



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:25 AM UTC

PDB ID : 2ECP / pdb_00002ecp
Title : THE CRYSTAL STRUCTURE OF THE E. COLI MALTODEXTRIN PHOSPHORYLASE COMPLEX
Authors : O'Reilly, M.; Watson, K.A.; Johnson, L.N.
Deposited on : 1998-10-27
Resolution : 2.95 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)
Xtrriage (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

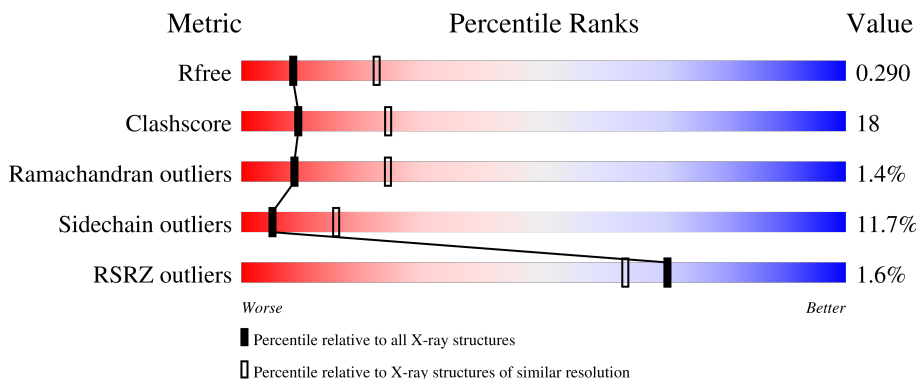
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	796	
1	B	796	
2	C	3	
2	D	3	

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	GLC	C	1	X	-	-	-
2	GLC	D	1	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12961 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 MALTODEXTRIN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	796	6369	4065	1127	1157	20	0	0	0
1	B	796	6369	4065	1127	1157	20	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	ALA	LYS	conflict	UNP P00490
A	532	ASP	GLN	conflict	UNP P00490
A	582	ARG	HIS	conflict	UNP P00490
A	716	LYS	GLU	conflict	UNP P00490
A	828	ALA	LYS	conflict	UNP P00490
B	205	ALA	LYS	conflict	UNP P00490
B	532	ASP	GLN	conflict	UNP P00490
B	582	ARG	HIS	conflict	UNP P00490
B	716	LYS	GLU	conflict	UNP P00490
B	828	ALA	LYS	conflict	UNP P00490

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose.

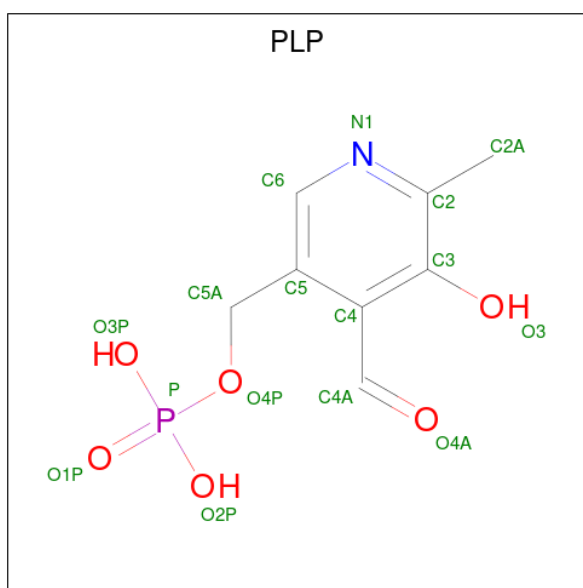
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	44	25	1	18	0	0	0
2	D	3	44	25	1	18	0	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

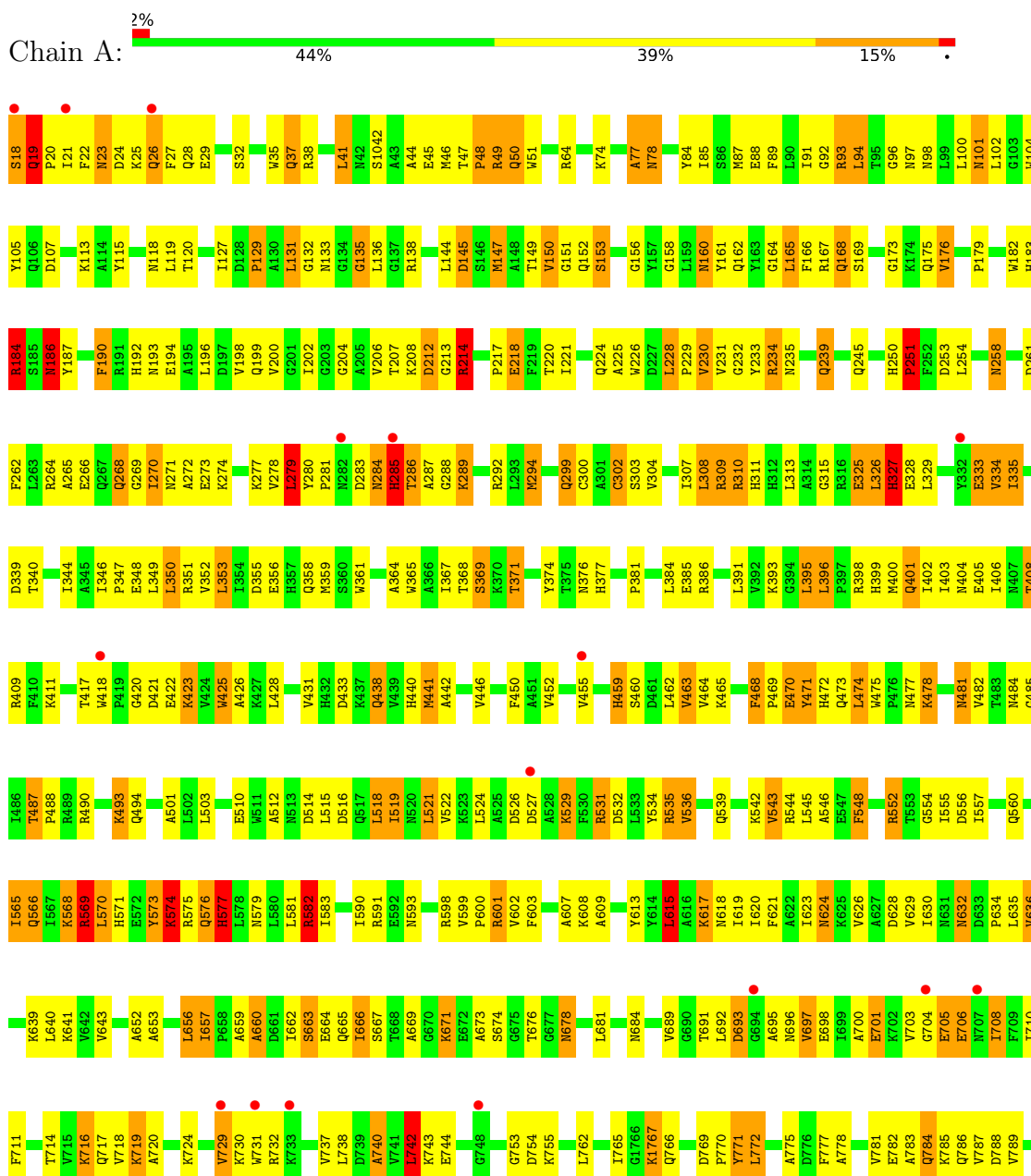
- Molecule 5 is water.

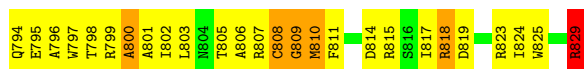
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	54	Total 54	O 54	0	0
5	B	39	Total 39	O 39	0	0

3 Residue-property plots i

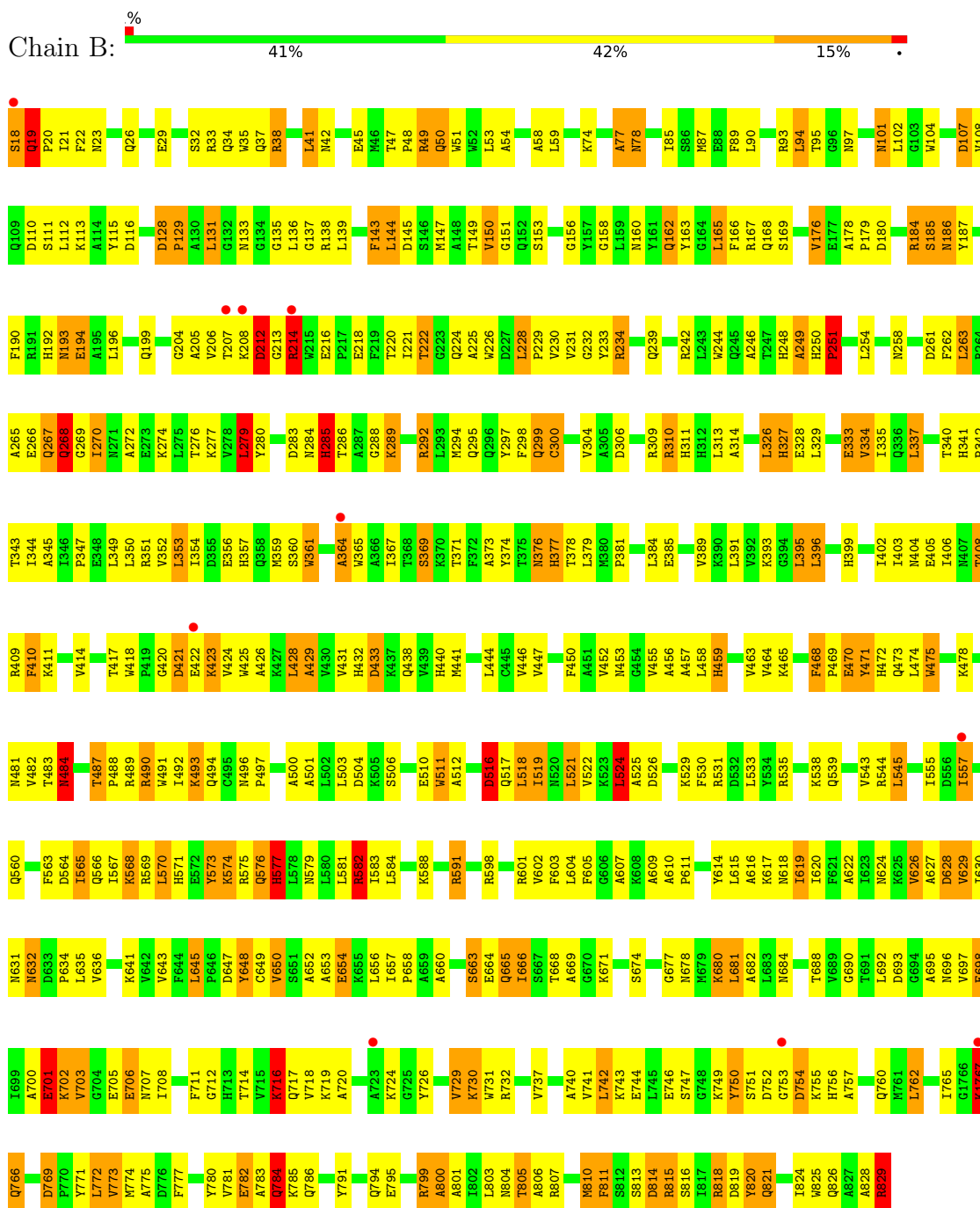
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MALTODEXTRIN PHOSPHORYLASE





● Molecule 1: MALTODEXTRIN PHOSPHORYLASE



● Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl}\}$ amino $\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose



GLC1
GLC2
AC13

- Molecule 2: 4,6-dideoxy-4-[[[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:  33% 67%

GLC1
GLC2
AC13

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.49Å 105.84Å 217.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.95 15.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	88.9 (15.00-2.95) 87.7 (15.00-2.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 2.96Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.293 0.242 , 0.290	Depositor DCC
R_{free} test set	852 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12961	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, AC1, PLP, GLC

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	1.02	6/6517 (0.1%)	2.26	294/8841 (3.3%)
1	B	1.00	6/6517 (0.1%)	2.31	332/8841 (3.8%)
All	All	1.01	12/13034 (0.1%)	2.28	626/17682 (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	B	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	HIS	CE1-NE2	-8.09	1.24	1.32
1	B	250	HIS	CE1-NE2	-8.05	1.24	1.32
1	A	250	HIS	CG-ND1	-6.82	1.30	1.38
1	A	569	ARG	NE-CZ	-6.81	1.25	1.33
1	A	250	HIS	CG-CD2	-6.32	1.28	1.35
1	B	292	ARG	CD-NE	-5.96	1.38	1.46
1	B	569	ARG	CD-NE	-5.91	1.38	1.46
1	B	569	ARG	NE-CZ	-5.90	1.26	1.33
1	A	569	ARG	CD-NE	-5.59	1.38	1.46
1	B	250	HIS	CG-ND1	-5.43	1.32	1.38
1	B	292	ARG	NE-CZ	-5.39	1.27	1.33
1	A	657	ILE	CA-CB	-5.17	1.51	1.54

All (626) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ARG	NE-CZ-NH2	37.34	152.80	119.20
1	A	292	ARG	NE-CZ-NH2	27.32	143.79	119.20
1	B	569	ARG	NE-CZ-NH2	25.73	142.35	119.20
1	B	569	ARG	NH1-CZ-NH2	-23.23	89.11	119.30
1	A	569	ARG	NH1-CZ-NH2	-22.23	90.41	119.30
1	B	569	ARG	CD-NE-CZ	19.68	151.96	124.40
1	B	292	ARG	NE-CZ-NH1	-17.28	104.22	121.50
1	B	292	ARG	CD-NE-CZ	15.98	146.77	124.40
1	A	569	ARG	NE-CZ-NH2	15.25	132.92	119.20
1	A	569	ARG	NE-CZ-NH1	15.17	136.67	121.50
1	A	250	HIS	ND1-CG-CD2	-14.38	91.72	106.10
1	A	569	ARG	CD-NE-CZ	14.17	144.24	124.40
1	A	250	HIS	CG-CD2-NE2	14.06	121.26	107.20
1	B	250	HIS	ND1-CG-CD2	-13.77	92.33	106.10
1	B	292	ARG	NH1-CZ-NH2	-12.57	102.95	119.30
1	A	292	ARG	NH1-CZ-NH2	-12.29	103.32	119.30
1	B	453	ASN	OD1-CG-ND2	-12.24	110.36	122.60
1	B	250	HIS	CG-CD2-NE2	12.20	119.40	107.20
1	A	164	GLY	CA-C-O	-11.43	107.49	121.67
1	A	168	GLN	OE1-CD-NE2	11.08	133.68	122.60
1	A	127	ILE	CA-C-O	-10.90	108.71	120.59
1	B	97	ASN	OD1-CG-ND2	-10.90	111.70	122.60
1	A	310	ARG	CD-NE-CZ	10.88	139.64	124.40
1	A	544	ARG	NE-CZ-NH2	-10.87	109.42	119.20
1	A	666	ILE	N-CA-C	10.65	121.39	111.91
1	A	271	ASN	CA-C-O	-10.58	109.33	120.55
1	B	481	ASN	OD1-CG-ND2	-10.56	112.03	122.60
1	A	268	GLN	OE1-CD-NE2	-10.29	112.31	122.60
1	A	621	PHE	CA-CB-CG	10.26	124.06	113.80
1	B	50	GLN	OE1-CD-NE2	10.23	132.83	122.60
1	A	28	GLN	OE1-CD-NE2	10.17	132.77	122.60
1	B	224	GLN	OE1-CD-NE2	-10.16	112.44	122.60
1	B	510	GLU	CA-C-O	-9.98	110.00	121.47
1	A	199	GLN	CA-C-O	-9.92	109.74	120.36
1	B	591	ARG	CD-NE-CZ	9.83	138.16	124.40
1	B	438	GLN	OE1-CD-NE2	9.68	132.28	122.60
1	B	693	ASP	CA-CB-CG	9.59	122.19	112.60
1	B	145	ASP	CA-CB-CG	9.57	122.17	112.60
1	B	577	HIS	CA-CB-CG	9.55	123.35	113.80
1	A	632	ASN	OD1-CG-ND2	9.49	132.09	122.60
1	B	309	ARG	NE-CZ-NH1	9.49	130.99	121.50
1	B	577	HIS	CA-C-O	9.46	130.85	119.97
1	B	214	ARG	NE-CZ-NH2	9.40	127.66	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ASP	CA-CB-CG	9.37	121.97	112.60
1	A	93	ARG	CA-C-O	-9.30	110.96	121.19
1	B	484	ASN	OD1-CG-ND2	9.30	131.90	122.60
1	A	258	ASN	OD1-CG-ND2	-9.27	113.33	122.60
1	A	535	ARG	NE-CZ-NH2	-9.22	110.91	119.20
1	B	285	HIS	CA-CB-CG	9.16	122.96	113.80
1	A	292	ARG	CG-CD-NE	9.00	131.80	112.00
1	B	565	ILE	N-CA-C	8.99	120.70	108.11
1	B	628	ASP	O-C-N	8.99	131.70	122.08
1	B	242	ARG	NH1-CZ-NH2	8.99	130.99	119.30
1	B	292	ARG	CG-CD-NE	8.97	131.74	112.00
1	B	250	HIS	CA-CB-CG	8.90	122.70	113.80
1	A	164	GLY	O-C-N	8.80	132.38	122.62
1	A	98	ASN	OD1-CG-ND2	8.79	131.38	122.60
1	B	156	GLY	CA-C-O	-8.77	113.65	120.76
1	A	815	ARG	NE-CZ-NH1	-8.64	112.86	121.50
1	A	292	ARG	NE-CZ-NH1	-8.61	112.89	121.50
1	A	535	ARG	NH1-CZ-NH2	8.60	130.47	119.30
1	A	325	GLU	O-C-N	-8.56	112.34	122.87
1	B	490	ARG	NE-CZ-NH2	-8.52	111.53	119.20
1	A	224	GLN	CA-C-O	-8.51	111.16	120.43
1	B	250	HIS	CB-CG-CD2	8.50	142.25	131.20
1	B	649	CYS	CA-C-O	-8.47	112.25	121.31
1	B	473	GLN	OE1-CD-NE2	8.46	131.06	122.60
1	B	786	GLN	OE1-CD-NE2	-8.44	114.16	122.60
1	A	199	GLN	OE1-CD-NE2	8.38	130.99	122.60
1	B	583	ILE	O-C-N	8.37	130.12	121.91
1	A	118	ASN	OD1-CG-ND2	-8.37	114.23	122.60
1	A	334	VAL	N-CA-CB	8.36	125.12	111.58
1	A	229	PRO	O-C-N	-8.34	113.60	123.03
1	A	147	MET	O-C-N	-8.31	113.44	122.09
1	B	268	GLN	CG-CD-NE2	8.29	128.83	116.40
1	A	133	ASN	OD1-CG-ND2	8.13	130.73	122.60
1	A	552	ARG	CD-NE-CZ	8.11	135.76	124.40
1	B	569	ARG	CG-CD-NE	8.08	129.78	112.00
1	B	624	ASN	OD1-CG-ND2	-8.08	114.52	122.60
1	A	294	MET	CA-C-O	8.05	128.96	120.42
1	A	115	TYR	CA-C-O	8.04	128.97	119.56
1	B	178	ALA	O-C-N	8.03	126.85	121.71
1	A	309	ARG	CD-NE-CZ	8.01	135.62	124.40
1	B	632	ASN	OD1-CG-ND2	7.99	130.59	122.60
1	B	272	ALA	CA-C-O	7.99	129.74	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	656	LEU	O-C-N	-7.96	113.50	122.09
1	B	628	ASP	CA-C-O	-7.92	112.36	121.07
1	A	101	ASN	CB-CG-ND2	-7.90	104.55	116.40
1	B	34	GLN	OE1-CD-NE2	7.87	130.47	122.60
1	A	701	GLU	CA-C-O	-7.86	112.09	120.42
1	A	574	LYS	CA-C-N	7.85	133.51	122.36
1	A	574	LYS	C-N-CA	7.85	133.51	122.36
1	B	129	PRO	CB-CA-C	7.73	121.76	111.71
1	B	431	VAL	CA-C-O	-7.72	112.27	120.53
1	B	143	PHE	CA-CB-CG	7.68	121.48	113.80
1	A	598	ARG	NE-CZ-NH1	-7.68	113.82	121.50
1	A	101	ASN	OD1-CG-ND2	7.66	130.26	122.60
1	B	115	TYR	CA-C-O	7.65	128.42	119.32
1	B	560	GLN	CA-C-O	7.64	127.45	119.05
1	B	160	ASN	OD1-CG-ND2	-7.61	114.99	122.60
1	A	543	VAL	O-C-N	7.61	129.66	121.83
1	B	199	GLN	CA-C-O	-7.60	112.23	120.36
1	B	167	ARG	O-C-N	-7.60	114.39	123.13
1	A	147	MET	CA-C-O	7.59	129.02	120.90
1	A	582	ARG	NH1-CZ-NH2	7.55	129.12	119.30
1	B	583	ILE	CA-C-O	-7.54	113.18	121.17
1	B	665	GLN	OE1-CD-NE2	7.53	130.13	122.60
1	A	401	GLN	CA-C-O	-7.49	113.13	121.00
1	B	101	ASN	CB-CG-ND2	-7.49	105.16	116.40
1	B	309	ARG	NE-CZ-NH2	-7.49	112.46	119.20
1	B	489	ARG	NE-CZ-NH2	7.49	125.94	119.20
1	A	229	PRO	CA-C-O	7.48	129.72	120.97
1	A	151	GLY	CA-C-O	7.44	127.62	119.06
1	B	133	ASN	OD1-CG-ND2	7.42	130.02	122.60
1	B	268	GLN	OE1-CD-NE2	-7.41	115.19	122.60
1	A	818	ARG	CA-C-O	-7.37	113.09	120.82
1	A	250	HIS	CE1-NE2-CD2	-7.36	101.64	109.00
1	A	325	GLU	CA-C-O	7.34	129.26	121.19
1	A	825	TRP	N-CA-C	7.32	120.19	111.33
1	A	693	ASP	CA-CB-CG	7.31	119.91	112.60
1	B	19	GLN	OE1-CD-NE2	7.31	129.91	122.60
1	A	271	ASN	O-C-N	7.30	129.86	122.12
1	A	786	GLN	OE1-CD-NE2	-7.28	115.32	122.60
1	B	627	ALA	O-C-N	-7.25	114.44	122.12
1	A	138	ARG	NE-CZ-NH1	7.23	128.73	121.50
1	A	245	GLN	OE1-CD-NE2	-7.22	115.38	122.60
1	A	334	VAL	CA-CB-CG2	7.18	122.60	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	ARG	NH1-CZ-NH2	-7.16	110.00	119.30
1	A	582	ARG	NE-CZ-NH2	-7.13	112.78	119.20
1	B	560	GLN	N-CA-C	-7.13	104.45	113.72
1	A	239	GLN	OE1-CD-NE2	7.12	129.72	122.60
1	A	468	PHE	CA-CB-CG	7.11	120.91	113.80
1	A	38	ARG	NE-CZ-NH2	7.10	125.59	119.20
1	B	393	LYS	CA-C-O	7.10	128.17	119.79
1	B	707	ASN	CB-CG-ND2	-7.07	105.80	116.40
1	A	576	GLN	CB-CG-CD	7.06	124.61	112.60
1	B	101	ASN	OD1-CG-ND2	7.05	129.65	122.60
1	B	38	ARG	CD-NE-CZ	7.03	134.25	124.40
1	A	115	TYR	O-C-N	-7.03	113.90	122.34
1	B	569	ARG	NE-CZ-NH1	7.01	128.51	121.50
1	A	251	PRO	CB-CA-C	-7.00	102.22	109.92
1	A	85	ILE	O-C-N	-7.00	114.09	122.77
1	B	682	ALA	CA-C-O	-7.00	113.65	121.00
1	B	653	ALA	N-CA-CB	7.00	120.41	110.12
1	A	84	TYR	CA-C-O	6.99	128.39	120.84
1	B	716	LYS	O-C-N	6.99	129.53	122.12
1	A	93	ARG	O-C-N	6.98	131.46	122.87
1	B	277	LYS	N-CA-CB	6.98	121.03	110.14
1	B	535	ARG	NE-CZ-NH1	-6.97	114.53	121.50
1	B	286	THR	CA-C-O	-6.96	112.88	121.02
1	B	749	LYS	O-C-N	6.96	130.08	122.15
1	A	167	ARG	NE-CZ-NH2	6.93	125.43	119.20
1	A	676	THR	CA-C-N	6.92	127.81	119.99
1	A	676	THR	C-N-CA	6.92	127.81	119.99
1	B	453	ASN	CB-CG-OD1	6.92	134.64	120.80
1	A	477	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	B	716	LYS	CA-C-O	-6.89	113.25	120.55
1	B	574	LYS	CA-C-N	6.87	132.11	122.36
1	B	574	LYS	C-N-CA	6.87	132.11	122.36
1	B	178	ALA	CA-C-O	-6.85	114.20	120.50
1	A	285	HIS	CA-CB-CG	6.84	120.64	113.80
1	A	19	GLN	OE1-CD-NE2	6.81	129.41	122.60
1	A	566	GLN	CB-CG-CD	6.80	124.17	112.60
1	B	821	GLN	O-C-N	-6.80	115.01	122.09
1	B	242	ARG	NE-CZ-NH2	-6.80	113.08	119.20
1	B	268	GLN	O-C-N	6.79	129.15	122.09
1	B	496	ASN	OD1-CG-ND2	6.74	129.34	122.60
1	B	272	ALA	N-CA-CB	6.72	120.28	110.26
1	B	292	ARG	CA-C-O	6.72	127.68	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	664	GLU	CA-C-O	6.71	128.37	120.58
1	A	404	ASN	OD1-CG-ND2	6.70	129.30	122.60
1	A	302	CYS	CA-C-N	6.67	129.55	120.54
1	A	302	CYS	C-N-CA	6.67	129.55	120.54
1	A	471	TYR	N-CA-C	-6.67	104.09	111.36
1	A	230	VAL	CB-CA-C	-6.63	102.73	111.81
1	B	193	ASN	CA-C-O	6.61	127.53	120.46
1	A	484	ASN	OD1-CG-ND2	6.58	129.18	122.60
1	A	808	CYS	O-C-N	-6.57	114.44	122.20
1	B	481	ASN	CB-CG-OD1	6.57	133.93	120.80
1	B	782	GLU	CA-C-O	-6.57	114.14	120.90
1	B	584	LEU	CA-C-O	-6.55	113.60	120.55
1	A	473	GLN	OE1-CD-NE2	6.55	129.15	122.60
1	A	277	LYS	N-CA-CB	6.54	121.97	110.27
1	A	459	HIS	CA-C-O	6.53	127.47	120.55
1	A	367	ILE	N-CA-C	-6.52	105.95	111.56
1	B	258	ASN	O-C-N	-6.52	113.92	122.39
1	A	744	GLU	O-C-N	-6.49	115.34	122.09
1	B	258	ASN	CB-CG-ND2	6.49	126.13	116.40
1	A	217	PRO	CA-C-O	-6.48	113.95	121.34
1	B	440	HIS	CA-C-O	6.48	127.84	120.84
1	B	334	VAL	N-CA-CB	6.48	122.07	111.58
1	A	560	GLN	N-CA-C	-6.47	105.54	113.50
1	A	25	LYS	CA-C-O	6.46	127.27	120.42
1	A	200	VAL	CA-C-N	6.43	128.59	122.36
1	A	200	VAL	C-N-CA	6.43	128.59	122.36
1	B	453	ASN	CA-C-O	-6.42	114.32	121.51
1	A	593	ASN	OD1-CG-ND2	6.42	129.02	122.60
1	A	632	ASN	O-C-N	-6.42	114.64	122.34
1	A	273	GLU	CA-C-O	-6.42	112.85	120.10
1	B	524	LEU	CA-C-O	6.40	127.30	119.11
1	A	652	ALA	CB-CA-C	6.39	122.39	110.70
1	A	431	VAL	CA-C-O	-6.38	113.64	120.59
1	A	97	ASN	CA-CB-CG	6.37	118.97	112.60
1	A	565	ILE	N-CA-C	6.37	117.03	108.11
1	B	799	ARG	NE-CZ-NH2	6.37	124.93	119.20
1	A	250	HIS	CA-CB-CG	6.36	120.16	113.80
1	A	334	VAL	CB-CA-C	-6.36	100.22	110.28
1	B	471	TYR	N-CA-C	-6.36	104.42	111.36
1	B	250	HIS	CG-ND1-CE1	6.36	120.11	109.30
1	A	575	ARG	N-CA-C	6.36	120.16	111.39
1	A	684	ASN	OD1-CG-ND2	6.35	128.95	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ALA	N-CA-C	6.35	118.91	110.53
1	A	184	ARG	CD-NE-CZ	6.35	133.29	124.40
1	A	566	GLN	OE1-CD-NE2	-6.34	116.26	122.60
1	B	295	GLN	CA-C-O	6.34	127.47	120.82
1	A	607	ALA	CB-CA-C	-6.32	97.84	110.42
1	B	814	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	615	LEU	CA-C-O	6.31	127.65	120.90
1	A	371	THR	O-C-N	6.30	130.54	122.10
1	B	343	THR	CA-C-N	6.30	133.30	121.97
1	B	343	THR	C-N-CA	6.30	133.30	121.97
1	B	351	ARG	NE-CZ-NH1	6.30	127.80	121.50
1	B	417	THR	CA-C-O	6.29	128.17	120.56
1	B	453	ASN	O-C-N	6.29	130.88	122.96
1	B	492	ILE	CA-C-N	6.29	129.03	120.54
1	B	492	ILE	C-N-CA	6.29	129.03	120.54
1	B	309	ARG	CD-NE-CZ	6.27	133.18	124.40
1	B	747	SER	CA-CB-OG	6.27	123.65	111.10
1	B	150	VAL	CA-CB-CG2	-6.27	99.74	110.40
1	B	576	GLN	CB-CG-CD	6.27	123.25	112.60
1	A	250	HIS	CG-ND1-CE1	6.26	119.94	109.30
1	A	719	LYS	CA-C-O	6.26	127.95	121.07
1	B	716	LYS	N-CA-CB	6.25	119.31	110.12
1	A	673	ALA	CA-C-O	-6.24	111.57	119.31
1	B	828	ALA	CA-C-O	6.24	127.72	120.49
1	A	127	ILE	O-C-N	6.22	131.18	122.97
1	B	737	VAL	CA-C-O	-6.22	113.56	120.96
1	A	333	GLU	N-CA-C	6.21	119.66	109.72
1	A	678	ASN	CA-C-O	-6.21	113.08	120.10
1	B	77	ALA	N-CA-C	6.20	118.92	110.55
1	B	631	ASN	OD1-CG-ND2	6.20	128.80	122.60
1	B	179	PRO	CA-C-O	-6.19	114.60	121.23
1	B	107	ASP	CA-CB-CG	6.18	118.78	112.60
1	B	828	ALA	O-C-N	-6.18	115.42	123.02
1	A	481	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	A	569	ARG	CB-CG-CD	-6.18	97.08	111.30
1	A	129	PRO	O-C-N	-6.16	114.33	122.64
1	B	429	ALA	CA-C-O	6.16	128.00	120.92
1	B	677	GLY	CA-C-O	6.15	127.38	121.05
1	B	821	GLN	CA-C-O	6.15	127.48	120.90
1	A	501	ALA	CA-C-O	6.14	127.06	120.55
1	A	278	VAL	CA-C-O	6.13	127.84	120.67
1	B	538	LYS	O-C-N	-6.13	115.62	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	773	VAL	N-CA-CB	6.13	117.31	110.51
1	A	335	ILE	CA-C-O	-6.12	113.74	120.48
1	A	272	ALA	CA-C-O	6.12	127.10	120.55
1	B	517	GLN	CA-C-O	6.12	126.90	119.31
1	B	510	GLU	O-C-N	6.11	129.87	122.96
1	A	510	GLU	CA-C-O	-6.11	114.90	121.56
1	B	404	ASN	O-C-N	6.10	128.59	122.12
1	A	701	GLU	O-C-N	6.09	129.10	122.15
1	B	251	PRO	N-CA-CB	-6.09	96.71	101.83
1	B	577	HIS	O-C-N	-6.09	114.78	122.27
1	A	691	THR	CA-CB-OG1	-6.08	100.47	109.60
1	A	636	VAL	N-CA-CB	6.07	118.09	111.41
1	B	410	PHE	CA-C-O	-6.04	114.14	120.55
1	B	289	LYS	O-C-N	-6.04	115.81	122.09
1	B	654	GLU	O-C-N	-6.02	115.18	122.22
1	A	554	GLY	CA-C-O	6.01	125.79	119.06
1	B	772	LEU	CA-C-N	6.01	128.35	120.60
1	B	772	LEU	C-N-CA	6.01	128.35	120.60
1	B	511	TRP	N-CA-C	-5.99	106.61	114.04
1	A	393	LYS	N-CA-C	5.99	117.89	111.36
1	B	726	TYR	O-C-N	-5.99	116.40	123.22
1	A	640	LEU	O-C-N	5.98	130.80	123.44
1	A	38	ARG	CA-C-O	5.97	126.84	119.97
1	A	829	ARG	NE-CZ-NH2	-5.97	113.83	119.20
1	A	818	ARG	O-C-N	5.97	128.22	122.07
1	A	289	LYS	CA-C-N	5.96	128.27	120.28
1	A	289	LYS	C-N-CA	5.96	128.27	120.28
1	B	38	ARG	NE-CZ-NH1	-5.96	115.54	121.50
1	A	149	THR	CA-CB-CG2	5.96	120.63	110.50
1	B	205	ALA	N-CA-CB	-5.96	100.97	111.39
1	B	607	ALA	CB-CA-C	-5.96	100.42	110.43
1	B	516	ASP	CA-CB-CG	5.94	118.54	112.60
1	B	453	ASN	CA-CB-CG	5.94	118.54	112.60
1	B	591	ARG	NE-CZ-NH2	5.94	124.54	119.20
1	B	769	ASP	CA-C-O	5.94	128.29	120.16
1	B	150	VAL	CA-CB-CG1	5.93	120.49	110.40
1	B	285	HIS	N-CA-CB	5.93	120.50	110.49
1	A	350	LEU	CA-C-N	5.92	128.54	120.54
1	A	350	LEU	C-N-CA	5.92	128.54	120.54
1	B	364	ALA	CA-C-O	5.92	127.04	120.82
1	A	481	ASN	CB-CG-OD1	5.92	132.64	120.80
1	B	49	ARG	CD-NE-CZ	5.92	132.69	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	773	VAL	CB-CA-C	-5.91	104.32	111.88
1	B	487	THR	CA-CB-OG1	-5.90	100.75	109.60
1	B	557	ILE	CA-C-O	-5.89	114.10	121.11
1	A	279	LEU	N-CA-C	-5.89	100.39	109.76
1	A	310	ARG	NE-CZ-NH1	-5.89	115.61	121.50
1	B	129	PRO	CA-C-O	5.88	127.44	121.27
1	B	149	THR	CA-CB-CG2	5.88	120.49	110.50
1	A	377	HIS	CA-CB-CG	5.87	119.67	113.80
1	A	408	THR	N-CA-CB	5.87	118.85	110.16
1	A	262	PHE	O-C-N	-5.87	115.75	122.09
1	B	357	HIS	CA-CB-CG	-5.86	107.94	113.80
1	A	377	HIS	CA-C-O	5.86	126.40	119.48
1	B	519	ILE	O-C-N	-5.86	115.98	121.90
1	B	128	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	582	ARG	NH1-CZ-NH2	5.86	126.92	119.30
1	A	441	MET	CA-C-O	5.85	126.75	120.55
1	B	800	ALA	CA-C-O	5.84	126.96	120.82
1	B	760	GLN	OE1-CD-NE2	-5.84	116.76	122.60
1	A	770	PRO	CB-CA-C	-5.83	103.57	111.85
1	B	475	TRP	O-C-N	-5.83	116.06	121.36
1	B	314	ALA	CA-C-N	5.82	131.29	120.87
1	B	314	ALA	C-N-CA	5.82	131.29	120.87
1	B	29	GLU	N-CA-C	-5.82	104.53	111.69
1	B	131	LEU	O-C-N	-5.82	115.33	122.25
1	A	214	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	A	485	GLY	CA-C-O	5.81	128.52	121.61
1	B	518	LEU	CA-C-N	5.80	130.13	120.62
1	B	518	LEU	C-N-CA	5.80	130.13	120.62
1	B	821	GLN	OE1-CD-NE2	5.79	128.39	122.60
1	A	602	VAL	O-C-N	5.79	128.65	123.03
1	A	573	TYR	CA-CB-CG	5.78	124.31	113.90
1	A	800	ALA	O-C-N	-5.78	116.12	122.07
1	A	308	LEU	CA-C-O	-5.77	114.43	120.55
1	B	212	ASP	CA-C-O	-5.77	114.58	121.56
1	B	108	VAL	CA-C-O	5.76	127.26	121.27
1	B	168	GLN	OE1-CD-NE2	5.76	128.36	122.60
1	B	242	ARG	CA-C-O	5.75	127.19	120.98
1	A	160	ASN	CB-CG-ND2	5.75	125.02	116.40
1	A	618	ASN	CA-C-O	5.74	126.58	119.97
1	B	179	PRO	CB-CA-C	-5.74	104.41	111.64
1	A	348	GLU	CA-C-O	-5.74	114.80	120.82
1	B	216	GLU	CA-C-O	5.73	127.47	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	613	TYR	CA-C-N	5.72	128.26	120.54
1	A	613	TYR	C-N-CA	5.72	128.26	120.54
1	A	624	ASN	O-C-N	-5.72	116.18	122.07
1	B	494	GLN	CB-CA-C	-5.71	101.19	110.79
1	A	591	ARG	O-C-N	5.71	128.25	122.09
1	A	615	LEU	O-C-N	-5.71	116.15	122.09
1	A	740	ALA	O-C-N	5.71	128.03	122.09
1	A	153	SER	N-CA-CB	5.70	118.79	109.95
1	B	151	GLY	CA-C-O	5.70	125.44	119.06
1	B	737	VAL	N-CA-C	-5.70	105.29	110.82
1	A	105	TYR	O-C-N	5.70	128.18	122.08
1	A	261	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	544	ARG	NH1-CZ-NH2	5.69	126.70	119.30
1	B	115	TYR	N-CA-C	-5.69	105.68	113.30
1	A	153	SER	CA-C-O	-5.69	114.21	120.69
1	B	780	TYR	O-C-N	-5.68	116.22	122.07
1	B	162	GLN	OE1-CD-NE2	5.68	128.28	122.60
1	A	151	GLY	O-C-N	-5.67	115.81	122.45
1	A	37	GLN	CA-C-O	5.67	126.48	119.79
1	B	575	ARG	CA-C-N	5.66	128.92	120.31
1	B	575	ARG	C-N-CA	5.66	128.92	120.31
1	B	712	GLY	O-C-N	5.66	128.74	122.68
1	B	500	ALA	N-CA-C	-5.66	105.19	111.36
1	A	167	ARG	NE-CZ-NH1	-5.66	115.84	121.50
1	A	179	PRO	CA-C-O	-5.66	114.97	121.36
1	A	281	PRO	CA-C-O	-5.66	114.84	122.08
1	B	1767	LYS	N-CA-C	5.66	117.44	111.28
1	B	459	HIS	CA-C-O	5.65	126.54	120.55
1	A	93	ARG	NE-CZ-NH2	5.65	124.28	119.20
1	B	784	GLN	CG-CD-NE2	5.65	124.87	116.40
1	A	671	LYS	CA-CB-CG	-5.64	102.83	114.10
1	A	105	TYR	CA-C-O	-5.63	114.87	121.07
1	B	58	ALA	O-C-N	-5.63	116.05	122.08
1	B	557	ILE	CA-CB-CG2	5.63	120.07	110.50
1	A	38	ARG	NE-CZ-NH1	-5.63	115.87	121.50
1	B	666	ILE	N-CA-C	5.63	121.05	109.34
1	B	233	TYR	CA-C-O	5.63	127.32	120.62
1	B	334	VAL	O-C-N	5.62	129.15	123.07
1	A	440	HIS	CA-C-O	5.62	126.91	120.84
1	A	786	GLN	CG-CD-NE2	5.61	124.81	116.40
1	A	481	ASN	O-C-N	5.60	130.33	123.44
1	A	186	ASN	OD1-CG-ND2	5.60	128.20	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLN	O-C-N	5.59	129.59	123.27
1	B	750	TYR	O-C-N	-5.59	115.47	122.35
1	B	800	ALA	N-CA-C	-5.59	105.08	111.07
1	B	444	LEU	CA-C-O	-5.59	114.62	120.55
1	B	688	THR	CA-C-O	5.59	126.86	120.54
1	B	276	THR	O-C-N	-5.58	114.41	121.95
1	A	96	GLY	CA-C-O	-5.58	114.97	121.00
1	A	264	ARG	CA-C-N	5.58	128.53	120.38
1	A	264	ARG	C-N-CA	5.58	128.53	120.38
1	B	627	ALA	CA-C-O	5.58	126.46	120.55
1	B	180	ASP	CA-C-O	-5.58	115.96	122.37
1	B	242	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	A	27	PHE	N-CA-C	5.56	117.15	111.14
1	A	534	TYR	O-C-N	5.56	128.73	122.22
1	B	468	PHE	CA-CB-CG	5.56	119.36	113.80
1	B	490	ARG	NE-CZ-NH1	5.56	127.06	121.50
1	B	730	LYS	O-C-N	-5.55	116.14	122.08
1	A	350	LEU	CA-C-O	5.55	126.65	120.82
1	A	487	THR	CA-C-N	5.55	125.38	119.28
1	A	487	THR	C-N-CA	5.55	125.38	119.28
1	B	538	LYS	CA-C-O	5.54	126.42	120.55
1	B	576	GLN	N-CA-C	-5.54	105.40	111.82
1	B	545	LEU	N-CA-C	-5.53	105.33	111.36
1	A	576	GLN	O-C-N	-5.53	115.75	122.22
1	B	310	ARG	CA-CB-CG	5.52	125.14	114.10
1	A	50	GLN	OE1-CD-NE2	5.52	128.12	122.60
1	A	23	ASN	CB-CG-ND2	-5.52	108.12	116.40
1	A	286	THR	O-C-N	5.51	129.91	122.59
1	A	88	GLU	CG-CD-OE2	5.50	131.06	118.40
1	A	598	ARG	NH1-CZ-NH2	5.50	126.45	119.30
1	B	95	THR	N-CA-CB	5.50	117.94	109.91
1	A	548	PHE	CA-CB-CG	5.49	119.29	113.80
1	B	49	ARG	NE-CZ-NH1	-5.49	116.01	121.50
1	B	766	GLN	N-CA-C	5.49	117.69	111.11
1	B	703	VAL	N-CA-CB	5.48	118.80	110.58
1	B	233	TYR	O-C-N	-5.47	115.38	122.77
1	A	160	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	B	408	THR	N-CA-CB	5.47	118.25	110.16
1	B	424	VAL	CA-C-O	5.46	127.09	121.41
1	A	284	ASN	CB-CG-ND2	-5.46	108.21	116.40
1	A	77	ALA	CA-C-O	5.45	128.20	121.87
1	A	199	GLN	CA-CB-CG	-5.45	103.20	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	PRO	O-C-N	-5.45	117.04	122.98
1	A	132	GLY	O-C-N	-5.45	115.62	122.70
1	B	825	TRP	N-CA-C	5.44	117.21	111.28
1	B	145	ASP	CA-C-O	5.44	126.71	121.00
1	B	229	PRO	N-CA-C	5.44	119.03	110.50
1	B	138	ARG	N-CA-C	-5.43	105.44	111.36
1	B	333	GLU	N-CA-C	5.43	118.09	109.50
1	A	557	ILE	CA-CB-CG2	5.43	119.74	110.50
1	A	310	ARG	CA-C-O	5.42	126.52	120.82
1	A	623	ILE	N-CA-C	5.42	115.87	110.23
1	B	680	LYS	CA-CB-CG	5.42	124.94	114.10
1	B	261	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	327	HIS	CA-CB-CG	5.42	119.22	113.80
1	A	463	VAL	N-CA-C	-5.42	105.25	110.72
1	B	77	ALA	CA-C-O	5.42	128.20	121.81
1	A	23	ASN	OD1-CG-ND2	5.41	128.01	122.60
1	B	137	GLY	O-C-N	5.41	127.43	122.19
1	B	250	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	B	702	LYS	O-C-N	-5.40	116.20	122.03
1	B	614	TYR	N-CA-C	5.39	117.58	111.11
1	A	45	GLU	CA-C-O	-5.39	112.96	119.27
1	B	145	ASP	O-C-N	-5.39	116.42	122.03
1	B	681	LEU	CA-C-O	5.39	126.26	120.55
1	A	250	HIS	CB-CG-CD2	5.39	138.21	131.20
1	B	632	ASN	CA-CB-CG	-5.39	107.21	112.60
1	B	649	CYS	O-C-N	5.39	128.76	122.99
1	B	504	ASP	O-C-N	5.38	128.71	122.20
1	B	605	PHE	O-C-N	5.38	129.84	123.27
1	A	49	ARG	CD-NE-CZ	5.38	131.94	124.40
1	B	354	ILE	O-C-N	-5.38	116.18	121.94
1	A	150	VAL	CA-CB-CG1	5.38	119.54	110.40
1	A	299	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	A	512	ALA	N-CA-C	5.38	117.84	111.33
1	B	636	VAL	N-CA-C	-5.37	107.55	111.90
1	B	234	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	B	258	ASN	CA-C-O	5.37	125.99	119.49
1	B	361	TRP	CA-C-O	5.37	126.46	120.82
1	B	143	PHE	CB-CA-C	5.37	119.97	110.85
1	A	190	PHE	N-CA-C	5.36	118.28	109.76
1	A	98	ASN	CA-C-O	-5.36	115.19	120.82
1	B	299	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	B	276	THR	CA-CB-OG1	5.35	117.63	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	618	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	B	811	PHE	CA-CB-CG	-5.35	108.45	113.80
1	A	152	GLN	OE1-CD-NE2	5.35	127.95	122.60
1	B	59	LEU	CA-C-O	-5.35	114.88	120.55
1	B	684	ASN	OD1-CG-ND2	5.35	127.95	122.60
1	A	183	HIS	CA-CB-CG	-5.34	108.46	113.80
1	B	493	LYS	N-CA-C	5.34	117.52	111.11
1	A	438	GLN	OE1-CD-NE2	5.33	127.93	122.60
1	B	820	TYR	N-CA-CB	5.33	118.05	110.16
1	A	478	LYS	CA-CB-CG	5.33	124.76	114.10
1	A	657	ILE	CA-C-N	5.33	125.04	119.82
1	A	657	ILE	C-N-CA	5.33	125.04	119.82
1	A	194	GLU	N-CA-CB	5.33	119.38	110.32
1	B	74	LYS	CA-C-O	5.32	124.76	119.49
1	A	199	GLN	O-C-N	5.32	129.28	123.22
1	B	313	LEU	CA-C-O	5.32	125.92	119.38
1	A	100	LEU	N-CA-C	5.31	117.07	111.28
1	B	603	PHE	CA-C-O	5.31	126.05	120.36
1	A	501	ALA	N-CA-CB	-5.31	102.31	110.12
1	B	573	TYR	CA-CB-CG	5.31	123.46	113.90
1	A	274	LYS	CA-C-O	-5.31	114.10	120.10
1	A	636	VAL	N-CA-C	-5.31	107.00	111.56
1	B	311	HIS	CA-C-O	5.31	126.58	120.90
1	B	762	LEU	N-CA-C	5.30	117.75	111.33
1	A	369	SER	CA-C-O	5.30	125.94	119.05
1	A	485	GLY	O-C-N	-5.30	117.84	123.45
1	B	475	TRP	CA-C-N	5.30	125.61	119.47
1	B	475	TRP	C-N-CA	5.30	125.61	119.47
1	A	29	GLU	CA-C-O	5.29	126.12	120.24
1	A	235	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	A	265	ALA	CA-C-N	5.29	131.12	122.65
1	A	265	ALA	C-N-CA	5.29	131.12	122.65
1	A	518	LEU	O-C-N	-5.29	116.03	122.22
1	B	815	ARG	CA-C-O	5.29	126.89	121.07
1	A	300	CYS	N-CA-CB	-5.29	102.06	109.94
1	A	313	LEU	O-C-N	-5.29	115.51	122.39
1	B	510	GLU	N-CA-C	-5.29	102.65	110.48
1	B	610	ALA	CA-C-N	5.29	126.45	119.84
1	B	610	ALA	C-N-CA	5.29	126.45	119.84
1	B	249	ALA	N-CA-C	-5.29	102.46	110.28
1	B	493	LYS	CA-C-O	-5.28	115.25	120.90
1	A	234	ARG	CA-C-O	-5.28	114.48	121.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	GLN	CG-CD-NE2	5.28	124.32	116.40
1	B	343	THR	O-C-N	-5.28	116.04	122.11
1	B	304	VAL	CA-C-O	5.27	126.76	121.17
1	A	778	ALA	CA-C-O	-5.27	115.27	121.07
1	B	263	LEU	O-C-N	-5.27	116.64	122.07
1	B	306	ASP	O-C-N	5.27	127.50	122.07
1	B	533	LEU	CA-C-O	5.27	126.35	120.82
1	B	618	ASN	CA-C-O	5.26	126.00	120.42
1	A	579	ASN	CA-C-O	5.26	126.53	121.00
1	B	51	TRP	O-C-N	5.26	128.14	122.15
1	B	251	PRO	CA-C-O	5.26	123.34	118.29
1	B	163	TYR	CA-C-O	-5.25	112.98	119.18
1	B	377	HIS	CA-CB-CG	5.25	119.05	113.80
1	A	708	ILE	CA-C-O	-5.25	115.79	121.19
1	A	441	MET	O-C-N	-5.24	116.56	122.12
1	B	483	THR	O-C-N	5.24	129.38	122.93
1	B	701	GLU	CA-C-O	-5.24	114.87	120.42
1	A	400	MET	O-C-N	-5.24	116.57	122.12
1	A	218	GLU	O-C-N	5.23	129.63	122.46
1	B	244	TRP	CA-C-N	5.23	130.15	122.77
1	B	244	TRP	C-N-CA	5.23	130.15	122.77
1	A	493	LYS	CA-CB-CG	5.23	124.56	114.10
1	B	49	ARG	NH1-CZ-NH2	5.23	126.10	119.30
1	B	501	ALA	O-C-N	-5.23	116.69	122.07
1	B	688	THR	N-CA-C	5.22	118.13	109.46
1	A	531	ARG	CA-C-O	5.22	126.26	120.63
1	A	482	VAL	CA-CB-CG1	-5.21	101.55	110.40
1	B	284	ASN	CB-CG-ND2	-5.21	108.59	116.40
1	B	645	LEU	CA-C-O	5.20	123.47	119.46
1	A	311	HIS	CA-C-O	5.19	126.45	120.90
1	A	554	GLY	O-C-N	-5.19	115.84	122.43
1	A	664	GLU	O-C-N	-5.19	116.42	122.96
1	B	780	TYR	CA-C-O	5.18	126.26	120.82
1	B	111	SER	O-C-N	-5.18	116.29	122.20
1	B	115	TYR	O-C-N	-5.18	115.97	122.24
1	B	563	PHE	CA-CB-CG	5.18	118.98	113.80
1	A	583	ILE	CA-C-O	-5.17	115.89	121.27
1	A	603	PHE	CA-C-O	5.17	126.22	120.43
1	A	284	ASN	OD1-CG-ND2	5.17	127.77	122.60
1	A	514	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	246	ALA	CA-C-O	5.17	126.58	120.69
1	B	757	ALA	O-C-N	-5.16	116.72	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	726	TYR	CA-C-O	5.16	125.88	120.36
1	A	474	LEU	CA-C-O	-5.16	115.40	120.82
1	B	698	GLU	CA-C-O	5.15	127.05	121.02
1	A	742	LEU	N-CA-CB	5.15	118.27	110.28
1	A	789	VAL	CA-CB-CG2	-5.15	101.64	110.40
1	A	230	VAL	N-CA-CB	5.15	117.78	111.60
1	A	771	TYR	CA-CB-CG	-5.15	104.63	113.90
1	B	37	GLN	OE1-CD-NE2	5.15	127.75	122.60
1	A	304	VAL	CA-C-O	5.15	126.30	120.95
1	B	360	SER	CA-C-O	-5.14	116.62	122.01
1	A	400	MET	CA-C-O	5.13	125.99	120.55
1	A	138	ARG	N-CA-C	-5.13	105.38	111.69
1	B	267	GLN	N-CA-C	5.12	117.26	111.11
1	B	791	TYR	CA-C-O	5.12	125.86	119.97
1	A	425	TRP	CA-C-O	-5.12	115.42	120.90
1	A	358	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	A	556	ASP	CA-C-N	5.12	127.94	120.98
1	A	556	ASP	C-N-CA	5.12	127.94	120.98
1	B	666	ILE	CA-C-O	-5.12	114.39	120.78
1	B	185	SER	CB-CA-C	-5.11	102.25	110.74
1	B	826	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	B	428	LEU	N-CA-C	5.10	119.49	113.16
1	A	233	TYR	CA-C-O	5.10	126.69	120.62
1	B	818	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	B	431	VAL	CB-CA-C	-5.10	103.52	110.96
1	A	577	HIS	CA-CB-CG	5.09	118.89	113.80
1	A	519	ILE	O-C-N	-5.09	116.26	122.06
1	A	581	LEU	CA-C-O	5.09	125.81	120.42
1	B	116	ASP	CA-C-O	-5.09	115.70	121.65
1	B	163	TYR	O-C-N	5.09	128.21	122.20
1	B	431	VAL	N-CA-CB	5.08	117.86	111.46
1	B	33	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	A	591	ARG	CA-C-O	-5.08	115.47	120.70
1	A	26	GLN	O-C-N	5.08	127.30	122.07
1	B	497	PRO	N-CA-CB	-5.08	97.75	103.44
1	A	135	GLY	O-C-N	5.08	129.30	122.70
1	B	429	ALA	N-CA-C	5.08	118.49	109.96
1	A	24	ASP	CA-C-O	-5.07	114.14	119.97
1	A	44	ALA	N-CA-CB	5.07	119.27	110.39
1	A	401	GLN	O-C-N	5.07	127.31	122.03
1	A	601	ARG	O-C-N	-5.07	117.00	123.24
1	B	760	GLN	O-C-N	5.07	127.36	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	752	ASP	CB-CA-C	-5.07	104.34	111.95
1	B	506	SER	CA-CB-OG	-5.07	100.97	111.10
1	B	85	ILE	N-CA-C	5.07	115.06	107.51
1	B	149	THR	CA-CB-OG1	-5.07	102.00	109.60
1	B	619	ILE	O-C-N	-5.06	116.75	121.87
1	B	805	THR	O-C-N	5.06	127.29	122.03
1	B	194	GLU	N-CA-CB	5.06	118.92	110.32
1	A	704	GLY	CA-C-O	-5.06	115.41	121.98
1	B	650	VAL	CB-CA-C	-5.06	105.42	112.04
1	B	648	TYR	O-C-N	5.05	129.12	123.06
1	A	315	GLY	CA-C-O	5.05	126.15	119.58
1	A	653	ALA	O-C-N	5.05	127.47	122.12
1	B	337	LEU	CA-C-O	-5.05	115.67	120.92
1	A	417	THR	CA-C-O	5.05	126.10	120.80
1	A	652	ALA	N-CA-C	-5.05	105.48	111.69
1	A	660	ALA	CA-C-O	-5.05	115.51	121.16
1	B	137	GLY	CA-C-N	5.05	127.46	120.29
1	B	137	GLY	C-N-CA	5.05	127.46	120.29
1	B	483	THR	CA-C-O	-5.04	115.01	120.81
1	B	279	LEU	CA-C-N	5.04	128.27	122.83
1	B	279	LEU	C-N-CA	5.04	128.27	122.83
1	A	74	LYS	CA-C-O	5.04	124.48	119.49
1	B	652	ALA	N-CA-C	-5.04	105.50	111.69
1	B	746	GLU	CG-CD-OE2	-5.03	106.83	118.40
1	B	702	LYS	CA-C-N	5.03	127.56	120.42
1	B	702	LYS	C-N-CA	5.03	127.56	120.42
1	B	500	ALA	CB-CA-C	5.03	119.39	110.85
1	A	253	ASP	OD1-CG-OD2	5.02	134.95	122.90
1	A	92	GLY	O-C-N	-5.02	117.31	122.68
1	B	544	ARG	NE-CZ-NH2	-5.02	114.68	119.20
1	B	829	ARG	NE-CZ-NH2	-5.02	114.68	119.20
1	A	579	ASN	O-C-N	-5.01	116.81	122.03
1	B	756	HIS	O-C-N	-5.01	116.18	122.24
1	B	295	GLN	O-C-N	-5.01	116.91	122.07
1	B	389	VAL	N-CA-CB	5.00	119.21	110.65
1	B	277	LYS	O-C-N	5.00	128.07	122.32
1	B	300	CYS	O-C-N	-5.00	116.89	122.09

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	516	ASP	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6369	0	6324	232	0
1	B	6369	0	6324	234	0
2	C	44	0	30	2	0
2	D	44	0	30	5	0
3	A	6	0	8	1	0
3	B	6	0	8	1	0
4	A	15	0	6	0	0
4	B	15	0	6	2	0
5	A	54	0	0	10	0
5	B	39	0	0	9	0
All	All	12961	0	12736	462	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 18.

All (462) 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:716:LYS:HE2	1:A:719:LYS:HD2	1.42	0.99
1:A:522:VAL:HG11	5:A:1777:HOH:O	1.61	0.97
1:B:310:ARG:HD2	5:B:1804:HOH:O	1.71	0.88
1:A:266:GLU:HG3	1:B:270:ILE:HD13	1.55	0.87
1:B:292:ARG:NH2	2:D:3:AC1:O2	2.09	0.85
1:B:716:LYS:HE2	1:B:719:LYS:HD2	1.58	0.84
1:B:403:ILE:HA	1:B:406:ILE:HD12	1.58	0.83
1:B:19:GLN:HB3	1:B:20:PRO:HD3	1.60	0.83
1:A:287:ALA:HB2	5:A:1793:HOH:O	1.80	0.81
1:A:283:ASP:HB2	1:A:289:LYS:HD3	1.63	0.81
1:A:18:SER:HB3	1:A:234:ARG:HD2	1.62	0.81
1:A:582:ARG:HH11	1:A:582:ARG:HB3	1.47	0.80
1:A:19:GLN:HB3	1:A:20:PRO:HD3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:SER:HB2	1:A:681:LEU:HD13	1.64	0.79
1:A:270:ILE:HD13	1:B:266:GLU:HG3	1.64	0.79
1:A:601:ARG:HH12	1:A:784:GLN:NE2	1.82	0.78
1:A:310:ARG:HD2	5:A:1807:HOH:O	1.84	0.77
1:B:582:ARG:HH11	1:B:582:ARG:HB3	1.48	0.76
1:B:601:ARG:HH12	1:B:784:GLN:NE2	1.84	0.76
1:B:294:MET:HG2	1:B:395:LEU:HD11	1.67	0.76
1:A:601:ARG:HH12	1:A:784:GLN:HE22	1.35	0.74
1:B:669:ALA:HB3	1:B:718:VAL:HG21	1.70	0.74
1:B:468:PHE:HB3	1:B:471:TYR:HB2	1.71	0.73
1:B:571:HIS:HD2	1:B:573:TYR:H	1.35	0.73
1:A:543:VAL:O	1:A:546:ALA:HB3	1.89	0.72
1:B:601:ARG:HH12	1:B:784:GLN:HE22	1.38	0.72
1:A:571:HIS:HD2	1:A:573:TYR:H	1.39	0.71
1:A:665:GLN:CD	1:A:678:ASN:HB3	2.16	0.71
1:B:18:SER:HB3	1:B:234:ARG:HD2	1.74	0.70
1:B:446:VAL:HG22	1:B:452:VAL:HG21	1.72	0.70
1:A:403:ILE:HA	1:A:406:ILE:HD12	1.72	0.70
1:B:777:PHE:O	1:B:781:VAL:HG23	1.93	0.69
1:B:518:LEU:HD23	1:B:805:THR:HG22	1.75	0.69
1:A:669:ALA:HB3	1:A:718:VAL:HG21	1.72	0.69
1:B:405:GLU:O	1:B:409:ARG:HG2	1.93	0.68
1:A:518:LEU:HD23	1:A:805:THR:HG22	1.76	0.68
1:A:158:GLY:HA2	1:A:299:GLN:NE2	2.09	0.68
1:A:446:VAL:HG22	1:A:452:VAL:HG21	1.76	0.68
1:B:422:GLU:O	1:B:423:LYS:C	2.37	0.68
1:A:20:PRO:HG2	1:A:102:LEU:HD22	1.77	0.67
1:A:270:ILE:HD12	1:B:263:LEU:HD12	1.76	0.67
1:A:422:GLU:O	1:A:423:LYS:C	2.37	0.67
1:B:283:ASP:HB2	1:B:289:LYS:HD3	1.78	0.66
1:A:777:PHE:O	1:A:781:VAL:HG23	1.95	0.66
1:B:516:ASP:O	5:B:1799:HOH:O	2.14	0.65
1:A:570:LEU:HD13	1:A:620:ILE:HG12	1.79	0.65
1:A:503:LEU:HD13	1:A:518:LEU:HD11	1.78	0.64
1:B:47:THR:OG1	1:B:50:GLN:HG3	1.96	0.64
1:B:300:CYS:SG	1:B:345:ALA:HB2	2.37	0.64
1:A:153:SER:HA	1:A:239:GLN:NE2	2.13	0.64
1:B:582:ARG:C	1:B:582:ARG:HD2	2.21	0.64
1:B:153:SER:HA	1:B:239:GLN:NE2	2.13	0.64
1:A:23:ASN:HB3	1:A:26:GLN:HE21	1.61	0.63
1:B:101:ASN:HB2	1:B:231:VAL:HG23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:LYS:HG2	5:B:1785:HOH:O	1.98	0.63
1:B:186:ASN:C	1:B:186:ASN:HD22	2.06	0.63
1:B:369:SER:O	1:B:450:PHE:HB3	1.98	0.63
1:A:674:SER:HB3	3:A:998:GOL:O2	1.98	0.62
1:B:327:HIS:HA	1:B:367:ILE:HD11	1.79	0.62
1:B:447:VAL:O	5:B:1779:HOH:O	2.16	0.62
1:B:418:TRP:CZ3	1:B:474:LEU:HD21	2.35	0.62
1:B:539:GLN:O	1:B:543:VAL:HG23	2.00	0.62
1:A:47:THR:OG1	1:A:50:GLN:HG3	2.00	0.62
1:B:582:ARG:HD2	1:B:582:ARG:O	2.00	0.62
1:A:162:GLN:HB2	1:A:184:ARG:CZ	2.30	0.61
1:B:663:SER:HB2	1:B:681:LEU:HD13	1.82	0.61
1:A:455:VAL:H	1:A:459:HIS:HD2	1.48	0.61
1:A:782:GLU:O	1:A:783:ALA:C	2.43	0.61
1:B:23:ASN:HB3	1:B:26:GLN:HE21	1.66	0.61
1:A:521:LEU:HA	1:A:524:LEU:HD12	1.84	0.60
1:A:784:GLN:HE21	1:A:784:GLN:HA	1.64	0.60
1:B:609:ALA:HB3	1:B:617:LYS:HG2	1.82	0.60
1:A:720:ALA:HB1	1:A:724:LYS:HE2	1.83	0.60
1:B:144:LEU:HD12	1:B:147:MET:HE3	1.83	0.60
1:B:565:ILE:HD12	1:B:660:ALA:HB2	1.84	0.59
1:A:352:VAL:HA	1:A:356:GLU:HG3	1.82	0.59
1:B:671:LYS:HZ3	1:B:771:TYR:HE1	1.50	0.59
1:B:720:ALA:HB1	1:B:724:LYS:HE2	1.84	0.59
1:A:566:GLN:HE22	1:A:576:GLN:HA	1.66	0.59
1:A:662:ILE:HG23	1:A:689:VAL:HG23	1.83	0.59
1:B:650:VAL:O	1:B:654:GLU:HG3	2.02	0.59
1:B:566:GLN:HE22	1:B:576:GLN:HA	1.67	0.59
1:B:193:ASN:HB3	1:B:196:LEU:HD12	1.84	0.58
1:B:428:LEU:HD21	1:B:470:GLU:HG2	1.83	0.58
1:A:582:ARG:HH11	1:A:582:ARG:CB	2.14	0.58
1:B:582:ARG:HH11	1:B:582:ARG:CB	2.16	0.58
1:A:158:GLY:HA2	1:A:299:GLN:HE21	1.68	0.58
1:A:284:ASN:O	1:A:285:HIS:HB3	2.04	0.58
1:A:165:LEU:O	1:A:166:PHE:HB3	2.03	0.58
1:B:503:LEU:HD13	1:B:518:LEU:HD11	1.85	0.58
1:A:101:ASN:HB2	1:A:231:VAL:HG23	1.85	0.58
1:A:381:PRO:HA	1:A:384:LEU:CD1	2.33	0.58
1:B:190:PHE:CE1	1:B:226:TRP:HB3	2.38	0.58
1:B:283:ASP:HA	1:B:288:GLY:HA3	1.84	0.57
1:B:753:GLY:O	1:B:755:LYS:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:LEU:HD23	1:B:364:ALA:HB1	1.86	0.57
1:B:714:THR:O	1:B:718:VAL:HG23	2.04	0.57
1:B:731:TRP:O	1:B:732:ARG:C	2.47	0.57
1:B:169:SER:OG	1:B:176:VAL:HG22	2.04	0.57
1:A:193:ASN:HB3	1:A:196:LEU:HD12	1.86	0.57
1:A:488:PRO:HG3	1:A:515:LEU:HD22	1.87	0.57
1:A:22:PHE:CD1	1:A:107:ASP:HB3	2.40	0.56
1:A:144:LEU:HD12	1:A:147:MET:CE	2.36	0.56
1:A:732:ARG:HD2	1:A:742:LEU:HD23	1.87	0.56
1:B:469:PRO:O	1:B:472:HIS:HB3	2.05	0.56
1:B:22:PHE:HB2	1:B:104:TRP:CG	2.41	0.56
1:A:186:ASN:C	1:A:186:ASN:HD22	2.14	0.56
1:B:42:ASN:HB2	1:B:45:GLU:OE2	2.04	0.56
1:B:144:LEU:HD12	1:B:147:MET:CE	2.36	0.56
1:B:248:HIS:HD2	1:B:249:ALA:O	1.87	0.56
1:A:169:SER:OG	1:A:176:VAL:HG22	2.06	0.56
1:B:186:ASN:C	1:B:186:ASN:ND2	2.64	0.56
1:A:455:VAL:H	1:A:459:HIS:CD2	2.24	0.55
1:A:526:ASP:HA	1:A:799:ARG:NH2	2.21	0.55
1:A:144:LEU:HD12	1:A:147:MET:HE3	1.87	0.55
1:A:719:LYS:HE2	5:A:1812:HOH:O	2.07	0.55
1:A:814:ASP:O	1:A:818:ARG:HG2	2.06	0.55
1:B:545:LEU:HD11	1:B:656:LEU:HD23	1.89	0.55
1:A:468:PHE:HB3	1:A:471:TYR:HB2	1.89	0.55
1:A:615:LEU:O	1:A:619:ILE:HG13	2.07	0.55
1:A:714:THR:O	1:A:718:VAL:HG23	2.05	0.55
1:A:22:PHE:HB2	1:A:104:TRP:CG	2.42	0.55
1:A:294:MET:HG2	1:A:395:LEU:HD11	1.88	0.55
1:B:665:GLN:CD	1:B:678:ASN:HB3	2.32	0.55
1:A:531:ARG:NH1	1:A:799:ARG:NH1	2.55	0.55
1:A:89:PHE:CE1	1:A:144:LEU:HD22	2.42	0.54
1:A:283:ASP:HA	1:A:288:GLY:HA3	1.89	0.54
1:A:101:ASN:HB3	1:A:232:GLY:O	2.07	0.54
1:B:101:ASN:HB3	1:B:232:GLY:O	2.08	0.54
1:A:19:GLN:CB	1:A:20:PRO:HD3	2.36	0.54
1:A:582:ARG:HB3	1:A:582:ARG:NH1	2.21	0.54
1:A:230:VAL:HG23	1:A:239:GLN:O	2.07	0.54
1:B:19:GLN:HB3	1:B:20:PRO:CD	2.36	0.53
1:A:19:GLN:HB3	1:A:20:PRO:CD	2.38	0.53
1:A:577:HIS:H	1:A:577:HIS:CD2	2.26	0.53
1:A:460:SER:OG	1:A:481:ASN:ND2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ASP:O	1:A:536:VAL:HG13	2.08	0.53
1:B:292:ARG:HH21	2:D:3:AC1:C2	2.21	0.53
1:B:456:ALA:HB1	5:B:1802:HOH:O	2.09	0.53
1:A:344:ILE:O	1:A:347:PRO:HG2	2.08	0.53
1:A:729:VAL:O	1:A:732:ARG:HB3	2.09	0.53
1:B:455:VAL:HB	1:B:484:ASN:ND2	2.24	0.53
1:A:671:LYS:HZ3	1:A:771:TYR:HE1	1.57	0.53
1:B:705:GLU:HG3	1:B:706:GLU:OE2	2.09	0.53
1:A:160:ASN:ND2	1:A:184:ARG:HD3	2.24	0.53
1:B:645:LEU:HD12	1:B:656:LEU:HD21	1.91	0.53
1:B:716:LYS:O	1:B:719:LYS:HB2	2.09	0.52
1:A:46:MET:HE3	1:A:51:TRP:CE2	2.44	0.52
1:A:129:PRO:HB3	1:A:182:TRP:CZ3	2.44	0.52
1:B:204:GLY:N	1:B:218:GLU:HG2	2.25	0.52
1:B:425:TRP:CZ2	1:B:429:ALA:HB2	2.43	0.52
1:A:204:GLY:N	1:A:218:GLU:HG2	2.25	0.52
1:A:422:GLU:HG2	1:A:426:ALA:HB2	1.91	0.52
1:A:285:HIS:CD2	1:A:287:ALA:HB3	2.44	0.52
1:A:335:ILE:HG13	1:A:371:THR:HG22	1.92	0.52
1:B:136:LEU:HD22	2:D:3:AC1:HCB2	1.91	0.52
1:A:570:LEU:HD13	1:A:620:ILE:CG1	2.40	0.52
1:A:64:ARG:NH1	1:B:38:ARG:HG3	2.24	0.52
1:B:475:TRP:CG	1:B:478:LYS:HE3	2.44	0.52
1:A:428:LEU:HD21	1:A:470:GLU:HG2	1.92	0.52
1:A:716:LYS:O	1:A:719:LYS:HB2	2.10	0.52
1:B:765:ILE:O	1:B:769:ASP:HB2	2.10	0.52
1:B:344:ILE:HD12	1:B:347:PRO:HG2	1.92	0.51
1:B:352:VAL:HA	1:B:356:GLU:HG3	1.91	0.51
1:B:465:LYS:O	1:B:469:PRO:HG3	2.10	0.51
1:A:32:SER:HA	1:A:35:TRP:NE1	2.25	0.51
1:B:186:ASN:O	1:B:187:TYR:C	2.53	0.51
1:A:212:ASP:O	1:A:214:ARG:N	2.44	0.51
1:A:369:SER:O	1:A:450:PHE:HB3	2.10	0.51
1:B:162:GLN:HB2	1:B:184:ARG:CZ	2.41	0.51
1:B:94:LEU:HB2	1:B:187:TYR:OH	2.11	0.51
1:A:519:ILE:HA	1:A:806:ALA:O	2.10	0.51
1:B:567:ILE:HG21	1:B:656:LEU:HD13	1.93	0.51
1:A:469:PRO:O	1:A:472:HIS:HB3	2.11	0.51
1:B:458:LEU:HB2	5:B:1803:HOH:O	2.09	0.51
1:A:798:THR:O	1:A:802:ILE:HG13	2.10	0.51
1:B:782:GLU:O	1:B:785:LYS:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:LEU:HD21	1:A:470:GLU:CG	2.41	0.50
1:B:77:ALA:O	1:B:78:ASN:C	2.54	0.50
1:A:411:LYS:HD2	1:A:425:TRP:CE2	2.46	0.50
1:B:731:TRP:CE3	1:B:775:ALA:HA	2.45	0.50
1:B:165:LEU:HD23	1:B:279:LEU:O	2.12	0.50
1:B:717:GLN:O	1:B:718:VAL:C	2.54	0.50
1:B:335:ILE:HG13	1:B:371:THR:HG22	1.93	0.50
1:A:349:LEU:HD23	1:A:368:THR:HG22	1.94	0.50
1:B:459:HIS:O	1:B:463:VAL:HG23	2.12	0.50
1:A:515:LEU:HG	1:A:809:GLY:HA2	1.93	0.49
1:A:173:GLY:O	1:A:624:ASN:ND2	2.41	0.49
1:A:288:GLY:O	1:A:289:LYS:C	2.51	0.49
1:A:518:LEU:CD2	1:A:805:THR:HG22	2.41	0.49
1:A:565:ILE:HD12	1:A:660:ALA:HB2	1.94	0.49
1:B:422:GLU:HG2	1:B:426:ALA:HB2	1.93	0.49
1:A:270:ILE:HG21	1:B:263:LEU:HA	1.93	0.49
1:A:539:GLN:O	1:A:543:VAL:HG23	2.12	0.49
1:A:545:LEU:HD11	1:A:656:LEU:HD23	1.95	0.49
1:B:410:PHE:O	1:B:414:VAL:HG23	2.13	0.49
1:A:636:VAL:O	1:A:639:LYS:HB2	2.13	0.49
1:A:327:HIS:CD2	1:A:328:GLU:HG3	2.48	0.49
1:A:361:TRP:CZ3	1:A:405:GLU:HG2	2.48	0.49
1:B:557:ILE:HD12	1:B:602:VAL:HG11	1.95	0.49
1:B:158:GLY:HA2	1:B:299:GLN:NE2	2.28	0.49
1:A:22:PHE:HB2	1:A:104:TRP:CD2	2.48	0.49
1:B:93:ARG:O	1:B:490:ARG:NH2	2.45	0.49
1:A:129:PRO:HA	1:A:182:TRP:CD2	2.47	0.48
1:A:309:ARG:HB2	5:A:1787:HOH:O	2.12	0.48
1:B:361:TRP:CH2	1:B:402:ILE:HG23	2.48	0.48
1:B:522:VAL:HG12	1:B:803:LEU:CD2	2.43	0.48
1:B:32:SER:HA	1:B:35:TRP:NE1	2.28	0.48
1:B:582:ARG:HB3	1:B:582:ARG:NH1	2.22	0.48
1:A:46:MET:HE3	1:A:51:TRP:CD2	2.48	0.48
1:A:693:ASP:O	1:A:696:ASN:HB2	2.13	0.48
1:B:193:ASN:HB3	1:B:196:LEU:CD1	2.43	0.48
1:B:194:GLU:N	5:B:1774:HOH:O	2.47	0.48
1:B:753:GLY:O	1:B:754:ASP:C	2.56	0.48
1:A:753:GLY:O	1:A:755:LYS:HG3	2.14	0.48
1:B:716:LYS:CE	1:B:719:LYS:HD2	2.38	0.48
1:B:753:GLY:O	1:B:755:LYS:HG3	2.13	0.48
1:A:346:ILE:N	1:A:347:PRO:HD2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TRP:O	1:A:41:LEU:HB2	2.13	0.48
1:A:129:PRO:HA	1:A:182:TRP:CE3	2.49	0.48
1:A:279:LEU:HD22	1:A:280:TYR:N	2.29	0.48
1:A:285:HIS:O	1:A:286:THR:C	2.56	0.48
1:A:632:ASN:O	1:A:634:PRO:HD3	2.13	0.48
1:A:705:GLU:HG3	1:A:706:GLU:OE2	2.14	0.48
1:A:740:ALA:O	1:A:743:LYS:HB2	2.14	0.48
1:B:475:TRP:CD2	1:B:478:LYS:HE3	2.49	0.48
1:B:794:GLN:O	1:B:795:GLU:C	2.56	0.48
1:A:258:ASN:O	1:B:285:HIS:CE1	2.67	0.48
1:A:350:LEU:HD11	1:A:365:TRP:CE3	2.49	0.48
1:B:22:PHE:CD1	1:B:107:ASP:HB3	2.49	0.48
1:B:20:PRO:HG2	1:B:102:LEU:HD22	1.96	0.47
1:A:459:HIS:N	5:A:1791:HOH:O	2.46	0.47
1:A:555:ILE:CD1	1:A:643:VAL:HG23	2.44	0.47
1:B:292:ARG:NH2	2:D:3:AC1:C2	2.78	0.47
1:A:93:ARG:O	1:A:490:ARG:NH2	2.47	0.47
1:A:516:ASP:O	1:A:519:ILE:HG22	2.14	0.47
1:A:629:VAL:O	1:A:630:ILE:C	2.56	0.47
1:A:753:GLY:O	1:A:755:LYS:N	2.47	0.47
1:B:570:LEU:HD13	1:B:620:ILE:CG1	2.45	0.47
1:B:657:ILE:HB	1:B:658:PRO:HD3	1.96	0.47
1:B:824:ILE:O	1:B:829:ARG:NH2	2.47	0.47
1:B:381:PRO:HA	1:B:384:LEU:CD1	2.44	0.47
1:A:198:VAL:HG11	1:A:302:CYS:HA	1.96	0.47
1:A:703:VAL:O	1:A:807:ARG:NH1	2.47	0.47
1:A:716:LYS:HD2	1:A:716:LYS:HA	1.71	0.47
1:A:729:VAL:CG1	1:A:1767:LYS:HG3	2.44	0.47
1:A:20:PRO:HG2	1:A:102:LEU:CD2	2.43	0.47
1:A:94:LEU:HB2	1:A:187:TYR:OH	2.14	0.47
1:A:731:TRP:O	1:A:732:ARG:C	2.58	0.47
1:B:557:ILE:HG23	1:B:602:VAL:HG21	1.96	0.47
1:A:101:ASN:O	1:A:234:ARG:HD3	2.15	0.47
1:A:503:LEU:CD1	1:A:518:LEU:HD11	2.44	0.47
1:B:262:PHE:O	1:B:265:ALA:HB3	2.15	0.47
1:B:577:HIS:O	1:B:581:LEU:HG	2.15	0.47
1:A:190:PHE:CD1	1:A:228:LEU:HD13	2.50	0.47
1:B:525:ALA:O	1:B:531:ARG:NH1	2.43	0.47
1:B:666:ILE:HG22	1:B:711:PHE:CE1	2.50	0.47
1:A:810:MET:HE3	1:A:810:MET:HB2	1.92	0.46
1:A:465:LYS:O	1:A:469:PRO:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:TYR:HD1	1:A:475:TRP:CZ3	2.32	0.46
1:A:656:LEU:O	1:A:657:ILE:C	2.57	0.46
1:A:166:PHE:CZ	1:A:608:LYS:HB3	2.50	0.46
1:A:695:ALA:O	1:A:696:ASN:C	2.55	0.46
1:B:89:PHE:CE1	1:B:144:LEU:HD22	2.50	0.46
1:B:377:HIS:ND1	3:B:998:GOL:O3	2.37	0.46
1:B:455:VAL:HB	1:B:484:ASN:CG	2.40	0.46
1:B:337:LEU:HD22	1:B:342:PRO:HG2	1.98	0.46
1:B:518:LEU:CD2	1:B:805:THR:HG22	2.45	0.46
1:B:706:GLU:CD	1:B:706:GLU:H	2.23	0.46
1:B:818:ARG:O	1:B:821:GLN:HB2	2.15	0.46
1:A:168:GLN:NE2	1:A:175:GLN:OE1	2.44	0.46
1:A:303:SER:O	1:A:307:ILE:HG13	2.15	0.46
1:A:441:MET:O	1:A:442:ALA:C	2.57	0.46
1:A:475:TRP:CG	1:A:478:LYS:HE3	2.51	0.46
1:B:698:GLU:HB3	1:B:811:PHE:HZ	1.81	0.46
1:A:144:LEU:HD21	1:A:156:GLY:HA3	1.97	0.46
1:B:101:ASN:CB	1:B:231:VAL:HG23	2.45	0.46
1:B:107:ASP:O	1:B:110:ASP:HB2	2.16	0.46
1:B:267:GLN:O	1:B:268:GLN:C	2.59	0.46
1:B:521:LEU:HA	1:B:524:LEU:HD12	1.98	0.46
1:A:542:LYS:HA	1:A:659:ALA:HB1	1.98	0.46
1:A:731:TRP:H	1:A:731:TRP:CD1	2.33	0.46
1:B:815:ARG:O	1:B:816:SER:C	2.57	0.46
1:A:47:THR:O	1:A:48:PRO:C	2.58	0.46
1:B:729:VAL:HG11	1:B:1767:LYS:HG3	1.98	0.46
1:A:77:ALA:O	1:A:78:ASN:C	2.58	0.45
1:A:251:PRO:HB2	1:A:269:GLY:HA3	1.98	0.45
1:B:230:VAL:HG23	1:B:239:GLN:O	2.16	0.45
1:A:190:PHE:CE1	1:A:226:TRP:HB3	2.51	0.45
1:B:701:GLU:OE2	1:B:702:LYS:HD3	2.16	0.45
1:A:23:ASN:HB3	1:A:26:GLN:HB3	1.99	0.45
1:A:446:VAL:HG11	1:A:471:TYR:CG	2.51	0.45
1:A:568:LYS:HD3	1:A:574:LYS:HG2	1.99	0.45
1:A:582:ARG:HD2	1:A:582:ARG:C	2.41	0.45
1:B:19:GLN:CB	1:B:20:PRO:HD3	2.36	0.45
1:B:112:LEU:HD23	1:B:112:LEU:HA	1.79	0.45
1:A:285:HIS:HD2	1:A:287:ALA:HB3	1.81	0.45
1:B:622:ALA:O	1:B:626:VAL:HG13	2.16	0.45
1:B:457:ALA:N	5:B:1802:HOH:O	2.50	0.45
1:B:814:ASP:O	1:B:818:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ASN:HB3	1:A:196:LEU:CD1	2.46	0.45
1:B:803:LEU:HD22	1:B:807:ARG:CZ	2.47	0.45
1:A:186:ASN:C	1:A:186:ASN:ND2	2.75	0.45
1:B:139:LEU:HD11	1:B:143:PHE:CZ	2.51	0.45
1:B:482:VAL:HG13	1:B:819:ASP:HB2	1.98	0.45
1:B:526:ASP:HA	1:B:799:ARG:NH2	2.32	0.45
1:B:629:VAL:O	1:B:630:ILE:C	2.57	0.45
1:B:800:ALA:O	1:B:801:ALA:C	2.58	0.45
1:A:350:LEU:HD23	1:A:364:ALA:HB1	1.98	0.44
1:B:555:ILE:HD12	1:B:643:VAL:HG23	1.99	0.44
1:B:598:ARG:HH12	1:B:785:LYS:HA	1.82	0.44
2:D:2:GLC:H62	2:D:3:AC1:C5	2.47	0.44
1:A:326:LEU:HD13	1:A:359:MET:CE	2.47	0.44
1:B:297:TYR:O	1:B:298:PHE:C	2.61	0.44
1:B:396:LEU:HB3	1:B:399:HIS:CD2	2.52	0.44
1:B:732:ARG:HD2	1:B:742:LEU:HD23	1.98	0.44
1:B:340:THR:OG1	1:B:385:GLU:HG3	2.17	0.44
1:A:490:ARG:HA	1:A:494:GLN:HB3	1.99	0.44
1:A:765:ILE:O	1:A:769:ASP:HB2	2.17	0.44
1:B:18:SER:HB3	1:B:234:ARG:CD	2.44	0.44
1:A:113:LYS:HA	1:A:113:LYS:HD3	1.67	0.44
1:A:325:GLU:OE1	1:A:327:HIS:CE1	2.70	0.44
1:B:555:ILE:CD1	1:B:643:VAL:HG23	2.47	0.44
1:B:716:LYS:HE2	1:B:719:LYS:CD	2.39	0.44
1:B:744:GLU:HB3	1:B:750:TYR:HE2	1.83	0.44
1:A:803:LEU:HD22	1:A:807:ARG:CZ	2.47	0.44
1:A:18:SER:N	1:A:102:LEU:O	2.51	0.44
1:A:487:THR:HA	1:A:488:PRO:HD3	1.77	0.44
1:A:794:GLN:O	1:A:795:GLU:C	2.57	0.44
1:B:192:HIS:HD2	1:B:225:ALA:O	2.01	0.44
1:B:251:PRO:HB2	1:B:269:GLY:HA3	1.99	0.44
1:B:588:LYS:HA	1:B:591:ARG:NH1	2.32	0.44
1:A:609:ALA:HB3	1:A:617:LYS:HG2	2.00	0.44
1:B:411:LYS:HD2	1:B:425:TRP:CE2	2.52	0.44
1:A:522:VAL:HG12	1:A:803:LEU:CD2	2.48	0.44
1:B:703:VAL:O	1:B:807:ARG:NH1	2.51	0.44
1:A:386:ARG:HD2	1:A:438:GLN:CD	2.43	0.43
1:A:698:GLU:HB3	1:A:811:PHE:HZ	1.83	0.43
1:B:378:THR:HG22	1:B:379:LEU:N	2.33	0.43
1:B:530:PHE:O	1:B:531:ARG:C	2.58	0.43
1:B:374:TYR:CZ	1:B:376:ASN:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:TRP:O	1:B:512:ALA:C	2.61	0.43
1:A:308:LEU:O	5:A:1788:HOH:O	2.21	0.43
1:A:527:ASP:OD1	1:A:529:LYS:HD2	2.18	0.43
1:A:782:GLU:O	1:A:785:LYS:N	2.51	0.43
1:B:632:ASN:O	1:B:634:PRO:HD3	2.19	0.43
1:A:775:ALA:O	5:A:1808:HOH:O	2.21	0.43
1:B:297:TYR:CD2	1:B:396:LEU:HD11	2.54	0.43
1:B:326:LEU:HD13	1:B:359:MET:CE	2.48	0.43
1:B:615:LEU:O	1:B:619:ILE:HG13	2.19	0.43
1:B:1767:LYS:HB2	1:B:1767:LYS:NZ	2.33	0.43
2:C:2:GLC:H62	2:C:3:AC1:C5	2.48	0.43
1:B:165:LEU:O	1:B:166:PHE:HB3	2.19	0.43
1:B:169:SER:HG	1:B:176:VAL:HG22	1.81	0.43
1:B:425:TRP:CE2	1:B:429:ALA:HB2	2.53	0.43
1:B:703:VAL:HG12	1:B:804:ASN:HA	2.01	0.43
1:A:144:LEU:HD12	1:A:144:LEU:HA	1.91	0.43
1:A:555:ILE:HD12	1:A:643:VAL:HG23	2.00	0.43
1:A:716:LYS:CE	1:A:719:LYS:HD2	2.30	0.43
1:B:22:PHE:HB2	1:B:104:TRP:CD2	2.53	0.43
1:B:279:LEU:HD22	1:B:280:TYR:N	2.34	0.43
1:B:310:ARG:NH1	1:B:333:GLU:OE2	2.52	0.43
1:A:418:TRP:CZ3	1:A:474:LEU:HD21	2.53	0.43
1:A:700:ALA:HA	1:A:708:ILE:HD13	2.00	0.43
1:B:576:GLN:O	1:B:579:ASN:HB3	2.19	0.43
1:B:784:GLN:HE21	1:B:784:GLN:HA	1.83	0.43
1:B:680:LYS:NZ	4:B:999:PLP:O3	2.52	0.43
1:B:773:VAL:HG12	1:B:774:MET:HE2	1.99	0.43
1:A:91:ILE:HD12	1:A:94:LEU:HD13	2.01	0.42
1:B:101:ASN:HB2	1:B:231:VAL:CG2	2.48	0.42
1:B:212:ASP:O	1:B:214:ARG:N	2.49	0.42
1:B:700:ALA:HA	1:B:708:ILE:HD13	2.00	0.42
1:A:398:ARG:HD2	1:A:401:GLN:OE1	2.19	0.42
1:B:564:ASP:OD1	1:B:664:GLU:OE2	2.37	0.42
1:A:340:THR:OG1	1:A:385:GLU:HG3	2.19	0.42
1:A:671:LYS:HA	1:A:671:LYS:HD3	1.74	0.42
1:B:248:HIS:CD2	1:B:249:ALA:O	2.71	0.42
1:A:717:GLN:O	1:A:718:VAL:C	2.61	0.42
1:A:824:ILE:O	1:A:829:ARG:NH2	2.53	0.42
1:B:128:ASP:O	1:B:129:PRO:C	2.61	0.42
1:B:190:PHE:CD1	1:B:228:LEU:HD13	2.55	0.42
1:A:800:ALA:O	1:A:801:ALA:C	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:VAL:HG11	1:B:471:TYR:CG	2.55	0.42
1:B:570:LEU:HD22	1:B:616:ALA:HB1	2.02	0.42
1:A:396:LEU:HB3	1:A:399:HIS:CD2	2.55	0.42
1:A:729:VAL:HG11	1:A:1767:LYS:HG3	2.02	0.42
1:B:729:VAL:CG1	1:B:1767:LYS:HG3	2.50	0.42
1:A:569:ARG:O	1:A:576:GLN:NE2	2.49	0.42
1:A:599:VAL:O	1:A:600:PRO:C	2.61	0.42
1:B:327:HIS:CD2	1:B:328:GLU:HG3	2.55	0.42
1:B:810:MET:HE3	1:B:810:MET:HB2	1.96	0.42
1:A:136:LEU:HD22	2:C:3:AC1:HCB2	2.02	0.42
1:A:662:ILE:HG23	1:A:689:VAL:CG2	2.48	0.42
1:A:666:ILE:HG22	1:A:711:PHE:CE1	2.55	0.42
1:B:35:TRP:O	1:B:41:LEU:HB2	2.19	0.42
1:B:349:LEU:O	1:B:353:LEU:HD22	2.19	0.42
1:B:519:ILE:HA	1:B:806:ALA:O	2.19	0.42
1:A:18:SER:HB3	1:A:234:ARG:HB3	2.02	0.42
1:B:567:ILE:O	1:B:568:LYS:HB3	2.19	0.42
1:A:808:CYS:O	1:A:810:MET:N	2.53	0.41
1:B:113:LYS:HD3	1:B:113:LYS:HA	1.90	0.41
1:B:491:TRP:CE2	1:B:680:LYS:HE2	2.54	0.41
1:B:696:ASN:O	1:B:697:VAL:C	2.63	0.41
1:A:353:LEU:HD12	1:A:359:MET:CE	2.50	0.41
1:A:361:TRP:CH2	1:A:402:ILE:HG23	2.56	0.41
1:A:535:ARG:HH11	1:A:535:ARG:HD2	1.72	0.41
1:A:772:LEU:HD12	1:A:775:ALA:HB3	2.01	0.41
1:B:221:ILE:HG22	1:B:222:THR:N	2.34	0.41
1:B:421:ASP:O	1:B:422:GLU:C	2.63	0.41
1:B:668:THR:OG1	1:B:771:TYR:HB3	2.20	0.41
1:B:695:ALA:O	1:B:696:ASN:C	2.62	0.41
1:A:32:SER:O	1:A:37:GLN:HG3	2.19	0.41
1:B:703:VAL:HG11	1:B:804:ASN:OD1	2.21	0.41
1:A:719:LYS:NZ	5:A:1819:HOH:O	2.54	0.41
1:B:577:HIS:CD2	1:B:577:HIS:H	2.38	0.41
1:B:23:ASN:HB3	1:B:26:GLN:HB2	2.02	0.41
1:B:557:ILE:HD13	1:B:557:ILE:HA	1.79	0.41
1:B:741:VAL:HA	1:B:744:GLU:OE1	2.21	0.41
1:A:202:ILE:HG12	1:A:221:ILE:HD12	2.02	0.41
1:B:740:ALA:O	1:B:743:LYS:HB2	2.19	0.41
1:A:129:PRO:HB2	1:A:131:LEU:HD22	2.03	0.41
1:A:310:ARG:NH1	1:A:333:GLU:OE2	2.54	0.41
1:A:714:THR:H	1:A:714:THR:HG23	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ALA:O	1:B:365:TRP:C	2.64	0.41
1:B:666:ILE:HG22	1:B:711:PHE:HE1	1.86	0.41
1:A:162:GLN:HB2	1:A:184:ARG:NH2	2.36	0.41
1:A:351:ARG:O	1:A:355:ASP:N	2.47	0.41
1:A:515:LEU:HD12	1:A:518:LEU:HD13	2.02	0.41
1:A:548:PHE:O	1:A:552:ARG:HG2	2.21	0.41
1:A:737:VAL:O	1:A:738:LEU:C	2.63	0.41
1:A:819:ASP:HB3	1:A:823:ARG:NH1	2.36	0.41
1:B:23:ASN:HB3	1:B:26:GLN:CB	2.50	0.41
1:B:90:LEU:HD21	4:B:999:PLP:H2A3	2.03	0.41
1:B:647:ASP:O	1:B:648:TYR:C	2.63	0.41
1:B:668:THR:O	1:B:669:ALA:C	2.64	0.41
1:B:782:GLU:O	1:B:783:ALA:C	2.64	0.41
1:A:119:LEU:O	1:A:120:THR:C	2.64	0.41
1:A:697:VAL:O	1:A:698:GLU:C	2.64	0.41
1:A:186:ASN:O	1:A:187:TYR:C	2.63	0.40
1:A:190:PHE:CE1	1:A:228:LEU:HD13	2.56	0.40
1:A:796:ALA:O	1:A:797:TRP:C	2.62	0.40
1:B:341:HIS:N	1:B:342:PRO:CD	2.84	0.40
1:B:418:TRP:CH2	1:B:474:LEU:HD21	2.55	0.40
1:B:503:LEU:CD1	1:B:518:LEU:HD11	2.49	0.40
1:B:629:VAL:HG11	1:B:750:TYR:CE1	2.56	0.40
1:B:671:LYS:HA	1:B:671:LYS:HD3	1.82	0.40
1:A:101:ASN:CB	1:A:231:VAL:HG23	2.51	0.40
1:A:192:HIS:HD2	1:A:225:ALA:O	2.05	0.40
1:A:405:GLU:O	1:A:409:ARG:HG2	2.22	0.40
1:A:590:ILE:HG21	1:A:636:VAL:HG12	2.02	0.40
1:B:53:LEU:O	1:B:54:ALA:C	2.62	0.40
1:B:373:ALA:HB1	5:B:1776:HOH:O	2.21	0.40
1:B:432:HIS:CD2	1:B:433:ASP:HB2	2.57	0.40
1:B:482:VAL:HG11	1:B:820:TYR:CD2	2.56	0.40
1:B:487:THR:HA	1:B:488:PRO:HD3	1.73	0.40
1:B:665:GLN:O	1:B:690:GLY:HA2	2.22	0.40
1:B:782:GLU:O	1:B:785:LYS:HB2	2.21	0.40
1:A:161:TYR:CD2	1:A:279:LEU:HB2	2.57	0.40
1:A:708:ILE:HG12	1:A:710:ILE:HG12	2.04	0.40
1:B:564:ASP:OD2	1:B:601:ARG:NH1	2.54	0.40
1:A:287:ALA:CB	5:A:1793:HOH:O	2.55	0.40
1:A:459:HIS:O	1:A:463:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	794/796 (100%)	729 (92%)	54 (7%)	11 (1%)	9	24
1	B	794/796 (100%)	725 (91%)	58 (7%)	11 (1%)	9	24
All	All	1588/1592 (100%)	1454 (92%)	112 (7%)	22 (1%)	9	24

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	LYS
1	B	423	LYS
1	A	285	HIS
1	A	421	ASP
1	B	207	THR
1	B	285	HIS
1	B	754	ASP
1	A	78	ASN
1	A	207	THR
1	A	754	ASP
1	B	78	ASN
1	A	809	GLY
1	B	674	SER
1	B	213	GLY
1	B	421	ASP
1	B	484	ASN
1	A	420	GLY
1	B	420	GLY
1	A	213	GLY
1	A	135	GLY
1	A	697	VAL
1	B	135	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	665/665 (100%)	586 (88%)	79 (12%)	5	15
1	B	665/665 (100%)	588 (88%)	77 (12%)	5	16
All	All	1330/1330 (100%)	1174 (88%)	156 (12%)	5	16

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	19	GLN
1	A	21	ILE
1	A	41	LEU
1	A	1042	SER
1	A	48	PRO
1	A	49	ARG
1	A	87	MET
1	A	94	LEU
1	A	131	LEU
1	A	145	ASP
1	A	150	VAL
1	A	165	LEU
1	A	176	VAL
1	A	184	ARG
1	A	186	ASN
1	A	206	VAL
1	A	208	LYS
1	A	212	ASP
1	A	214	ARG
1	A	220	THR
1	A	228	LEU
1	A	251	PRO
1	A	254	LEU
1	A	268	GLN
1	A	270	ILE
1	A	279	LEU

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Mol	Chain	Res	Type
1	A	326	LEU
1	A	327	HIS
1	A	329	LEU
1	A	334	VAL
1	A	339	ASP
1	A	353	LEU
1	A	374	TYR
1	A	376	ASN
1	A	391	LEU
1	A	395	LEU
1	A	396	LEU
1	A	408	THR
1	A	433	ASP
1	A	462	LEU
1	A	464	VAL
1	A	470	GLU
1	A	493	LYS
1	A	521	LEU
1	A	529	LYS
1	A	536	VAL
1	A	568	LYS
1	A	569	ARG
1	A	570	LEU
1	A	574	LYS
1	A	577	HIS
1	A	582	ARG
1	A	615	LEU
1	A	617	LYS
1	A	626	VAL
1	A	628	ASP
1	A	635	LEU
1	A	641	LYS
1	A	663	SER
1	A	667	SER
1	A	692	LEU
1	A	701	GLU
1	A	705	GLU
1	A	706	GLU
1	A	716	LYS
1	A	729	VAL
1	A	730	LYS
1	A	742	LEU

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Mol	Chain	Res	Type
1	A	762	LEU
1	A	1767	LYS
1	A	766	GLN
1	A	772	LEU
1	A	784	GLN
1	A	787	VAL
1	A	788	ASP
1	A	810	MET
1	A	817	ILE
1	A	829	ARG
1	B	18	SER
1	B	19	GLN
1	B	21	ILE
1	B	41	LEU
1	B	48	PRO
1	B	49	ARG
1	B	87	MET
1	B	94	LEU
1	B	131	LEU
1	B	144	LEU
1	B	150	VAL
1	B	165	LEU
1	B	176	VAL
1	B	184	ARG
1	B	185	SER
1	B	186	ASN
1	B	206	VAL
1	B	208	LYS
1	B	212	ASP
1	B	214	ARG
1	B	220	THR
1	B	222	THR
1	B	228	LEU
1	B	251	PRO
1	B	254	LEU
1	B	268	GLN
1	B	270	ILE
1	B	274	LYS
1	B	279	LEU
1	B	326	LEU
1	B	327	HIS
1	B	329	LEU

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Mol	Chain	Res	Type
1	B	334	VAL
1	B	353	LEU
1	B	369	SER
1	B	376	ASN
1	B	391	LEU
1	B	395	LEU
1	B	396	LEU
1	B	408	THR
1	B	433	ASP
1	B	441	MET
1	B	464	VAL
1	B	470	GLU
1	B	493	LYS
1	B	521	LEU
1	B	524	LEU
1	B	529	LYS
1	B	568	LYS
1	B	570	LEU
1	B	574	LYS
1	B	577	HIS
1	B	582	ARG
1	B	604	LEU
1	B	611	PRO
1	B	626	VAL
1	B	628	ASP
1	B	629	VAL
1	B	635	LEU
1	B	641	LYS
1	B	663	SER
1	B	692	LEU
1	B	701	GLU
1	B	706	GLU
1	B	716	LYS
1	B	729	VAL
1	B	730	LYS
1	B	742	LEU
1	B	751	SER
1	B	762	LEU
1	B	1767	LYS
1	B	766	GLN
1	B	772	LEU
1	B	784	GLN

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Mol	Chain	Res	Type
1	B	810	MET
1	B	813	SER
1	B	829	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	83	ASN
1	A	133	ASN
1	A	160	ASN
1	A	186	ASN
1	A	192	HIS
1	A	245	GLN
1	A	250	HIS
1	A	271	ASN
1	A	285	HIS
1	A	327	HIS
1	A	432	HIS
1	A	459	HIS
1	A	481	ASN
1	A	520	ASN
1	A	566	GLN
1	A	571	HIS
1	A	577	HIS
1	A	756	HIS
1	A	784	GLN
1	B	26	GLN
1	B	37	GLN
1	B	42	ASN
1	B	109	GLN
1	B	133	ASN
1	B	160	ASN
1	B	186	ASN
1	B	192	HIS
1	B	245	GLN
1	B	271	ASN
1	B	285	HIS
1	B	299	GLN
1	B	327	HIS
1	B	399	HIS
1	B	440	HIS

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Mol	Chain	Res	Type
1	B	459	HIS
1	B	481	ASN
1	B	494	GLN
1	B	566	GLN
1	B	571	HIS
1	B	577	HIS
1	B	624	ASN
1	B	696	ASN
1	B	756	HIS
1	B	760	GLN
1	B	763	HIS
1	B	766	GLN
1	B	784	GLN

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](#)

6 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	GLC	C	1	2	12,12,12	0.78	0	17,17,17	2.12	4 (23%)
2	GLC	C	2	2	11,11,12	1.43	1 (9%)	15,15,17	2.29	7 (46%)
2	AC1	C	3	2	21,22,23	1.28	2 (9%)	22,32,34	2.67	10 (45%)
2	GLC	D	1	2	12,12,12	0.76	0	17,17,17	2.07	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	D	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.79	3 (20%)
2	AC1	D	3	2	21,22,23	1.76	6 (28%)	22,32,34	2.20	7 (31%)

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	GLC	C	1	2	1/1/5/5	1/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	AC1	C	3	2	-	3/6/43/46	0/2/2/2
2	GLC	D	1	2	1/1/5/5	1/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	AC1	D	3	2	-	3/6/43/46	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	AC1	C7B-C5B	3.80	1.38	1.32
2	D	3	AC1	C4A-C5B	3.57	1.54	1.51
2	C	2	GLC	C2-C3	3.22	1.57	1.52
2	C	3	AC1	C7B-C5B	2.99	1.37	1.32
2	D	3	AC1	O4-C4A	2.90	1.47	1.42
2	D	3	AC1	O6B-C6B	2.46	1.49	1.41
2	D	2	GLC	C2-C3	2.35	1.56	1.52
2	D	3	AC1	C3B-C4A	2.33	1.56	1.53
2	D	3	AC1	C2B-C1B	2.31	1.56	1.53
2	C	3	AC1	C1B-C7B	-2.23	1.47	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	AC1	C7B-C1B-N4A	7.04	121.05	110.68
2	C	1	GLC	O3-C3-C4	5.28	122.82	110.38
2	D	1	GLC	O4-C4-C3	-5.17	98.18	110.38
2	C	2	GLC	C1-O5-C5	4.91	118.77	112.19
2	D	3	AC1	C7B-C1B-N4A	4.79	117.72	110.68
2	C	3	AC1	O3B-C3B-C4A	4.65	118.85	109.64
2	D	3	AC1	O4-C4A-C3B	-4.30	101.59	110.53
2	C	3	AC1	O2B-C2B-C3B	-4.14	100.62	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	C1-O5-C5	4.12	117.71	112.19
2	D	3	AC1	O2B-C2B-C3B	-3.76	101.51	110.38
2	C	1	GLC	O2-C2-C3	-3.75	101.53	110.38
2	C	2	GLC	C2-C3-C4	-3.74	104.29	110.86
2	C	2	GLC	O2-C2-C1	3.69	117.68	109.22
2	D	3	AC1	C1-C2-C3	3.67	114.99	109.64
2	C	3	AC1	O2B-C2B-C1B	3.58	116.12	109.08
2	D	2	GLC	O5-C5-C6	-3.53	100.80	107.66
2	C	3	AC1	O4-C4A-C3B	-3.51	103.24	110.53
2	D	2	GLC	C2-C3-C4	-2.81	105.93	110.86
2	D	3	AC1	C5-C4-N4A	-2.77	104.12	111.74
2	D	1	GLC	O2-C2-C1	2.76	115.62	109.25
2	D	3	AC1	O3B-C3B-C4A	2.70	114.98	109.64
2	D	1	GLC	O3-C3-C2	2.63	116.58	110.38
2	C	1	GLC	O4-C4-C3	-2.63	104.17	110.38
2	C	2	GLC	C3-C4-C5	2.58	114.90	110.23
2	C	3	AC1	C6-C5-C4	-2.54	108.91	113.57
2	D	1	GLC	C6-C5-C4	2.53	119.23	113.02
2	C	3	AC1	C5-C4-N4A	-2.47	104.95	111.74
2	D	3	AC1	C6-C5-C4	-2.46	109.07	113.57
2	C	2	GLC	O5-C5-C6	-2.43	102.93	107.66
2	C	2	GLC	C1-C2-C3	-2.36	106.21	109.64
2	C	3	AC1	C1-C2-C3	2.34	113.05	109.64
2	C	3	AC1	C4A-C5B-C7B	-2.21	118.60	122.23
2	C	2	GLC	O3-C3-C2	2.12	114.38	110.05
2	C	1	GLC	O1-C1-O5	2.11	116.67	110.41
2	D	1	GLC	O5-C5-C6	-2.09	101.27	106.44
2	C	3	AC1	O2-C2-C1	2.07	113.97	109.22
2	D	1	GLC	C4-C3-C2	-2.07	107.19	110.83
2	D	1	GLC	C1-C2-C3	-2.03	106.21	110.36

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	GLC	C1
2	D	1	GLC	C1

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	AC1	C5-C4-N4A-C1B
2	D	3	AC1	C2B-C1B-N4A-C4

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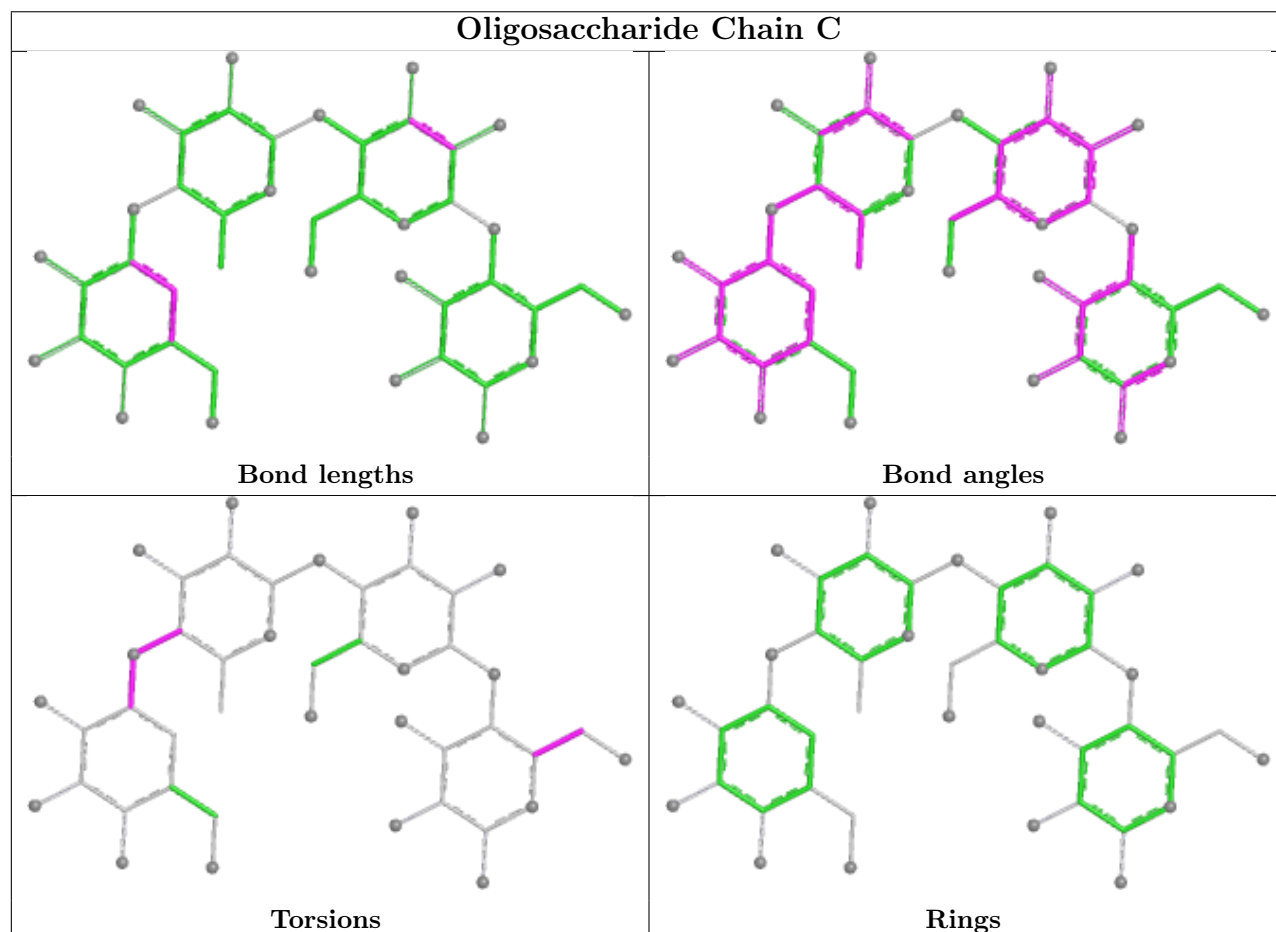
Mol	Chain	Res	Type	Atoms
2	D	1	GLC	O5-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	C	3	AC1	C2B-C1B-N4A-C4
2	C	3	AC1	C3-C4-N4A-C1B
2	C	3	AC1	C5-C4-N4A-C1B
2	D	3	AC1	C3-C4-N4A-C1B

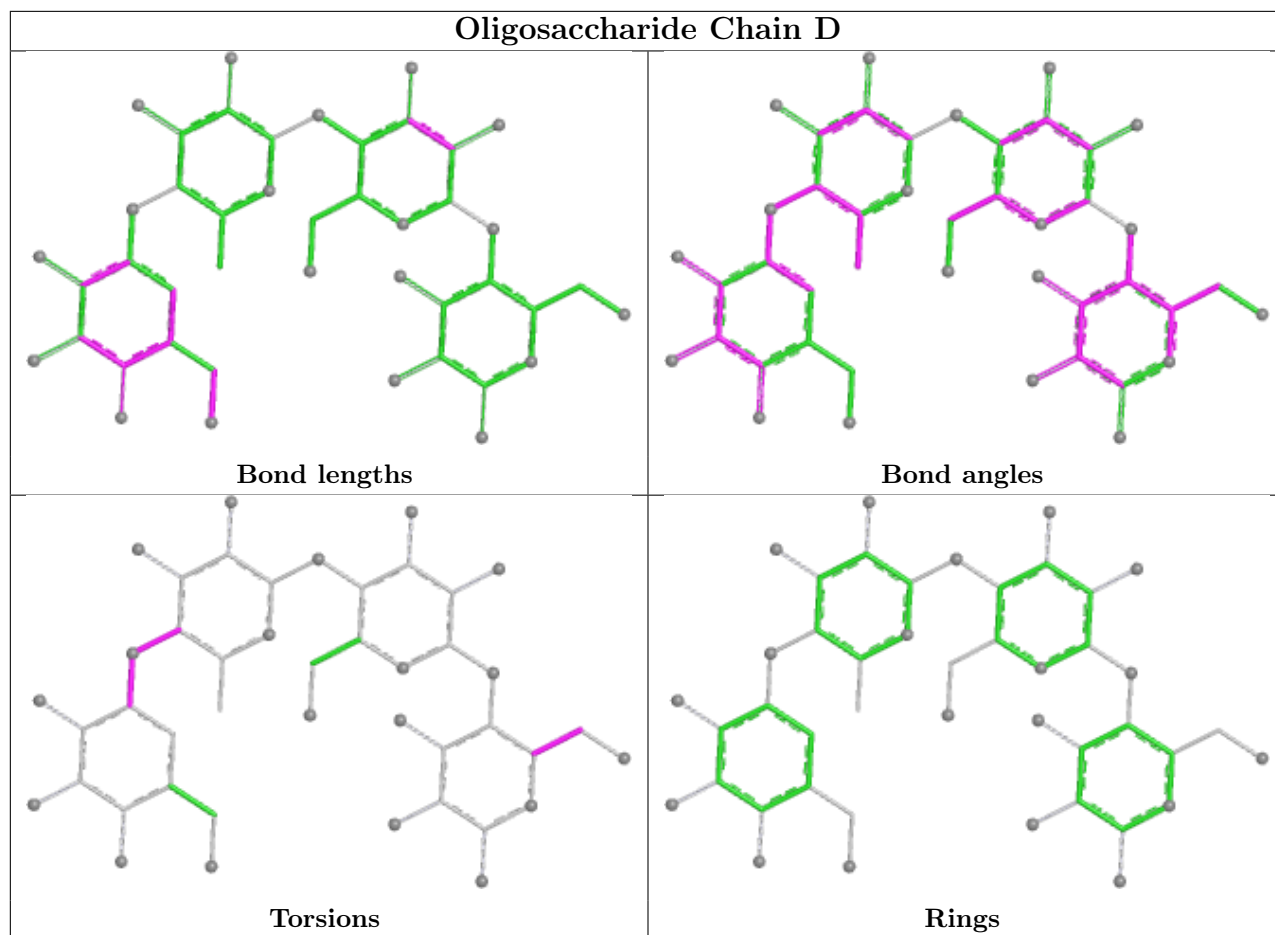
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	AC1	2	0
2	D	3	AC1	5	0
2	D	2	GLC	1	0
2	C	2	GLC	1	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.





5.6 Ligand geometry [i](#)

4 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	GOL	A	998	-	5,5,5	0.78	0	5,5,5	0.88	0
3	GOL	B	998	-	5,5,5	0.50	0	5,5,5	0.56	0
4	PLP	A	999	1	15,15,16	1.87	3 (20%)	21,22,23	1.95	5 (23%)
4	PLP	B	999	1	15,15,16	2.61	4 (26%)	21,22,23	1.91	6 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	998	-	-	1/4/4/4	-
3	GOL	B	998	-	-	2/4/4/4	-
4	PLP	A	999	1	-	3/6/6/8	0/1/1/1
4	PLP	B	999	1	-	2/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	999	PLP	C3-C2	-8.29	1.32	1.41
4	A	999	PLP	C3-C2	-4.37	1.36	1.41
4	B	999	PLP	P-O3P	-3.34	1.42	1.54
4	A	999	PLP	P-O3P	-3.25	1.42	1.54
4	B	999	PLP	C3-C4	-2.62	1.35	1.40
4	A	999	PLP	C3-C4	-2.44	1.35	1.40
4	B	999	PLP	C5A-C5	2.11	1.56	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	PLP	C2A-C2-C3	-5.23	114.68	120.80
4	B	999	PLP	C4A-C4-C5	4.08	125.14	120.94
4	B	999	PLP	O3P-P-O1P	3.38	124.02	110.83
4	B	999	PLP	C2A-C2-C3	-3.28	116.96	120.80
4	A	999	PLP	O2P-P-O1P	-3.02	99.05	110.83
4	A	999	PLP	C2A-C2-N1	2.89	123.09	117.64
4	A	999	PLP	O3P-P-O4P	2.71	113.74	106.67
4	A	999	PLP	O4P-C5A-C5	-2.55	104.58	109.36
4	B	999	PLP	O3-C3-C2	2.51	122.78	117.58
4	B	999	PLP	C4A-C4-C3	-2.28	116.72	120.52
4	B	999	PLP	O2P-P-O1P	-2.09	102.70	110.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	998	GOL	O1-C1-C2-C3
4	A	999	PLP	C5A-O4P-P-O1P
4	A	999	PLP	C5A-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
4	A	999	PLP	C5A-O4P-P-O3P
4	B	999	PLP	C5A-O4P-P-O3P
3	B	998	GOL	O1-C1-C2-O2
3	A	998	GOL	O1-C1-C2-O2
4	B	999	PLP	C5A-O4P-P-O2P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	998	GOL	1	0
3	B	998	GOL	1	0
4	B	999	PLP	2	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	796/796 (100%)	0.31	16 (2%) 65 57	41, 50, 76, 114	0
1	B	796/796 (100%)	0.07	10 (1%) 75 69	41, 50, 76, 114	0
All	All	1592/1592 (100%)	0.19	26 (1%) 70 63	41, 50, 76, 114	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1767	LYS	5.4
1	A	18	SER	3.6
1	A	418	TRP	3.4
1	A	748	GLY	3.3
1	B	207	THR	3.0
1	B	422	GLU	2.9
1	A	733	LYS	2.7
1	B	557	ILE	2.7
1	B	753	GLY	2.6
1	A	729	VAL	2.4
1	B	18	SER	2.4
1	A	694	GLY	2.3
1	A	704	GLY	2.3
1	A	26	GLN	2.3
1	A	285	HIS	2.3
1	A	731	TRP	2.3
1	A	707	ASN	2.2
1	B	208	LYS	2.2
1	A	21	ILE	2.1
1	A	332	TYR	2.1
1	B	214	ARG	2.1
1	A	527	ASP	2.1
1	B	364	ALA	2.1
1	B	723	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	455	VAL	2.0
1	A	282	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

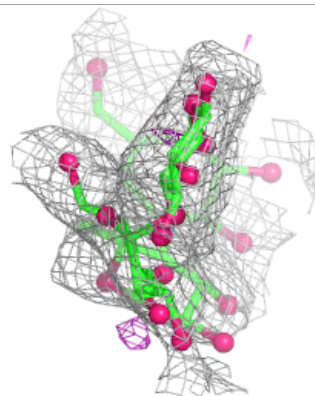
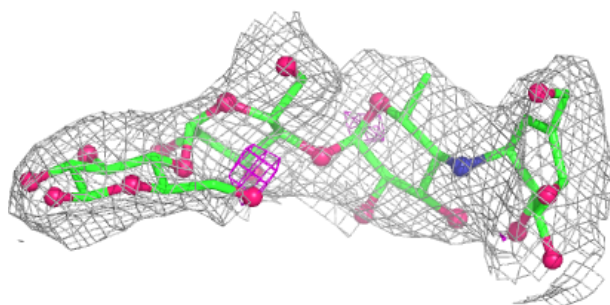
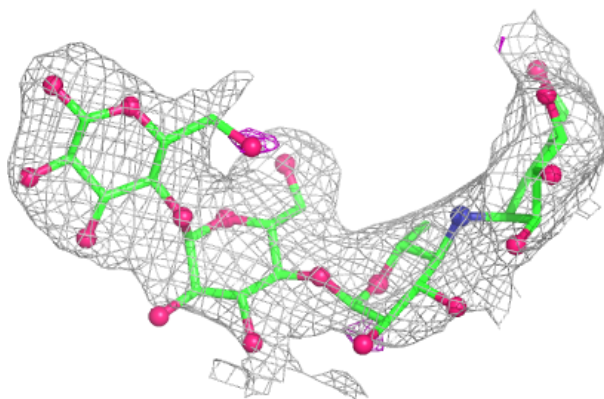
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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	GLC	C	1	12/12	0.80	0.12	58,59,59,60	0
2	AC1	C	3	21/22	0.80	0.12	58,58,59,59	0
2	GLC	C	2	11/12	0.81	0.10	58,58,59,59	0
2	GLC	D	1	12/12	0.82	0.08	58,59,59,59	0
2	AC1	D	3	21/22	0.86	0.10	58,58,59,60	0
2	GLC	D	2	11/12	0.89	0.09	58,58,59,59	0

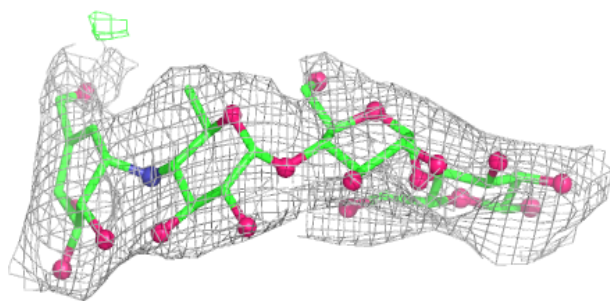
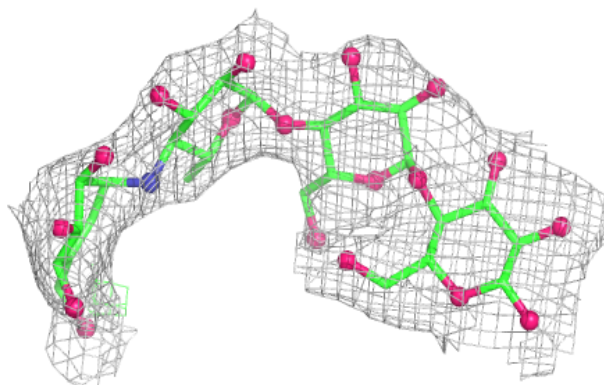
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain D:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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
3	GOL	B	998	6/6	0.89	0.10	58,58,59,59	0
3	GOL	A	998	6/6	0.90	0.11	58,58,59,59	0
4	PLP	A	999	15/16	0.91	0.12	37,42,47,51	0
4	PLP	B	999	15/16	0.95	0.07	41,43,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.