP:OD1	2.32	0.48
1:A:151:LEU:O	1:A:152:LYS:HB2	2.13	0.48
1:A:318:THR:CG2	2:A:806:NAG:H5	2.34	0.48
1:A:367:LEU:HB2	1:A:413:THR:O	2.12	0.48
1:A:481:LEU:HD12	1:A:481:LEU:HA	1.50	0.48
1:A:250:PRO:O	1:A:255:TRP:CE3	2.66	0.48
1:A:117:VAL:O	1:A:212:THR:N	2.46	0.48
1:A:150:ILE:HD11	1:A:165:ILE:HB	1.96	0.48
1:A:151:LEU:HD12	1:A:151:LEU:H	1.78	0.48
1:A:281:ILE:O	1:A:281:ILE:HG23	2.13	0.48
1:A:518:ASN:C	1:A:520:PRO:CD	2.87	0.48
2:A:809:NAG:C6	2:A:810:NAG:C6	2.92	0.48
1:A:192:GLN:HA	1:A:203:VAL:O	2.13	0.48
1:A:418:SER:O	1:A:419:VAL:HG23	2.14	0.48
1:A:449:ASP:CB	1:A:532:CYS:H	2.22	0.48
1:A:537:ILE:CG1	1:A:538:LYS:N	2.77	0.48
1:A:290:PHE:CE2	1:A:293:ARG:CB	2.92	0.48
1:A:310:VAL:HG12	1:A:312:LEU:HG	1.95	0.48
1:A:468:THR:C	1:A:469:TYR:O	2.54	0.48
1:A:138:ASN:C	1:A:138:ASN:ND2	2.73	0.47
1:A:186:GLU:OE1	2:A:801:NAG:C6	2.59	0.47
1:A:365:GLN:HA	1:A:416:GLY:HA3	1.95	0.47
1:A:50:VAL:HB	1:A:51:PHE:CD1	2.50	0.47
1:A:282:LEU:CD2	1:A:283:THR:N	2.76	0.47
1:A:286:LYS:C	1:A:287:GLY:O	2.55	0.47
1:A:300:ILE:HD12	1:A:300:ILE:N	2.30	0.47
1:A:333:VAL:CB	1:A:334:PRO:CD	2.88	0.47
1:A:335:ALA:CB	3:A:811:NDG:C6	2.90	0.47
1:A:36:TYR:O	1:A:55:TRP:HA	2.15	0.47
1:A:41:GLN:HA	1:A:45:ASN:HB2	1.95	0.47
1:A:225:THR:HA	1:A:318:THR:O	2.14	0.47
1:A:241:ARG:HE	1:A:281:ILE:CD1	2.24	0.47
1:A:268:PHE:CA	1:A:285:ALA:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:THR:CB	2:A:807:NAG:N2	2.78	0.47
1:A:266:GLY:N	1:A:268:PHE:CE2	2.76	0.47
1:A:344:ASP:CG	1:A:344:ASP:O	2.57	0.46
1:A:511:VAL:N	1:A:523:THR:O	2.46	0.46
1:A:522:LEU:HA	1:A:522:LEU:HD23	1.36	0.46
1:A:3:VAL:HB	1:A:4:ILE:H	1.51	0.46
1:A:23:GLN:HB2	1:A:59:TRP:CE3	2.50	0.46
1:A:227:THR:N	2:A:812:NAG:H2	2.31	0.46
1:A:270:ASN:OD1	1:A:271:ILE:N	2.49	0.46
1:A:272:THR:HG23	2:A:803:NAG:HN2	1.80	0.46
1:A:301:THR:CG2	1:A:316:THR:HG23	2.45	0.46
1:A:421:THR:HG21	2:A:809:NAG:H61	1.98	0.46
1:A:514:SER:CA	1:A:517:GLN:O	2.62	0.46
1:A:67:ASP:CG	1:A:69:GLU:HB2	2.40	0.46
1:A:100:ASP:OD1	1:A:101:GLN:N	2.49	0.46
1:A:54:GLU:HB2	1:A:57:THR:OG1	2.16	0.46
1:A:400:TYR:O	1:A:401:VAL:C	2.59	0.46
1:A:451:ASN:O	1:A:534:GLY:CA	2.60	0.46
1:A:461:ASP:HB3	1:A:468:THR:CG2	2.46	0.46
1:A:298:LEU:N	1:A:298:LEU:CD2	2.75	0.45
1:A:381:VAL:HA	1:A:387:ILE:O	2.17	0.45
1:A:155:PRO:O	1:A:157:GLU:N	2.43	0.45
1:A:459:ILE:N	1:A:459:ILE:HD12	2.31	0.45
1:A:473:VAL:CG2	1:A:487:LEU:HD21	2.47	0.45
1:A:187:TYR:HE1	1:A:211:ILE:HD11	1.81	0.45
1:A:271:ILE:O	1:A:271:ILE:HG23	2.15	0.45
1:A:109:THR:CB	1:A:131:SER:HB2	2.46	0.45
1:A:194:THR:CG2	1:A:195:ASP:N	2.79	0.45
1:A:482:THR:O	1:A:483:TRP:CD2	2.70	0.45
1:A:262:ARG:HG3	1:A:299:GLN:HB2	1.98	0.45
1:A:448:CYS:SG	1:A:537:ILE:CG2	3.01	0.45
1:A:380:THR:CG2	1:A:381:VAL:N	2.79	0.45
1:A:152:LYS:O	1:A:189:LEU:HA	2.17	0.45
1:A:187:TYR:CE1	1:A:211:ILE:HD11	2.52	0.45
1:A:312:LEU:O	3:A:804:NDG:H8C1	2.17	0.45
1:A:408:VAL:O	1:A:426:LEU:N	2.49	0.45
1:A:109:THR:HB	1:A:131:SER:HB2	1.99	0.45
1:A:299:GLN:CG	1:A:318:THR:HG23	2.42	0.45
1:A:339:VAL:HG11	1:A:351:ILE:HG23	1.98	0.45
1:A:310:VAL:HG12	1:A:311:PRO:O	2.15	0.44
1:A:352:ILE:CG1	1:A:388:VAL:HB	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:805:NAG:H62	2:A:806:NAG:N2	2.31	0.44
1:A:226:TYR:O	1:A:227:THR:HG23	2.15	0.44
1:A:227:THR:HG22	1:A:320:THR:HB	1.98	0.44
1:A:365:GLN:O	1:A:365:GLN:CG	2.54	0.44
1:A:432:ASP:CG	1:A:433:VAL:N	2.74	0.44
1:A:448:CYS:C	1:A:452:PRO:HG3	2.40	0.44
1:A:22:VAL:CG2	1:A:23:GLN:N	2.81	0.44
1:A:336:VAL:HG12	1:A:338:ARG:CB	2.47	0.44
1:A:380:THR:HG22	1:A:381:VAL:N	2.32	0.44
1:A:108:PHE:HE1	1:A:203:VAL:HG23	1.80	0.44
1:A:155:PRO:CB	2:A:801:NAG:C8	2.94	0.44
1:A:162:LEU:HB2	1:A:163:PHE:CE1	2.52	0.44
1:A:194:THR:HG23	1:A:201:LEU:O	2.18	0.44
1:A:276:GLU:HG3	1:A:277:SER:N	2.25	0.44
1:A:450:GLN:CB	1:A:533:GLU:OE2	2.65	0.44
1:A:181:ARG:NH1	1:A:249:MET:HE3	2.33	0.44
1:A:220:ILE:O	1:A:220:ILE:HG22	2.18	0.44
1:A:442:PRO:HD2	1:A:457:LEU:HD12	2.00	0.44
1:A:247:LEU:HD12	1:A:247:LEU:N	2.33	0.43
1:A:368:SER:CB	1:A:370:PHE:HE1	2.31	0.43
1:A:489:SER:C	1:A:491:GLY:H	2.26	0.43
1:A:90:GLU:O	1:A:91:PRO:O	2.37	0.43
1:A:250:PRO:C	1:A:252:THR:H	2.26	0.43
1:A:232:GLU:HA	1:A:288:LEU:HD12	1.99	0.43
1:A:290:PHE:CD2	1:A:293:ARG:O	2.71	0.43
1:A:151:LEU:HD12	1:A:151:LEU:N	2.33	0.43
1:A:421:THR:CG2	1:A:422:GLY:N	2.81	0.43
1:A:289:ASP:C	1:A:290:PHE:CD1	2.97	0.43
1:A:354:LEU:HD12	1:A:386:GLY:O	2.18	0.43
1:A:449:ASP:N	1:A:532:CYS:HB3	2.19	0.43
1:A:482:THR:C	1:A:483:TRP:CG	2.96	0.43
1:A:483:TRP:CZ2	1:A:507:TYR:CE1	2.87	0.43
2:A:805:NAG:C5	2:A:806:NAG:H83	2.46	0.43
1:A:134:ASP:HB2	1:A:146:LEU:HD11	1.99	0.43
1:A:439:VAL:HA	1:A:440:PRO:HD3	1.81	0.43
1:A:441:SER:CB	1:A:442:PRO:HD3	2.47	0.43
1:A:260:LYS:HB3	1:A:260:LYS:HE3	1.81	0.43
1:A:188:THR:H	2:A:801:NAG:H83	1.84	0.43
1:A:371:ILE:HD12	1:A:371:ILE:HA	1.65	0.43
1:A:277:SER:O	1:A:278:ASN:C	2.62	0.42
1:A:371:ILE:HG13	1:A:410:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASP:OD1	1:A:69:GLU:HB2	2.18	0.42
1:A:232:GLU:CG	1:A:289:ASP:C	2.92	0.42
1:A:250:PRO:HA	1:A:255:TRP:CG	2.54	0.42
1:A:339:VAL:HG21	1:A:351:ILE:HG22	2.01	0.42
1:A:343:GLU:CD	1:A:395:ASP:HA	2.44	0.42
1:A:409:ILE:HD13	3:A:811:NDG:H8C3	2.01	0.42
1:A:40:GLY:O	1:A:45:ASN:HB2	2.19	0.42
1:A:175:ILE:CG2	1:A:176:GLY:N	2.82	0.42
1:A:524:VAL:HG21	2:A:904:NAG:C8	2.44	0.42
1:A:195:ASP:HB3	1:A:196:LEU:HG	2.01	0.42
1:A:419:VAL:HG13	1:A:420:GLY:N	2.33	0.42
1:A:458:THR:C	1:A:459:ILE:HD12	2.44	0.42
1:A:461:ASP:HB3	1:A:468:THR:HG22	2.00	0.42
1:A:7:ILE:O	1:A:96:ILE:HG23	2.20	0.42
1:A:108:PHE:HA	1:A:132:ALA:CB	2.50	0.42
1:A:264:ASN:HB3	1:A:267:GLY:HA2	2.01	0.42
1:A:333:VAL:HG23	1:A:334:PRO:HD3	2.01	0.42
1:A:373:ASN:O	1:A:374:ASP:CB	2.64	0.42
1:A:385:ASN:O	1:A:386:GLY:C	2.62	0.42
1:A:347:ARG:HD2	1:A:392:GLY:CA	2.50	0.42
1:A:371:ILE:HA	1:A:410:MET:HB3	2.02	0.42
1:A:515:ASP:OD1	1:A:516:ALA:N	2.53	0.42
1:A:226:TYR:C	1:A:227:THR:CG2	2.92	0.41
1:A:274:ASP:HA	1:A:275:PRO:HD3	1.93	0.41
1:A:347:ARG:HG3	1:A:392:GLY:N	2.33	0.41
1:A:474:SER:N	1:A:512:LEU:O	2.53	0.41
1:A:23:GLN:HA	1:A:58:GLY:O	2.21	0.41
1:A:230:VAL:O	1:A:323:VAL:HA	2.20	0.41
1:A:297:VAL:HG21	2:A:807:NAG:H62	2.01	0.41
1:A:119:GLU:CG	1:A:214:ALA:HB3	2.51	0.41
1:A:154:ASP:HB3	2:A:801:NAG:C7	2.48	0.41
1:A:239:VAL:HG11	1:A:282:LEU:HD22	2.02	0.41
1:A:231:PRO:O	1:A:288:LEU:HD12	2.20	0.41
1:A:237:PHE:N	1:A:284:THR:OG1	2.42	0.41
1:A:297:VAL:HG22	2:A:807:NAG:H62	2.03	0.41
1:A:367:LEU:H	1:A:367:LEU:HG	1.41	0.41
1:A:440:PRO:HB3	1:A:457:LEU:CD2	2.43	0.41
1:A:27:ASN:C	1:A:29:ASP:N	2.79	0.41
1:A:68:ARG:HD3	1:A:100:ASP:CB	2.51	0.41
1:A:118:ARG:CA	1:A:212:THR:HB	2.51	0.41
1:A:227:THR:C	2:A:812:NAG:O5	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:THR:C	1:A:254:ALA:H	2.28	0.41
1:A:409:ILE:C	1:A:410:MET:HG2	2.46	0.41
1:A:519:ASN:O	1:A:520:PRO:C	2.59	0.41
1:A:42:GLY:CA	1:A:47:PRO:O	2.69	0.41
1:A:108:PHE:HA	1:A:132:ALA:HB2	2.03	0.41
1:A:193:ALA:O	1:A:202:SER:HA	2.21	0.40
1:A:316:THR:OG1	2:A:806:NAG:H83	2.21	0.40
1:A:371:ILE:HD13	1:A:381:VAL:HG11	1.95	0.40
1:A:23:GLN:HB2	1:A:59:TRP:CD2	2.55	0.40
1:A:108:PHE:CZ	1:A:191:VAL:HG23	2.56	0.40
1:A:239:VAL:HG13	1:A:240:GLN:N	2.33	0.40
1:A:438:PRO:HB2	1:A:513:LEU:CD1	2.51	0.40
1:A:522:LEU:HB3	1:A:523:THR:H	1.57	0.40
1:A:111:ASP:O	1:A:112:VAL:HG13	2.21	0.40
1:A:222:ASP:H	1:A:243:SER:C	2.30	0.40
1:A:231:PRO:O	1:A:235:ILE:HD13	2.21	0.40
1:A:409:ILE:HD13	3:A:811:NDG:C8	2.52	0.40
1:A:505:GLY:H	1:A:529:VAL:HB	1.85	0.40
1:A:127:VAL:HG22	1:A:128:MET:HG3	2.03	0.40
1:A:223:PRO:HB2	1:A:226:TYR:CZ	2.56	0.40
1:A:290:PHE:CG	1:A:292:LEU:HB2	2.56	0.40
1:A:423:THR:CG2	2:A:810:NAG:N2	2.84	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	538/546 (98%)	401 (74%)	92 (17%)	45 (8%)	0 3

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
1	A	155	PRO
1	A	235	ILE
1	A	347	ARG
1	A	363	GLN
1	A	364	ILE
1	A	374	ASP
1	A	404	ASN
1	A	467	ASN
1	A	476	SER
1	A	502	LEU
1	A	517	GLN
1	A	518	ASN
1	A	519	ASN
1	A	3	VAL
1	A	156	GLU
1	A	260	LYS
1	A	287	GLY
1	A	470	PRO
1	A	503	LYS
1	A	55	TRP
1	A	212	THR
1	A	250	PRO
1	A	333	VAL
1	A	360	ASP
1	A	372	GLY
1	A	377	ARG
1	A	506	ASP
1	A	152	LYS
1	A	223	PRO
1	A	359	PRO
1	A	375	PRO
1	A	160	PRO
1	A	265	GLU
1	A	278	ASN
1	A	289	ASP
1	A	482	THR
1	A	498	PRO
1	A	523	THR
1	A	154	ASP
1	A	307	PRO
1	A	222	ASP
1	A	200	GLY

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Mol	Chain	Res	Type
1	A	47	PRO
1	A	158	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	438/486 (90%)	346 (79%)	92 (21%)	1 4

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	18	PRO
1	A	19	LYS
1	A	27	ASN
1	A	61	LEU
1	A	66	LEU
1	A	68	ARG
1	A	88	VAL
1	A	91	PRO
1	A	92	MET
1	A	109	THR
1	A	117	VAL
1	A	121	VAL
1	A	138	ASN
1	A	146	LEU
1	A	151	LEU
1	A	155	PRO
1	A	161	ASN
1	A	163	PHE
1	A	189	LEU
1	A	195	ASP
1	A	196	LEU
1	A	202	SER
1	A	216	ASP

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Mol	Chain	Res	Type
1	A	217	ASN
1	A	220	ILE
1	A	223	PRO
1	A	226	TYR
1	A	231	PRO
1	A	233	ASN
1	A	234	GLU
1	A	235	ILE
1	A	237	PHE
1	A	239	VAL
1	A	250	PRO
1	A	253	PRO
1	A	268	PHE
1	A	273	THR
1	A	278	ASN
1	A	282	LEU
1	A	284	THR
1	A	288	LEU
1	A	298	LEU
1	A	303	GLU
1	A	309	SER
1	A	310	VAL
1	A	315	SER
1	A	316	THR
1	A	318	THR
1	A	333	VAL
1	A	336	VAL
1	A	339	VAL
1	A	353	SER
1	A	354	LEU
1	A	360	ASP
1	A	361	LYS
1	A	363	GLN
1	A	365	GLN
1	A	371	ILE
1	A	375	PRO
1	A	379	LEU
1	A	382	ASN
1	A	384	ASP
1	A	394	LEU
1	A	395	ASP
1	A	399	GLU

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Mol	Chain	Res	Type
1	A	405	THR
1	A	407	THR
1	A	419	VAL
1	A	423	THR
1	A	425	THR
1	A	427	ILE
1	A	433	VAL
1	A	436	ASN
1	A	447	MET
1	A	448	CYS
1	A	457	LEU
1	A	461	ASP
1	A	465	PRO
1	A	466	PRO
1	A	470	PRO
1	A	477	HIS
1	A	492	THR
1	A	509	ILE
1	A	511	VAL
1	A	512	LEU
1	A	517	GLN
1	A	520	PRO
1	A	522	LEU
1	A	523	THR
1	A	532	CYS
1	A	539	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	27	ASN
1	A	45	ASN
1	A	97	ASN
1	A	104	ASN
1	A	110	GLN
1	A	122	GLN
1	A	138	ASN
1	A	217	ASN
1	A	240	GLN
1	A	278	ASN
1	A	299	GLN

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Mol	Chain	Res	Type
1	A	373	ASN
1	A	385	ASN
1	A	391	ASN
1	A	455	GLN
1	A	467	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 for Mogul analysis.

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	NDG	A	811	1	14,14,15	0.87	0	17,19,21	1.96	1 (5%)
2	NAG	A	803	1	14,14,15	1.00	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	A	806	1	14,14,15	0.56	0	17,19,21	1.39	3 (17%)
2	NAG	A	808	1	14,14,15	0.67	0	17,19,21	0.70	0
2	NAG	A	812	1	14,14,15	0.83	1 (7%)	17,19,21	0.76	1 (5%)
2	NAG	A	809	1	14,14,15	0.77	1 (7%)	17,19,21	0.94	0
2	NAG	A	903	1	14,14,15	0.55	0	17,19,21	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	904	1	14,14,15	0.77	1 (7%)	17,19,21	0.70	1 (5%)
3	NDG	A	804	1	14,14,15	0.65	0	17,19,21	0.78	0
2	NAG	A	810	1	14,14,15	0.67	0	17,19,21	1.33	4 (23%)
2	NAG	A	902	1	14,14,15	1.14	1 (7%)	17,19,21	1.09	2 (11%)
2	NAG	A	801	1	14,14,15	0.70	0	17,19,21	0.98	1 (5%)
2	NAG	A	802	1	14,14,15	0.77	1 (7%)	17,19,21	0.85	0
2	NAG	A	807	1	14,14,15	0.64	0	17,19,21	1.19	2 (11%)
2	NAG	A	805	1	14,14,15	0.71	0	17,19,21	1.05	1 (5%)

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	NDG	A	811	1	-	2/6/23/26	0/1/1/1
2	NAG	A	806	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	803	1	-	2/6/23/26	0/1/1/1
2	NAG	A	808	1	-	3/6/23/26	0/1/1/1
2	NAG	A	812	1	-	4/6/23/26	0/1/1/1
2	NAG	A	903	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	809	1	-	2/6/23/26	0/1/1/1
2	NAG	A	904	1	-	3/6/23/26	0/1/1/1
3	NDG	A	804	1	-	0/6/23/26	0/1/1/1
2	NAG	A	902	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	810	1	-	3/6/23/26	0/1/1/1
2	NAG	A	801	1	-	4/6/23/26	0/1/1/1
2	NAG	A	802	1	-	2/6/23/26	0/1/1/1
2	NAG	A	807	1	-	5/6/23/26	0/1/1/1
2	NAG	A	805	1	1/1/5/7	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	NAG	C1-C2	3.40	1.57	1.52
2	A	803	NAG	O5-C5	2.64	1.48	1.43
2	A	904	NAG	C1-C2	-2.41	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	812	NAG	C1-C2	-2.32	1.49	1.52
2	A	802	NAG	C1-C2	2.08	1.55	1.52
2	A	809	NAG	C1-C2	-2.02	1.49	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	811	NDG	C2-N2-C7	-7.42	112.95	122.90
2	A	806	NAG	C2-N2-C7	-3.62	118.04	122.90
2	A	805	NAG	C2-N2-C7	-3.16	118.66	122.90
2	A	807	NAG	C2-N2-C7	-3.06	118.80	122.90
2	A	803	NAG	C2-N2-C7	-3.00	118.88	122.90
2	A	810	NAG	C1-C2-N2	2.52	114.41	110.43
2	A	810	NAG	C4-C3-C2	-2.46	107.42	111.02
2	A	803	NAG	C1-O5-C5	2.45	115.47	112.19
2	A	806	NAG	C4-C3-C2	-2.44	107.44	111.02
2	A	810	NAG	O5-C1-C2	-2.36	107.64	111.29
2	A	810	NAG	C1-O5-C5	-2.24	109.19	112.19
2	A	812	NAG	C2-N2-C7	-2.16	120.00	122.90
2	A	801	NAG	C1-C2-N2	-2.15	107.05	110.43
2	A	902	NAG	O5-C1-C2	2.14	114.60	111.29
2	A	807	NAG	O5-C1-C2	-2.06	108.10	111.29
2	A	904	NAG	C2-N2-C7	-2.03	120.17	122.90
2	A	902	NAG	C1-O5-C5	2.02	114.90	112.19
2	A	806	NAG	O5-C1-C2	-2.02	108.16	111.29

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	805	NAG	C1
2	A	806	NAG	C1
2	A	902	NAG	C1
2	A	903	NAG	C1

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	807	NAG	C3-C2-N2-C7
2	A	808	NAG	C1-C2-N2-C7
2	A	810	NAG	C1-C2-N2-C7
2	A	812	NAG	C1-C2-N2-C7
2	A	902	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	A	904	NAG	C3-C2-N2-C7
3	A	811	NDG	C4-C5-C6-O6
2	A	802	NAG	C4-C5-C6-O6
2	A	807	NAG	C4-C5-C6-O6
3	A	811	NDG	O5-C5-C6-O6
2	A	809	NAG	O5-C5-C6-O6
2	A	809	NAG	C4-C5-C6-O6
2	A	807	NAG	O5-C5-C6-O6
2	A	807	NAG	C8-C7-N2-C2
2	A	805	NAG	O5-C5-C6-O6
2	A	802	NAG	O5-C5-C6-O6
2	A	904	NAG	C4-C5-C6-O6
2	A	805	NAG	C4-C5-C6-O6
2	A	810	NAG	C4-C5-C6-O6
2	A	812	NAG	O5-C5-C6-O6
2	A	807	NAG	O7-C7-N2-C2
2	A	803	NAG	C4-C5-C6-O6
2	A	810	NAG	O5-C5-C6-O6
2	A	904	NAG	O5-C5-C6-O6
2	A	801	NAG	C4-C5-C6-O6
2	A	803	NAG	O5-C5-C6-O6
2	A	903	NAG	C4-C5-C6-O6
2	A	808	NAG	C4-C5-C6-O6
2	A	806	NAG	C4-C5-C6-O6
2	A	801	NAG	C3-C2-N2-C7
2	A	903	NAG	C3-C2-N2-C7
2	A	801	NAG	O5-C5-C6-O6
2	A	801	NAG	C1-C2-N2-C7
2	A	902	NAG	C1-C2-N2-C7
2	A	806	NAG	O5-C5-C6-O6
2	A	808	NAG	C3-C2-N2-C7
2	A	812	NAG	C3-C2-N2-C7
2	A	812	NAG	C4-C5-C6-O6

There are no ring outliers.

13 monomers are involved in 95 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	811	NDG	7	0
2	A	803	NAG	4	0
2	A	806	NAG	9	0
2	A	808	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	812	NAG	3	0
2	A	809	NAG	8	0
2	A	904	NAG	6	0
3	A	804	NDG	2	0
2	A	810	NAG	12	0
2	A	902	NAG	7	0
2	A	801	NAG	22	0
2	A	807	NAG	16	0
2	A	805	NAG	7	0

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	540/546 (98%)	0.62	49 (9%) 15 8	6, 68, 100, 100	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	478	GLY	4.6
1	A	516	ALA	4.4
1	A	374	ASP	4.2
1	A	507	TYR	4.2
1	A	327	ASN	3.9
1	A	417	VAL	3.8
1	A	471	TYR	3.6
1	A	523	THR	3.6
1	A	450	GLN	3.3
1	A	418	SER	3.3
1	A	527	ALA	3.2
1	A	485	ALA	3.1
1	A	510	TYR	3.1
1	A	375	PRO	3.1
1	A	506	ASP	3.0
1	A	537	ILE	3.0
1	A	524	VAL	2.9
1	A	482	THR	2.8
1	A	536	ALA	2.8
1	A	371	ILE	2.8
1	A	508	SER	2.6
1	A	393	ASN	2.6
1	A	38	ILE	2.6
1	A	365	GLN	2.6
1	A	430	VAL	2.6
1	A	398	SER	2.6
1	A	328	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	540	GLN	2.5
1	A	459	ILE	2.5
1	A	135	GLU	2.5
1	A	461	ASP	2.5
1	A	413	THR	2.5
1	A	344	ASP	2.4
1	A	277	SER	2.4
1	A	305	ALA	2.4
1	A	481	LEU	2.3
1	A	469	TYR	2.3
1	A	534	GLY	2.3
1	A	495	LEU	2.3
1	A	362	GLN	2.3
1	A	539	CYS	2.3
1	A	445	PHE	2.2
1	A	337	SER	2.2
1	A	431	LEU	2.2
1	A	308	PHE	2.2
1	A	233	ASN	2.2
1	A	519	ASN	2.0
1	A	448	CYS	2.0
1	A	525	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	903	14/15	0.40	0.29	56,56,56,56	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	904	14/15	0.41	0.24	27,27,27,27	14
2	NAG	A	812	14/15	0.50	0.29	67,67,67,67	14
2	NAG	A	807	14/15	0.53	0.27	62,62,62,62	14
2	NAG	A	902	14/15	0.57	0.18	37,37,37,37	14
2	NAG	A	802	14/15	0.60	0.20	99,99,99,99	14
2	NAG	A	801	14/15	0.60	0.31	39,39,39,39	14
3	NDG	A	811	14/15	0.61	0.28	100,100,100,100	14
2	NAG	A	806	14/15	0.62	0.23	64,64,64,64	14
2	NAG	A	810	14/15	0.63	0.34	78,78,78,78	14
2	NAG	A	805	14/15	0.64	0.24	89,89,89,89	0
3	NDG	A	804	14/15	0.71	0.21	51,51,51,51	14
2	NAG	A	809	14/15	0.72	0.16	100,100,100,100	0
2	NAG	A	803	14/15	0.78	0.25	63,63,63,63	14
2	NAG	A	808	14/15	0.81	0.26	83,83,83,83	14
4	CA	A	611	1/1	0.92	0.08	85,85,85,85	0
4	CA	A	610	1/1	0.94	0.04	70,70,70,70	0
4	CA	A	607	1/1	0.94	0.06	90,90,90,90	0
4	CA	A	602	1/1	0.97	0.09	15,15,15,15	0
4	CA	A	609	1/1	0.97	0.04	69,69,69,69	0
4	CA	A	606	1/1	0.98	0.05	37,37,37,37	0
4	CA	A	603	1/1	0.99	0.03	10,10,10,10	0
4	CA	A	608	1/1	0.99	0.02	34,34,34,34	0
4	CA	A	604	1/1	0.99	0.06	12,12,12,12	0
4	CA	A	605	1/1	0.99	0.03	10,10,10,10	0
4	CA	A	600	1/1	0.99	0.02	22,22,22,22	0
4	CA	A	601	1/1	1.00	0.05	5,5,5,5	0

6.5 Other polymers [i](#)

There are no such residues in this entry.