



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:35 AM UTC

PDB ID : 2GRX / pdb_00002grx
Title : Crystal structure of TonB in complex with FhuA, E. coli outer membrane receptor for ferrichrome
Authors : Pawelek, P.D.; Allaire, M.; Coulton, J.W.
Deposited on : 2006-04-25
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

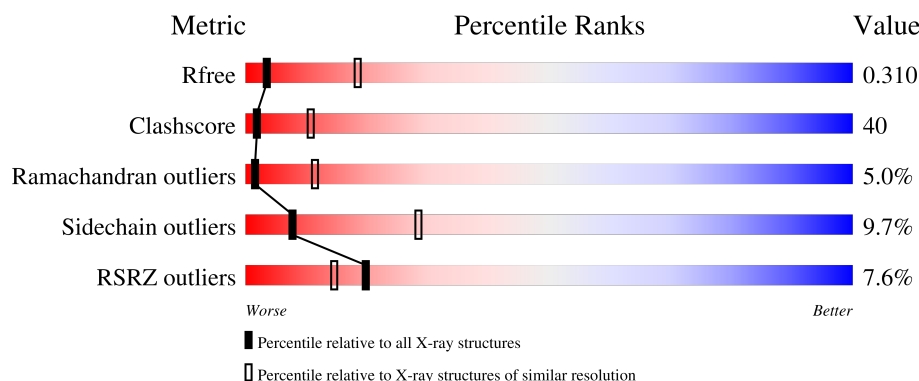
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	725	3% 43% 46% 7% • •
1	B	725	12% 43% 44% 7% • 5%
2	C	229	12% 17% 5% 66%
2	D	229	3% 12% 17% • 66%
3	E	5	40% 60%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	5	

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
3	GCN	E	1	-	-	X	-
3	GCN	F	1	-	-	X	-
3	GCN	F	2	-	-	X	-
3	KDO	F	4	-	-	X	-
5	FTT	A	900	-	-	X	-
5	FTT	A	901	-	-	X	-
5	FTT	B	900	-	-	X	-
5	FTT	B	901	-	-	X	-
5	FTT	B	902	-	-	X	-
5	FTT	B	903	-	-	X	-
6	DPO	A	910	-	-	X	-
6	DPO	B	910	-	-	X	-
7	DAO	B	930	-	-	X	-
9	FCI	A	1050	X	-	-	-
9	FCI	B	1050	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12533 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 Ferrichrome-iron receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	702	Total	C	N	O	S	0	0	0
			5466	3444	926	1082	14			
1	B	691	Total	C	N	O	S	0	0	0
			5394	3398	914	1068	14			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	SEE REMARK 999	UNP P06971
A	407	SER	-	SEE REMARK 999	UNP P06971
A	408	HIS	-	SEE REMARK 999	UNP P06971
A	409	HIS	-	SEE REMARK 999	UNP P06971
A	410	HIS	-	SEE REMARK 999	UNP P06971
A	411	HIS	-	SEE REMARK 999	UNP P06971
A	412	HIS	-	SEE REMARK 999	UNP P06971
A	413	HIS	-	SEE REMARK 999	UNP P06971
A	414	GLY	-	SEE REMARK 999	UNP P06971
A	415	SER	-	SEE REMARK 999	UNP P06971
A	416	SER	-	SEE REMARK 999	UNP P06971
B	406	SER	-	SEE REMARK 999	UNP P06971
B	407	SER	-	SEE REMARK 999	UNP P06971
B	408	HIS	-	SEE REMARK 999	UNP P06971
B	409	HIS	-	SEE REMARK 999	UNP P06971
B	410	HIS	-	SEE REMARK 999	UNP P06971
B	411	HIS	-	SEE REMARK 999	UNP P06971
B	412	HIS	-	SEE REMARK 999	UNP P06971
B	413	HIS	-	SEE REMARK 999	UNP P06971
B	414	GLY	-	SEE REMARK 999	UNP P06971
B	415	SER	-	SEE REMARK 999	UNP P06971
B	416	SER	-	SEE REMARK 999	UNP P06971

- Molecule 2 is a protein called Protein tonB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	78	Total 624	C 393	N 120	O 109	S 2	0	0	0
2	D	78	Total 624	C 393	N 120	O 109	S 2	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

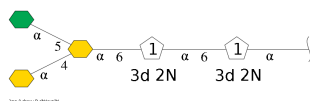
Chain	Residue	Modelled	Actual	Comment	Reference
C	11	GLY	-	SEE REMARK 999	UNP P94739
C	12	SER	-	SEE REMARK 999	UNP P94739
C	13	SER	-	SEE REMARK 999	UNP P94739
C	14	HIS	-	SEE REMARK 999	UNP P94739
C	15	HIS	-	SEE REMARK 999	UNP P94739
C	16	HIS	-	SEE REMARK 999	UNP P94739
C	17	HIS	-	SEE REMARK 999	UNP P94739
C	18	HIS	-	SEE REMARK 999	UNP P94739
C	19	HIS	-	SEE REMARK 999	UNP P94739
C	20	SER	-	SEE REMARK 999	UNP P94739
C	21	SER	-	SEE REMARK 999	UNP P94739
C	22	GLY	-	SEE REMARK 999	UNP P94739
C	23	LEU	-	SEE REMARK 999	UNP P94739
C	24	VAL	-	SEE REMARK 999	UNP P94739
C	25	PRO	-	SEE REMARK 999	UNP P94739
C	26	ARG	-	SEE REMARK 999	UNP P94739
C	27	GLY	-	SEE REMARK 999	UNP P94739
C	28	SER	-	SEE REMARK 999	UNP P94739
C	29	HIS	-	SEE REMARK 999	UNP P94739
C	30	MET	-	SEE REMARK 999	UNP P94739
C	31	SER	-	SEE REMARK 999	UNP P94739
C	32	VAL	-	SEE REMARK 999	UNP P94739
D	11	GLY	-	SEE REMARK 999	UNP P94739
D	12	SER	-	SEE REMARK 999	UNP P94739
D	13	SER	-	SEE REMARK 999	UNP P94739
D	14	HIS	-	SEE REMARK 999	UNP P94739
D	15	HIS	-	SEE REMARK 999	UNP P94739
D	16	HIS	-	SEE REMARK 999	UNP P94739
D	17	HIS	-	SEE REMARK 999	UNP P94739
D	18	HIS	-	SEE REMARK 999	UNP P94739
D	19	HIS	-	SEE REMARK 999	UNP P94739
D	20	SER	-	SEE REMARK 999	UNP P94739
D	21	SER	-	SEE REMARK 999	UNP P94739
D	22	GLY	-	SEE REMARK 999	UNP P94739
D	23	LEU	-	SEE REMARK 999	UNP P94739

Continued on next page...

Continued from previous page...

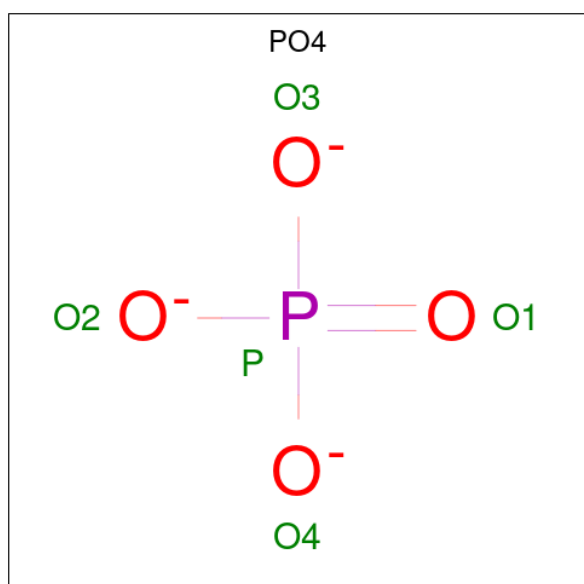
Chain	Residue	Modelled	Actual	Comment	Reference
D	24	VAL	-	SEE REMARK 999	UNP P94739
D	25	PRO	-	SEE REMARK 999	UNP P94739
D	26	ARG	-	SEE REMARK 999	UNP P94739
D	27	GLY	-	SEE REMARK 999	UNP P94739
D	28	SER	-	SEE REMARK 999	UNP P94739
D	29	HIS	-	SEE REMARK 999	UNP P94739
D	30	MET	-	SEE REMARK 999	UNP P94739
D	31	SER	-	SEE REMARK 999	UNP P94739
D	32	VAL	-	SEE REMARK 999	UNP P94739

- Molecule 3 is an oligosaccharide called 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-[L-glycero-alpha-D-manno-heptopyranose-(1-5)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2,3-dideoxy-alpha-D-glucopyranose-(1-6)-2-amino-2,3-dideoxy-alpha-D-glucopyranose.



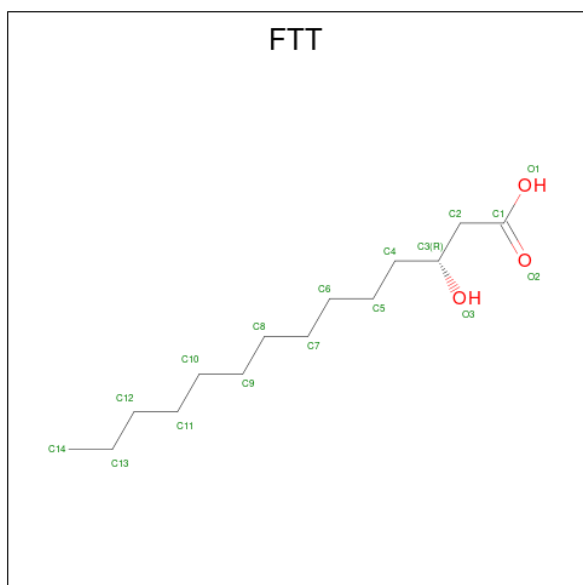
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			63	35	2	26			
3	F	5	Total	C	N	O	0	0	0
			63	35	2	26			

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



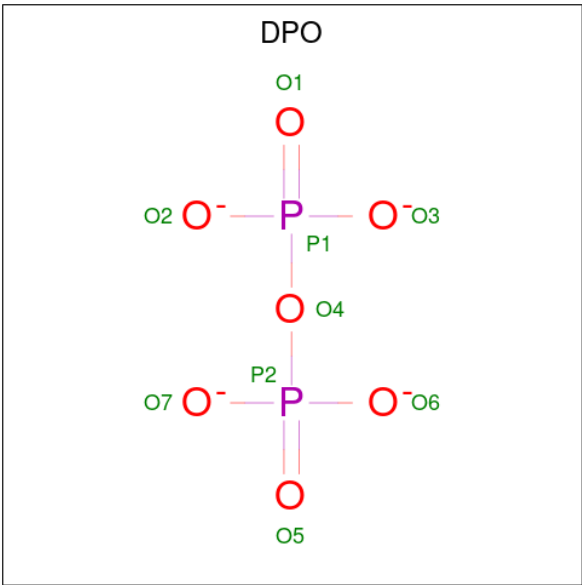
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			4	3	1		
4	B	1	Total	O	P	0	0
			4	3	1		

- Molecule 5 is 3-HYDROXY-TETRADECANOIC ACID (CCD ID: FTT) (formula: $C_{14}H_{28}O_3$).



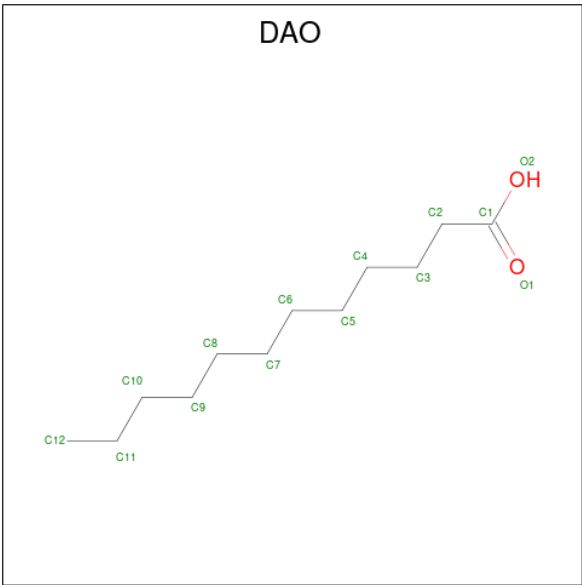
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	14	2		
5	A	1	Total	C	O	0	0
			16	14	2		
5	A	1	Total	C	O	0	0
			16	14	2		
5	A	1	Total	C	O	0	0
			16	14	2		
5	B	1	Total	C	O	0	0
			16	14	2		
5	B	1	Total	C	O	0	0
			16	14	2		
5	B	1	Total	C	O	0	0
			16	14	2		
5	B	1	Total	C	O	0	0
			16	14	2		

- Molecule 6 is DIPHOSPHATE (CCD ID: DPO) (formula: O_7P_2).



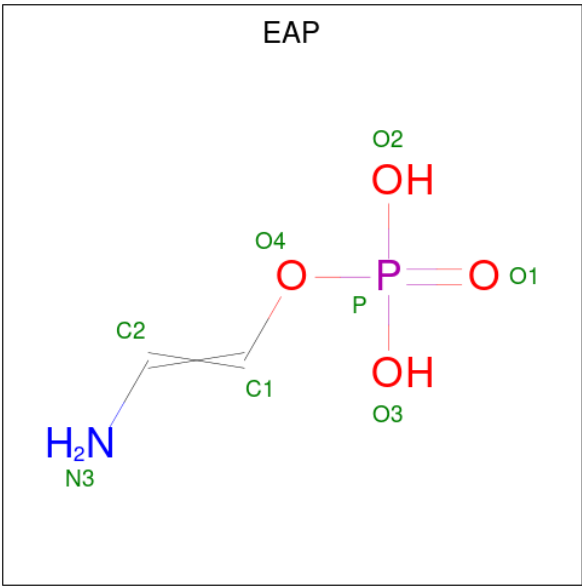
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			8	6	2		
6	B	1	Total	O	P	0	0
			8	6	2		

- Molecule 7 is LAURIC ACID (CCD ID: DAO) (formula: C₁₂H₂₄O₂).



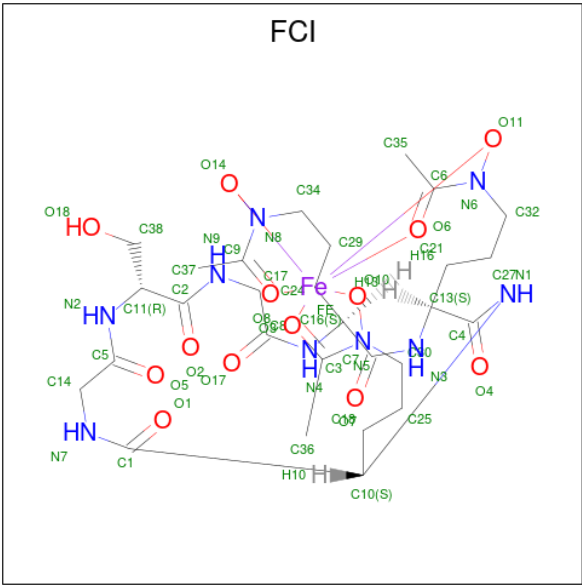
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	12	1		
7	B	1	Total	C	O	0	0
			13	12	1		

- Molecule 8 is 2-AMINO-VINYL-PHOSPHATE (CCD ID: EAP) (formula: C₂H₆NO₄P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			7	2	1	3	1		
8	B	1	Total	C	N	O	P	0	0
			7	2	1	3	1		

- Molecule 9 is FERRICROCIN-IRON (CCD ID: FCI) (formula: C₂₈H₄₄FeN₉O₁₃).



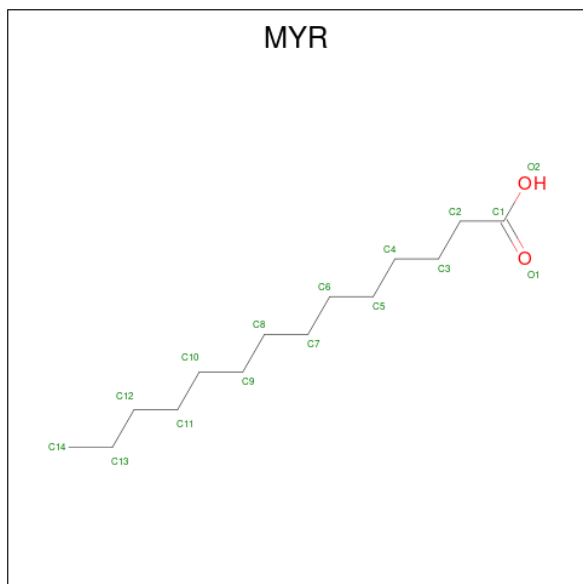
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	O	0	0
			46	24	1	9	12		

Continued on next page...

Continued from previous page...

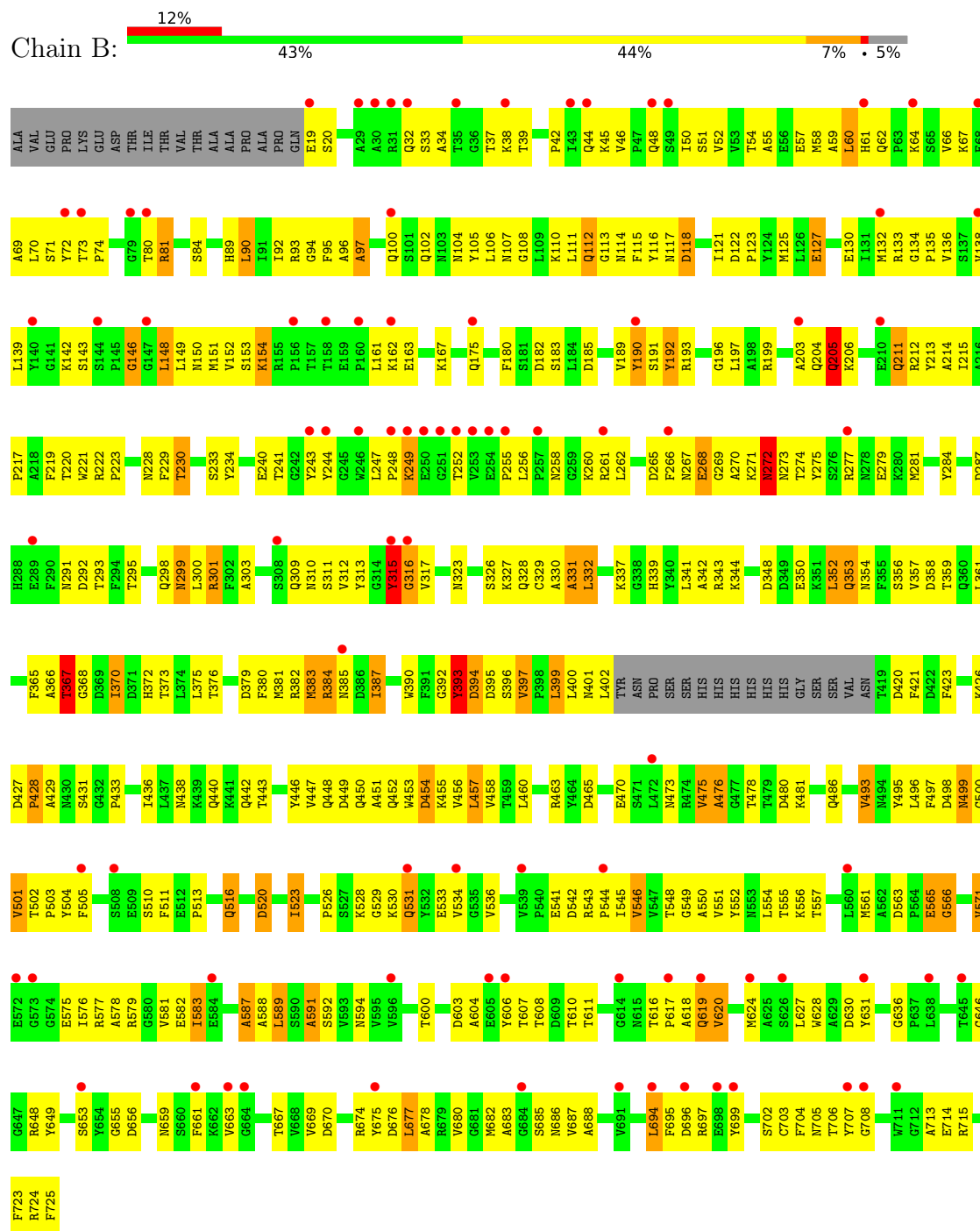
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	Fe	N	O	
			46	24	1	9	12	
							0	0

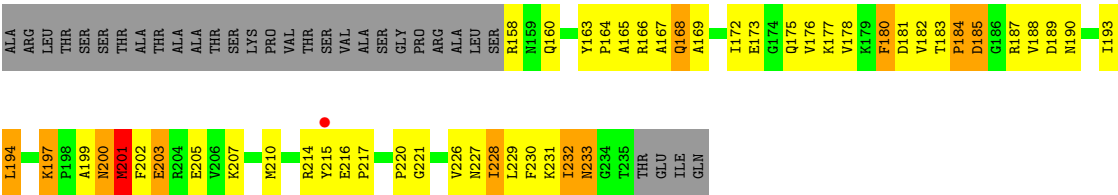
- Molecule 10 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



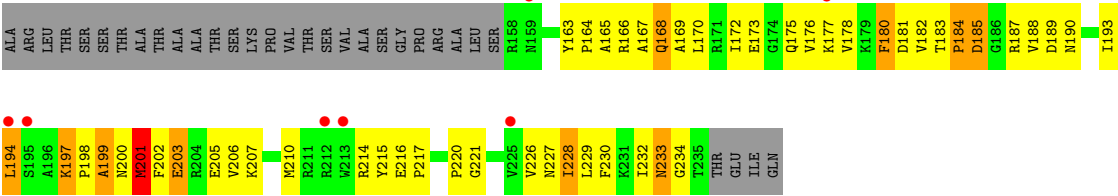
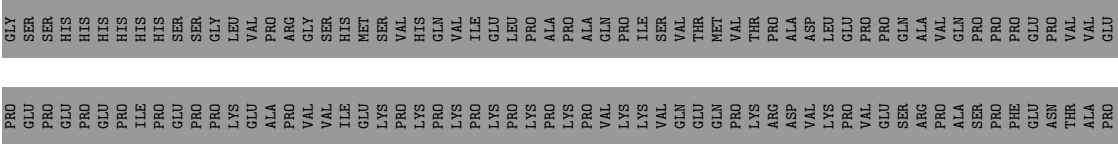
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O		
			15	14	1	0	0

● Molecule 1: Ferrichrome-iron receptor





• Molecule 2: Protein tonB



• Molecule 3: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-[L-glycero-alpha-D-manno-heptopyranose-(1-5)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2,3-dideoxy-alpha-D-glucopyranose-(1-6)-2-amino-2,3-dideoxy-alpha-D-glucopyranose



• Molecule 3: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-[L-glycero-alpha-D-manno-heptopyranose-(1-5)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2,3-dideoxy-alpha-D-glucopyranose-(1-6)-2-amino-2,3-dideoxy-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	234.32Å 91.84Å 138.51Å 90.00° 118.86° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 50.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-3.30) 99.2 (50.00-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.284 , 0.329 0.262 , 0.310	Depositor DCC
R_{free} test set	2325 reflections (6.01%)	wwPDB-VP
Wilson B-factor (Å ²)	93.6	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12533	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DAO, KDO, GMH, GCN, DPO, EAP, FCI, MYR, FTT, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	0/5599	1.04	25/7609 (0.3%)
1	B	0.48	0/5525	0.98	22/7504 (0.3%)
2	C	0.45	0/636	0.86	1/857 (0.1%)
2	D	0.37	0/636	0.84	1/857 (0.1%)
All	All	0.55	0/12396	1.00	49/16827 (0.3%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ALA	CA-C-N	13.30	136.47	119.84
1	A	16	ALA	C-N-CA	13.30	136.47	119.84
1	A	496	LEU	N-CA-C	7.91	121.48	109.62
1	A	591	ALA	N-CA-C	-7.87	101.89	114.09
1	B	591	ALA	N-CA-C	-7.58	102.34	114.09
1	B	496	LEU	N-CA-C	7.53	120.91	109.62
1	B	73	THR	CA-C-N	6.92	126.89	119.76
1	B	73	THR	C-N-CA	6.92	126.89	119.76
1	A	73	THR	CA-C-N	6.87	126.83	119.76
1	A	73	THR	C-N-CA	6.87	126.83	119.76
1	A	541	GLU	N-CA-C	-6.55	105.17	113.43
1	A	17	PRO	N-CA-C	6.55	125.96	112.47
1	B	61	HIS	N-CA-C	-6.51	105.07	114.12
1	A	61	HIS	N-CA-C	-6.31	105.35	114.12
1	B	55	ALA	N-CA-C	-6.29	104.34	111.07
1	B	587	ALA	N-CA-C	6.19	117.92	108.52
2	C	180	PHE	N-CA-C	6.15	116.68	108.38
1	A	587	ALA	N-CA-C	6.14	117.86	108.52
1	A	154	LYS	N-CA-C	-6.12	102.03	110.35
1	A	13	ALA	N-CA-C	6.11	119.12	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	348	ASP	N-CA-C	6.07	119.40	108.48
2	D	180	PHE	N-CA-C	6.02	116.51	108.38
1	B	230	THR	N-CA-C	5.98	118.49	108.02
1	A	348	ASP	N-CA-C	5.96	119.21	108.48
1	A	230	THR	N-CA-C	5.92	118.37	108.02
1	A	393	TYR	N-CA-C	5.92	119.12	109.24
1	B	541	GLU	N-CA-C	-5.91	105.98	113.43
1	A	55	ALA	N-CA-C	-5.84	104.82	111.07
1	B	127	GLU	N-CA-C	-5.76	106.39	113.41
1	A	272	ASN	N-CA-C	5.62	119.13	112.72
1	B	272	ASN	N-CA-C	5.62	119.12	112.72
1	B	636	GLY	CA-C-N	5.58	125.05	119.24
1	B	636	GLY	C-N-CA	5.58	125.05	119.24
1	A	249	LYS	N-CA-C	-5.57	105.59	112.38
1	B	154	LYS	N-CA-C	-5.53	102.83	110.35
1	A	636	GLY	CA-C-N	5.50	124.96	119.24
1	A	636	GLY	C-N-CA	5.50	124.96	119.24
1	B	393	TYR	N-CA-C	5.50	118.42	109.24
1	B	249	LYS	N-CA-C	-5.41	105.78	112.38
1	B	74	PRO	N-CA-C	5.40	119.57	111.14
1	A	699	TYR	N-CA-C	5.29	117.23	109.24
1	A	562	ALA	N-CA-C	5.21	117.26	110.43
1	B	619	GLN	CA-C-N	-5.11	118.91	122.59
1	B	619	GLN	C-N-CA	-5.11	118.91	122.59
1	B	699	TYR	N-CA-C	5.05	116.86	109.24
1	A	88	ASP	N-CA-C	-5.04	102.61	109.71
1	A	315	TYR	N-CA-C	-5.02	102.27	110.20
1	A	74	PRO	N-CA-C	5.01	118.96	111.14
1	B	315	TYR	N-CA-C	-5.01	101.80	109.76

There are no chirality outliers.

There are no planarity outliers.

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	5466	0	5193	380	0
1	B	5394	0	5120	363	0
2	C	624	0	640	56	0
2	D	624	0	640	52	0
3	E	63	0	50	18	0
3	F	63	0	51	24	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	64	0	107	30	0
5	B	64	0	107	100	0
6	A	8	0	0	8	0
6	B	8	0	0	8	0
7	A	13	0	23	5	0
7	B	13	0	23	7	0
8	A	7	0	4	2	0
8	B	7	0	4	3	0
9	A	46	0	31	2	0
9	B	46	0	31	1	0
10	B	15	0	27	4	0
All	All	12533	0	12051	970	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 40.

All (970) 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)
5:B:902:FTT:H92	5:B:903:FTT:C8	1.28	1.55
3:F:4:KDO:O1B	3:F:4:KDO:C1	1.70	1.39
5:B:902:FTT:C9	5:B:903:FTT:H82	1.52	1.39
5:B:902:FTT:C13	5:B:903:FTT:H131	1.55	1.34
5:B:901:FTT:C14	5:B:903:FTT:H112	1.58	1.33
5:B:901:FTT:C14	5:B:903:FTT:C11	2.06	1.32
5:B:901:FTT:C1	3:F:1:GCN:H31	1.58	1.32
5:A:901:FTT:C1	3:E:1:GCN:H31	1.59	1.31
5:B:903:FTT:C1	3:F:2:GCN:H31	1.62	1.29
5:A:903:FTT:C1	3:E:2:GCN:H31	1.64	1.27
5:B:901:FTT:H143	5:B:903:FTT:C11	1.61	1.27
5:B:901:FTT:C14	5:B:903:FTT:C13	2.16	1.24
5:B:901:FTT:C14	5:B:903:FTT:H132	1.69	1.19
6:A:910:DPO:O6	6:B:910:DPO:O6	1.58	1.17
5:B:902:FTT:H72	5:B:903:FTT:H62	1.25	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:901:FTT:H143	5:B:903:FTT:H111	1.24	1.12
5:B:901:FTT:H142	5:B:903:FTT:H112	1.24	1.10
3:E:4:KDO:C1	3:E:4:KDO:O1A	2.01	1.08
6:A:910:DPO:P1	3:E:1:GCN:C1	2.42	1.07
6:B:910:DPO:P1	3:F:1:GCN:C1	2.42	1.07
5:B:902:FTT:H112	5:B:903:FTT:H92	1.32	1.07
5:B:902:FTT:H131	5:B:903:FTT:H131	1.20	1.07
2:C:164:PRO:HG3	2:C:205:GLU:HG3	1.35	1.07
5:B:902:FTT:H132	5:B:903:FTT:H131	1.35	1.05
1:A:390:TRP:HE1	1:A:431:SER:HB3	1.22	1.05
1:B:390:TRP:HE1	1:B:431:SER:HB3	1.17	1.05
5:B:902:FTT:C11	5:B:903:FTT:H111	1.86	1.05
5:B:902:FTT:H111	5:B:903:FTT:H111	1.37	1.05
5:B:901:FTT:C1	3:F:1:GCN:C3	2.35	1.05
6:A:910:DPO:O6	6:B:910:DPO:P2	2.14	1.04
2:D:164:PRO:HG3	2:D:205:GLU:HG3	1.36	1.03
5:B:902:FTT:H72	5:B:903:FTT:C6	1.87	1.03
1:A:516:GLN:HE21	1:A:516:GLN:HA	1.24	1.01
1:B:142:LYS:HE3	1:B:440:GLN:HE21	1.23	1.01
5:B:902:FTT:C9	5:B:903:FTT:C8	2.22	1.01
5:A:901:FTT:C1	3:E:1:GCN:C3	2.38	1.00
5:B:903:FTT:C1	3:F:2:GCN:C3	2.39	0.99
1:B:516:GLN:HE21	1:B:516:GLN:HA	1.23	0.99
5:B:900:FTT:C9	5:B:900:FTT:C8	2.41	0.99
5:B:901:FTT:H142	5:B:903:FTT:H132	1.43	0.98
1:A:81:ARG:HG3	1:A:84:SER:HB3	1.46	0.97
5:A:903:FTT:C1	3:E:2:GCN:C3	2.42	0.97
1:B:81:ARG:HG3	1:B:84:SER:HB3	1.47	0.96
1:A:11:VAL:HB	2:C:228:ILE:HG22	1.48	0.96
1:A:579:ARG:HG3	1:A:603:ASP:HB3	1.47	0.95
1:B:579:ARG:HG3	1:B:603:ASP:HB3	1.44	0.95
1:A:204:GLN:HE22	1:A:713:ALA:HA	1.31	0.95
1:A:343:ARG:NH1	1:A:400:LEU:HD22	1.79	0.95
1:A:353:GLN:HE21	1:A:384:ARG:HD2	1.32	0.95
1:B:343:ARG:NH1	1:B:400:LEU:HD22	1.81	0.95
1:A:38:LYS:HD2	1:A:139:LEU:HD22	1.49	0.95
1:B:353:GLN:HE21	1:B:384:ARG:HD2	1.31	0.94
1:B:204:GLN:HE22	1:B:713:ALA:HA	1.30	0.94
5:B:902:FTT:H132	5:B:903:FTT:C13	1.98	0.94
1:B:284:TYR:CD2	5:B:902:FTT:H143	2.04	0.93
5:B:901:FTT:C12	5:B:903:FTT:H112	1.98	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:THR:HG22	1:A:447:VAL:HG12	1.51	0.92
5:B:902:FTT:C13	5:B:903:FTT:C13	2.46	0.92
1:B:273:ASN:HD21	1:B:312:VAL:H	1.16	0.92
1:B:376:THR:HG22	1:B:447:VAL:HG12	1.50	0.92
1:A:678:ALA:HB2	1:A:683:ALA:HA	1.51	0.92
1:A:142:LYS:HE3	1:A:440:GLN:HE21	1.32	0.92
1:B:284:TYR:HD2	5:B:902:FTT:H143	1.34	0.91
1:A:52:VAL:HG22	1:A:130:GLU:HG2	1.52	0.91
1:B:298:GLN:C	1:B:299:ASN:HD22	1.79	0.91
1:B:273:ASN:ND2	1:B:312:VAL:H	1.68	0.90
1:B:38:LYS:HD2	1:B:139:LEU:HD22	1.51	0.90
1:A:273:ASN:ND2	1:A:312:VAL:H	1.69	0.90
5:B:901:FTT:H111	7:B:930:DAO:H92	1.54	0.90
1:B:342:ALA:O	1:B:343:ARG:HG3	1.72	0.90
1:A:342:ALA:O	1:A:343:ARG:HG3	1.72	0.90
1:B:135:PRO:HB3	1:B:510:SER:HB3	1.52	0.89
5:B:902:FTT:H92	5:B:903:FTT:H81	1.52	0.89
1:A:284:TYR:HD2	5:A:902:FTT:H143	1.37	0.89
5:B:901:FTT:H141	5:B:903:FTT:H132	1.50	0.89
1:A:273:ASN:HD21	1:A:312:VAL:H	1.17	0.89
1:B:142:LYS:H	1:B:442:GLN:HE22	1.20	0.88
1:A:298:GLN:C	1:A:299:ASN:HD22	1.80	0.88
2:D:184:PRO:HG3	2:D:220:PRO:HG3	1.56	0.87
1:B:678:ALA:HB2	1:B:683:ALA:HA	1.55	0.87
1:A:284:TYR:CD2	5:A:902:FTT:H143	2.10	0.86
1:A:9:ILE:HD12	2:C:158:ARG:NH1	1.91	0.85
1:B:134:GLY:CA	1:B:146:GLY:HA2	2.06	0.85
5:B:901:FTT:C14	5:B:903:FTT:C12	2.54	0.85
2:C:184:PRO:HG3	2:C:220:PRO:HG3	1.56	0.85
1:B:116:TYR:HB2	1:B:350:GLU:OE2	1.77	0.84
1:A:142:LYS:HG2	1:A:442:GLN:NE2	1.92	0.83
1:A:134:GLY:CA	1:A:146:GLY:HA2	2.08	0.83
1:A:135:PRO:HB3	1:A:510:SER:HB3	1.58	0.83
1:A:284:TYR:HE1	1:A:298:GLN:HG2	1.44	0.82
1:A:9:ILE:HD13	1:A:10:THR:H	1.44	0.82
1:A:11:VAL:HB	2:C:228:ILE:CG2	2.09	0.82
1:A:343:ARG:HH11	1:A:400:LEU:HD22	1.44	0.82
5:B:901:FTT:H143	5:B:903:FTT:C13	2.03	0.82
1:A:9:ILE:HD12	2:C:158:ARG:HH12	1.39	0.82
1:A:680:VAL:HG12	1:A:680:VAL:O	1.80	0.82
3:F:2:GCN:H62	3:F:3:KDO:O1A	1.77	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:910:DPO:O6	6:B:910:DPO:O7	1.99	0.81
1:B:70:LEU:HD12	1:B:90:LEU:HD21	1.62	0.81
1:A:142:LYS:H	1:A:442:GLN:HE22	1.25	0.80
1:A:533:GLU:HG3	1:A:552:TYR:HB3	1.63	0.80
5:B:901:FTT:C12	5:B:903:FTT:C11	2.60	0.80
1:B:52:VAL:HG22	1:B:130:GLU:HG2	1.62	0.80
1:B:343:ARG:HH11	1:B:400:LEU:HD22	1.45	0.79
5:B:901:FTT:H122	5:B:903:FTT:C11	2.13	0.79
1:A:116:TYR:HB2	1:A:350:GLU:OE2	1.82	0.79
5:B:902:FTT:C7	5:B:903:FTT:H62	2.11	0.79
1:A:70:LEU:HD12	1:A:90:LEU:HD21	1.64	0.78
1:B:533:GLU:HG3	1:B:552:TYR:HB3	1.63	0.78
5:B:901:FTT:H143	5:B:902:FTT:H131	1.64	0.78
5:B:901:FTT:C13	5:B:903:FTT:H112	2.12	0.78
5:B:902:FTT:H112	5:B:903:FTT:C9	2.12	0.77
1:B:284:TYR:HE1	1:B:298:GLN:HG2	1.49	0.77
5:B:901:FTT:H142	5:B:903:FTT:C13	2.01	0.77
1:A:107:ASN:HD21	1:A:153:SER:H	1.32	0.77
5:B:901:FTT:H142	5:B:903:FTT:C11	1.87	0.77
1:A:397:VAL:HB	1:A:421:PHE:CE1	2.20	0.77
1:B:134:GLY:C	1:B:146:GLY:HA2	2.10	0.77
1:B:142:LYS:HG2	1:B:442:GLN:NE2	2.00	0.76
5:B:901:FTT:H141	5:B:903:FTT:C13	2.10	0.76
1:A:57:GLU:O	1:A:60:LEU:HB3	1.86	0.76
1:B:370:ILE:HD13	1:B:370:ILE:H	1.50	0.76
1:B:616:THR:H	1:B:659:ASN:HD21	1.33	0.76
5:B:901:FTT:C14	5:B:903:FTT:H131	2.15	0.76
5:B:902:FTT:H112	5:B:903:FTT:H111	1.67	0.76
1:A:17:PRO:O	1:A:18:GLN:HB2	1.85	0.76
3:F:2:GCN:C6	3:F:3:KDO:O1A	2.34	0.76
1:B:680:VAL:HG12	1:B:680:VAL:O	1.86	0.75
5:A:900:FTT:O2	7:A:930:DAO:H22	1.86	0.75
5:B:901:FTT:H142	5:B:903:FTT:C12	2.14	0.75
5:B:902:FTT:H131	5:B:903:FTT:C13	2.11	0.75
3:F:4:KDO:C1	3:F:4:KDO:O1A	2.34	0.75
1:A:134:GLY:C	1:A:146:GLY:HA2	2.12	0.75
1:B:600:THR:HB	1:B:624:MET:HB2	1.67	0.75
1:A:262:LEU:HD21	1:A:402:LEU:HD12	1.69	0.75
1:B:107:ASN:HD21	1:B:153:SER:H	1.35	0.75
1:B:309:GLN:HE21	1:B:311:SER:HB2	1.52	0.75
5:B:900:FTT:O2	7:B:930:DAO:H22	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:GLU:O	1:B:60:LEU:HB3	1.87	0.74
1:A:370:ILE:HD13	1:A:370:ILE:H	1.51	0.74
1:A:62:GLN:HG3	1:A:167:LYS:HZ3	1.53	0.74
1:B:262:LEU:HD21	1:B:402:LEU:HD12	1.69	0.74
1:A:397:VAL:HB	1:A:421:PHE:HE1	1.52	0.73
1:B:267:ASN:ND2	1:B:269:GLY:H	1.85	0.73
1:B:397:VAL:HB	1:B:421:PHE:CE1	2.23	0.73
1:A:267:ASN:ND2	1:A:269:GLY:H	1.86	0.73
1:A:309:GLN:HE21	1:A:311:SER:HB2	1.51	0.73
1:A:99:GLY:HA2	9:A:1050:FCI:H16	1.70	0.73
1:A:600:THR:HB	1:A:624:MET:HB2	1.70	0.73
1:B:142:LYS:H	1:B:442:GLN:NE2	1.87	0.73
5:B:902:FTT:H92	5:B:903:FTT:C9	2.18	0.72
5:B:901:FTT:H143	5:B:903:FTT:C12	2.16	0.72
1:A:616:THR:H	1:A:659:ASN:HD21	1.35	0.72
1:B:197:LEU:C	1:B:197:LEU:HD12	2.14	0.72
1:B:551:VAL:HB	1:B:581:VAL:HG12	1.72	0.72
1:A:133:ARG:NE	1:A:582:GLU:OE2	2.21	0.72
1:A:316:GLY:H	1:A:707:TYR:HB2	1.55	0.72
1:B:19:GLU:HG2	1:B:20:SER:N	2.05	0.72
1:A:551:VAL:HB	1:A:581:VAL:HG12	1.72	0.72
1:B:604:ALA:O	1:B:616:THR:HG22	1.90	0.71
1:A:197:LEU:C	1:A:197:LEU:HD12	2.15	0.71
1:B:162:LYS:HA	1:B:180:PHE:HD1	1.54	0.71
1:A:451:ALA:HB3	1:A:458:VAL:HG23	1.73	0.71
1:A:604:ALA:O	1:A:616:THR:HG22	1.89	0.71
1:B:401:ASN:C	1:B:402:LEU:HD22	2.14	0.71
1:B:451:ALA:HB3	1:B:458:VAL:HG23	1.72	0.71
1:A:281:MET:HB3	1:A:303:ALA:HB2	1.71	0.71
1:A:401:ASN:C	1:A:402:LEU:HD22	2.16	0.71
2:D:214:ARG:HB3	2:D:214:ARG:NH1	2.05	0.70
1:B:142:LYS:HE3	1:B:440:GLN:NE2	2.03	0.70
1:B:397:VAL:HB	1:B:421:PHE:HE1	1.56	0.70
1:A:162:LYS:HA	1:A:180:PHE:HD1	1.56	0.70
2:C:214:ARG:NH1	2:C:214:ARG:HB3	2.06	0.70
1:A:50:ILE:HG22	1:A:51:SER:N	2.06	0.70
2:D:215:TYR:HD1	2:D:216:GLU:H	1.38	0.70
1:B:281:MET:HB3	1:B:303:ALA:HB2	1.74	0.69
1:B:390:TRP:NE1	1:B:431:SER:HB3	2.01	0.69
2:D:193:ILE:HD11	2:D:207:LYS:HD3	1.72	0.69
2:C:215:TYR:HD1	2:C:216:GLU:H	1.38	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:193:ILE:HD11	2:C:207:LYS:HD3	1.74	0.69
1:A:704:PHE:CE2	1:A:708:GLY:HA3	2.28	0.69
1:B:316:GLY:H	1:B:707:TYR:HB2	1.58	0.69
5:A:900:FTT:H111	5:B:900:FTT:H111	1.74	0.69
1:B:205:GLN:HG3	1:B:243:TYR:CB	2.23	0.68
5:A:900:FTT:H142	5:B:900:FTT:H122	1.74	0.68
5:A:901:FTT:H143	7:A:930:DAO:H111	1.74	0.68
1:B:503:PRO:HA	1:B:536:VAL:HG12	1.76	0.68
5:B:901:FTT:C14	5:B:902:FTT:H131	2.23	0.68
1:A:142:LYS:H	1:A:442:GLN:NE2	1.91	0.68
6:A:910:DPO:P2	6:B:910:DPO:O6	2.51	0.68
1:B:339:HIS:O	1:B:402:LEU:HD23	1.93	0.68
1:B:50:ILE:HG22	1:B:51:SER:N	2.08	0.68
1:A:9:ILE:CD1	1:A:10:THR:H	2.05	0.68
1:A:475:VAL:HG22	1:A:475:VAL:O	1.94	0.68
1:B:678:ALA:CB	1:B:683:ALA:HA	2.24	0.68
1:A:205:GLN:HG3	1:A:243:TYR:CB	2.24	0.67
1:B:499:ASN:OD1	1:B:501:VAL:HG22	1.95	0.67
1:B:594:ASN:HB2	1:B:630:ASP:OD2	1.94	0.67
1:B:110:LYS:HG2	1:B:112:GLN:HG2	1.76	0.67
1:B:215:ILE:O	1:B:217:PRO:HD3	1.94	0.67
1:A:544:PRO:HG2	1:A:588:ALA:HB3	1.76	0.67
1:B:70:LEU:CD1	1:B:90:LEU:HD21	2.25	0.67
1:B:133:ARG:NE	1:B:582:GLU:OE2	2.24	0.67
1:B:704:PHE:CE2	1:B:708:GLY:HA3	2.30	0.67
3:E:2:GCN:H62	3:E:3:KDO:O1A	1.95	0.67
1:A:134:GLY:N	1:A:146:GLY:HA2	2.10	0.67
1:A:401:ASN:CG	1:A:402:LEU:H	2.03	0.67
1:A:148:LEU:C	1:A:148:LEU:HD23	2.21	0.66
1:A:678:ALA:CB	1:A:683:ALA:HA	2.22	0.66
1:A:11:VAL:CB	2:C:228:ILE:HG22	2.25	0.66
1:A:503:PRO:HA	1:A:536:VAL:HG12	1.77	0.66
1:B:373:THR:HB	1:B:450:GLN:HB2	1.78	0.66
1:A:299:ASN:HD22	1:A:299:ASN:N	1.92	0.66
1:A:352:LEU:C	1:A:352:LEU:HD12	2.20	0.66
1:A:211:GLN:NE2	1:A:213:TYR:OH	2.29	0.66
1:B:134:GLY:N	1:B:146:GLY:HA2	2.09	0.66
5:B:902:FTT:H112	5:B:903:FTT:C11	2.25	0.66
1:A:392:GLY:HA3	1:A:396:SER:OG	1.96	0.66
1:B:475:VAL:HG22	1:B:475:VAL:O	1.95	0.66
1:A:339:HIS:O	1:A:402:LEU:HD23	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ASN:HD22	1:B:299:ASN:N	1.90	0.66
1:B:549:GLY:CA	1:B:583:ILE:HG22	2.26	0.66
1:B:204:GLN:NE2	1:B:713:ALA:HA	2.07	0.66
5:B:901:FTT:H143	5:B:903:FTT:H131	1.78	0.66
1:A:281:MET:HB3	1:A:303:ALA:CB	2.26	0.65
1:A:12:THR:O	2:C:160:GLN:NE2	2.30	0.65
1:A:373:THR:HB	1:A:450:GLN:HB2	1.78	0.65
1:B:105:TYR:CE2	1:B:110:LYS:HB2	2.31	0.65
1:A:204:GLN:NE2	1:A:713:ALA:HA	2.08	0.65
1:A:284:TYR:CE1	1:A:298:GLN:HG2	2.30	0.65
1:A:353:GLN:HE21	1:A:384:ARG:CD	2.07	0.65
1:A:655:GLY:HA3	1:A:661:PHE:CZ	2.31	0.65
8:B:980:EAP:H11	3:F:5:GMH:H6	1.78	0.65
1:A:70:LEU:CD1	1:A:90:LEU:HD21	2.26	0.65
1:A:594:ASN:HB2	1:A:630:ASP:OD2	1.97	0.65
1:B:189:VAL:HG13	1:B:190:TYR:CD2	2.32	0.65
1:A:499:ASN:OD1	1:A:501:VAL:HG22	1.95	0.65
1:A:531:GLN:HG3	1:A:554:LEU:HB2	1.79	0.65
1:A:107:ASN:ND2	1:A:153:SER:H	1.95	0.64
1:A:549:GLY:CA	1:A:583:ILE:HG22	2.27	0.64
2:C:164:PRO:HG3	2:C:205:GLU:CG	2.21	0.64
2:C:177:LYS:HB3	2:C:194:LEU:HB2	1.78	0.64
1:A:110:LYS:HG2	1:A:112:GLN:HG2	1.77	0.64
1:B:544:PRO:HG2	1:B:588:ALA:HB3	1.79	0.64
1:A:125:MET:HG3	1:A:234:TYR:HE1	1.62	0.64
8:A:980:EAP:H11	3:E:5:GMH:H6	1.79	0.64
1:B:392:GLY:HA3	1:B:396:SER:OG	1.97	0.64
6:B:910:DPO:O3	3:F:1:GCN:C1	2.46	0.64
1:A:401:ASN:CG	1:A:402:LEU:N	2.53	0.64
1:B:352:LEU:C	1:B:352:LEU:HD12	2.22	0.64
5:A:900:FTT:H42	5:B:900:FTT:H22	1.80	0.64
1:B:495:TYR:O	1:B:503:PRO:HD2	1.98	0.64
1:B:211:GLN:NE2	1:B:213:TYR:OH	2.31	0.64
1:A:352:LEU:HD12	1:A:353:GLN:N	2.13	0.64
1:B:352:LEU:HD12	1:B:353:GLN:N	2.13	0.64
1:B:380:PHE:CZ	5:B:900:FTT:H51	2.33	0.64
1:B:655:GLY:HA3	1:B:661:PHE:CZ	2.32	0.64
1:A:495:TYR:O	1:A:503:PRO:HD2	1.98	0.63
1:B:104:ASN:ND2	1:B:149:LEU:HD23	2.13	0.63
1:B:401:ASN:CG	1:B:402:LEU:N	2.56	0.63
1:A:189:VAL:HG13	1:A:190:TYR:CD2	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LYS:HD3	1:A:193:ARG:NH2	2.13	0.63
2:C:226:VAL:O	2:C:227:ASN:HB3	1.98	0.63
2:D:164:PRO:HG3	2:D:205:GLU:CG	2.21	0.63
2:D:177:LYS:HB3	2:D:194:LEU:HB2	1.79	0.63
5:B:902:FTT:H92	5:B:903:FTT:H82	0.65	0.63
6:A:910:DPO:O3	3:E:1:GCN:C1	2.46	0.63
1:B:551:VAL:CB	1:B:581:VAL:HG12	2.29	0.63
1:B:353:GLN:HE21	1:B:384:ARG:CD	2.07	0.63
1:B:401:ASN:CG	1:B:402:LEU:H	2.06	0.63
1:B:531:GLN:HG3	1:B:554:LEU:HB2	1.78	0.63
2:D:226:VAL:O	2:D:227:ASN:HB3	1.99	0.63
1:A:309:GLN:HE21	1:A:311:SER:CB	2.11	0.62
5:B:903:FTT:O3	10:B:940:MYR:C2	2.47	0.62
1:B:125:MET:HG3	1:B:234:TYR:HE1	1.63	0.62
1:B:281:MET:HB3	1:B:303:ALA:CB	2.29	0.62
5:B:901:FTT:H121	5:B:903:FTT:H112	1.81	0.62
1:B:523:ILE:HD13	1:B:523:ILE:H	1.63	0.62
1:A:215:ILE:O	1:A:217:PRO:HD3	1.99	0.62
1:B:154:LYS:HD3	1:B:193:ARG:NH2	2.14	0.62
1:A:33:SER:OG	1:A:34:ALA:N	2.32	0.62
1:A:105:TYR:CE2	1:A:110:LYS:HB2	2.35	0.62
1:A:46:VAL:HG12	1:A:48:GLN:H	1.65	0.62
1:A:315:TYR:O	1:A:316:GLY:O	2.18	0.62
1:A:676:ASP:OD2	2:C:200:ASN:HB2	2.00	0.62
1:B:46:VAL:HG12	1:B:48:GLN:H	1.64	0.62
1:A:50:ILE:CG2	1:A:51:SER:N	2.63	0.62
5:A:901:FTT:H71	5:B:900:FTT:H72	1.82	0.62
1:B:516:GLN:HA	1:B:516:GLN:NE2	2.07	0.62
1:A:42:PRO:HB2	1:A:44:GLN:OE1	2.00	0.61
1:A:93:ARG:HH21	1:A:582:GLU:CD	2.09	0.61
1:A:104:ASN:ND2	1:A:149:LEU:HD23	2.15	0.61
1:B:107:ASN:ND2	1:B:153:SER:H	1.97	0.61
1:B:205:GLN:HG3	1:B:243:TYR:CG	2.35	0.61
5:B:901:FTT:H131	7:B:930:DAO:H112	1.82	0.61
1:A:205:GLN:HG3	1:A:243:TYR:HB2	1.81	0.61
1:B:148:LEU:HD23	1:B:148:LEU:C	2.26	0.61
1:A:95:PHE:HE1	1:A:578:ALA:HB2	1.66	0.61
1:A:199:ARG:HH22	1:A:212:ARG:NH1	1.98	0.61
1:A:523:ILE:HD13	1:A:523:ILE:H	1.66	0.61
1:A:551:VAL:CB	1:A:581:VAL:HG12	2.31	0.61
1:B:274:THR:HG22	1:B:310:ASN:HB2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:ILE:CD1	2:D:207:LYS:HD3	2.31	0.60
1:B:328:GLN:HE21	1:B:395:ASP:HB3	1.67	0.60
1:A:221:TRP:CE2	1:A:223:PRO:HG3	2.36	0.60
1:B:134:GLY:H	1:B:146:GLY:HA2	1.66	0.60
1:A:11:VAL:HG12	1:A:12:THR:N	2.16	0.60
1:A:563:ASP:HA	1:A:571:VAL:HG21	1.82	0.60
1:B:205:GLN:HG3	1:B:243:TYR:HB2	1.84	0.60
2:C:232:ILE:O	2:C:233:ASN:C	2.44	0.60
1:B:42:PRO:HB2	1:B:44:GLN:OE1	2.02	0.60
1:B:197:LEU:HD12	1:B:197:LEU:O	2.02	0.60
1:B:284:TYR:CE1	1:B:298:GLN:HG2	2.33	0.60
2:C:167:ALA:C	2:C:169:ALA:H	2.10	0.60
1:B:380:PHE:CE1	5:B:900:FTT:H51	2.37	0.60
5:B:902:FTT:C9	5:B:903:FTT:H81	2.21	0.60
1:A:252:THR:O	1:A:261:ARG:HD3	2.01	0.60
1:A:516:GLN:HE21	1:A:516:GLN:CA	2.01	0.60
1:B:309:GLN:HE21	1:B:311:SER:CB	2.14	0.60
1:B:62:GLN:HG3	1:B:167:LYS:HZ3	1.67	0.59
1:B:476:ALA:C	1:B:478:THR:H	2.10	0.59
1:B:549:GLY:HA2	1:B:583:ILE:HG22	1.84	0.59
2:D:163:TYR:HD2	2:D:164:PRO:HD2	1.67	0.59
1:A:380:PHE:CZ	5:A:900:FTT:H51	2.36	0.59
1:A:516:GLN:HA	1:A:516:GLN:NE2	2.08	0.59
6:A:910:DPO:P2	6:B:910:DPO:P2	3.01	0.59
1:A:295:THR:O	1:A:361:LEU:HD12	2.03	0.59
1:B:563:ASP:HA	1:B:571:VAL:HG21	1.84	0.59
1:A:134:GLY:H	1:A:146:GLY:HA2	1.67	0.59
1:B:315:TYR:O	1:B:316:GLY:O	2.19	0.59
1:A:9:ILE:CG1	1:A:10:THR:H	2.15	0.59
1:A:37:THR:HA	1:A:139:LEU:HD11	1.85	0.59
1:A:60:LEU:HD11	1:A:628:TRP:CH2	2.37	0.59
1:B:366:ALA:O	1:B:367:THR:HG23	2.02	0.59
2:D:180:PHE:HE2	2:D:226:VAL:HG23	1.68	0.59
1:A:291:ASN:ND2	1:A:293:THR:H	2.01	0.59
1:A:576:ILE:HD11	1:A:606:TYR:CE1	2.38	0.59
1:B:108:GLY:H	1:B:150:ASN:HD21	1.50	0.59
1:B:291:ASN:ND2	1:B:293:THR:H	2.01	0.59
1:A:274:THR:HG22	1:A:310:ASN:HB2	1.84	0.58
1:B:44:GLN:HG2	1:B:45:LYS:N	2.16	0.58
1:A:44:GLN:HG2	1:A:45:LYS:N	2.18	0.58
1:A:148:LEU:HD23	1:A:148:LEU:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ILE:CG2	1:B:51:SER:N	2.65	0.58
1:B:60:LEU:HD11	1:B:628:TRP:CH2	2.38	0.58
1:B:685:SER:OG	1:B:723:PHE:HA	2.03	0.58
1:A:685:SER:OG	1:A:723:PHE:HA	2.04	0.58
1:B:516:GLN:HE21	1:B:516:GLN:CA	1.99	0.58
1:A:453:TRP:O	1:A:455:LYS:N	2.36	0.58
2:C:193:ILE:CD1	2:C:207:LYS:HD3	2.33	0.58
2:C:232:ILE:HD12	2:C:232:ILE:H	1.68	0.58
3:E:2:GCN:C6	3:E:3:KDO:O1A	2.52	0.58
1:A:99:GLY:HA2	9:A:1050:FCI:O17	2.04	0.58
1:B:167:LYS:HB2	1:B:175:GLN:HB3	1.85	0.58
1:A:476:ALA:C	1:A:478:THR:H	2.09	0.58
1:A:205:GLN:HG3	1:A:243:TYR:CG	2.39	0.58
1:A:274:THR:CG2	1:A:310:ASN:HB2	2.34	0.58
1:B:274:THR:CG2	1:B:310:ASN:HB2	2.34	0.58
1:B:95:PHE:HE1	1:B:578:ALA:HB2	1.68	0.57
1:B:453:TRP:O	1:B:455:LYS:N	2.36	0.57
1:A:142:LYS:HE3	1:A:440:GLN:NE2	2.12	0.57
1:A:167:LYS:HB2	1:A:175:GLN:HB3	1.86	0.57
1:A:291:ASN:O	1:A:293:THR:N	2.37	0.57
1:A:328:GLN:HE21	1:A:395:ASP:HB3	1.68	0.57
1:A:329:CYS:O	1:A:332:LEU:HG	2.04	0.57
1:B:221:TRP:CE2	1:B:223:PRO:HG3	2.39	0.57
1:B:617:PRO:O	1:B:620:VAL:HG13	2.04	0.57
8:B:980:EAP:C1	3:F:5:GMH:H6	2.35	0.57
2:D:167:ALA:C	2:D:169:ALA:H	2.13	0.57
1:A:108:GLY:H	1:A:150:ASN:HD21	1.50	0.57
1:B:93:ARG:HH21	1:B:582:GLU:CD	2.11	0.57
1:B:199:ARG:HH22	1:B:212:ARG:NH1	2.01	0.57
2:C:163:TYR:HD2	2:C:164:PRO:HD2	1.68	0.57
5:B:903:FTT:O3	10:B:940:MYR:H22	2.05	0.57
2:D:215:TYR:O	2:D:217:PRO:HD3	2.05	0.57
5:A:900:FTT:C11	5:B:900:FTT:H111	2.35	0.57
2:C:180:PHE:HE2	2:C:226:VAL:HG23	1.70	0.57
1:A:617:PRO:O	1:A:620:VAL:HG13	2.05	0.56
5:A:900:FTT:H81	5:B:900:FTT:H82	1.87	0.56
8:A:980:EAP:C1	3:E:5:GMH:H6	2.35	0.56
1:B:252:THR:O	1:B:261:ARG:HD3	2.05	0.56
1:A:52:VAL:HG22	1:A:130:GLU:CG	2.32	0.56
1:A:71:SER:HB3	1:A:648:ARG:HD2	1.88	0.56
1:A:163:GLU:HB2	1:A:724:ARG:HG2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ALA:O	1:A:367:THR:HG23	2.04	0.56
1:A:380:PHE:CE1	5:A:900:FTT:H51	2.39	0.56
1:A:549:GLY:HA2	1:A:583:ILE:HG22	1.85	0.56
2:C:188:VAL:HG22	2:C:189:ASP:N	2.20	0.56
2:C:215:TYR:O	2:C:217:PRO:HD3	2.05	0.56
3:E:4:KDO:O1A	3:E:4:KDO:O1B	2.23	0.56
1:B:575:GLU:HG2	1:B:607:THR:HB	1.87	0.56
1:B:675:TYR:HD2	1:B:676:ASP:N	2.04	0.56
1:A:575:GLU:HG2	1:A:607:THR:HB	1.87	0.56
5:A:900:FTT:H21	6:A:910:DPO:O5	2.05	0.56
1:B:162:LYS:HA	1:B:180:PHE:CD1	2.38	0.56
5:A:901:FTT:H122	7:A:930:DAO:H91	1.87	0.56
1:A:675:TYR:HD2	1:A:676:ASP:N	2.03	0.56
1:B:591:ALA:C	2:D:166:ARG:HH22	2.14	0.56
1:A:11:VAL:HG12	1:A:12:THR:H	1.71	0.55
1:A:327:LYS:HB2	1:A:395:ASP:OD2	2.07	0.55
1:B:37:THR:HA	1:B:139:LEU:HD11	1.87	0.55
1:B:352:LEU:HB3	1:B:385:ASN:OD1	2.06	0.55
5:B:900:FTT:H21	6:B:910:DPO:O5	2.05	0.55
1:A:62:GLN:HG3	1:A:167:LYS:NZ	2.20	0.55
1:A:163:GLU:HA	1:A:723:PHE:O	2.07	0.55
1:B:62:GLN:HG3	1:B:167:LYS:NZ	2.21	0.55
2:D:188:VAL:HG22	2:D:189:ASP:N	2.20	0.55
5:B:902:FTT:C7	5:B:903:FTT:C6	2.74	0.55
2:C:164:PRO:CG	2:C:205:GLU:HG3	2.25	0.55
2:D:164:PRO:CG	2:D:205:GLU:HG3	2.25	0.55
1:A:182:ASP:HB3	1:A:192:TYR:HE1	1.71	0.55
1:B:33:SER:OG	1:B:34:ALA:N	2.39	0.55
1:B:185:ASP:CG	1:B:189:VAL:HG12	2.32	0.55
1:B:549:GLY:HA3	1:B:583:ILE:HG22	1.88	0.55
1:A:352:LEU:HB3	1:A:385:ASN:OD1	2.07	0.55
2:C:215:TYR:HD1	2:C:216:GLU:N	2.05	0.55
1:B:343:ARG:HH12	1:B:400:LEU:HD22	1.71	0.55
5:B:902:FTT:C11	5:B:903:FTT:H92	2.22	0.55
1:A:309:GLN:NE2	1:A:311:SER:HB2	2.20	0.55
1:A:354:ASN:C	1:A:354:ASN:ND2	2.64	0.55
2:C:177:LYS:HB3	2:C:194:LEU:HD12	1.89	0.55
1:A:549:GLY:HA3	1:A:583:ILE:HG22	1.89	0.54
2:C:178:VAL:HG11	2:C:210:MET:SD	2.47	0.54
1:A:501:VAL:O	1:A:501:VAL:HG23	2.08	0.54
1:A:661:PHE:HD1	1:A:661:PHE:H	1.55	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:LYS:N	1:B:442:GLN:HE22	1.99	0.54
1:B:284:TYR:HB3	5:B:902:FTT:C14	2.38	0.54
1:A:217:PRO:HD2	1:A:233:SER:OG	2.07	0.54
1:B:72:TYR:CE2	1:B:628:TRP:HB2	2.42	0.54
1:B:295:THR:O	1:B:361:LEU:HD12	2.06	0.54
1:A:72:TYR:CE2	1:A:628:TRP:HB2	2.42	0.54
1:B:66:VAL:O	1:B:70:LEU:HG	2.08	0.54
1:B:523:ILE:HD13	1:B:523:ILE:N	2.23	0.54
1:A:162:LYS:HA	1:A:180:PHE:CD1	2.39	0.54
1:A:451:ALA:O	1:A:457:LEU:HD23	2.08	0.54
1:B:182:ASP:HB3	1:B:192:TYR:HE1	1.73	0.54
1:A:9:ILE:HD13	1:A:10:THR:N	2.17	0.54
1:A:262:LEU:HD23	1:A:266:PHE:CD2	2.43	0.54
1:A:500:GLY:O	1:A:501:VAL:C	2.50	0.54
3:F:4:KDO:H32	3:F:5:GMH:H71	1.89	0.54
1:A:197:LEU:HD12	1:A:197:LEU:O	2.06	0.54
3:F:4:KDO:O1B	3:F:4:KDO:O1A	2.26	0.54
1:B:329:CYS:O	1:B:332:LEU:HG	2.07	0.54
2:D:215:TYR:HD1	2:D:216:GLU:N	2.05	0.54
3:E:4:KDO:H32	3:E:5:GMH:H71	1.89	0.54
1:A:648:ARG:NH1	1:A:670:ASP:OD2	2.40	0.53
1:B:327:LYS:HB2	1:B:395:ASP:OD2	2.08	0.53
1:B:546:VAL:O	1:B:546:VAL:HG12	2.07	0.53
2:D:177:LYS:HB3	2:D:194:LEU:HD12	1.90	0.53
1:B:497:PHE:C	1:B:499:ASN:H	2.17	0.53
2:D:178:VAL:HG11	2:D:210:MET:SD	2.48	0.53
2:D:227:ASN:C	2:D:227:ASN:HD22	2.16	0.53
1:B:102:GLN:HG2	1:B:118:ASP:OD2	2.09	0.53
1:B:262:LEU:HD23	1:B:266:PHE:CD2	2.44	0.53
1:A:393:TYR:O	1:A:395:ASP:N	2.41	0.53
1:A:433:PRO:HG2	1:A:475:VAL:HG21	1.90	0.53
1:A:546:VAL:HG12	1:A:546:VAL:O	2.07	0.53
1:B:163:GLU:HB2	1:B:724:ARG:HG2	1.90	0.53
1:B:576:ILE:HD11	1:B:606:TYR:CE1	2.43	0.53
1:A:113:GLY:O	1:A:114:ASN:HB2	2.08	0.53
1:A:185:ASP:CG	1:A:189:VAL:HG12	2.33	0.53
1:B:500:GLY:O	1:B:501:VAL:C	2.51	0.53
1:A:284:TYR:OH	1:A:298:GLN:NE2	2.42	0.53
1:B:309:GLN:NE2	1:B:311:SER:HB2	2.22	0.53
2:C:178:VAL:HG11	2:C:210:MET:HE1	1.91	0.53
1:B:291:ASN:O	1:B:293:THR:N	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLN:HG2	1:A:118:ASP:OD2	2.09	0.53
2:C:167:ALA:C	2:C:169:ALA:N	2.64	0.53
1:A:628:TRP:CD1	1:A:646:GLY:HA3	2.44	0.53
1:B:354:ASN:C	1:B:354:ASN:HD22	2.17	0.53
1:A:354:ASN:C	1:A:354:ASN:HD22	2.17	0.52
1:B:189:VAL:HG13	1:B:190:TYR:H	1.75	0.52
1:B:451:ALA:O	1:B:457:LEU:HD23	2.09	0.52
2:D:214:ARG:HB3	2:D:214:ARG:HH11	1.73	0.52
1:A:543:ARG:HG3	1:A:543:ARG:HH11	1.75	0.52
2:C:167:ALA:O	2:C:169:ALA:N	2.42	0.52
1:A:563:ASP:HA	1:A:571:VAL:CG2	2.39	0.52
1:A:401:ASN:O	1:A:402:LEU:HD22	2.10	0.52
1:B:298:GLN:HE22	5:B:900:FTT:H142	1.73	0.52
1:B:426:LYS:O	1:B:428:PRO:HD3	2.09	0.52
1:A:483:ASP:OD1	3:F:4:KDO:H7	2.10	0.52
1:A:497:PHE:C	1:A:499:ASN:H	2.18	0.52
1:B:339:HIS:C	1:B:402:LEU:HD23	2.33	0.52
1:B:354:ASN:C	1:B:354:ASN:ND2	2.65	0.52
1:B:433:PRO:HG2	1:B:475:VAL:HG21	1.90	0.52
1:B:661:PHE:HD1	1:B:661:PHE:H	1.57	0.52
5:B:903:FTT:H21	10:B:940:MYR:C1	2.39	0.52
2:D:178:VAL:HG11	2:D:210:MET:HE1	1.92	0.52
1:B:312:VAL:HG23	1:B:423:PHE:CZ	2.45	0.52
1:A:523:ILE:HD13	1:A:523:ILE:N	2.25	0.52
1:B:563:ASP:HA	1:B:571:VAL:CG2	2.40	0.52
1:A:331:ALA:C	1:A:332:LEU:HD23	2.35	0.52
1:B:113:GLY:O	1:B:114:ASN:HB2	2.09	0.52
1:B:284:TYR:OH	1:B:298:GLN:NE2	2.43	0.52
1:B:648:ARG:NH1	1:B:670:ASP:OD2	2.42	0.52
1:A:182:ASP:CG	1:A:183:SER:H	2.18	0.51
1:A:370:ILE:H	1:A:370:ILE:CD1	2.23	0.51
1:A:608:THR:HG22	1:A:608:THR:O	2.10	0.51
1:B:628:TRP:CD1	1:B:646:GLY:HA3	2.45	0.51
2:C:227:ASN:HD22	2:C:227:ASN:C	2.16	0.51
1:A:390:TRP:CZ3	1:A:433:PRO:HB3	2.45	0.51
1:B:267:ASN:C	1:B:267:ASN:HD22	2.19	0.51
2:C:183:THR:O	2:C:185:ASP:N	2.44	0.51
1:A:339:HIS:C	1:A:402:LEU:HD23	2.36	0.51
1:A:446:TYR:HB3	1:A:463:ARG:HB2	1.93	0.51
2:D:183:THR:O	2:D:185:ASP:N	2.44	0.51
1:A:58:MET:O	1:A:60:LEU:N	2.37	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LEU:HB2	1:A:384:ARG:O	2.11	0.51
1:B:343:ARG:HH11	1:B:400:LEU:CD2	2.20	0.51
1:B:60:LEU:HD23	1:B:60:LEU:C	2.35	0.51
2:C:214:ARG:HB3	2:C:214:ARG:HH11	1.73	0.51
1:A:95:PHE:CE1	1:A:578:ALA:HB2	2.45	0.51
1:B:543:ARG:HG3	1:B:543:ARG:HH11	1.75	0.51
1:B:591:ALA:O	2:D:166:ARG:NH2	2.43	0.51
1:B:71:SER:HB3	1:B:648:ARG:HD2	1.91	0.51
1:B:217:PRO:HD2	1:B:233:SER:OG	2.10	0.51
1:B:608:THR:O	1:B:608:THR:HG22	2.11	0.51
1:A:426:LYS:O	1:A:428:PRO:HD3	2.11	0.51
5:B:902:FTT:C11	5:B:903:FTT:C11	2.72	0.51
2:D:167:ALA:C	2:D:169:ALA:N	2.67	0.51
1:A:343:ARG:HH11	1:A:400:LEU:CD2	2.19	0.51
1:B:284:TYR:HD2	5:B:902:FTT:C14	2.16	0.51
5:B:900:FTT:O2	7:B:930:DAO:C2	2.57	0.51
1:B:299:ASN:N	1:B:299:ASN:ND2	2.57	0.50
1:A:312:VAL:HG23	1:A:423:PHE:CZ	2.46	0.50
1:A:687:VAL:HG23	1:A:687:VAL:O	2.10	0.50
1:B:393:TYR:O	1:B:395:ASP:N	2.44	0.50
1:B:501:VAL:HG23	1:B:501:VAL:O	2.12	0.50
1:A:262:LEU:HD23	1:A:266:PHE:CG	2.47	0.50
1:A:628:TRP:HD1	1:A:646:GLY:HA3	1.76	0.50
1:B:182:ASP:CG	1:B:183:SER:H	2.19	0.50
1:A:503:PRO:CA	1:A:536:VAL:HG12	2.41	0.50
1:B:196:GLY:HA2	1:B:214:ALA:O	2.12	0.50
1:B:163:GLU:HA	1:B:723:PHE:O	2.11	0.50
1:B:592:SER:O	1:B:631:TYR:HA	2.11	0.50
1:A:189:VAL:HG13	1:A:190:TYR:H	1.77	0.50
1:B:561:MET:O	1:B:571:VAL:N	2.37	0.50
1:A:130:GLU:O	1:A:149:LEU:HD12	2.12	0.50
5:B:902:FTT:H132	5:B:903:FTT:C12	2.41	0.50
1:A:695:PHE:O	1:A:696:ASP:C	2.55	0.50
1:B:148:LEU:HD23	1:B:148:LEU:O	2.11	0.50
1:B:300:LEU:HD21	5:B:902:FTT:H102	1.94	0.50
1:A:17:PRO:O	1:A:18:GLN:CB	2.58	0.49
1:A:284:TYR:HB3	5:A:902:FTT:C14	2.42	0.49
1:A:189:VAL:HG13	1:A:190:TYR:N	2.27	0.49
1:A:511:PHE:CD1	1:A:511:PHE:C	2.90	0.49
1:B:19:GLU:HG2	1:B:20:SER:H	1.74	0.49
1:B:106:LEU:HD12	1:B:151:MET:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:C	1:A:60:LEU:HD23	2.36	0.49
1:B:248:PRO:HB3	1:B:316:GLY:HA2	1.94	0.49
1:B:503:PRO:CA	1:B:536:VAL:HG12	2.40	0.49
1:A:66:VAL:O	1:A:70:LEU:HG	2.13	0.49
1:B:344:LYS:HE2	1:B:394:ASP:H	1.76	0.49
1:B:331:ALA:C	1:B:332:LEU:HD23	2.38	0.49
1:A:592:SER:O	1:A:631:TYR:HA	2.12	0.49
1:B:115:PHE:CD2	1:B:387:ILE:HD13	2.47	0.49
1:A:343:ARG:HH12	1:A:400:LEU:HD22	1.70	0.49
5:A:900:FTT:H101	5:B:900:FTT:C9	2.43	0.49
1:B:401:ASN:O	1:B:402:LEU:HD22	2.12	0.49
1:B:446:TYR:HB3	1:B:463:ARG:HB2	1.94	0.49
1:A:182:ASP:CG	1:A:183:SER:N	2.70	0.49
1:B:110:LYS:HG3	1:B:112:GLN:N	2.27	0.49
1:A:106:LEU:HD22	1:A:121:ILE:HG13	1.93	0.49
1:A:133:ARG:NH2	1:A:582:GLU:OE2	2.46	0.49
1:A:618:ALA:O	1:A:619:GLN:HB2	2.13	0.49
1:B:130:GLU:O	1:B:149:LEU:HD12	2.12	0.49
1:B:649:TYR:HD1	1:B:667:THR:OG1	1.96	0.49
1:A:196:GLY:HA2	1:A:214:ALA:O	2.13	0.49
1:A:523:ILE:H	1:A:523:ILE:CD1	2.24	0.49
1:A:667:THR:H	1:A:697:ARG:HH12	1.61	0.49
1:B:628:TRP:HD1	1:B:646:GLY:HA3	1.77	0.49
5:B:901:FTT:C1	3:F:1:GCN:H32	2.38	0.49
2:D:214:ARG:HH11	2:D:214:ARG:CB	2.26	0.49
1:A:381:MET:SD	1:A:381:MET:C	2.95	0.48
5:A:901:FTT:C1	3:E:1:GCN:H32	2.39	0.48
1:A:390:TRP:NE1	1:A:431:SER:HB3	2.06	0.48
1:B:189:VAL:HG13	1:B:190:TYR:N	2.27	0.48
1:B:695:PHE:O	1:B:696:ASP:C	2.56	0.48
1:A:110:LYS:HG3	1:A:112:GLN:N	2.28	0.48
1:B:281:MET:CB	1:B:303:ALA:HB2	2.43	0.48
2:D:167:ALA:O	2:D:169:ALA:N	2.47	0.48
1:A:281:MET:CB	1:A:303:ALA:HB2	2.41	0.48
1:B:81:ARG:CG	1:B:84:SER:HB3	2.33	0.48
1:B:262:LEU:HD23	1:B:266:PHE:CG	2.48	0.48
1:B:628:TRP:CH2	1:B:630:ASP:HB3	2.48	0.48
1:A:60:LEU:HD21	1:A:628:TRP:CZ2	2.48	0.48
1:B:95:PHE:CE1	1:B:578:ALA:HB2	2.48	0.48
1:B:273:ASN:HD21	1:B:312:VAL:N	1.98	0.48
1:B:313:TYR:CZ	9:B:1050:FCI:H302	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LEU:C	1:B:197:LEU:CD1	2.84	0.48
1:B:240:GLU:HA	1:B:240:GLU:OE1	2.14	0.48
1:B:344:LYS:HA	1:B:396:SER:HB3	1.96	0.48
1:A:627:LEU:HD23	1:A:628:TRP:N	2.29	0.48
5:A:900:FTT:O2	7:A:930:DAO:C2	2.57	0.48
1:A:576:ILE:HG22	1:A:577:ARG:N	2.29	0.48
1:B:529:GLY:C	1:B:530:LYS:HD2	2.38	0.48
1:A:529:GLY:C	1:A:530:LYS:HD2	2.39	0.48
1:B:273:ASN:ND2	1:B:312:VAL:N	2.51	0.48
1:B:436:ILE:HD13	1:B:473:ASN:HA	1.96	0.48
2:C:176:VAL:O	2:C:227:ASN:HA	2.14	0.48
1:A:72:TYR:CE1	1:A:648:ARG:HD3	2.48	0.48
1:A:142:LYS:N	1:A:442:GLN:HE22	2.04	0.48
1:B:106:LEU:HD22	1:B:121:ILE:HG13	1.95	0.48
1:B:215:ILE:N	1:B:215:ILE:HD12	2.29	0.48
1:B:381:MET:SD	1:B:381:MET:C	2.96	0.48
1:A:32:GLN:HG2	1:A:42:PRO:HA	1.96	0.47
1:A:694:LEU:O	1:A:715:ARG:NH1	2.47	0.47
1:B:694:LEU:O	1:B:715:ARG:NH1	2.48	0.47
1:A:106:LEU:HD12	1:A:151:MET:O	2.14	0.47
1:B:192:TYR:CD1	1:B:192:TYR:C	2.92	0.47
1:B:37:THR:HB	1:B:448:GLN:HE22	1.78	0.47
1:B:58:MET:O	1:B:60:LEU:N	2.38	0.47
1:B:161:LEU:O	1:B:180:PHE:HA	2.14	0.47
1:B:190:TYR:CD2	1:B:190:TYR:N	2.82	0.47
1:B:511:PHE:CD1	1:B:511:PHE:C	2.92	0.47
1:B:277:ARG:HG3	1:B:277:ARG:HH11	1.79	0.47
2:D:176:VAL:O	2:D:227:ASN:HA	2.15	0.47
2:D:197:LYS:HB2	2:D:197:LYS:NZ	2.29	0.47
1:A:15:PRO:O	1:A:16:ALA:CB	2.63	0.47
1:A:228:ASN:OD1	1:A:229:PHE:N	2.48	0.47
1:B:241:THR:OG1	1:B:275:TYR:HB3	2.15	0.47
1:B:520:ASP:OD1	1:B:520:ASP:N	2.46	0.47
5:B:901:FTT:H122	5:B:903:FTT:C10	2.44	0.47
2:C:229:LEU:N	2:C:229:LEU:HD12	2.29	0.47
3:F:4:KDO:C1	3:F:4:KDO:H1B	2.13	0.47
1:A:10:THR:HG22	1:A:11:VAL:N	2.30	0.47
1:A:110:LYS:HG3	1:A:111:LEU:N	2.27	0.47
1:A:248:PRO:HB3	1:A:316:GLY:HA2	1.96	0.47
1:A:675:TYR:HD2	1:A:676:ASP:H	1.63	0.47
1:B:182:ASP:CG	1:B:183:SER:N	2.71	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LEU:CD2	1:B:268:GLU:HG3	2.45	0.47
1:B:352:LEU:HB2	1:B:384:ARG:O	2.14	0.47
1:B:375:LEU:O	1:B:447:VAL:HA	2.14	0.47
1:B:618:ALA:O	1:B:619:GLN:HB2	2.15	0.47
2:C:214:ARG:HH11	2:C:214:ARG:CB	2.27	0.47
1:A:190:TYR:CD2	1:A:190:TYR:N	2.83	0.47
1:A:436:ILE:HD13	1:A:473:ASN:HA	1.96	0.47
1:A:545:ILE:HG22	1:A:546:VAL:N	2.29	0.47
1:A:678:ALA:C	1:A:680:VAL:H	2.23	0.47
5:A:903:FTT:C1	3:E:2:GCN:H32	2.42	0.47
5:B:901:FTT:H122	5:B:903:FTT:H111	1.93	0.47
1:B:228:ASN:OD1	1:B:229:PHE:N	2.48	0.47
1:B:379:ASP:O	1:B:443:THR:HA	2.15	0.47
5:B:902:FTT:C8	5:B:903:FTT:C8	2.90	0.47
1:B:627:LEU:HD23	1:B:628:TRP:N	2.30	0.46
5:B:903:FTT:C1	3:F:2:GCN:H32	2.37	0.46
2:C:197:LYS:HB2	2:C:197:LYS:NZ	2.30	0.46
1:A:115:PHE:CD2	1:A:387:ILE:HD13	2.50	0.46
1:A:219:PHE:CD2	1:A:220:THR:N	2.84	0.46
1:A:344:LYS:HE2	1:A:394:ASP:H	1.79	0.46
1:A:649:TYR:HD1	1:A:667:THR:OG1	1.98	0.46
1:B:133:ARG:NH2	1:B:582:GLU:OE2	2.47	0.46
1:B:530:LYS:HD2	1:B:530:LYS:N	2.30	0.46
1:A:16:ALA:HA	1:A:17:PRO:HD2	1.67	0.46
1:A:270:ALA:O	1:A:272:ASN:N	2.48	0.46
1:B:105:TYR:CZ	1:B:110:LYS:HB2	2.51	0.46
1:B:370:ILE:H	1:B:370:ILE:CD1	2.23	0.46
1:B:667:THR:H	1:B:697:ARG:HH12	1.61	0.46
1:A:14:ALA:HB1	1:A:15:PRO:HD2	1.97	0.46
1:B:32:GLN:HG2	1:B:42:PRO:HA	1.97	0.46
1:B:60:LEU:HD21	1:B:628:TRP:CZ2	2.51	0.46
1:B:122:ASP:CG	1:B:123:PRO:HD2	2.40	0.46
1:B:190:TYR:N	1:B:190:TYR:HD2	2.12	0.46
5:B:901:FTT:H122	5:B:903:FTT:H101	1.98	0.46
5:B:901:FTT:H91	7:B:930:DAO:H72	1.96	0.46
5:B:901:FTT:O2	3:F:1:GCN:C3	2.61	0.46
2:C:181:ASP:OD1	2:C:190:ASN:CG	2.58	0.46
1:A:58:MET:C	1:A:60:LEU:H	2.22	0.46
1:A:724:ARG:HG3	1:A:724:ARG:HH11	1.81	0.46
1:A:50:ILE:CG2	1:A:51:SER:H	2.28	0.46
1:B:52:VAL:HG22	1:B:130:GLU:CG	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:TYR:CE1	1:B:648:ARG:HD3	2.51	0.46
1:B:678:ALA:C	1:B:680:VAL:H	2.23	0.46
5:B:901:FTT:O2	3:F:1:GCN:H32	2.15	0.46
1:A:436:ILE:CG2	1:A:438:ASN:HD21	2.29	0.46
1:B:675:TYR:HD2	1:B:676:ASP:H	1.64	0.46
2:D:227:ASN:C	2:D:227:ASN:ND2	2.73	0.46
1:A:189:VAL:HG13	1:A:190:TYR:HD2	1.78	0.46
1:A:240:GLU:OE1	1:A:240:GLU:HA	2.15	0.46
1:A:344:LYS:HA	1:A:396:SER:HB3	1.97	0.46
1:A:528:LYS:O	1:A:556:LYS:HA	2.15	0.46
1:B:89:HIS:CD2	1:B:100:GLN:HE21	2.34	0.46
1:B:545:ILE:HG22	1:B:546:VAL:N	2.31	0.46
2:D:229:LEU:N	2:D:229:LEU:HD12	2.30	0.46
1:B:352:LEU:HD12	1:B:353:GLN:C	2.41	0.46
5:B:901:FTT:H143	5:B:902:FTT:C13	2.39	0.46
5:B:901:FTT:H143	5:B:902:FTT:H111	1.98	0.46
1:A:142:LYS:O	1:A:143:SER:HB3	2.16	0.46
5:A:901:FTT:O2	3:E:1:GCN:C3	2.64	0.46
1:B:313:TYR:H	1:B:313:TYR:HD1	1.64	0.46
2:C:227:ASN:C	2:C:227:ASN:ND2	2.73	0.46
1:A:92:ILE:N	1:A:92:ILE:HD12	2.31	0.45
1:A:136:VAL:C	1:A:138:VAL:N	2.73	0.45
1:A:199:ARG:O	1:A:211:GLN:HA	2.16	0.45
1:A:493:VAL:O	1:A:504:TYR:HB2	2.16	0.45
1:B:219:PHE:CD2	1:B:220:THR:N	2.84	0.45
1:B:219:PHE:O	1:B:230:THR:HG23	2.15	0.45
1:A:190:TYR:N	1:A:190:TYR:HD2	2.13	0.45
1:B:528:LYS:O	1:B:556:LYS:HA	2.16	0.45
2:C:165:ALA:O	2:C:166:ARG:C	2.58	0.45
1:A:357:VAL:HG22	1:A:358:ASP:N	2.32	0.45
1:B:687:VAL:O	1:B:687:VAL:HG23	2.16	0.45
1:A:117:ASN:CG	1:A:352:LEU:HD23	2.41	0.45
1:A:161:LEU:O	1:A:180:PHE:HA	2.16	0.45
1:A:476:ALA:C	1:A:478:THR:N	2.74	0.45
1:A:616:THR:N	1:A:659:ASN:HD21	2.10	0.45
1:B:382:ARG:HG2	1:B:383:MET:N	2.31	0.45
1:B:516:GLN:O	1:B:523:ILE:HG22	2.17	0.45
1:A:687:VAL:O	1:A:687:VAL:CG2	2.63	0.45
5:A:901:FTT:H71	5:B:900:FTT:C7	2.46	0.45
2:D:181:ASP:OD1	2:D:190:ASN:CG	2.60	0.45
1:A:323:ASN:O	1:A:326:SER:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:PHE:CD1	1:A:365:PHE:C	2.95	0.45
1:A:199:ARG:NH2	1:A:212:ARG:NH1	2.65	0.45
1:A:368:GLY:H	1:A:370:ILE:CD1	2.30	0.45
1:A:653:SER:HB3	1:A:663:VAL:HG12	1.99	0.45
1:A:677:LEU:HB2	1:A:685:SER:O	2.17	0.45
1:B:256:LEU:HB2	1:B:260:LYS:O	2.17	0.45
1:B:452:GLN:HA	1:B:456:VAL:O	2.17	0.45
1:B:545:ILE:HG23	1:B:587:ALA:HB2	1.99	0.45
5:B:900:FTT:C13	7:B:930:DAO:H102	2.47	0.45
1:A:452:GLN:HA	1:A:456:VAL:O	2.17	0.44
1:A:516:GLN:O	1:A:523:ILE:HG22	2.16	0.44
2:C:182:VAL:HG23	2:C:221:GLY:O	2.18	0.44
1:B:189:VAL:HG13	1:B:190:TYR:HD2	1.78	0.44
1:A:241:THR:OG1	1:A:275:TYR:HB3	2.17	0.44
1:A:291:ASN:C	1:A:293:THR:N	2.76	0.44
1:A:530:LYS:HD2	1:A:530:LYS:N	2.32	0.44
1:B:365:PHE:CD1	1:B:365:PHE:C	2.96	0.44
1:B:493:VAL:O	1:B:504:TYR:HB2	2.17	0.44
1:A:267:ASN:C	1:A:267:ASN:HD22	2.24	0.44
1:A:300:LEU:HD21	5:A:902:FTT:H102	1.99	0.44
1:B:343:ARG:O	1:B:397:VAL:HG13	2.16	0.44
1:B:576:ILE:HG22	1:B:577:ARG:N	2.32	0.44
2:D:165:ALA:O	2:D:166:ARG:C	2.61	0.44
2:D:198:PRO:O	2:D:199:ALA:O	2.36	0.44
3:E:3:KDO:H7	3:E:5:GMH:C1	2.48	0.44
1:A:316:GLY:C	1:A:341:LEU:HD12	2.41	0.44
1:B:270:ALA:O	1:B:272:ASN:N	2.51	0.44
1:B:316:GLY:C	1:B:341:LEU:HD12	2.43	0.44
3:F:3:KDO:H7	3:F:5:GMH:C1	2.48	0.44
1:A:365:PHE:CE1	1:A:372:HIS:CG	3.05	0.44
1:B:92:ILE:N	1:B:92:ILE:HD12	2.32	0.44
1:B:127:GLU:HB2	1:B:154:LYS:HA	1.99	0.44
1:B:199:ARG:O	1:B:211:GLN:HA	2.18	0.44
1:B:300:LEU:HD23	1:B:301:ARG:N	2.33	0.44
1:B:317:VAL:HA	1:B:341:LEU:HA	1.99	0.44
5:B:903:FTT:O2	3:F:2:GCN:H32	2.17	0.44
1:A:111:LEU:HD23	1:A:301:ARG:HH12	1.83	0.44
5:A:901:FTT:O2	3:E:1:GCN:H32	2.17	0.44
1:B:323:ASN:O	1:B:326:SER:HB3	2.18	0.44
1:B:368:GLY:H	1:B:370:ILE:CD1	2.30	0.44
1:B:449:ASP:OD2	1:B:451:ALA:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:724:ARG:HH11	1:B:724:ARG:HG3	1.82	0.44
1:A:122:ASP:CG	1:A:123:PRO:HD2	2.43	0.44
1:A:317:VAL:HA	1:A:341:LEU:HA	1.99	0.44
1:B:256:LEU:HD11	1:B:262:LEU:HD11	2.00	0.44
1:B:616:THR:N	1:B:659:ASN:HD21	2.08	0.44
1:B:694:LEU:O	1:B:715:ARG:HD3	2.18	0.44
5:B:902:FTT:C8	5:B:903:FTT:H82	2.38	0.44
1:A:247:LEU:CD2	1:A:268:GLU:HG3	2.48	0.43
1:A:256:LEU:HB2	1:A:260:LYS:O	2.18	0.43
1:A:299:ASN:N	1:A:299:ASN:ND2	2.58	0.43
2:C:202:PHE:O	2:C:203:GLU:C	2.61	0.43
1:A:273:ASN:HD21	1:A:312:VAL:N	1.99	0.43
1:A:352:LEU:HD12	1:A:353:GLN:C	2.43	0.43
1:A:365:PHE:CD1	1:A:372:HIS:HB2	2.53	0.43
1:A:449:ASP:OD2	1:A:451:ALA:HB2	2.18	0.43
1:A:468:ASP:N	1:A:468:ASP:OD2	2.50	0.43
1:A:470:GLU:HG3	1:A:481:LYS:HB3	2.00	0.43
1:B:110:LYS:HG3	1:B:111:LEU:N	2.29	0.43
1:B:543:ARG:HG3	1:B:543:ARG:NH1	2.33	0.43
1:A:192:TYR:CD1	1:A:192:TYR:C	2.95	0.43
1:A:628:TRP:CH2	1:A:630:ASP:HB3	2.53	0.43
1:B:94:GLY:HA2	1:B:620:VAL:HB	1.99	0.43
1:B:523:ILE:H	1:B:523:ILE:CD1	2.22	0.43
1:B:591:ALA:CA	2:D:166:ARG:HH22	2.32	0.43
1:A:10:THR:CG2	1:A:11:VAL:N	2.80	0.43
1:A:189:VAL:HG23	1:A:222:ARG:O	2.18	0.43
1:A:554:LEU:HB3	1:A:578:ALA:HB3	1.99	0.43
1:B:470:GLU:HG3	1:B:481:LYS:HB3	2.00	0.43
1:B:678:ALA:HA	1:B:682:MET:C	2.44	0.43
1:B:703:CYS:HA	1:B:708:GLY:O	2.19	0.43
2:D:226:VAL:O	2:D:227:ASN:CB	2.67	0.43
1:A:81:ARG:CG	1:A:84:SER:HB3	2.31	0.43
1:A:182:ASP:HB3	1:A:192:TYR:CE1	2.52	0.43
1:A:256:LEU:HD11	1:A:262:LEU:HD11	2.00	0.43
1:A:483:ASP:OD1	3:F:4:KDO:O8	2.30	0.43
1:B:58:MET:C	1:B:60:LEU:H	2.21	0.43
1:B:96:ALA:C	1:B:97:ALA:O	2.60	0.43
1:B:112:GLN:CA	1:B:112:GLN:NE2	2.82	0.43
1:A:94:GLY:HA2	1:A:620:VAL:HB	2.00	0.43
1:A:132:MET:SD	1:A:136:VAL:HG11	2.59	0.43
1:A:375:LEU:O	1:A:447:VAL:HA	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ASP:OD1	1:A:520:ASP:N	2.48	0.43
1:A:579:ARG:CG	1:A:603:ASP:HB3	2.34	0.43
1:A:672:LEU:HD12	1:A:673:VAL:H	1.84	0.43
1:B:357:VAL:HG22	1:B:358:ASP:N	2.33	0.43
1:B:591:ALA:HA	2:D:166:ARG:NH2	2.33	0.43
1:B:677:LEU:HB2	1:B:685:SER:O	2.19	0.43
1:A:112:GLN:CA	1:A:112:GLN:NE2	2.81	0.43
1:A:197:LEU:C	1:A:197:LEU:CD1	2.85	0.43
1:A:273:ASN:ND2	1:A:312:VAL:N	2.52	0.43
1:A:370:ILE:HG22	1:A:453:TRP:CG	2.53	0.43
1:A:436:ILE:CG2	1:A:438:ASN:ND2	2.82	0.43
1:A:454:ASP:OD1	1:A:455:LYS:HE2	2.19	0.43
1:B:675:TYR:O	1:B:686:ASN:HB2	2.19	0.43
2:C:226:VAL:O	2:C:227:ASN:CB	2.65	0.43
2:D:164:PRO:HG2	2:D:202:PHE:CD2	2.54	0.43
1:A:291:ASN:C	1:A:293:THR:H	2.26	0.43
1:A:382:ARG:HG2	1:A:383:MET:N	2.34	0.43
1:A:550:ALA:O	1:A:581:VAL:HA	2.19	0.43
1:B:206:LYS:HE3	1:B:265:ASP:OD1	2.19	0.43
1:B:255:PRO:HA	1:B:261:ARG:HG2	2.01	0.43
2:C:232:ILE:H	2:C:232:ILE:CD1	2.29	0.43
2:D:202:PHE:O	2:D:203:GLU:C	2.61	0.43
2:D:232:ILE:O	2:D:233:ASN:C	2.62	0.43
1:A:15:PRO:HG3	2:C:233:ASN:H	1.83	0.43
1:A:694:LEU:O	1:A:715:ARG:HD3	2.19	0.43
1:B:268:GLU:N	1:B:268:GLU:OE1	2.52	0.43
1:B:365:PHE:CD1	1:B:372:HIS:HB2	2.54	0.43
1:B:365:PHE:CE1	1:B:372:HIS:CG	3.07	0.43
1:B:117:ASN:CG	1:B:352:LEU:HD23	2.44	0.42
1:A:93:ARG:O	1:A:95:PHE:CD1	2.72	0.42
1:A:96:ALA:C	1:A:97:ALA:O	2.60	0.42
1:A:555:THR:HG22	1:A:577:ARG:HA	2.01	0.42
1:B:554:LEU:HB3	1:B:578:ALA:HB3	2.00	0.42
1:A:105:TYR:CZ	1:A:110:LYS:HB2	2.53	0.42
1:A:127:GLU:HB2	1:A:154:LYS:HA	2.00	0.42
1:A:341:LEU:HG	1:A:342:ALA:O	2.19	0.42
1:A:354:ASN:HD22	1:A:355:PHE:N	2.17	0.42
1:A:678:ALA:HA	1:A:682:MET:C	2.44	0.42
1:B:214:ALA:C	1:B:215:ILE:HD12	2.44	0.42
2:C:215:TYR:CD1	2:C:216:GLU:N	2.83	0.42
1:A:37:THR:HB	1:A:448:GLN:HE22	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:MET:C	1:A:60:LEU:N	2.78	0.42
1:A:255:PRO:HA	1:A:261:ARG:HG2	2.02	0.42
1:A:543:ARG:HG3	1:A:543:ARG:NH1	2.33	0.42
1:B:249:LYS:HA	1:B:252:THR:OG1	2.18	0.42
5:B:903:FTT:O2	3:F:2:GCN:C3	2.66	0.42
1:A:656:ASP:HB3	1:A:705:ASN:HA	2.02	0.42
1:B:58:MET:C	1:B:60:LEU:N	2.77	0.42
1:B:454:ASP:OD1	1:B:455:LYS:HE2	2.20	0.42
2:D:182:VAL:HG23	2:D:221:GLY:O	2.18	0.42
1:A:93:ARG:O	1:A:95:PHE:HD1	2.02	0.42
1:A:215:ILE:HD12	1:A:215:ILE:N	2.34	0.42
1:A:672:LEU:HD12	1:A:673:VAL:N	2.35	0.42
1:B:135:PRO:HD3	1:B:554:LEU:HD13	1.99	0.42
1:B:142:LYS:O	1:B:143:SER:HB3	2.19	0.42
1:B:189:VAL:HG23	1:B:222:ARG:O	2.20	0.42
1:B:332:LEU:HD11	1:B:399:LEU:CD1	2.50	0.42
2:C:175:GLN:HB3	2:C:229:LEU:HG	2.02	0.42
1:A:142:LYS:HG2	1:A:442:GLN:HE21	1.80	0.42
1:A:545:ILE:HG23	1:A:587:ALA:HB2	2.02	0.42
1:A:561:MET:O	1:A:571:VAL:N	2.40	0.42
1:B:50:ILE:CG2	1:B:51:SER:H	2.31	0.42
1:B:93:ARG:O	1:B:95:PHE:CD1	2.72	0.42
1:B:436:ILE:CG2	1:B:438:ASN:HD21	2.33	0.42
1:B:552:TYR:CD1	1:B:552:TYR:C	2.98	0.42
2:D:172:ILE:HD11	2:D:201:MET:SD	2.60	0.42
2:D:232:ILE:O	2:D:234:GLY:N	2.52	0.42
1:A:147:GLY:O	1:A:148:LEU:HB2	2.20	0.42
1:A:203:ALA:O	1:A:204:GLN:C	2.61	0.42
1:A:277:ARG:HG3	1:A:277:ARG:HH11	1.83	0.42
1:B:267:ASN:HD22	1:B:269:GLY:H	1.67	0.42
1:B:427:ASP:C	1:B:429:ALA:H	2.28	0.42
1:B:531:GLN:HB2	1:B:554:LEU:HD12	2.00	0.42
1:A:327:LYS:O	1:A:328:GLN:C	2.62	0.42
1:B:93:ARG:O	1:B:95:PHE:HD1	2.02	0.42
1:B:273:ASN:ND2	1:B:311:SER:HA	2.35	0.42
1:B:463:ARG:NE	1:B:465:ASP:OD1	2.52	0.42
2:C:173:GLU:HB2	2:C:230:PHE:O	2.20	0.42
2:D:173:GLU:HB2	2:D:230:PHE:O	2.19	0.42
1:A:675:TYR:O	1:A:686:ASN:HB2	2.20	0.42
1:B:497:PHE:C	1:B:499:ASN:N	2.78	0.42
1:A:206:LYS:HE3	1:A:265:ASP:OD1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:SER:O	1:A:330:ALA:HB3	2.20	0.41
1:B:284:TYR:HB3	5:B:902:FTT:H142	2.00	0.41
2:D:173:GLU:OE2	2:D:232:ILE:HG22	2.20	0.41
1:B:44:GLN:HG2	1:B:45:LYS:H	1.86	0.41
1:B:653:SER:HB3	1:B:663:VAL:HG12	2.02	0.41
1:A:27:THR:HG22	2:C:166:ARG:HD2	2.02	0.41
1:A:67:LYS:C	1:A:69:ALA:H	2.28	0.41
1:A:256:LEU:HD11	1:A:262:LEU:CD1	2.51	0.41
1:B:44:GLN:OE1	1:B:44:GLN:N	2.49	0.41
1:B:67:LYS:C	1:B:69:ALA:H	2.28	0.41
1:B:132:MET:SD	1:B:136:VAL:HG11	2.60	0.41
1:A:249:LYS:HA	1:A:252:THR:OG1	2.20	0.41
1:A:273:ASN:ND2	1:A:311:SER:HA	2.35	0.41
1:A:427:ASP:C	1:A:429:ALA:H	2.27	0.41
1:B:341:LEU:HG	1:B:342:ALA:O	2.21	0.41
1:B:656:ASP:HB3	1:B:705:ASN:HA	2.03	0.41
2:C:178:VAL:HG11	2:C:210:MET:CE	2.49	0.41
1:A:433:PRO:CG	1:A:475:VAL:HG21	2.51	0.41
1:A:481:LYS:NZ	8:B:980:EAP:H21	2.36	0.41
1:A:619:GLN:NE2	1:A:702:SER:OG	2.53	0.41
1:B:60:LEU:HD23	1:B:60:LEU:O	2.20	0.41
1:B:204:GLN:NE2	1:B:714:GLU:H	2.19	0.41
1:A:185:ASP:OD1	1:A:189:VAL:HG12	2.21	0.41
1:A:300:LEU:HD23	1:A:301:ARG:N	2.36	0.41
1:A:497:PHE:O	1:A:499:ASN:N	2.53	0.41
1:A:678:ALA:C	1:A:680:VAL:N	2.78	0.41
1:B:185:ASP:OD1	1:B:189:VAL:HG12	2.21	0.41
1:B:272:ASN:HB3	1:B:420:ASP:OD1	2.20	0.41
1:B:497:PHE:O	1:B:499:ASN:N	2.53	0.41
1:B:724:ARG:O	1:B:725:PHE:C	2.64	0.41
1:A:81:ARG:HA	1:A:81:ARG:HD3	1.93	0.41
1:B:505:PHE:CD1	1:B:505:PHE:C	2.99	0.41
1:B:550:ALA:O	1:B:581:VAL:HA	2.19	0.41
1:B:555:THR:CG2	1:B:577:ARG:HG3	2.51	0.41
2:C:183:THR:HG23	2:C:189:ASP:HB2	2.03	0.41
2:D:175:GLN:HB3	2:D:229:LEU:HG	2.02	0.41
2:D:215:TYR:CD1	2:D:216:GLU:N	2.83	0.41
1:A:284:TYR:HD2	5:A:902:FTT:C14	2.20	0.41
1:A:565:GLU:O	1:A:566:GLY:C	2.64	0.41
1:A:638:LEU:O	1:A:639:SER:C	2.63	0.41
1:A:724:ARG:O	1:A:725:PHE:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:LEU:HD23	1:B:301:ARG:HH12	1.85	0.41
1:B:199:ARG:NH2	1:B:212:ARG:NH1	2.68	0.41
1:B:291:ASN:C	1:B:293:THR:H	2.29	0.41
1:B:291:ASN:C	1:B:293:THR:N	2.78	0.41
1:B:565:GLU:O	1:B:566:GLY:C	2.64	0.41
1:B:589:LEU:HD12	1:B:589:LEU:HA	1.86	0.41
1:B:674:ARG:CB	1:B:688:ALA:HB2	2.51	0.41
5:B:902:FTT:H51	7:B:930:DAO:C1	2.51	0.41
2:C:164:PRO:HG2	2:C:202:PHE:CD2	2.55	0.41
2:C:172:ILE:HD11	2:C:201:MET:SD	2.61	0.41
2:D:181:ASP:O	2:D:188:VAL:HG23	2.21	0.41
1:A:132:MET:SD	1:A:136:VAL:CG1	3.09	0.41
1:A:490:ARG:HG3	1:A:507:TYR:O	2.21	0.41
1:A:504:TYR:CD2	1:A:535:GLY:O	2.74	0.41
1:B:327:LYS:O	1:B:328:GLN:C	2.63	0.41
1:B:350:GLU:HG2	1:B:387:ILE:HG23	2.02	0.41
1:B:619:GLN:NE2	1:B:702:SER:OG	2.53	0.41
1:A:9:ILE:CG1	1:A:10:THR:N	2.82	0.40
1:A:268:GLU:N	1:A:268:GLU:OE1	2.54	0.40
1:A:463:ARG:NE	1:A:465:ASP:OD1	2.51	0.40
1:B:182:ASP:HB3	1:B:192:TYR:CE1	2.54	0.40
1:B:390:TRP:CZ3	1:B:433:PRO:HB3	2.56	0.40
1:B:436:ILE:CG2	1:B:438:ASN:ND2	2.84	0.40
5:B:901:FTT:C14	5:B:903:FTT:H111	2.02	0.40
5:B:903:FTT:C2	10:B:940:MYR:C1	2.99	0.40
2:D:228:ILE:C	2:D:229:LEU:HD12	2.47	0.40
1:B:203:ALA:O	1:B:204:GLN:C	2.62	0.40
1:B:326:SER:O	1:B:330:ALA:HB3	2.21	0.40
1:B:513:PRO:HA	1:B:526:PRO:HA	2.03	0.40
1:B:646:GLY:O	1:B:669:VAL:HG13	2.20	0.40
2:C:232:ILE:O	2:C:232:ILE:HD12	2.21	0.40
1:A:99:GLY:C	1:A:101:SER:N	2.78	0.40
1:A:270:ALA:O	1:A:271:LYS:C	2.65	0.40
1:A:497:PHE:C	1:A:499:ASN:N	2.78	0.40
1:A:555:THR:CG2	1:A:577:ARG:HG3	2.51	0.40
5:A:900:FTT:H112	5:B:900:FTT:H102	2.02	0.40
5:A:902:FTT:H51	7:A:930:DAO:C1	2.51	0.40
1:B:475:VAL:O	1:B:475:VAL:CG2	2.66	0.40
2:C:228:ILE:C	2:C:229:LEU:HD12	2.46	0.40
1:A:19:GLU:HG3	1:A:20:SER:N	2.36	0.40
1:A:505:PHE:CD1	1:A:505:PHE:C	2.99	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:LEU:HD12	1:A:642:THR:H	1.86	0.40
1:B:72:TYR:HE2	1:B:628:TRP:HB2	1.87	0.40
1:B:433:PRO:CG	1:B:475:VAL:HG21	2.51	0.40
1:B:714:GLU:O	1:B:715:ARG:C	2.64	0.40
2:C:188:VAL:HG22	2:C:189:ASP:H	1.86	0.40
2:D:183:THR:HG23	2:D:189:ASP:HB2	2.04	0.40
1:A:313:TYR:H	1:A:313:TYR:HD1	1.64	0.40
1:A:531:GLN:HB2	1:A:554:LEU:HD12	2.04	0.40
1:B:136:VAL:C	1:B:138:VAL:N	2.76	0.40
1:B:502:THR:O	1:B:536:VAL:HA	2.22	0.40
2:D:170:LEU:O	2:D:172:ILE:HG23	2.21	0.40
2:D:178:VAL:HG21	2:D:206:VAL:HG11	2.03	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	698/725 (96%)	590 (84%)	77 (11%)	31 (4%)	2	13
1	B	687/725 (95%)	582 (85%)	79 (12%)	26 (4%)	2	16
2	C	76/229 (33%)	55 (72%)	11 (14%)	10 (13%)	0	1
2	D	76/229 (33%)	53 (70%)	13 (17%)	10 (13%)	0	1
All	All	1537/1908 (81%)	1280 (83%)	180 (12%)	77 (5%)	1	11

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ALA
1	A	18	GLN
1	A	316	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	331	ALA
1	A	367	THR
1	B	316	GLY
1	B	331	ALA
1	B	367	THR
1	B	394	ASP
2	C	185	ASP
2	C	187	ARG
2	C	199	ALA
2	C	203	GLU
2	D	185	ASP
2	D	187	ARG
2	D	199	ALA
2	D	203	GLU
2	D	233	ASN
1	A	148	LEU
1	A	244	TYR
1	A	271	LYS
1	A	292	ASP
1	A	337	LYS
1	A	394	ASP
1	A	454	ASP
1	A	498	ASP
1	A	501	VAL
1	A	566	GLY
1	B	148	LEU
1	B	244	TYR
1	B	271	LYS
1	B	292	ASP
1	B	337	LYS
1	B	498	ASP
1	B	501	VAL
1	B	566	GLY
2	C	194	LEU
2	C	233	ASN
2	D	194	LEU
1	A	146	GLY
1	A	205	GLN
1	A	399	LEU
1	A	476	ALA
1	B	97	ALA
1	B	146	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	205	GLN
1	B	399	LEU
1	B	454	ASP
1	B	476	ALA
1	B	706	THR
2	C	168	GLN
2	C	184	PRO
2	C	200	ASN
2	D	168	GLN
2	D	184	PRO
2	D	200	ASN
1	A	15	PRO
1	A	97	ALA
1	A	301	ARG
1	A	706	THR
1	B	301	ARG
1	B	677	LEU
2	C	201	MET
2	D	201	MET
1	A	17	PRO
1	A	59	ALA
1	A	542	ASP
1	A	677	LEU
1	B	59	ALA
1	B	542	ASP
1	A	9	ILE
1	A	475	VAL
1	A	428	PRO
1	A	546	VAL
1	B	475	VAL
1	B	428	PRO
1	B	546	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	579/601 (96%)	519 (90%)	60 (10%)	7	25
1	B	572/601 (95%)	517 (90%)	55 (10%)	8	29
2	C	66/200 (33%)	60 (91%)	6 (9%)	9	31
2	D	66/200 (33%)	62 (94%)	4 (6%)	17	45
All	All	1283/1602 (80%)	1158 (90%)	125 (10%)	8	28

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	18	GLN
1	A	19	GLU
1	A	39	THR
1	A	54	THR
1	A	60	LEU
1	A	64	LYS
1	A	80	THR
1	A	81	ARG
1	A	90	LEU
1	A	110	LYS
1	A	112	GLN
1	A	118	ASP
1	A	152	VAL
1	A	190	TYR
1	A	191	SER
1	A	192	TYR
1	A	205	GLN
1	A	211	GLN
1	A	258	ASN
1	A	268	GLU
1	A	272	ASN
1	A	279	GLU
1	A	287	ASP
1	A	299	ASN
1	A	315	TYR
1	A	332	LEU
1	A	352	LEU
1	A	353	GLN
1	A	356	SER
1	A	359	THR
1	A	367	THR
1	A	370	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	383	MET
1	A	384	ARG
1	A	387	ILE
1	A	393	TYR
1	A	397	VAL
1	A	457	LEU
1	A	460	LEU
1	A	468	ASP
1	A	480	ASP
1	A	486	GLN
1	A	493	VAL
1	A	499	ASN
1	A	516	GLN
1	A	520	ASP
1	A	523	ILE
1	A	531	GLN
1	A	534	VAL
1	A	548	THR
1	A	557	THR
1	A	565	GLU
1	A	571	VAL
1	A	583	ILE
1	A	589	LEU
1	A	610	THR
1	A	611	THR
1	A	620	VAL
1	A	694	LEU
1	B	39	THR
1	B	54	THR
1	B	60	LEU
1	B	64	LYS
1	B	80	THR
1	B	81	ARG
1	B	90	LEU
1	B	112	GLN
1	B	118	ASP
1	B	152	VAL
1	B	190	TYR
1	B	191	SER
1	B	192	TYR
1	B	205	GLN
1	B	211	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	258	ASN
1	B	268	GLU
1	B	272	ASN
1	B	279	GLU
1	B	287	ASP
1	B	299	ASN
1	B	315	TYR
1	B	332	LEU
1	B	352	LEU
1	B	353	GLN
1	B	356	SER
1	B	359	THR
1	B	367	THR
1	B	370	ILE
1	B	383	MET
1	B	384	ARG
1	B	387	ILE
1	B	393	TYR
1	B	397	VAL
1	B	457	LEU
1	B	460	LEU
1	B	480	ASP
1	B	486	GLN
1	B	493	VAL
1	B	499	ASN
1	B	516	GLN
1	B	520	ASP
1	B	523	ILE
1	B	531	GLN
1	B	534	VAL
1	B	548	THR
1	B	557	THR
1	B	565	GLU
1	B	571	VAL
1	B	583	ILE
1	B	589	LEU
1	B	610	THR
1	B	611	THR
1	B	620	VAL
1	B	694	LEU
2	C	168	GLN
2	C	197	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	201	MET
2	C	228	ILE
2	C	231	LYS
2	C	232	ILE
2	D	168	GLN
2	D	197	LYS
2	D	201	MET
2	D	228	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	32	GLN
1	A	62	GLN
1	A	100	GLN
1	A	112	GLN
1	A	204	GLN
1	A	211	GLN
1	A	267	ASN
1	A	272	ASN
1	A	273	ASN
1	A	291	ASN
1	A	298	GLN
1	A	299	ASN
1	A	309	GLN
1	A	310	ASN
1	A	328	GLN
1	A	353	GLN
1	A	354	ASN
1	A	372	HIS
1	A	388	ASN
1	A	424	ASN
1	A	438	ASN
1	A	440	GLN
1	A	442	GLN
1	A	448	GLN
1	A	452	GLN
1	A	469	GLN
1	A	486	GLN
1	A	516	GLN
1	A	531	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	615	ASN
1	A	619	GLN
1	A	623	HIS
1	A	659	ASN
1	A	692	ASN
1	B	32	GLN
1	B	62	GLN
1	B	100	GLN
1	B	112	GLN
1	B	204	GLN
1	B	211	GLN
1	B	267	ASN
1	B	272	ASN
1	B	273	ASN
1	B	291	ASN
1	B	298	GLN
1	B	299	ASN
1	B	309	GLN
1	B	310	ASN
1	B	328	GLN
1	B	353	GLN
1	B	354	ASN
1	B	372	HIS
1	B	388	ASN
1	B	424	ASN
1	B	438	ASN
1	B	440	GLN
1	B	442	GLN
1	B	448	GLN
1	B	452	GLN
1	B	516	GLN
1	B	594	ASN
1	B	615	ASN
1	B	619	GLN
1	B	623	HIS
1	B	659	ASN
1	B	692	ASN
2	C	160	GLN
2	C	208	ASN
2	C	227	ASN
2	C	233	ASN
2	D	168	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	208	ASN
2	D	227	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

10 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$
3	GCN	E	1	5,3	10,10,11	0.83	0	13,13,15	0.78	0
3	GCN	E	2	5,4,3	10,10,11	1.06	1 (10%)	13,13,15	2.65	2 (15%)
3	KDO	E	3	3	15,15,16	3.67	2 (13%)	17,21,24	2.76	2 (11%)
3	KDO	E	4	3	15,15,16	7.09	2 (13%)	17,21,24	5.88	3 (17%)
3	GMH	E	5	8,3	13,13,14	0.79	0	16,18,20	0.65	0
3	GCN	F	1	5,3	10,10,11	0.84	0	13,13,15	0.78	0
3	GCN	F	2	5,4,3	10,10,11	1.07	1 (10%)	13,13,15	2.64	2 (15%)
3	KDO	F	3	3	15,15,16	1.56	1 (6%)	17,21,24	3.18	3 (17%)
3	KDO	F	4	3	15,15,16	10.31	2 (13%)	17,21,24	7.63	2 (11%)
3	GMH	F	5	8,3	13,13,14	0.79	0	16,18,20	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GCN	E	1	5,3	-	2/2/15/18	0/1/1/1
3	GCN	E	2	5,4,3	-	0/2/15/18	0/1/1/1
3	KDO	E	3	3	-	2/10/26/30	0/1/1/1
3	KDO	E	4	3	-	7/10/26/30	0/1/1/1
3	GMH	E	5	8,3	-	2/6/23/26	0/1/1/1
3	GCN	F	1	5,3	-	2/2/15/18	0/1/1/1
3	GCN	F	2	5,4,3	-	0/2/15/18	0/1/1/1
3	KDO	F	3	3	-	2/10/26/30	0/1/1/1
3	KDO	F	4	3	-	7/10/26/30	0/1/1/1
3	GMH	F	5	8,3	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	KDO	O1A-C1	37.87	2.34	1.22
3	E	4	KDO	O1A-C1	26.83	2.01	1.22
3	F	4	KDO	O1B-C1	12.55	1.70	1.30
3	E	3	KDO	O1A-C1	12.18	1.58	1.22
3	E	3	KDO	O1B-C1	-6.83	1.08	1.30
3	E	4	KDO	O1B-C1	5.52	1.48	1.30
3	F	3	KDO	O1B-C1	5.26	1.47	1.30
3	F	2	GCN	C1-C2	2.85	1.55	1.52
3	E	2	GCN	C1-C2	2.81	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	KDO	O1B-C1-O1A	-25.71	65.75	124.08
3	E	4	KDO	O1B-C1-O1A	-20.41	77.78	124.08
3	F	4	KDO	O1B-C1-C2	17.87	159.21	112.71
3	E	4	KDO	O1B-C1-C2	12.22	144.52	112.71
3	F	3	KDO	O1A-C1-C2	-10.04	101.15	122.85
3	E	3	KDO	O1A-C1-C2	-9.36	102.62	122.85
3	E	2	GCN	C3-C2-C1	8.73	116.92	109.87
3	F	2	GCN	C3-C2-C1	8.69	116.90	109.87
3	F	3	KDO	O1B-C1-C2	-6.45	95.93	112.71
3	E	3	KDO	O1B-C1-O1A	-5.64	111.29	124.08
3	F	3	KDO	O1B-C1-O1A	-4.47	113.94	124.08
3	E	4	KDO	O1A-C1-C2	-3.62	115.03	122.85
3	E	2	GCN	C1-O5-C5	2.59	115.65	112.19
3	F	2	GCN	C1-O5-C5	2.55	115.61	112.19

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	3	KDO	O1A-C1-C2-O6
3	E	4	KDO	C5-C6-C7-O7
3	E	4	KDO	C5-C6-C7-C8
3	E	4	KDO	O6-C6-C7-O7
3	E	4	KDO	O6-C6-C7-C8
3	E	5	GMH	O6-C6-C7-O7
3	F	3	KDO	O1A-C1-C2-C3
3	F	4	KDO	O1B-C1-C2-C3
3	F	4	KDO	C5-C6-C7-O7
3	F	4	KDO	C5-C6-C7-C8
3	F	4	KDO	O6-C6-C7-O7
3	F	4	KDO	O6-C6-C7-C8
3	F	5	GMH	O6-C6-C7-O7
3	E	1	GCN	C4-C5-C6-O6
3	F	1	GCN	C4-C5-C6-O6
3	E	1	GCN	O5-C5-C6-O6
3	F	1	GCN	O5-C5-C6-O6
3	E	5	GMH	C5-C6-C7-O7
3	F	5	GMH	C5-C6-C7-O7
3	E	4	KDO	O7-C7-C8-O8
3	F	4	KDO	O7-C7-C8-O8
3	F	3	KDO	O1A-C1-C2-O6
3	E	4	KDO	C6-C7-C8-O8
3	F	4	KDO	C6-C7-C8-O8
3	E	3	KDO	O1A-C1-C2-C3
3	E	4	KDO	O1B-C1-C2-C3

There are no ring outliers.

10 monomers are involved in 42 short contacts:

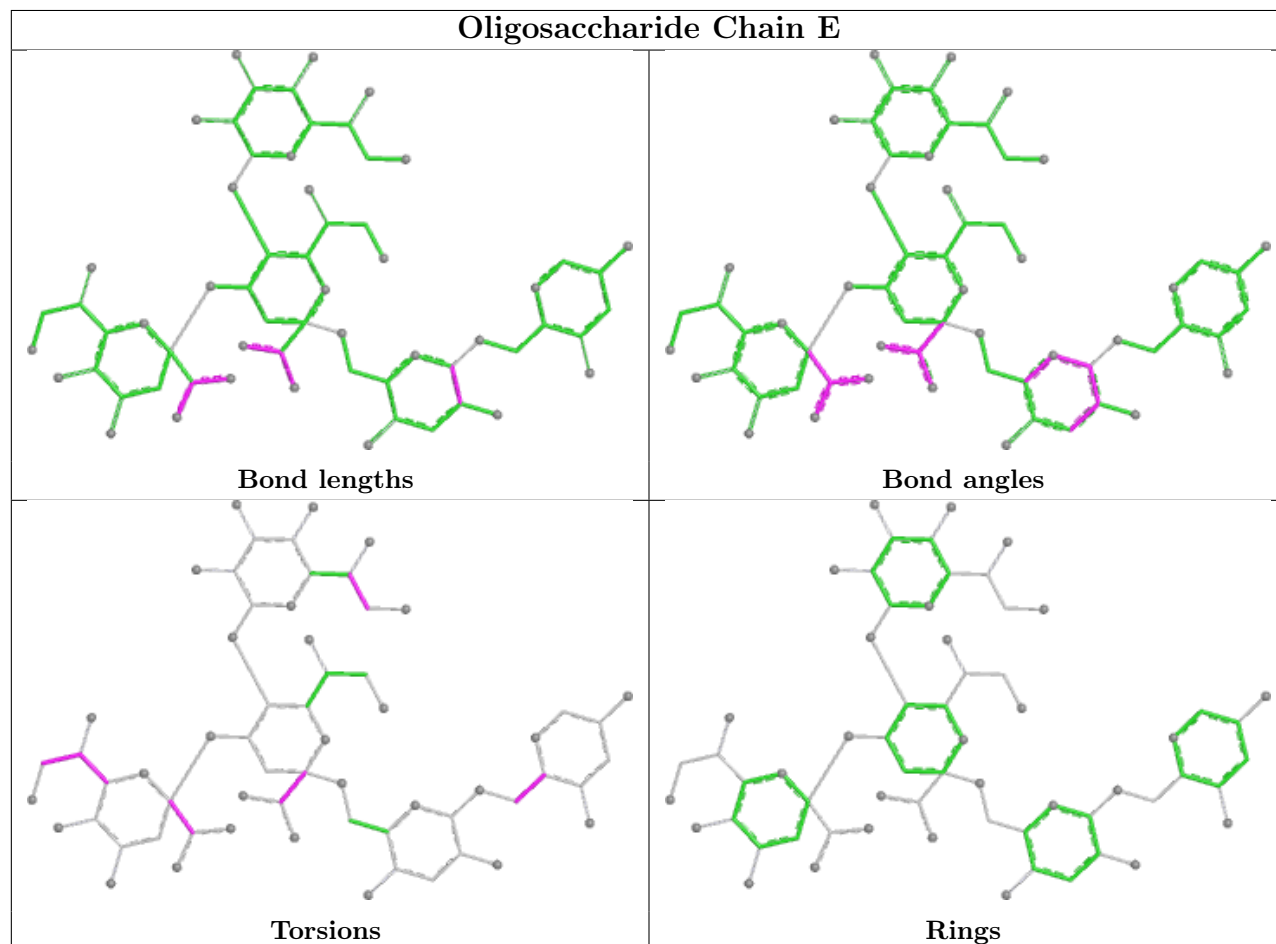
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5	GMH	4	0
3	E	2	GCN	5	0
3	F	2	GCN	7	0
3	E	3	KDO	3	0
3	F	5	GMH	4	0
3	F	4	KDO	7	0
3	F	1	GCN	7	0
3	F	3	KDO	3	0
3	E	1	GCN	7	0

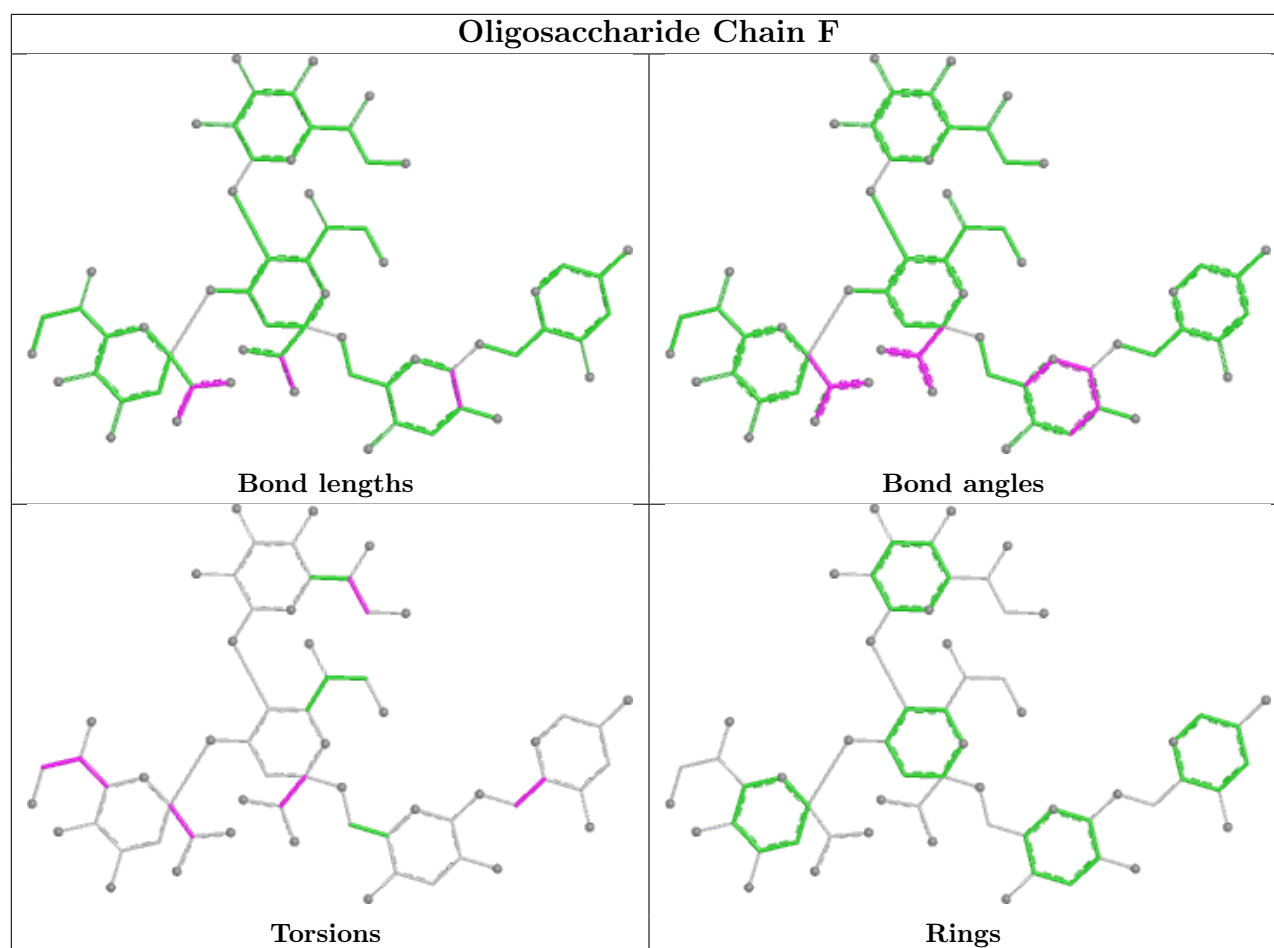
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	4	KDO	3	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](#)

19 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
10	MYR	B	940	5	14,14,15	1.00	1 (7%)	13,13,15	0.83	1 (7%)
9	FCI	A	1050	-	45,51,56	1.45	4 (8%)	51,78,87	1.19	5 (9%)
4	PO4	A	950	3	0,3,4	-	-	0,3,6	-	-
7	DAO	A	930	5	12,12,13	1.06	1 (8%)	11,11,13	0.82	1 (9%)
5	FTT	B	900	3	14,15,16	4.81	1 (7%)	15,15,17	2.28	3 (20%)
5	FTT	B	902	7,3	14,15,16	0.32	0	15,15,17	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FTT	A	902	7,3	14,15,16	0.32	0	15,15,17	0.81	0
6	DPO	A	910	-	4,7,8	2.50	1 (25%)	5,10,13	0.96	0
5	FTT	B	901	-	14,15,16	0.31	0	15,15,17	0.81	0
5	FTT	B	903	10	14,15,16	0.45	0	15,15,17	0.50	0
5	FTT	A	903	-	14,15,16	0.45	0	15,15,17	0.50	0
5	FTT	A	900	3	14,15,16	0.41	0	15,15,17	0.69	1 (6%)
8	EAP	A	980	3	3,6,7	3.09	2 (66%)	0,6,9	-	-
5	FTT	A	901	-	14,15,16	0.31	0	15,15,17	0.81	0
7	DAO	B	930	5	12,12,13	1.06	1 (8%)	11,11,13	0.82	1 (9%)
6	DPO	B	910	-	4,7,8	2.51	1 (25%)	5,10,13	0.96	0
4	PO4	B	950	3	0,3,4	-	-	0,3,6	-	-
9	FCI	B	1050	-	45,51,56	1.46	4 (8%)	51,78,87	1.19	5 (9%)
8	EAP	B	980	3	3,6,7	3.08	2 (66%)	0,6,9	-	-

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
5	FTT	B	903	10	-	2/14/14/15	-
10	MYR	B	940	5	-	2/12/12/13	-
9	FCI	A	1050	-	3/3/13/23	11/57/102/116	0/4/6/6
7	DAO	A	930	5	-	1/10/10/11	-
5	FTT	B	900	3	-	2/14/14/15	-
6	DPO	A	910	-	-	0/2/5/6	-
8	EAP	A	980	3	-	0/0/4/5	-
5	FTT	A	901	-	-	2/14/14/15	-
7	DAO	B	930	5	-	1/10/10/11	-
5	FTT	B	902	7,3	-	3/14/14/15	-
9	FCI	B	1050	-	3/3/13/23	11/57/102/116	0/4/6/6
6	DPO	B	910	-	-	0/2/5/6	-
5	FTT	A	902	7,3	-	3/14/14/15	-
8	EAP	B	980	3	-	0/0/4/5	-
5	FTT	A	903	-	-	2/14/14/15	-
5	FTT	A	900	3	-	0/14/14/15	-
5	FTT	B	901	-	-	5/14/14/15	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	900	FTT	C9-C8	17.95	2.41	1.51
9	A	1050	FCI	O10-FE	5.97	2.12	1.99
9	B	1050	FCI	O10-FE	5.95	2.12	1.99
9	B	1050	FCI	O3-FE	5.33	2.19	2.04
9	A	1050	FCI	O3-FE	5.28	2.19	2.04
8	A	980	EAP	P-O4	-4.72	1.49	1.63
8	B	980	EAP	P-O4	-4.70	1.49	1.63
6	B	910	DPO	P1-O4	-4.49	1.50	1.63
6	A	910	DPO	P1-O4	-4.47	1.50	1.63
10	B	940	MYR	O2-C1	-3.71	1.23	1.42
7	A	930	DAO	O2-C1	-3.63	1.23	1.42
7	B	930	DAO	O2-C1	-3.62	1.23	1.42
9	A	1050	FCI	O11-FE	3.07	2.05	1.99
9	B	1050	FCI	O11-FE	3.07	2.05	1.99
9	A	1050	FCI	O14-FE	2.61	2.04	1.99
9	B	1050	FCI	O14-FE	2.59	2.04	1.99
8	A	980	EAP	O4-C1	2.51	1.44	1.37
8	B	980	EAP	O4-C1	2.51	1.44	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	900	FTT	C9-C8-C7	8.00	154.83	114.37
9	A	1050	FCI	C1-C10-N1	3.50	120.58	111.11
9	B	1050	FCI	C1-C10-N1	3.50	120.57	111.11
9	A	1050	FCI	C34-N8-C9	2.52	130.56	125.58
9	B	1050	FCI	C34-N8-C9	2.52	130.56	125.58
9	B	1050	FCI	C30-N5-C3	2.41	130.35	125.58
9	A	1050	FCI	C30-N5-C3	2.41	130.34	125.58
9	B	1050	FCI	C32-N6-C6	2.28	130.09	125.58
9	A	1050	FCI	C32-N6-C6	2.26	130.05	125.58
7	B	930	DAO	O2-C1-C2	2.19	125.34	111.44
7	A	930	DAO	O2-C1-C2	2.19	125.34	111.44
10	B	940	MYR	O2-C1-C2	2.17	125.23	111.44
9	A	1050	FCI	O17-C8-N4	-2.14	119.33	122.95
9	B	1050	FCI	O17-C8-N4	-2.12	119.36	122.95
5	A	900	FTT	O2-C1-C2	-2.10	119.26	125.38
5	B	900	FTT	O2-C1-C2	-2.10	119.26	125.38
5	B	900	FTT	C10-C9-C8	2.07	124.82	114.37

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	1050	FCI	N8
9	A	1050	FCI	N6
9	A	1050	FCI	N5
9	B	1050	FCI	N8
9	B	1050	FCI	N6
9	B	1050	FCI	N5

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	901	FTT	C2-C3-C4-C5
5	B	901	FTT	C1-C2-C3-O3
9	A	1050	FCI	C25-C30-N5-C3
9	B	1050	FCI	C25-C30-N5-C3
5	A	901	FTT	O3-C3-C4-C5
9	A	1050	FCI	C24-C16-C7-N3
9	B	1050	FCI	C24-C16-C7-N3
9	A	1050	FCI	C24-C16-C7-O7
9	B	1050	FCI	C24-C16-C7-O7
5	A	902	FTT	O3-C3-C4-C5
5	B	902	FTT	O3-C3-C4-C5
5	B	900	FTT	C7-C8-C9-C10
5	A	903	FTT	C11-C10-C9-C8
5	B	903	FTT	C11-C10-C9-C8
5	B	900	FTT	C6-C7-C8-C9
7	A	930	DAO	O2-C1-C2-C3
7	B	930	DAO	O2-C1-C2-C3
9	A	1050	FCI	C25-C30-N5-O10
9	B	1050	FCI	C25-C30-N5-O10
9	A	1050	FCI	N2-C11-C2-N9
9	B	1050	FCI	N2-C11-C2-N9
5	B	901	FTT	O3-C3-C4-C5
5	B	901	FTT	C1-C2-C3-C4
9	A	1050	FCI	N4-C16-C7-O7
9	B	1050	FCI	N4-C16-C7-O7
5	A	903	FTT	C1-C2-C3-O3
5	B	903	FTT	C1-C2-C3-O3
5	A	902	FTT	O2-C1-C2-C3
5	B	902	FTT	O2-C1-C2-C3
9	A	1050	FCI	N2-C11-C2-O2
9	B	1050	FCI	N2-C11-C2-O2
9	B	1050	FCI	N4-C16-C7-N3
9	A	1050	FCI	N4-C16-C7-N3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	901	FTT	C2-C3-C4-C5
9	B	1050	FCI	C29-C34-N8-C9
9	A	1050	FCI	C29-C34-N8-C9
10	B	940	MYR	C2-C3-C4-C5
9	A	1050	FCI	C2-C11-N2-C5
9	B	1050	FCI	C2-C11-N2-C5
5	B	901	FTT	C3-C4-C5-C6
5	A	902	FTT	C2-C3-C4-C5
5	B	902	FTT	C2-C3-C4-C5
10	B	940	MYR	O2-C1-C2-C3
9	A	1050	FCI	O1-C1-C10-C18
9	B	1050	FCI	O1-C1-C10-C18

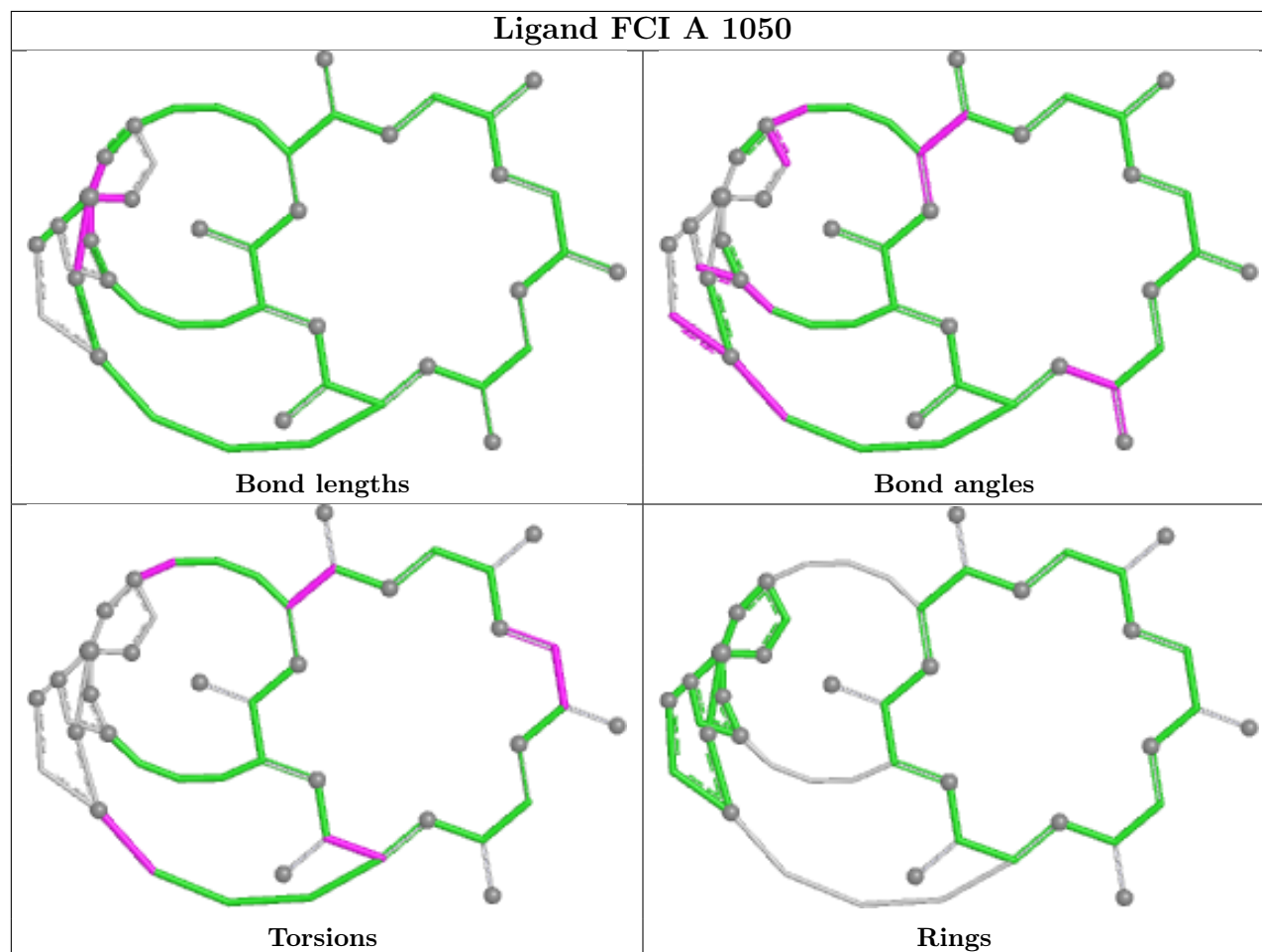
There are no ring outliers.

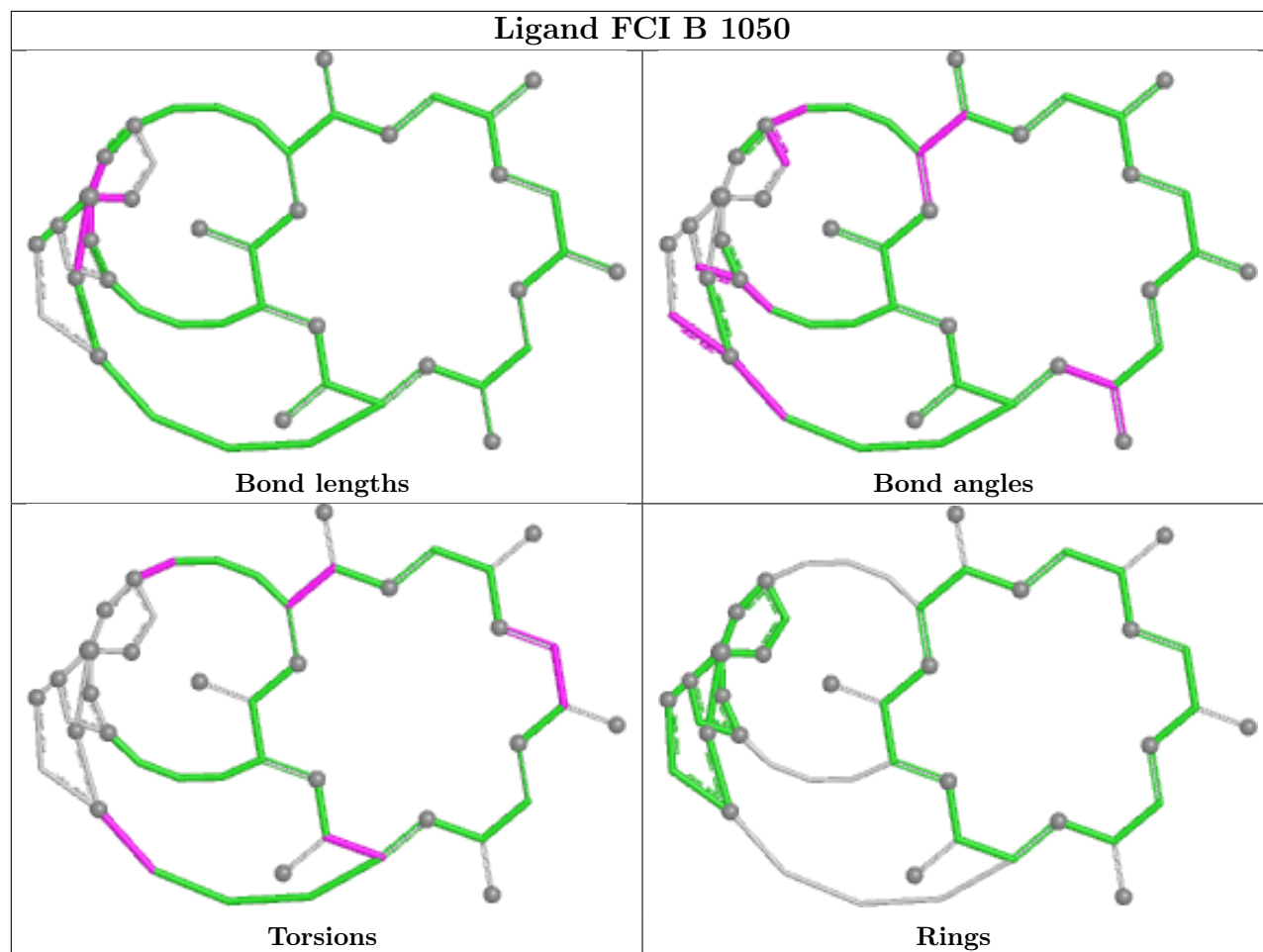
17 monomers are involved in 138 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	940	MYR	4	0
9	A	1050	FCI	2	0
7	A	930	DAO	5	0
5	B	900	FTT	17	0
5	B	902	FTT	39	0
5	A	902	FTT	6	0
6	A	910	DPO	8	0
5	B	901	FTT	39	0
5	B	903	FTT	64	0
5	A	903	FTT	3	0
5	A	900	FTT	12	0
8	A	980	EAP	2	0
5	A	901	FTT	9	0
7	B	930	DAO	7	0
6	B	910	DPO	8	0
9	B	1050	FCI	1	0
8	B	980	EAP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	702/725 (96%)	0.06	21 (2%) 52 35	24, 61, 110, 177	0
1	B	691/725 (95%)	0.77	88 (12%) 8 6	44, 115, 186, 210	0
2	C	78/229 (34%)	0.19	1 (1%) 75 56	43, 112, 179, 209	0
2	D	78/229 (34%)	0.68	7 (8%) 15 11	102, 187, 210, 210	0
All	All	1549/1908 (81%)	0.42	117 (7%) 20 14	24, 88, 186, 210	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	TYR	7.9
1	B	250	GLU	7.4
1	B	30	ALA	6.1
1	B	210	GLU	5.9
1	B	664	GLY	5.6
1	A	391	PHE	5.0
1	B	663	VAL	5.0
1	B	645	THR	4.1
1	B	572	GLU	3.9
1	B	255	PRO	3.9
1	B	252	THR	3.9
1	B	385	ASN	3.8
1	B	80	THR	3.7
1	B	249	LYS	3.7
1	B	251	GLY	3.7
1	B	38	LYS	3.6
1	B	73	THR	3.5
1	B	31	ARG	3.4
1	B	638	LEU	3.4
1	B	32	GLN	3.3
1	B	44	GLN	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	225	ASP	3.3
1	B	244	TYR	3.2
1	B	29	ALA	3.2
1	B	316	GLY	3.2
1	B	605	GLU	3.1
1	B	606	TYR	3.1
1	A	224	ASP	3.0
1	B	100	GLN	3.0
1	B	711	TRP	3.0
1	B	508	SER	3.0
1	A	315	TYR	2.9
2	D	225	VAL	2.9
1	B	472	LEU	2.9
1	B	35	THR	2.9
1	A	622	LYS	2.9
1	B	248	PRO	2.8
2	C	215	TYR	2.8
1	B	61	HIS	2.8
1	B	707	TYR	2.8
1	A	226	LYS	2.8
1	A	239	PRO	2.8
1	B	534	VAL	2.8
1	B	584	GLU	2.8
1	B	505	PHE	2.8
1	B	624	MET	2.8
1	B	49	SER	2.8
1	B	560	LEU	2.8
1	A	287	ASP	2.7
1	B	619	GLN	2.7
1	B	308	SER	2.7
1	B	64	LYS	2.7
1	B	144	SER	2.7
1	A	683	ALA	2.7
1	B	190	TYR	2.7
2	D	159	ASN	2.7
1	B	257	PRO	2.6
1	B	162	LYS	2.6
1	A	470	GLU	2.6
1	B	132	MET	2.6
1	B	246	TRP	2.6
1	B	158	THR	2.6
1	B	675	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	573	GLY	2.5
1	B	243	TYR	2.5
2	D	194	LEU	2.5
1	B	160	PRO	2.4
1	B	531	GLN	2.4
1	A	505	PHE	2.4
1	B	147	GLY	2.4
1	B	253	VAL	2.4
1	B	48	GLN	2.4
1	B	68	GLU	2.4
1	A	348	ASP	2.4
1	A	313	TYR	2.4
1	B	661	PHE	2.4
1	B	699	TYR	2.3
1	B	684	GLY	2.3
1	B	43	ILE	2.3
1	A	541	GLU	2.3
1	B	696	ASP	2.3
1	B	261	ARG	2.3
1	A	526	PRO	2.3
1	A	59	ALA	2.3
1	B	156	PRO	2.2
1	B	694	LEU	2.2
1	B	626	SER	2.2
2	D	195	SER	2.2
1	B	175	GLN	2.2
1	A	401	ASN	2.2
1	B	315	TYR	2.2
1	B	691	VAL	2.2
1	B	544	PRO	2.2
1	A	494	ASN	2.2
1	A	139	LEU	2.1
1	B	653	SER	2.1
1	B	617	PRO	2.1
1	B	539	VAL	2.1
1	B	631	TYR	2.1
2	D	177	LYS	2.1
1	B	277	ARG	2.1
1	B	19	GLU	2.1
1	B	614	GLY	2.1
1	B	266	PHE	2.1
1	A	489	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	596	VAL	2.1
1	B	203	ALA	2.1
1	B	289	GLU	2.1
2	D	213	TRP	2.1
1	B	138	VAL	2.1
1	B	72	TYR	2.1
2	D	212	ARG	2.0
1	A	211	GLN	2.0
1	B	254	GLU	2.0
1	B	79	GLY	2.0
1	B	708	GLY	2.0
1	B	698	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

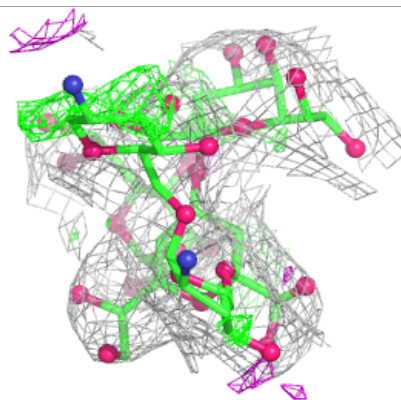
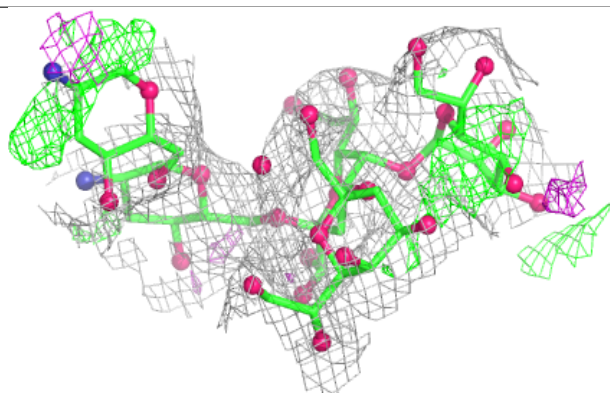
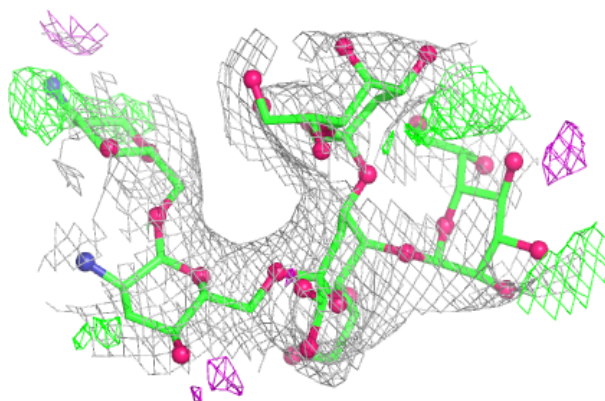
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	KDO	F	4	15/16	0.63	0.16	73,80,98,98	0
3	GMH	F	5	13/14	0.71	0.15	62,67,79,81	0
3	KDO	E	4	15/16	0.75	0.10	73,80,98,98	0
3	GMH	E	5	13/14	0.75	0.12	62,67,79,81	0
3	GCN	E	1	10/11	0.84	0.13	62,74,79,87	0
3	KDO	F	3	15/16	0.86	0.12	65,72,98,98	0
3	GCN	F	1	10/11	0.87	0.10	62,74,79,87	0
3	GCN	E	2	10/11	0.88	0.10	49,60,64,74	0
3	KDO	E	3	15/16	0.88	0.12	65,72,98,98	0
3	GCN	F	2	10/11	0.89	0.07	49,60,64,74	0

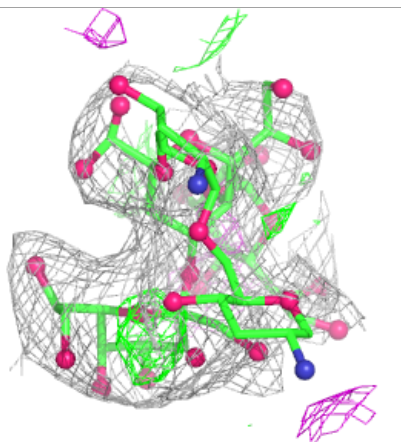
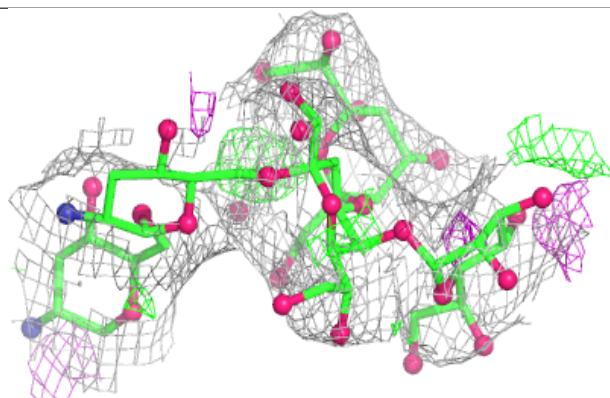
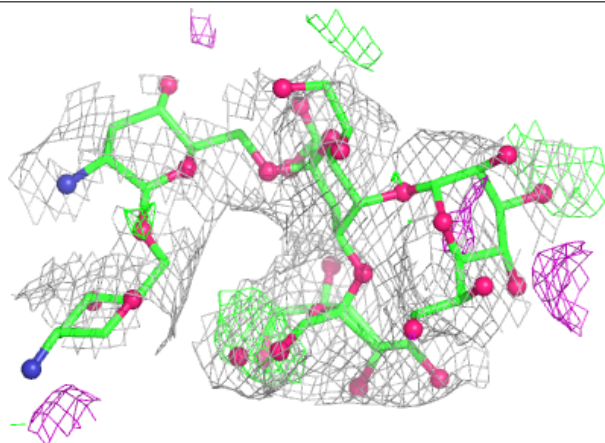
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

**Electron density around Chain F:**

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



6.4 Ligands ⓘ

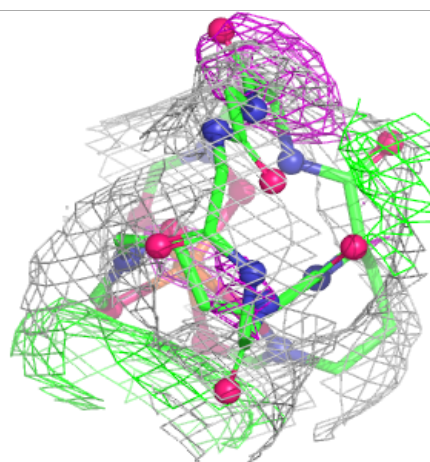
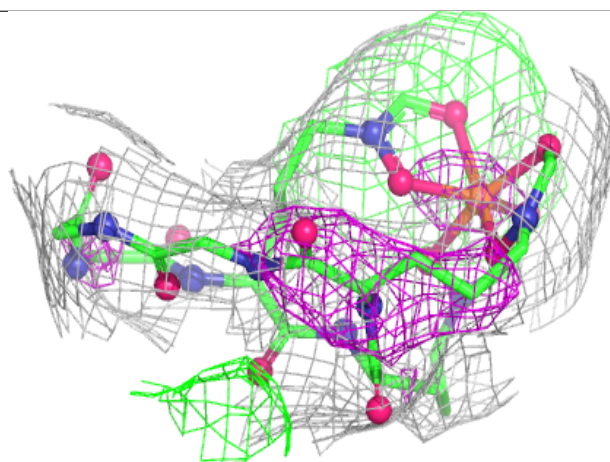
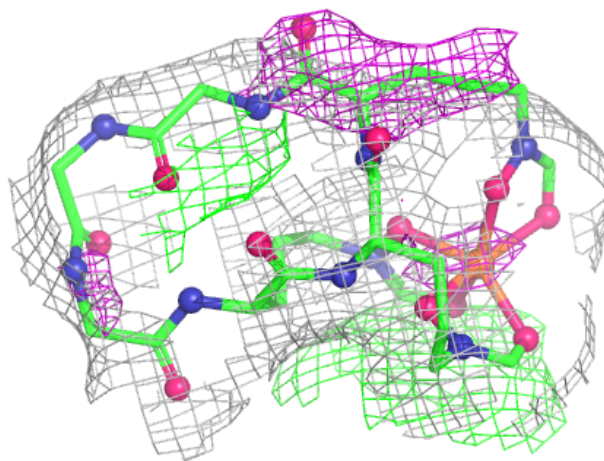
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FTT	B	903	16/17	0.62	0.20	75,88,92,97	0
7	DAO	A	930	13/14	0.68	0.28	69,75,82,86	0
6	DPO	A	910	8/9	0.70	0.13	62,80,93,95	0
8	EAP	A	980	7/8	0.71	0.14	81,87,93,95	0
6	DPO	B	910	8/9	0.73	0.15	62,80,93,95	0
5	FTT	B	901	16/17	0.77	0.21	63,70,78,79	0
8	EAP	B	980	7/8	0.77	0.15	81,87,93,95	0
7	DAO	B	930	13/14	0.79	0.22	69,75,82,86	0
4	PO4	B	950	4/5	0.80	0.12	71,74,76,81	0
5	FTT	A	903	16/17	0.80	0.23	75,88,92,97	0
10	MYR	B	940	15/16	0.80	0.22	69,86,94,95	0
5	FTT	A	901	16/17	0.81	0.22	63,70,78,79	0
9	FCI	B	1050	46/51	0.82	0.13	44,57,70,81	0
5	FTT	A	900	16/17	0.83	0.27	76,87,96,102	0
5	FTT	B	900	16/17	0.83	0.28	84,95,98,102	0
5	FTT	A	902	16/17	0.84	0.20	63,70,78,79	0
5	FTT	B	902	16/17	0.85	0.14	63,70,78,79	0
9	FCI	A	1050	46/51	0.85	0.15	44,57,70,81	0
4	PO4	A	950	4/5	0.91	0.13	71,74,76,81	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

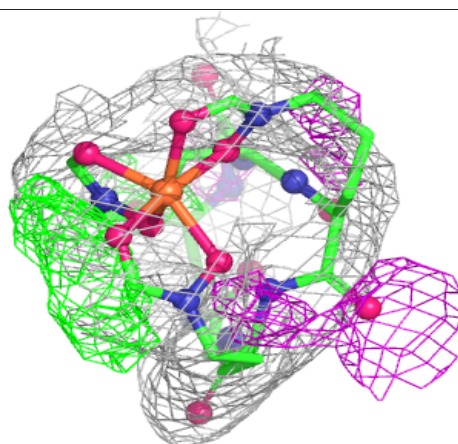
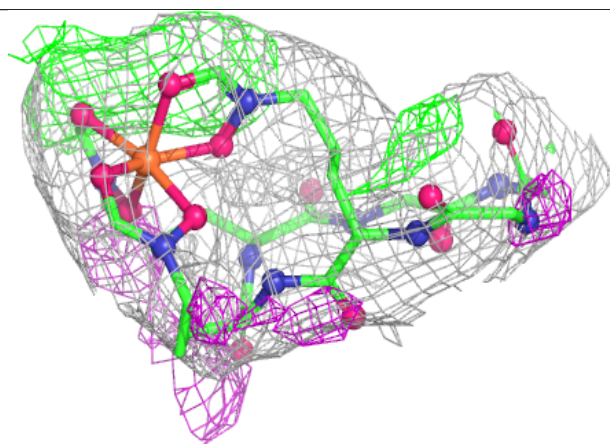
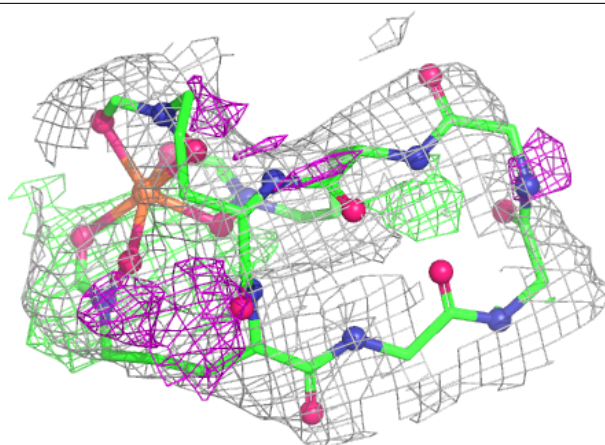
Electron density around FCI B 1050:

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



Electron density around FCI A 1050:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.