



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2020 – 04:53 PM BST

PDB ID : 2ECP
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

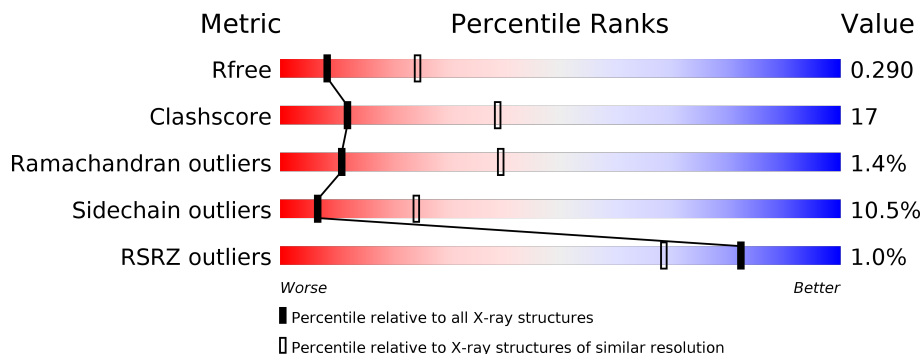
1 Overall quality at a glance

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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	 53% 36% 10% .
1	B	796	 51% 39% 7% .
2	C	3	 33% 67%
2	D	3	 33% 67%

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 crite-

ria:

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.

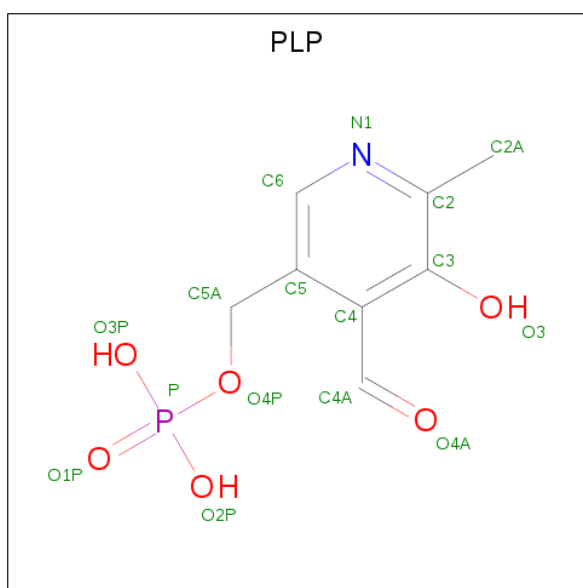
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	44	25	1	18	0	0	0
2	D	3	44	25	1	18	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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		

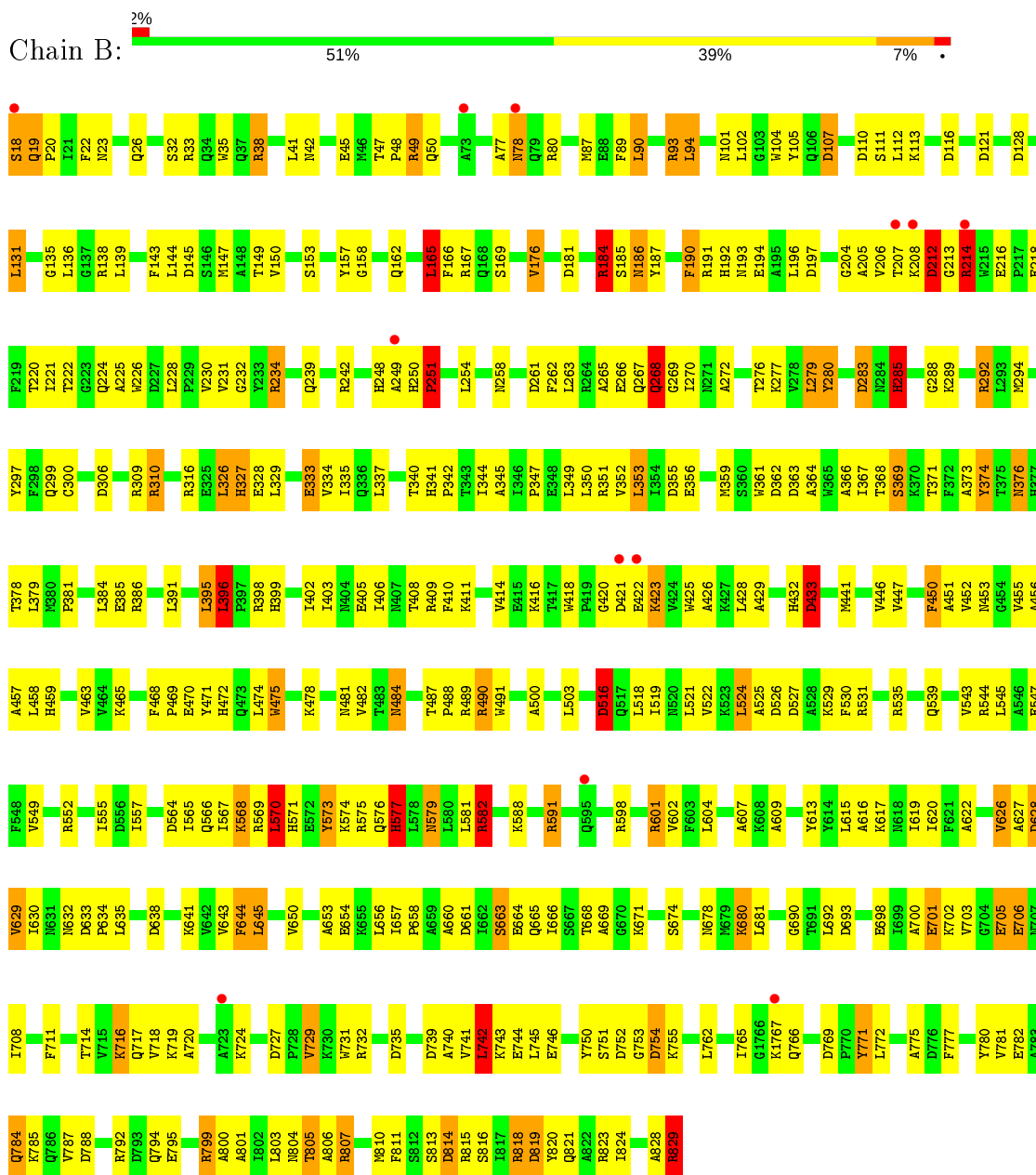
- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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



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



GLC1
GLC2
AC13

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) 88.5 (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)	0.28 , 59.6	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, GLC, PLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.77	1/6517 (0.0%)	1.99	165/8841 (1.9%)
1	B	0.75	1/6517 (0.0%)	2.12	163/8841 (1.8%)
All	All	0.76	2/13034 (0.0%)	2.05	328/17682 (1.9%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	569	ARG	NE-CZ	-5.76	1.25	1.33
1	B	292	ARG	CD-NE	-5.03	1.38	1.46

All (328) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ARG	NE-CZ-NH2	65.00	152.80	120.30
1	A	292	ARG	NE-CZ-NH2	46.98	143.79	120.30
1	B	569	ARG	NE-CZ-NH2	44.11	142.35	120.30
1	A	569	ARG	NE-CZ-NH1	32.74	136.67	120.30
1	B	292	ARG	NE-CZ-NH1	-32.15	104.22	120.30
1	B	569	ARG	NH1-CZ-NH2	-27.54	89.11	119.40
1	A	569	ARG	NH1-CZ-NH2	-26.36	90.41	119.40
1	A	569	ARG	NE-CZ-NH2	25.25	132.92	120.30
1	A	544	ARG	NE-CZ-NH2	-21.76	109.42	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	ARG	NE-CZ-NH1	21.38	130.99	120.30
1	B	569	ARG	CD-NE-CZ	20.25	151.96	123.60
1	A	535	ARG	NE-CZ-NH2	-18.79	110.91	120.30
1	B	490	ARG	NE-CZ-NH2	-17.54	111.53	120.30
1	A	138	ARG	NE-CZ-NH1	16.86	128.73	120.30
1	B	292	ARG	CD-NE-CZ	16.55	146.77	123.60
1	B	569	ARG	NE-CZ-NH1	16.43	128.51	120.30
1	B	309	ARG	NE-CZ-NH2	-15.68	112.46	120.30
1	A	582	ARG	NE-CZ-NH2	-15.03	112.78	120.30
1	B	351	ARG	NE-CZ-NH1	14.99	127.80	120.30
1	B	292	ARG	NH1-CZ-NH2	-14.95	102.95	119.40
1	A	815	ARG	NE-CZ-NH1	-14.88	112.86	120.30
1	A	292	ARG	NE-CZ-NH1	-14.82	112.89	120.30
1	A	569	ARG	CD-NE-CZ	14.74	144.24	123.60
1	B	214	ARG	NE-CZ-NH2	14.71	127.66	120.30
1	A	292	ARG	NH1-CZ-NH2	-14.62	103.32	119.40
1	B	242	ARG	NE-CZ-NH2	-14.44	113.08	120.30
1	B	490	ARG	NE-CZ-NH1	13.53	127.06	120.30
1	A	598	ARG	NE-CZ-NH1	-12.96	113.82	120.30
1	A	829	ARG	NE-CZ-NH2	-12.95	113.83	120.30
1	B	752	ASP	CB-CG-OD1	-12.66	106.90	118.30
1	A	504	ASP	CB-CG-OD1	12.66	129.69	118.30
1	B	544	ARG	NE-CZ-NH1	11.92	126.26	120.30
1	B	535	ARG	NE-CZ-NH1	-11.54	114.53	120.30
1	A	310	ARG	CD-NE-CZ	11.45	139.64	123.60
1	B	33	ARG	NE-CZ-NH2	-11.35	114.63	120.30
1	B	489	ARG	NE-CZ-NH2	11.28	125.94	120.30
1	B	544	ARG	NE-CZ-NH2	-11.24	114.68	120.30
1	B	829	ARG	NE-CZ-NH2	-11.23	114.68	120.30
1	A	33	ARG	NE-CZ-NH1	11.01	125.80	120.30
1	A	64	ARG	NE-CZ-NH2	-10.89	114.86	120.30
1	A	38	ARG	NE-CZ-NH2	10.59	125.59	120.30
1	B	242	ARG	NH1-CZ-NH2	10.53	130.99	119.40
1	B	591	ARG	CD-NE-CZ	10.40	138.16	123.60
1	B	362	ASP	CB-CG-OD1	10.28	127.55	118.30
1	A	167	ARG	NE-CZ-NH2	10.27	125.43	120.30
1	A	250	HIS	ND1-CG-CD2	-10.20	91.72	106.00
1	A	309	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	A	535	ARG	NH1-CZ-NH2	10.07	130.47	119.40
1	B	575	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	754	ASP	CB-CG-OD2	9.76	127.09	118.30
1	B	250	HIS	ND1-CG-CD2	-9.76	92.33	106.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	726	TYR	CB-CG-CD2	9.71	126.82	121.00
1	A	807	ARG	NE-CZ-NH1	9.68	125.14	120.30
1	A	292	ARG	CG-CD-NE	9.52	131.80	111.80
1	B	38	ARG	NE-CZ-NH1	-9.52	115.54	120.30
1	B	386	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	B	292	ARG	CG-CD-NE	9.49	131.74	111.80
1	A	310	ARG	NE-CZ-NH1	-9.37	115.61	120.30
1	B	355	ASP	CB-CG-OD2	-9.34	109.89	118.30
1	B	799	ARG	NE-CZ-NH2	9.26	124.93	120.30
1	B	107	ASP	CB-CG-OD2	9.14	126.53	118.30
1	A	167	ARG	NE-CZ-NH1	-8.92	115.84	120.30
1	B	661	ASP	CB-CG-OD1	-8.92	110.27	118.30
1	A	38	ARG	NE-CZ-NH1	-8.86	115.87	120.30
1	B	823	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	A	582	ARG	NH1-CZ-NH2	8.84	129.12	119.40
1	B	242	ARG	NE-CZ-NH1	-8.74	115.93	120.30
1	A	125	GLU	OE1-CD-OE2	8.71	133.75	123.30
1	A	552	ARG	CD-NE-CZ	8.68	135.76	123.60
1	B	191	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	309	ARG	CD-NE-CZ	8.59	135.62	123.60
1	B	49	ARG	NE-CZ-NH1	-8.58	116.01	120.30
1	B	582	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	A	261	ASP	CB-CG-OD2	-8.56	110.59	118.30
1	B	569	ARG	CG-CD-NE	8.56	129.78	111.80
1	A	138	ARG	NH1-CZ-NH2	-8.55	110.00	119.40
1	B	250	HIS	CG-ND1-CE1	8.51	120.11	108.20
1	B	591	ARG	NE-CZ-NH2	8.49	124.54	120.30
1	B	819	ASP	CB-CG-OD1	8.41	125.87	118.30
1	B	93	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	250	HIS	CG-ND1-CE1	8.38	119.94	108.20
1	B	234	ARG	NE-CZ-NH1	-8.34	116.13	120.30
1	A	601	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	B	633	ASP	CB-CG-OD1	-8.32	110.81	118.30
1	B	788	ASP	CB-CG-OD1	8.31	125.78	118.30
1	A	792	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	214	ARG	NE-CZ-NH2	8.26	124.43	120.30
1	B	351	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	A	652	ALA	CB-CA-C	8.20	122.39	110.10
1	A	807	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	A	607	ALA	CB-CA-C	-8.17	97.84	110.10
1	B	739	ASP	CB-CG-OD2	8.16	125.64	118.30
1	A	351	ARG	NE-CZ-NH1	8.13	124.36	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	GLU	OE1-CD-OE2	8.11	133.03	123.30
1	B	107	ASP	CB-CG-OD1	-8.09	111.02	118.30
1	B	261	ASP	CB-CG-OD1	8.09	125.58	118.30
1	B	138	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	A	93	ARG	NE-CZ-NH2	7.97	124.28	120.30
1	A	197	ASP	CB-CG-OD1	-7.97	111.13	118.30
1	B	157	TYR	CB-CG-CD2	-7.95	116.23	121.00
1	A	253	ASP	CB-CG-OD2	-7.94	111.16	118.30
1	B	829	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	334	VAL	CA-CB-CG2	7.80	122.60	110.90
1	B	818	ARG	NE-CZ-NH1	-7.80	116.40	120.30
1	A	242	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	B	807	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	B	181	ASP	CB-CG-OD1	7.73	125.26	118.30
1	A	362	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	795	GLU	OE1-CD-OE2	7.67	132.50	123.30
1	A	693	ASP	CB-CG-OD1	7.63	125.17	118.30
1	B	38	ARG	CD-NE-CZ	7.60	134.25	123.60
1	B	197	ASP	CB-CG-OD1	-7.60	111.46	118.30
1	B	771	TYR	CB-CG-CD2	7.59	125.56	121.00
1	A	49	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	A	306	ASP	CB-CG-OD1	7.55	125.09	118.30
1	A	726	TYR	CB-CG-CD1	-7.52	116.49	121.00
1	B	693	ASP	CB-CG-OD1	7.51	125.06	118.30
1	B	150	VAL	CA-CB-CG2	-7.44	99.74	110.90
1	B	450	PHE	CB-CG-CD1	7.38	125.96	120.80
1	B	653	ALA	N-CA-CB	7.36	120.41	110.10
1	A	351	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	164	GLY	CA-C-O	-7.28	107.49	120.60
1	B	272	ALA	N-CA-CB	7.27	120.28	110.10
1	A	544	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	B	433	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	A	461	ASP	CB-CG-OD2	7.13	124.72	118.30
1	B	184	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	B	145	ASP	CB-CG-OD1	-7.11	111.90	118.30
1	B	283	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	814	ASP	CB-CG-OD1	-7.05	111.95	118.30
1	B	792	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	B	138	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	B	167	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	363	ASP	CB-CG-OD2	-6.96	112.03	118.30
1	A	184	ARG	CD-NE-CZ	6.92	133.29	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	B	333	GLU	OE1-CD-OE2	-6.91	115.01	123.30
1	B	309	ARG	CD-NE-CZ	6.84	133.18	123.60
1	B	582	ARG	NH1-CZ-NH2	6.83	126.92	119.40
1	A	752	ASP	CB-CG-OD1	-6.80	112.17	118.30
1	A	310	ARG	NE-CZ-NH2	6.77	123.68	120.30
1	B	601	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	591	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	A	478	LYS	CD-CE-NZ	6.65	126.99	111.70
1	A	544	ARG	NH1-CZ-NH2	6.63	126.70	119.40
1	A	180	ASP	CB-CG-OD2	6.62	124.25	118.30
1	A	638	ASP	CB-CG-OD2	6.59	124.23	118.30
1	B	157	TYR	CB-CG-CD1	6.57	124.94	121.00
1	B	165	LEU	CA-CB-CG	6.55	130.38	115.30
1	A	44	ALA	N-CA-CB	6.55	119.27	110.10
1	B	814	ASP	CB-CG-OD1	6.53	124.18	118.30
1	B	205	ALA	N-CA-CB	-6.52	100.97	110.10
1	B	453	ASN	CB-CG-OD1	6.52	134.64	121.60
1	A	732	ARG	NE-CZ-NH1	-6.51	117.05	120.30
1	B	49	ARG	CD-NE-CZ	6.49	132.69	123.60
1	A	325	GLU	O-C-N	-6.48	112.34	122.70
1	A	309	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	582	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	B	607	ALA	CB-CA-C	-6.45	100.42	110.10
1	A	386	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	80	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	A	598	ARG	NH1-CZ-NH2	6.41	126.45	119.40
1	B	150	VAL	CA-CB-CG1	6.39	120.49	110.90
1	A	325	GLU	OE1-CD-OE2	-6.38	115.64	123.30
1	A	88	GLU	CG-CD-OE2	6.38	131.06	118.30
1	A	788	ASP	CB-CG-OD1	6.35	124.02	118.30
1	A	250	HIS	CG-CD2-NE2	6.35	121.26	109.20
1	A	57	GLU	OE1-CD-OE2	6.32	130.88	123.30
1	A	277	LYS	N-CA-CB	6.32	121.97	110.60
1	B	628	ASP	CB-CG-OD2	-6.32	112.62	118.30
1	B	547	GLU	OE1-CD-OE2	-6.31	115.73	123.30
1	B	638	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	746	GLU	OE1-CD-OE2	6.28	130.84	123.30
1	B	727	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	482	VAL	CA-CB-CG1	-6.23	101.55	110.90
1	B	500	ALA	CB-CA-C	6.20	119.39	110.10
1	A	334	VAL	N-CA-CB	6.19	125.12	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	789	VAL	CA-CB-CG2	-6.17	101.64	110.90
1	B	527	ASP	CB-CG-OD1	6.17	123.85	118.30
1	B	481	ASN	CB-CG-OD1	6.17	133.93	121.60
1	A	184	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	253	ASP	OD1-CG-OD2	6.13	134.95	123.30
1	B	316	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	B	368	THR	CA-CB-CG2	-6.13	103.82	112.40
1	A	613	TYR	CB-CG-CD1	6.11	124.66	121.00
1	B	49	ARG	NH1-CZ-NH2	6.09	126.10	119.40
1	A	164	GLY	O-C-N	6.05	132.38	122.70
1	A	128	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	A	333	GLU	OE1-CD-OE2	-6.02	116.08	123.30
1	B	121	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	88	GLU	OE1-CD-OE2	-6.00	116.10	123.30
1	B	629	VAL	CA-CB-CG2	-5.98	101.93	110.90
1	B	742	LEU	CA-CB-CG	5.98	129.05	115.30
1	A	396	LEU	CA-CB-CG	5.97	129.03	115.30
1	A	49	ARG	CD-NE-CZ	5.95	131.94	123.60
1	B	105	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	B	310	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	334	VAL	CB-CA-C	-5.88	100.22	111.40
1	A	149	THR	CA-CB-CG2	5.88	120.63	112.40
1	B	145	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	145	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	214	ARG	NH1-CZ-NH2	-5.82	113.00	119.40
1	A	527	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	535	ARG	NE-CZ-NH2	5.81	123.21	120.30
1	A	591	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	277	LYS	N-CA-CB	5.80	121.03	110.60
1	A	772	LEU	CA-CB-CG	5.79	128.62	115.30
1	B	216	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	A	147	MET	O-C-N	-5.79	113.44	122.70
1	B	149	THR	CA-CB-CG2	5.78	120.49	112.40
1	A	531	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	150	VAL	CA-CB-CG1	5.76	119.54	110.90
1	A	334	VAL	CA-CB-CG1	-5.75	102.27	110.90
1	A	356	GLU	OE1-CD-OE2	5.75	130.20	123.30
1	A	656	LEU	O-C-N	-5.75	113.50	122.70
1	B	745	LEU	CB-CG-CD2	-5.75	101.22	111.00
1	B	128	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	B	450	PHE	CB-CG-CD2	-5.75	116.78	120.80
1	A	573	TYR	CA-CB-CG	5.74	124.31	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	577	HIS	CA-CB-CG	5.74	123.35	113.60
1	B	746	GLU	CG-CD-OE2	-5.73	106.83	118.30
1	A	64	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	668	THR	CA-CB-CG2	-5.71	104.41	112.40
1	A	591	ARG	NH1-CZ-NH2	-5.71	113.12	119.40
1	A	33	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	229	PRO	O-C-N	-5.69	113.60	122.70
1	A	212	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	409	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	131	LEU	CA-CB-CG	5.65	128.29	115.30
1	B	628	ASP	O-C-N	5.63	131.70	122.70
1	A	788	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	165	LEU	CA-CB-CG	5.59	128.17	115.30
1	A	569	ARG	CB-CG-CD	-5.58	97.08	111.60
1	B	116	ASP	CB-CG-OD1	-5.57	113.28	118.30
1	A	501	ALA	N-CA-CB	-5.56	102.31	110.10
1	B	366	ALA	CB-CA-C	-5.56	101.76	110.10
1	A	90	LEU	CB-CG-CD2	5.55	120.43	111.00
1	B	451	ALA	CB-CA-C	5.53	118.39	110.10
1	A	153	SER	N-CA-CB	5.53	118.79	110.50
1	A	481	ASN	CB-CG-OD1	5.52	132.64	121.60
1	B	628	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	355	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	93	ARG	CD-NE-CZ	5.51	131.31	123.60
1	B	285	HIS	CA-CB-CG	5.51	122.96	113.60
1	A	706	GLU	OE1-CD-OE2	-5.50	116.70	123.30
1	B	285	HIS	N-CA-CB	5.50	120.50	110.60
1	A	115	TYR	O-C-N	-5.50	113.90	122.70
1	B	258	ASN	O-C-N	-5.49	113.92	122.70
1	B	805	THR	CA-CB-CG2	-5.49	104.72	112.40
1	B	111	SER	N-CA-CB	-5.48	102.29	110.50
1	A	93	ARG	O-C-N	5.47	131.46	122.70
1	A	628	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	B	280	TYR	CB-CG-CD1	5.46	124.28	121.00
1	B	398	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	769	ASP	CB-CG-OD1	5.44	123.19	118.30
1	B	396	LEU	CA-CB-CG	5.43	127.80	115.30
1	A	127	ILE	CA-C-O	-5.42	108.71	120.10
1	A	227	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	B	386	ARG	CD-NE-CZ	5.39	131.15	123.60
1	A	85	ILE	O-C-N	-5.38	114.09	122.70
1	A	504	ASP	OD1-CG-OD2	-5.38	113.07	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	613	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	A	669	ALA	N-CA-CB	-5.37	102.58	110.10
1	B	250	HIS	CG-CD2-NE2	5.37	119.40	109.20
1	B	250	HIS	CA-CB-CG	5.35	122.70	113.60
1	B	251	PRO	N-CA-CB	-5.35	96.71	102.60
1	B	197	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	745	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	B	735	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	B	310	ARG	CA-CB-CG	5.34	125.14	113.40
1	B	191	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	B	212	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	362	ASP	OD1-CG-OD2	-5.32	113.19	123.30
1	A	363	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	177	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	A	127	ILE	O-C-N	5.30	131.18	122.70
1	B	573	TYR	CA-CB-CG	5.29	123.46	113.40
1	B	184	ARG	CD-NE-CZ	5.28	130.99	123.60
1	A	815	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	B	280	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	A	80	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	A	259	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	B	680	LYS	CA-CB-CG	5.25	124.94	113.40
1	B	570	LEU	CB-CG-CD1	5.25	119.92	111.00
1	B	90	LEU	CB-CG-CD2	5.24	119.90	111.00
1	A	129	PRO	O-C-N	-5.23	114.33	122.70
1	A	673	ALA	N-CA-CB	5.22	117.41	110.10
1	B	552	ARG	CD-NE-CZ	5.22	130.91	123.60
1	B	355	ASP	OD1-CG-OD2	5.21	133.20	123.30
1	B	644	PHE	CB-CG-CD1	5.21	124.45	120.80
1	B	828	ALA	N-CA-CB	-5.21	102.81	110.10
1	A	150	VAL	CA-CB-CG2	-5.19	103.11	110.90
1	A	216	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	B	167	ARG	O-C-N	-5.19	114.39	122.70
1	B	276	THR	O-C-N	-5.18	114.41	122.70
1	B	627	ALA	O-C-N	-5.17	114.44	122.70
1	B	374	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	A	478	LYS	CA-CB-CG	5.16	124.76	113.40
1	B	306	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	A	490	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	A	808	CYS	O-C-N	-5.15	114.44	123.20
1	A	271	ASN	CA-C-O	-5.13	109.33	120.10
1	B	549	VAL	CA-CB-CG2	-5.12	103.22	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	GLN	OE1-CD-NE2	5.12	133.68	121.90
1	B	645	LEU	CA-CB-CG	5.12	127.08	115.30
1	B	577	HIS	CA-C-O	5.12	130.85	120.10
1	B	261	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	759	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	527	ASP	OD1-CG-OD2	-5.11	113.59	123.30
1	B	780	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	A	744	GLU	OE1-CD-OE2	5.10	129.43	123.30
1	B	516	ASP	O-C-N	-5.10	114.53	122.70
1	A	527	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	234	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	493	LYS	CA-CB-CG	5.07	124.56	113.40
1	A	101	ASN	CB-CG-ND2	-5.07	104.55	116.70
1	A	640	LEU	O-C-N	5.06	130.80	122.70
1	B	787	VAL	CA-CB-CG2	-5.06	103.31	110.90
1	B	268	GLN	CG-CD-NE2	5.05	128.83	116.70
1	A	651	SER	N-CA-CB	-5.04	102.94	110.50
1	A	632	ASN	O-C-N	-5.04	114.64	122.70
1	A	368	THR	CA-CB-CG2	-5.03	105.36	112.40
1	A	316	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	138	ARG	CD-NE-CZ	5.02	130.62	123.60
1	B	453	ASN	OD1-CG-ND2	-5.02	110.36	121.90
1	A	50	GLN	CG-CD-OE1	-5.01	111.58	121.60
1	A	131	LEU	CA-CB-CG	5.00	126.81	115.30
1	A	576	GLN	CB-CG-CD	5.00	124.61	111.60

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

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	223	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6369	0	6324	220	0
2	C	44	0	30	2	0
2	D	44	0	30	5	0
3	A	6	0	8	2	0
3	B	6	0	8	0	0
4	A	15	0	6	1	0
4	B	15	0	6	3	0
5	A	54	0	0	11	0
5	B	39	0	0	9	0
All	All	12961	0	12736	439	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 17.

All (439) 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
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:HB3	1:B:582:ARG:HH11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:HD21	4:B:999:PLP:H2A3	1.71	0.72
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: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: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: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:A:665:GLN:CD	1:A:678:ASN:HB3	2.16	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: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
1:B:422:GLU:O	1:B:423:LYS:C	2.37	0.63
1:B:716:LYS:HG2	5:B:1785:HOH:O	1.98	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:A:422:GLU:O	1:A:423:LYS:C	2.37	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:VAL:H	1:A:459:HIS:HD2	1.48	0.61
1:B:144:LEU:HD12	1:B:147:MET:HE3	1.81	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:HA	1:A:784:GLN:HE21	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: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:582:ARG:C	1:B:582:ARG:HD2	2.21	0.59
1:B:720:ALA:HB1	1:B:724:LYS:HE2	1.84	0.59
1:B:671:LYS:HZ3	1:B:771:TYR:HE1	1.50	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:CB	1:B:582:ARG:HH11	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:B:186:ASN:HD22	1:B:186:ASN:C	2.06	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
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: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:782:GLU:O	1:A:783:ALA:C	2.43	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:A:144:LEU:HD12	1:A:147:MET:HE3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:PHE:HB2	1:B:104:TRP:CG	2.41	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: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: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: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:CD2	1:A:577:HIS:H	2.26	0.53
1:A:671:LYS:HZ3	1:A:771:TYR:HE1	1.56	0.53
1:A:460:SER:OG	1:A:481:ASN:ND2	2.38	0.53
1:A:532:ASP:O	1:A:536:VAL:HG13	2.08	0.53
1:B:456:ALA:HB1	5:B:1802:HOH:O	2.09	0.53
1:B:292:ARG:HH21	2:D:3:AC1:C2	2.21	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:719:LYS:NZ	5:A:1792:HOH:O	2.41	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:731:TRP:O	1:B:732:ARG:C	2.47	0.53
1:B:716:LYS:O	1:B:719:LYS:HB2	2.09	0.52
1:A:129:PRO:HB3	1:A:182:TRP:CZ3	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:186:ASN:ND2	1:B:186:ASN:C	2.64	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
1:A:428:LEU:HD21	1:A:470:GLU:CG	2.41	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:335:ILE:HG13	1:B:371:THR:HG22	1.93	0.50
1:B:665:GLN:CD	1:B:678:ASN:HB3	2.32	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:186:ASN:C	1:A:186:ASN:HD22	2.14	0.49
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:565:ILE:HD12	1:A:660:ALA:HB2	1.94	0.49
1:A:518:LEU:CD2	1:A:805:THR:HG22	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	1:B:582:ARG:HB3	2.22	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: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
1:A:129:PRO:HA	1:A:182:TRP:CE3	2.49	0.48
1:A:35:TRP:O	1:A:41:LEU:HB2	2.13	0.48
1:A:279:LEU:HD22	1:A:280:TYR:N	2.29	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: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:90:LEU:CD2	4:B:999:PLP:H2A3	2.42	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ASP:O	1:A:519:ILE:HG22	2.14	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:729:VAL:CG1	1:A:1767:LYS:HG3	2.44	0.47
1:A:716:LYS:HA	1:A:716:LYS:HD2	1.71	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:94:LEU:HB2	1:A:187:TYR:OH	2.14	0.47
1:A:20:PRO:HG2	1:A:102:LEU:CD2	2.43	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:186:ASN:O	1:B:187:TYR:C	2.53	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:465:LYS:O	1:A:469:PRO:HG3	2.15	0.46
1:A:471:TYR:HD1	1:A:475:TRP:CZ3	2.32	0.46
1:A:166:PHE:CZ	1:A:608:LYS:HB3	2.50	0.46
1:B:89:PHE:CE1	1:B:144:LEU:HD22	2.50	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: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: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:107:ASP:O	1:B:110:ASP:HB2	2.16	0.46
1:B:101:ASN:CB	1:B:231:VAL:HG23	2.45	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:B:717:GLN:O	1:B:718:VAL:C	2.54	0.46
1:B:77:ALA:O	1:B:78:ASN:C	2.54	0.46
1:A:288:GLY:O	1:A:289:LYS:C	2.51	0.46
1:B:729:VAL:HG11	1:B:1767:LYS:HG3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:112:LEU:HA	1:B:112:LEU:HD23	1.79	0.45
1:B:19:GLN:CB	1:B:20:PRO:HD3	2.36	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
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: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: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: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:695:ALA:O	1:A:696:ASN:C	2.55	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:HD3	1:A:113:LYS:HA	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:753:GLY:O	1:B:754:ASP:C	2.56	0.43
1:B:374:TYR:CZ	1:B:376:ASN:HB2	2.53	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:629:VAL:O	1:A:630:ILE:C	2.56	0.43
1:A:775:ALA:O	5:A:1808:HOH:O	2.21	0.43
1:B:1767:LYS:NZ	1:B:1767:LYS:HB2	2.33	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
2:C:2:GLC:H62	2:C:3:AC1:C5	2.48	0.43
1:A:285:HIS:O	1:A:286:THR:C	2.56	0.43
1:B:794:GLN:O	1:B:795:GLU:C	2.56	0.43
1:B:165:LEU:O	1:B:166:PHE:HB3	2.19	0.43
1:B:425:TRP:CE2	1:B:429:ALA:HB2	2.53	0.43
1:B:567:ILE:O	1:B:568:LYS:HB3	2.19	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:A:656:LEU:O	1:A:657:ILE:C	2.57	0.42
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:HD2	1:A:401:GLN:OE1	2.19	0.42
1:A:377:HIS:CE1	3:A:998:GOL:HO3	2.26	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:46:MET:HE1	1:A:51:TRP:CE3	2.54	0.42
1:A:824:ILE:O	1:A:829:ARG:NH2	2.53	0.42
1:B:190:PHE:CD1	1:B:228:LEU:HD13	2.55	0.42
1:A:90:LEU:HD21	4:A:999:PLP:H2A3	2.02	0.42
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:729:VAL:HG11	1:A:1767:LYS:HG3	2.02	0.42
1:A:396:LEU:HB3	1:A:399:HIS:CD2	2.55	0.42
1:A:731:TRP:O	1:A:732:ARG:C	2.58	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:794:GLN:O	1:A:795:GLU:C	2.57	0.42
1:B:327:HIS:CD2	1:B:328:GLU:HG3	2.55	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:349:LEU:O	1:B:353:LEU:HD22	2.19	0.42
1:B:35:TRP:O	1:B:41:LEU:HB2	2.19	0.42
1:B:519:ILE:HA	1:B:806:ALA:O	2.19	0.42
1:A:136:LEU:HD22	2:C:3:AC1:HCB2	2.02	0.42
1:A:18:SER:HB3	1:A:234:ARG:HB3	2.02	0.42
1:A:441:MET:O	1:A:442:ALA:C	2.57	0.41
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:455:VAL:HB	1:B:484:ASN:CG	2.40	0.41
1:B:491:TRP:CE2	1:B:680:LYS:HE2	2.54	0.41
1:B:706:GLU:CD	1:B:706:GLU:H	2.23	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:668:THR:OG1	1:B:771:TYR:HB3	2.20	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:B:800:ALA:O	1:B:801:ALA:C	2.58	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:LYS:NZ	5:A:1819:HOH:O	2.54	0.41
1:B:267:GLN:O	1:B:268:GLN:C	2.59	0.41
1:B:577:HIS:H	1:B:577:HIS:CD2	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:A:582:ARG:C	1:A:582:ARG:HD2	2.41	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:47:THR:O	1:A:48:PRO:C	2.58	0.41
1:A:714:THR:HG23	1:A:714:THR:H	1.64	0.41
1:B:666:ILE:HG22	1:B:711:PHE:HE1	1.86	0.41
1:B:815:ARG:O	1:B:816:SER:C	2.57	0.41
1:A:162:GLN:HB2	1:A:184:ARG:NH2	2.36	0.41
1:A:294:MET:HE3	1:A:294:MET:HB2	1.95	0.41
1:A:77:ALA:O	1:A:78:ASN:C	2.58	0.41
1:B:23:ASN:HB3	1:B:26:GLN:CB	2.50	0.41
1:B:530:PHE:O	1:B:531:ARG:C	2.58	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:819:ASP:HB3	1:A:823:ARG:NH1	2.36	0.41
1:A:190:PHE:CE1	1:A:228:LEU:HD13	2.56	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:HD3	1:B:671:LYS:HA	1.82	0.40
1:A:192:HIS:HD2	1:A:225:ALA:O	2.05	0.40
1:A:101:ASN:CB	1:A:231:VAL:HG23	2.51	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: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: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:B:482:VAL:HG11	1:B:820:TYR:CD2	2.56	0.40
1:A:161:TYR:CD2	1:A:279:LEU:HB2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:VAL:O	1:B:630:ILE:C	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 [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	794/796 (100%)	729 (92%)	54 (7%)	11 (1%)	11	39
1	B	794/796 (100%)	725 (91%)	58 (7%)	11 (1%)	11	39
All	All	1588/1592 (100%)	1454 (92%)	112 (7%)	22 (1%)	11	39

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	594 (89%)	71 (11%)	6	23
1	B	665/665 (100%)	596 (90%)	69 (10%)	7	24
All	All	1330/1330 (100%)	1190 (90%)	140 (10%)	7	24

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	19	GLN
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	186	ASN
1	A	190	PHE
1	A	206	VAL
1	A	208	LYS
1	A	212	ASP
1	A	214	ARG
1	A	220	THR
1	A	251	PRO
1	A	254	LEU
1	A	268	GLN
1	A	279	LEU
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	493	LYS
1	A	524	LEU
1	A	529	LYS
1	A	569	ARG
1	A	570	LEU
1	A	573	TYR
1	A	577	HIS
1	A	579	ASN
1	A	582	ARG
1	A	613	TYR
1	A	615	LEU
1	A	626	VAL
1	A	628	ASP
1	A	635	LEU
1	A	641	LYS
1	A	644	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	663	SER
1	A	667	SER
1	A	692	LEU
1	A	701	GLU
1	A	705	GLU
1	A	716	LYS
1	A	729	VAL
1	A	742	LEU
1	A	762	LEU
1	A	766	GLN
1	A	772	LEU
1	A	784	GLN
1	A	788	ASP
1	A	810	MET
1	A	829	ARG
1	B	18	SER
1	B	19	GLN
1	B	48	PRO
1	B	49	ARG
1	B	87	MET
1	B	94	LEU
1	B	131	LEU
1	B	165	LEU
1	B	176	VAL
1	B	184	ARG
1	B	185	SER
1	B	186	ASN
1	B	190	PHE
1	B	206	VAL
1	B	208	LYS
1	B	212	ASP
1	B	214	ARG
1	B	220	THR
1	B	224	GLN
1	B	251	PRO
1	B	254	LEU
1	B	268	GLN
1	B	279	LEU
1	B	326	LEU
1	B	327	HIS
1	B	329	LEU
1	B	334	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	416	LYS
1	B	433	ASP
1	B	441	MET
1	B	475	TRP
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	579	ASN
1	B	582	ARG
1	B	604	LEU
1	B	613	TYR
1	B	626	VAL
1	B	628	ASP
1	B	635	LEU
1	B	641	LYS
1	B	644	PHE
1	B	663	SER
1	B	692	LEU
1	B	701	GLU
1	B	705	GLU
1	B	706	GLU
1	B	716	LYS
1	B	729	VAL
1	B	742	LEU
1	B	751	SER
1	B	762	LEU
1	B	766	GLN
1	B	772	LEU
1	B	784	GLN
1	B	810	MET
1	B	813	SER
1	B	829	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	133	ASN
1	A	186	ASN
1	A	192	HIS
1	A	250	HIS
1	A	271	ASN
1	A	285	HIS
1	A	296	GLN
1	A	327	HIS
1	A	399	HIS
1	A	440	HIS
1	A	459	HIS
1	A	481	ASN
1	A	494	GLN
1	A	566	GLN
1	A	571	HIS
1	A	577	HIS
1	A	579	ASN
1	A	784	GLN
1	B	26	GLN
1	B	109	GLN
1	B	133	ASN
1	B	183	HIS
1	B	186	ASN
1	B	192	HIS
1	B	248	HIS
1	B	271	ASN
1	B	285	HIS
1	B	327	HIS
1	B	399	HIS
1	B	440	HIS
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	579	ASN
1	B	760	GLN
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	0.79	0	17,17,17	2.14	5 (29%)
2	GLC	C	2	2	11,11,12	1.47	1 (9%)	15,15,17	2.44	7 (46%)
2	AC1	C	3	2	21,22,23	1.31	2 (9%)	22,32,34	2.64	9 (40%)
2	GLC	D	1	2	12,12,12	0.76	0	17,17,17	2.10	6 (35%)
2	GLC	D	2	2	11,11,12	1.08	1 (9%)	15,15,17	1.90	3 (20%)
2	AC1	D	3	2	21,22,23	1.77	6 (28%)	22,32,34	2.37	8 (36%)

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	3.90	1.38	1.32
2	D	3	AC1	C4A-C5B	3.56	1.54	1.51
2	C	2	GLC	C2-C3	3.34	1.57	1.52
2	C	3	AC1	C7B-C5B	3.09	1.37	1.32
2	D	3	AC1	O4-C4A	2.80	1.47	1.42
2	D	2	GLC	C2-C3	2.42	1.56	1.52
2	D	3	AC1	O6B-C6B	2.33	1.49	1.41
2	D	3	AC1	C2B-C1B	2.32	1.56	1.52
2	D	3	AC1	C3B-C4A	2.24	1.56	1.53
2	C	3	AC1	C1B-C7B	-2.14	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	6.91	121.05	110.68
2	C	1	GLC	O3-C3-C4	5.39	122.82	110.35
2	D	1	GLC	O4-C4-C3	-5.26	98.18	110.35
2	C	2	GLC	C1-O5-C5	4.85	118.77	112.19
2	C	3	AC1	O3B-C3B-C4A	4.80	118.85	109.68
2	D	3	AC1	C7B-C1B-N4A	4.69	117.72	110.68
2	D	3	AC1	C1-C2-C3	4.33	114.99	109.67
2	D	3	AC1	O4-C4A-C3B	-4.33	101.59	110.53
2	C	3	AC1	O2B-C2B-C3B	-4.21	100.62	110.35
2	C	2	GLC	O2-C2-C1	4.17	117.68	109.15
2	D	2	GLC	O5-C5-C6	-4.08	100.80	107.20
2	D	3	AC1	C2-C3-C4	-4.08	107.03	110.63
2	D	2	GLC	C1-O5-C5	4.07	117.71	112.19
2	D	3	AC1	O2B-C2B-C3B	-3.82	101.51	110.35
2	C	2	GLC	C2-C3-C4	-3.82	104.29	110.89
2	C	1	GLC	O2-C2-C3	-3.82	101.53	110.35
2	C	3	AC1	O4-C4A-C3B	-3.53	103.24	110.53
2	C	3	AC1	O2B-C2B-C1B	3.49	116.12	109.12
2	D	2	GLC	C2-C3-C4	-2.87	105.93	110.89
2	C	2	GLC	C1-C2-C3	-2.81	106.21	109.67
2	D	1	GLC	O2-C2-C1	2.79	115.62	109.16
2	D	3	AC1	O3B-C3B-C4A	2.77	114.98	109.68
2	D	3	AC1	C5-C4-N4A	-2.77	104.12	111.74
2	C	3	AC1	C1-C2-C3	2.75	113.05	109.67
2	C	2	GLC	O5-C5-C6	-2.73	102.93	107.20
2	D	1	GLC	O3-C3-C2	2.70	116.58	110.35
2	C	1	GLC	O4-C4-C3	-2.67	104.17	110.35
2	D	1	GLC	C6-C5-C4	2.66	119.23	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	GLC	C3-C4-C5	2.62	114.90	110.24
2	C	3	AC1	C5-C4-N4A	-2.47	104.95	111.74
2	C	3	AC1	O2-C2-C1	2.36	113.97	109.15
2	C	2	GLC	O3-C3-C2	2.29	114.38	109.99
2	C	3	AC1	C4A-C5B-C7B	-2.21	118.60	122.23
2	C	1	GLC	C6-C5-C4	2.10	117.92	113.00
2	C	1	GLC	O1-C1-O5	2.09	116.67	110.38
2	D	1	GLC	C4-C3-C2	-2.08	107.19	110.82
2	D	1	GLC	O5-C5-C6	-2.08	101.27	106.44
2	D	3	AC1	O6B-C6B-C5B	2.04	117.37	112.50

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:

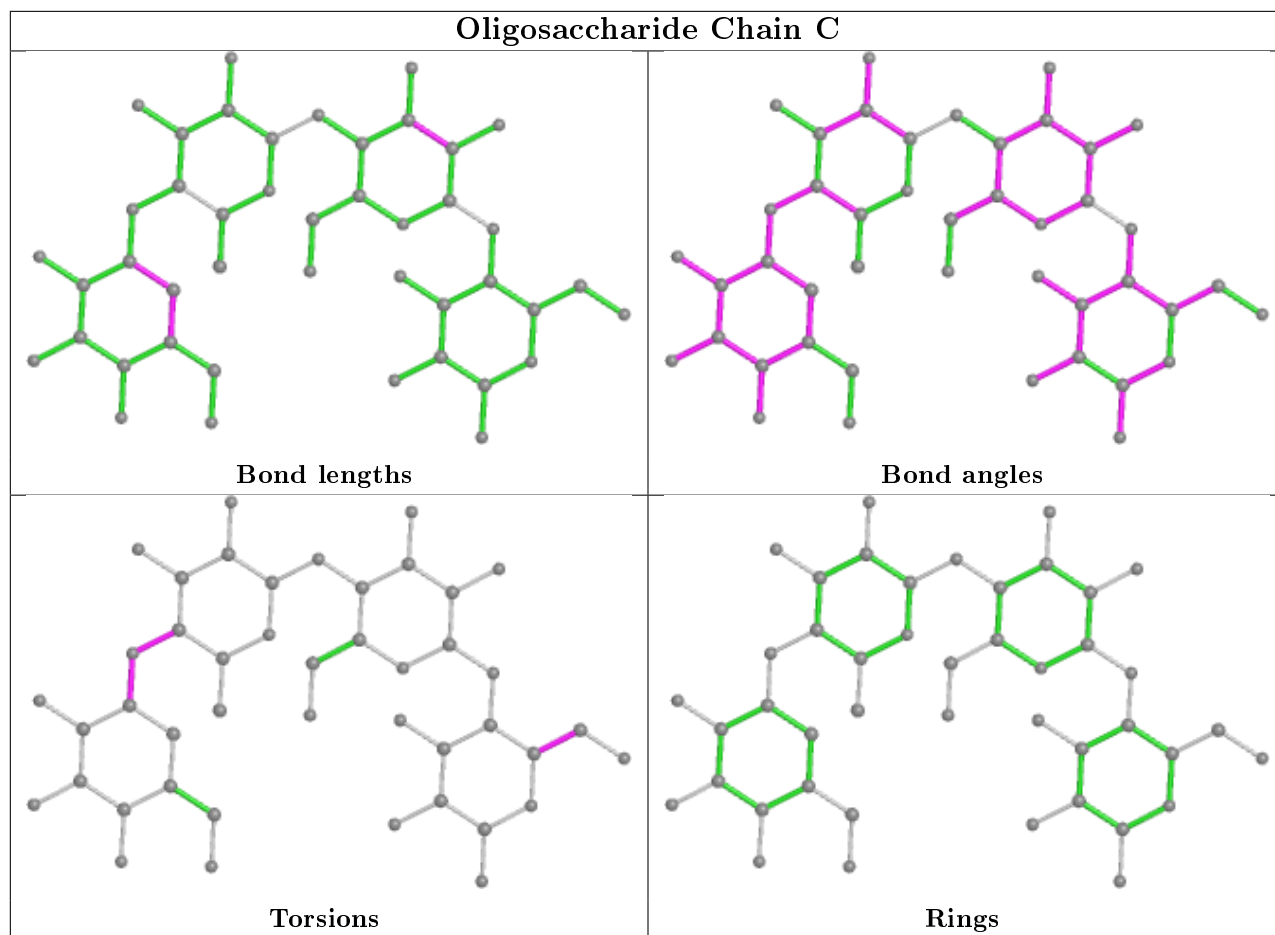
Mol	Chain	Res	Type	Atoms
2	D	3	AC1	C5-C4-N4A-C1B
2	D	3	AC1	C2B-C1B-N4A-C4
2	D	1	GLC	O5-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	C	3	AC1	C2B-C1B-N4A-C4
2	C	3	AC1	C3-C4-N4A-C1B
2	C	3	AC1	C5-C4-N4A-C1B
2	D	3	AC1	C3-C4-N4A-C1B

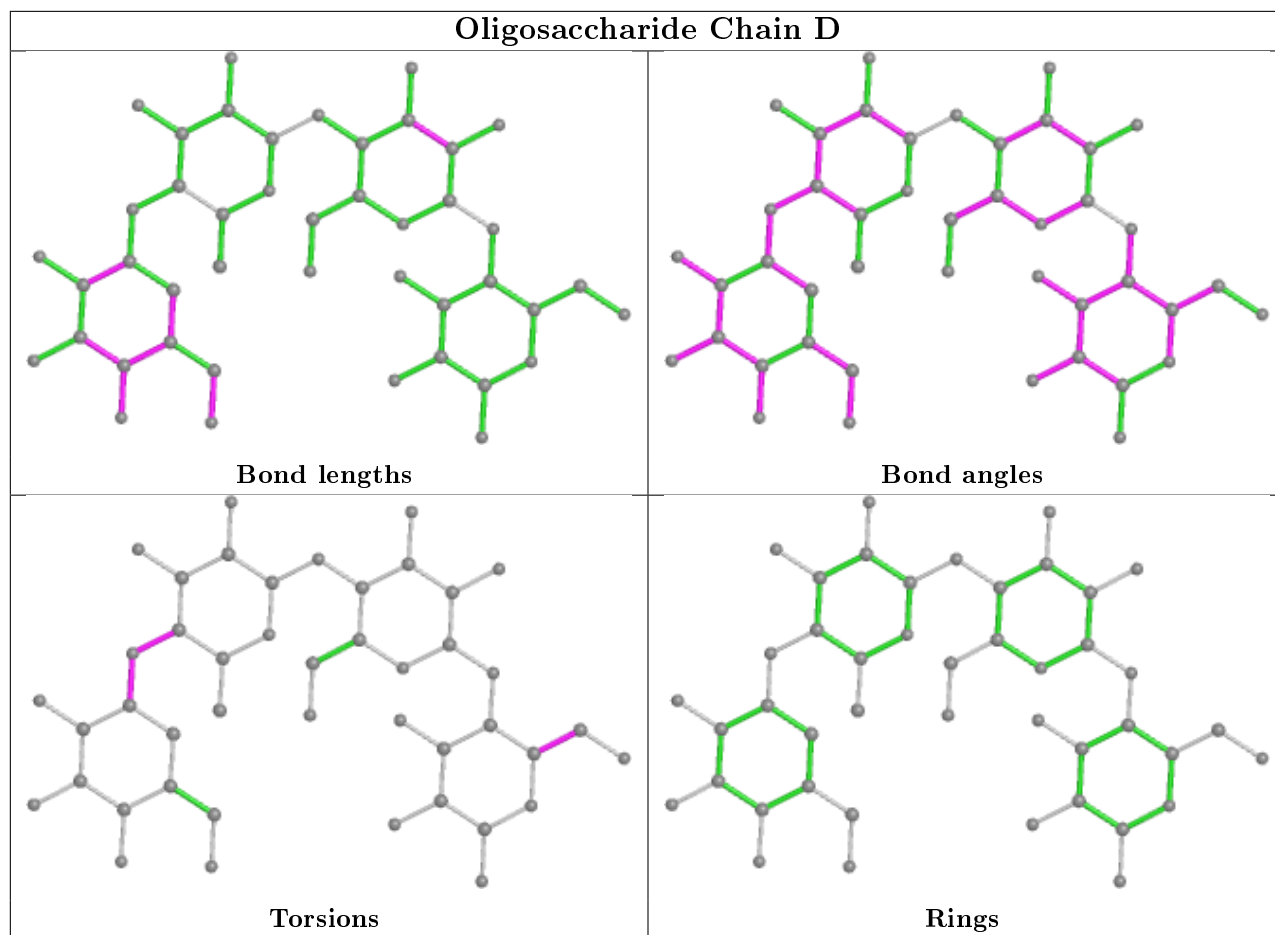
There are no ring outliers.

4 monomers are involved in 7 short contacts:

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

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





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$
4	PLP	B	999	1	15,15,16	2.62	4 (26%)	20,22,23	1.91	6 (30%)
3	GOL	A	998	-	5,5,5	0.75	0	5,5,5	0.83	0
3	GOL	B	998	-	5,5,5	0.48	0	5,5,5	0.53	0
4	PLP	A	999	1	15,15,16	1.83	3 (20%)	20,22,23	1.92	5 (25%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PLP	B	999	1	-	2/6/6/8	0/1/1/1
3	GOL	A	998	-	-	2/4/4/4	-
3	GOL	B	998	-	-	2/4/4/4	-
4	PLP	A	999	1	-	3/6/6/8	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	-8.53	1.32	1.40
4	A	999	PLP	C3-C2	-4.47	1.36	1.40
4	B	999	PLP	P-O3P	-3.23	1.42	1.54
4	A	999	PLP	P-O3P	-3.14	1.42	1.54
4	B	999	PLP	C3-C4	-2.39	1.35	1.40
4	A	999	PLP	C3-C4	-2.23	1.35	1.40
4	B	999	PLP	C5A-C5	2.03	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	-5.03	114.68	120.89
4	B	999	PLP	C4A-C4-C5	4.08	125.14	120.94
4	B	999	PLP	O3P-P-O1P	3.41	124.02	110.68
4	B	999	PLP	C2A-C2-C3	-3.18	116.96	120.89
4	A	999	PLP	O2P-P-O1P	-2.97	99.05	110.68
4	A	999	PLP	C2A-C2-N1	2.77	123.09	117.67
4	A	999	PLP	O3P-P-O4P	2.63	113.74	106.73
4	A	999	PLP	O4P-C5A-C5	-2.50	104.58	109.35
4	B	999	PLP	O3-C3-C2	2.42	122.78	117.49
4	B	999	PLP	C4A-C4-C3	-2.23	116.72	120.50
4	B	999	PLP	O2P-P-O1P	-2.04	102.70	110.68

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	999	PLP	C5A-O4P-P-O3P
3	B	998	GOL	O1-C1-C2-C3
4	A	999	PLP	C5A-O4P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	999	PLP	C5A-O4P-P-O2P
4	A	999	PLP	C5A-O4P-P-O3P
3	B	998	GOL	O1-C1-C2-O2
3	A	998	GOL	O1-C1-C2-O2
3	A	998	GOL	O1-C1-C2-C3
4	B	999	PLP	C5A-O4P-P-O2P

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	999	PLP	3	0
3	A	998	GOL	2	0
4	A	999	PLP	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.18	4 (0%) 91 81	41, 50, 76, 114	0
1	B	796/796 (100%)	-0.29	12 (1%) 73 57	41, 50, 76, 114	0
All	All	1592/1592 (100%)	-0.24	16 (1%) 82 68	41, 50, 76, 114	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	18	SER	5.3
1	B	207	THR	4.1
1	B	723	ALA	3.7
1	B	208	LYS	3.3
1	B	421	ASP	3.0
1	B	214	ARG	2.9
1	A	214	ARG	2.7
1	B	78	ASN	2.5
1	B	1767	LYS	2.5
1	B	73	ALA	2.5
1	A	18	SER	2.5
1	A	733	LYS	2.3
1	B	595	GLN	2.2
1	B	422	GLU	2.1
1	A	421	ASP	2.1
1	B	249	ALA	2.1

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

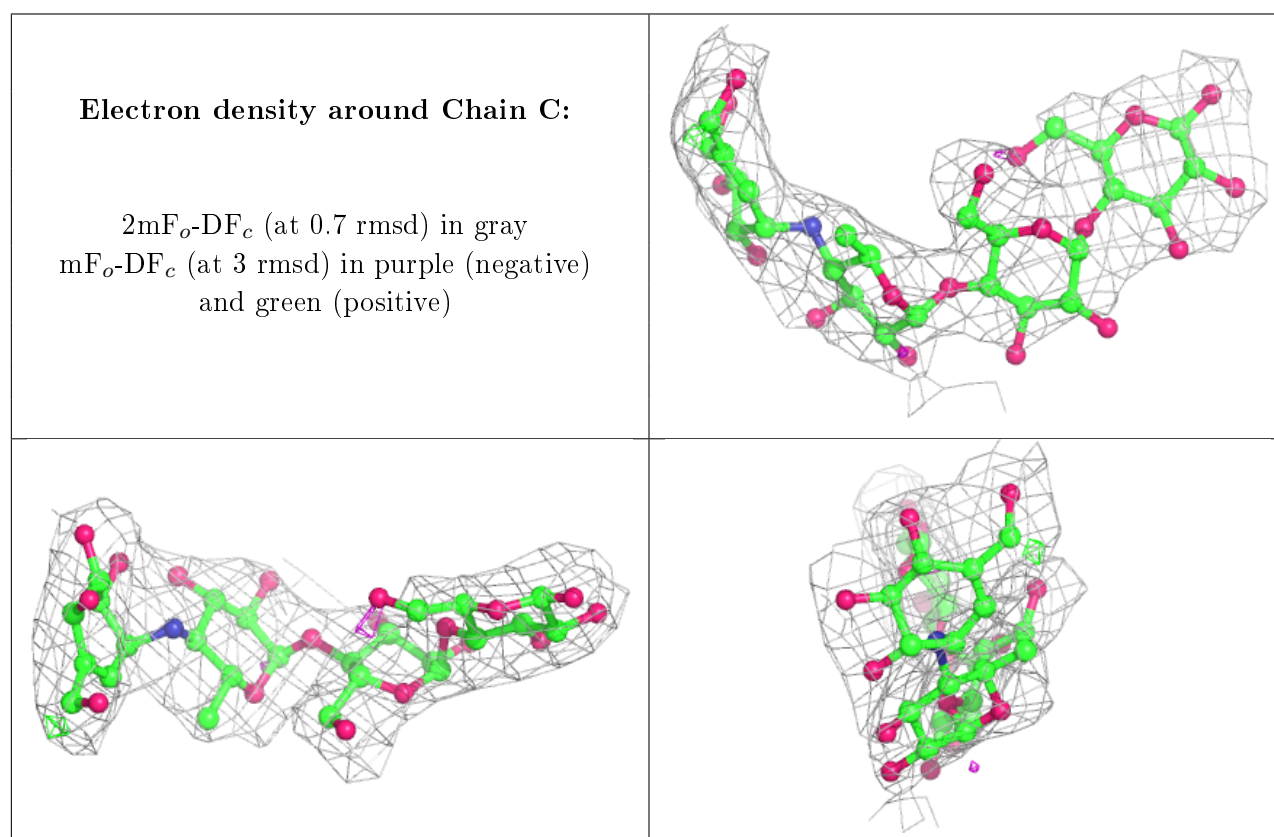
There are no non-standard protein/DNA/RNA residues in this entry.

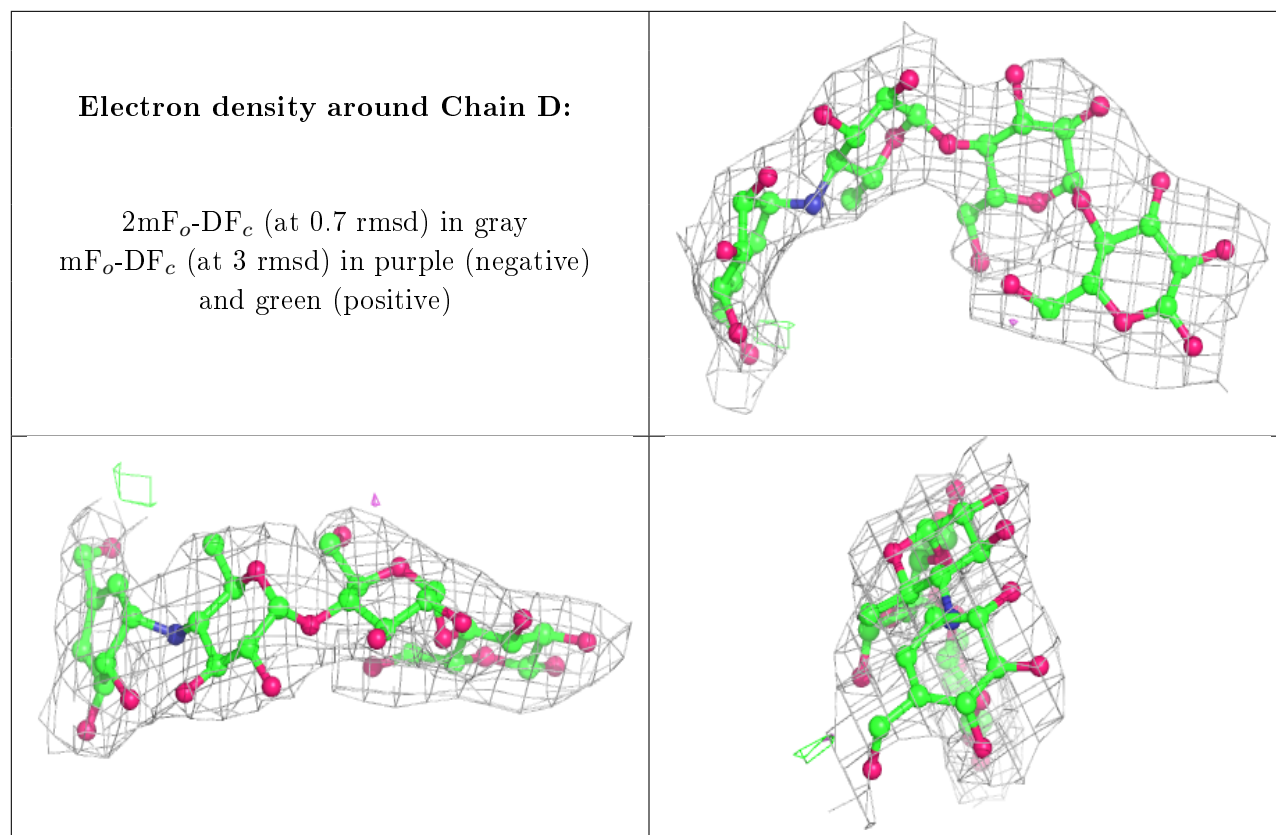
6.3 Carbohydrates [i](#)

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	AC1	C	3	21/22	0.89	0.20	58,58,59,59	0
2	AC1	D	3	21/22	0.89	0.20	58,58,59,60	0
2	GLC	D	1	12/12	0.90	0.19	58,59,59,59	0
2	GLC	C	2	11/12	0.90	0.24	58,58,59,59	0
2	GLC	C	1	12/12	0.91	0.25	58,59,59,60	0
2	GLC	D	2	11/12	0.92	0.23	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.





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	0.21	58,58,59,59	0
3	GOL	A	998	6/6	0.91	0.27	58,58,59,59	0
4	PLP	A	999	15/16	0.95	0.17	37,42,47,51	0
4	PLP	B	999	15/16	0.97	0.12	41,43,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.