



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:05 PM BST

PDB ID : 2GRX
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 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 : 2.13.1
buster-report : 1.1.7 (2018)
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) : 2.13.1

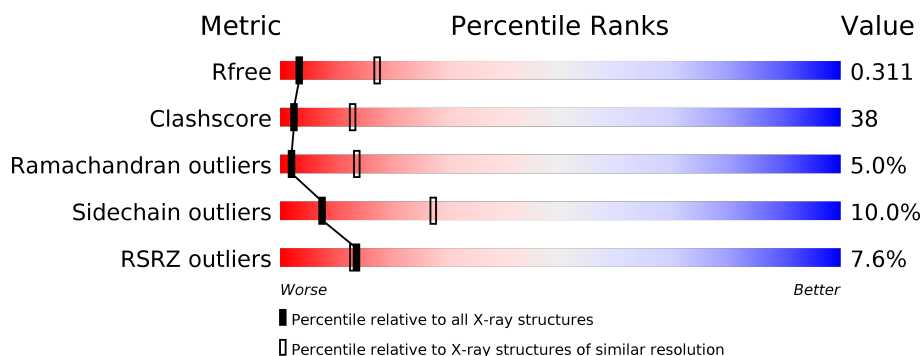
1 Overall quality at a glance

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	725	
1	B	725	
2	C	229	
2	D	229	
3	E	5	
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
10	MYR	B	940	-	-	-	X
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	X
5	FTT	A	903	-	-	-	X
5	FTT	B	900	-	-	X	-
5	FTT	B	901	-	-	X	X
5	FTT	B	902	-	-	X	-
5	FTT	B	903	-	-	X	X
6	DPO	A	910	-	-	X	-
6	DPO	B	910	-	-	X	-
7	DAO	A	930	-	-	-	X
7	DAO	B	930	-	-	X	-

2 Entry composition [i](#)

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:

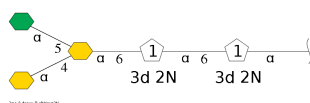
Chain	Residue	Modelled	Actual	Comment	Reference
C	11	GLY	-	SEE REMARK 999	UNP P94739
C	12	SER	-	SEE REMARK 999	UNP P94739
C	13	SER	-	SEE REMARK 999	UNP P94739
C	14	HIS	-	SEE REMARK 999	UNP P94739
C	15	HIS	-	SEE REMARK 999	UNP P94739
C	16	HIS	-	SEE REMARK 999	UNP P94739
C	17	HIS	-	SEE REMARK 999	UNP P94739
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...

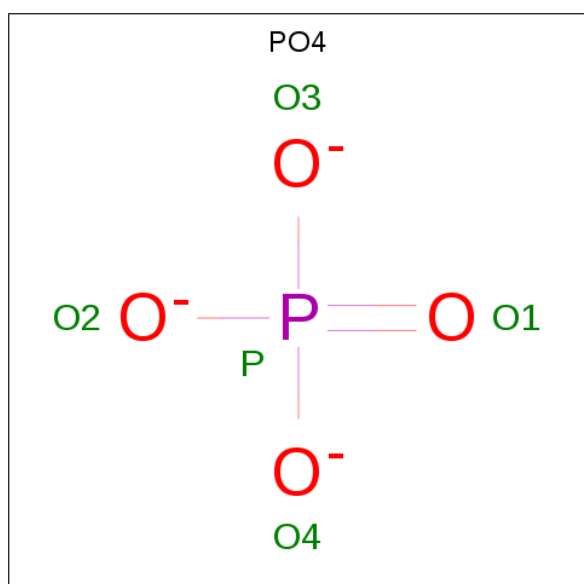
Chain	Residue	Modelled	Actual	Comment	Reference
D	24	VAL	-	SEE REMARK 999	UNP P94739
D	25	PRO	-	SEE REMARK 999	UNP P94739
D	26	ARG	-	SEE REMARK 999	UNP P94739
D	27	GLY	-	SEE REMARK 999	UNP P94739
D	28	SER	-	SEE REMARK 999	UNP P94739
D	29	HIS	-	SEE REMARK 999	UNP P94739
D	30	MET	-	SEE REMARK 999	UNP P94739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



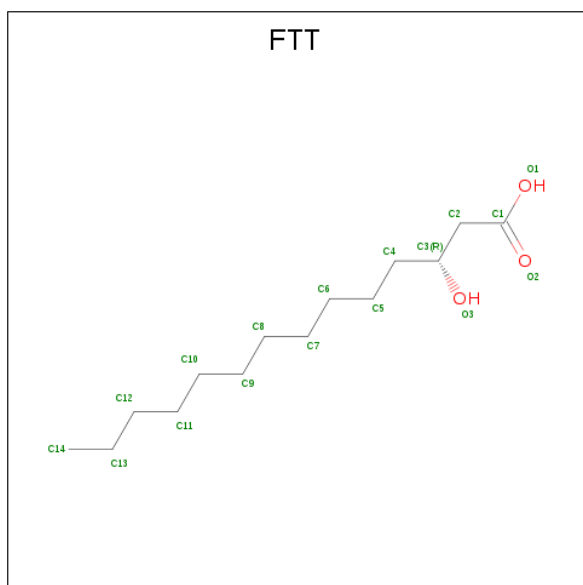
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			63	35	2	26			
3	F	5	Total	C	N	O	0	0	0
			63	35	2	26			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



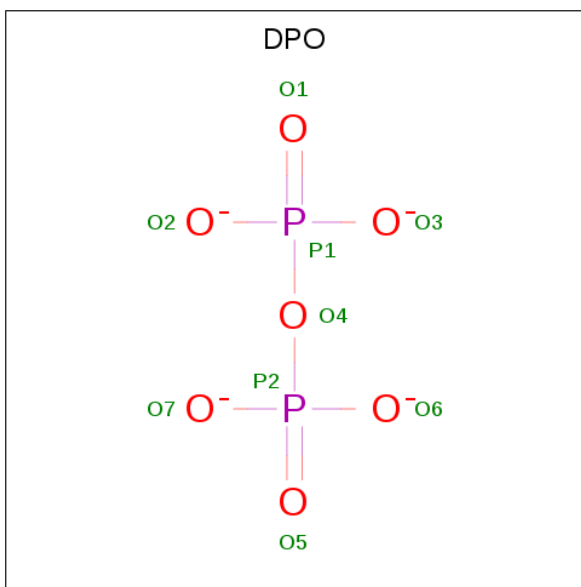
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 4 3 1	0	0
4	B	1	Total O P 4 3 1	0	0

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



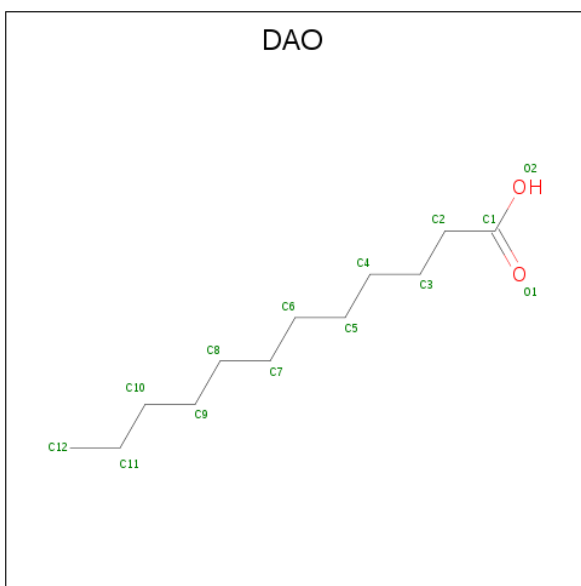
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 16 14 2	0	0
5	A	1	Total C O 16 14 2	0	0
5	A	1	Total C O 16 14 2	0	0
5	A	1	Total C O 16 14 2	0	0
5	B	1	Total C O 16 14 2	0	0
5	B	1	Total C O 16 14 2	0	0
5	B	1	Total C O 16 14 2	0	0
5	B	1	Total C O 16 14 2	0	0

- Molecule 6 is DIPHOSPHATE (three-letter code: DPO) (formula: O_7P_2).



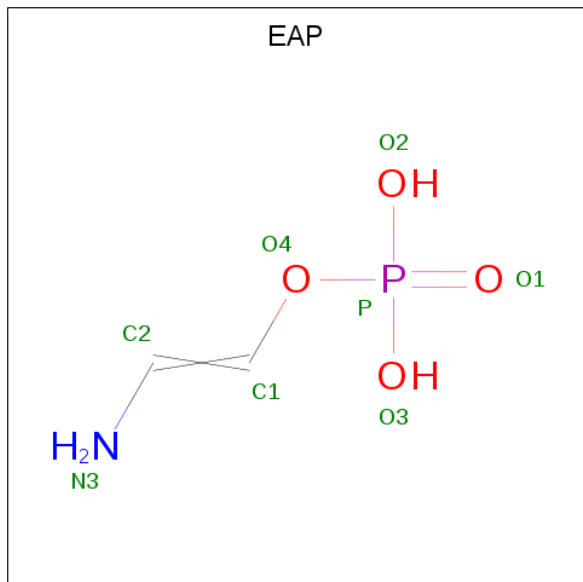
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			8	6	2		
6	B	1	Total	O	P	0	0
			8	6	2		

- Molecule 7 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



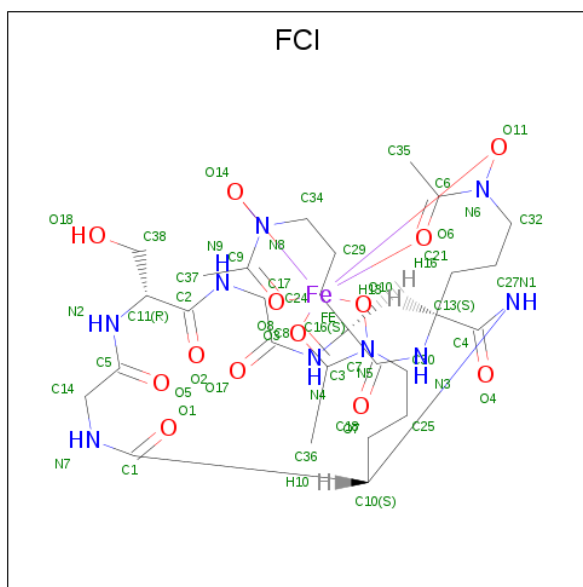
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	12	1		
7	B	1	Total	C	O	0	0
			13	12	1		

- Molecule 8 is 2-AMINO-VINYLP-HOSPHATE (three-letter code: EAP) (formula: $C_2H_6NO_4P$).



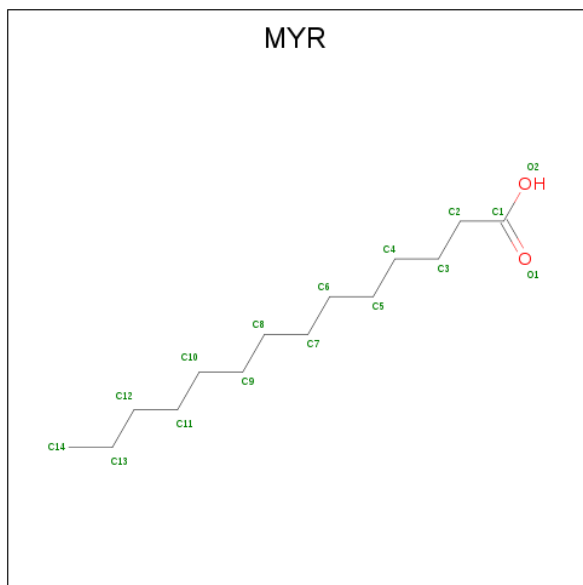
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			7	2	1	3	1		
8	B	1	Total	C	N	O	P	0	0
			7	2	1	3	1		

- Molecule 9 is FERRICROCIN-IRON (three-letter code: FCI) (formula: $C_{28}H_{44}FeN_9O_{13}$).



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

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

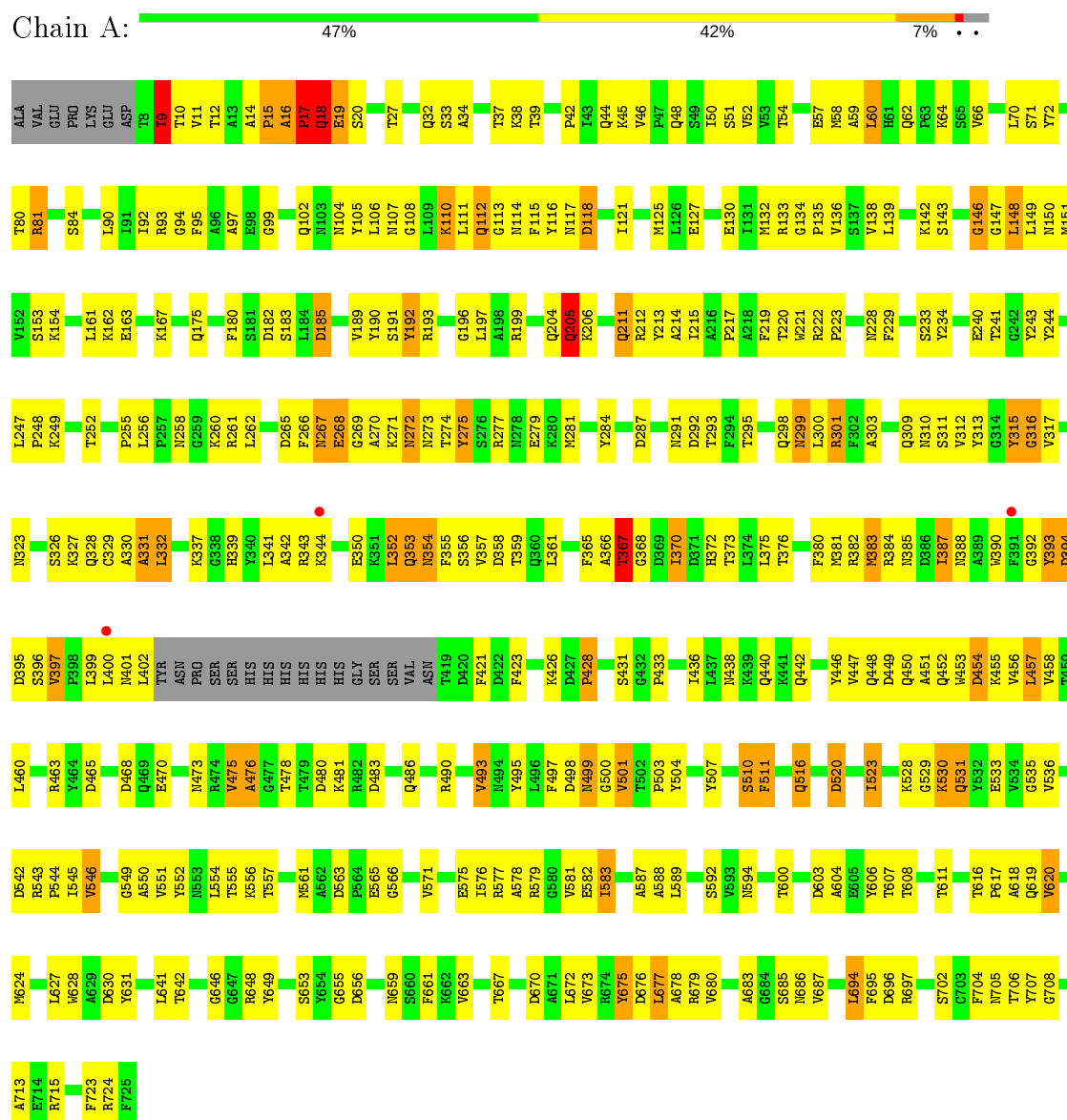


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O		
			15	14	1	0	0

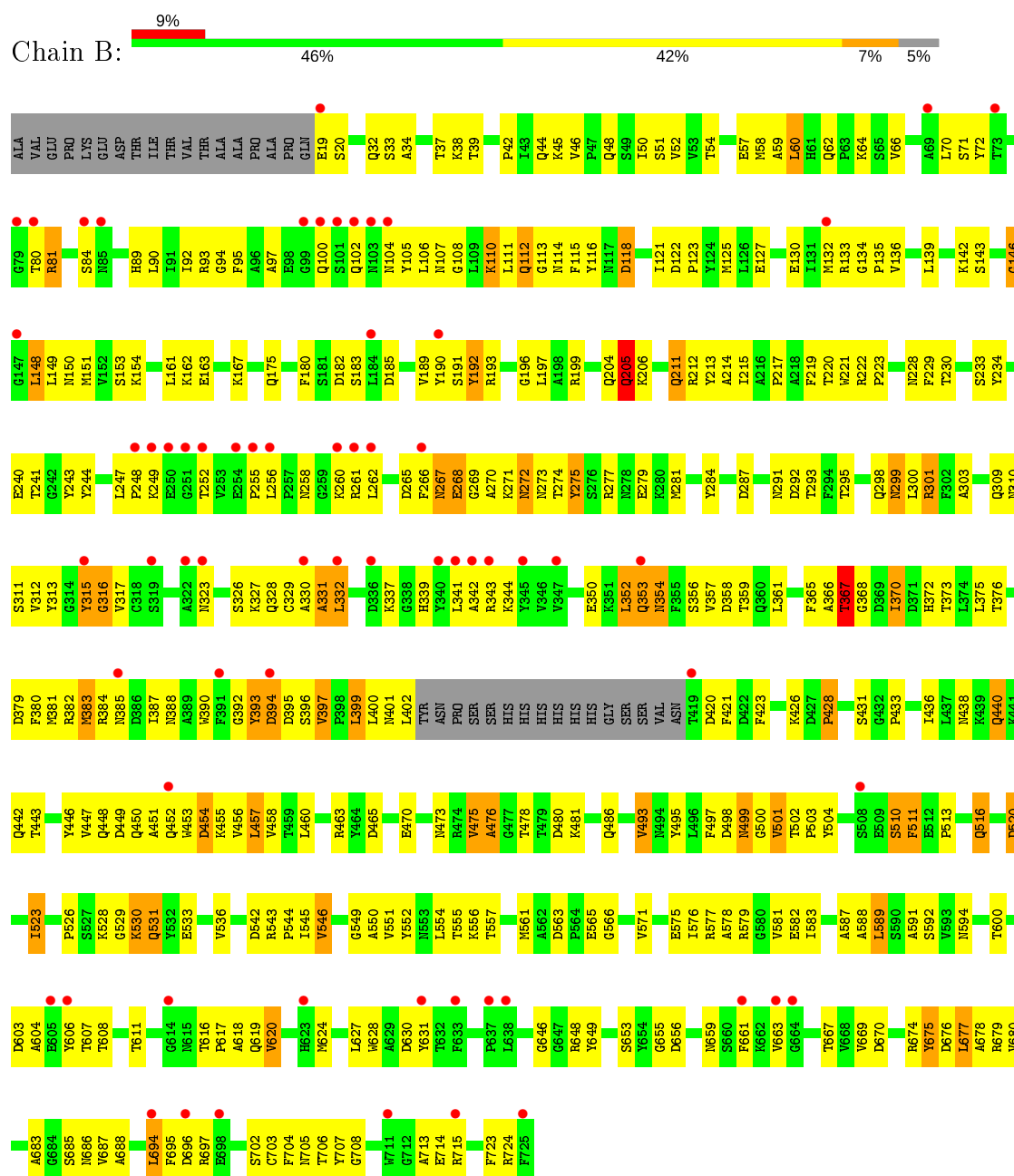
3 Residue-property plots

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

- Molecule 1: Ferrichrome-iron receptor

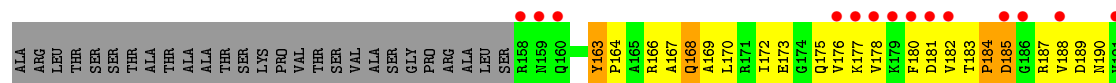


- Molecule 1: Ferrichrome-iron receptor

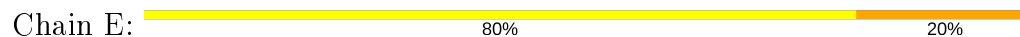




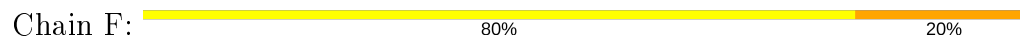
● Molecule 2: Protein tonB



● 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 45.94 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-3.30) 99.2 (45.94-3.30)	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 0.260 , 0.311	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)	0.25 , 68.4	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.50	0/5599	0.69	1/7609 (0.0%)
1	B	0.40	0/5525	0.66	0/7504
2	C	0.35	0/636	0.56	0/857
2	D	0.31	0/636	0.54	0/857
All	All	0.44	0/12396	0.66	1/16827 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	PRO	N-CA-C	5.33	125.96	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5466	0	5193	358	0
1	B	5394	0	5120	344	0
2	C	624	0	640	53	0
2	D	624	0	640	48	0
3	E	63	0	50	18	0
3	F	63	0	51	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	922	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 38.

All (922) 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
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:O1A	3:E:4:KDO:C1	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:390:TRP:HE1	1:B:431:SER:HB3	1.17	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:B:142:LYS:HE3	1:B:440:GLN:HE21	1.23	1.01
1:A:516:GLN:HE21	1:A:516:GLN:HA	1.24	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:298:GLN:C	1:B:299:ASN:HD22	1.79	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:298:GLN:C	1:A:299:ASN:HD22	1.80	0.83
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:343:ARG:HH11	1:A:400:LEU:HD22	1.44	0.82
1:A:11:VAL:HB	2:C:228:ILE:CG2	2.09	0.82
5:B:901:FTT:H143	5:B:903:FTT:C13	2.03	0.82
1:A:680:VAL:HG12	1:A:680:VAL:O	1.80	0.82
1:A:9:ILE:HD12	2:C:158:ARG:HH12	1.39	0.82
3:F:2:GCN:H62	3:F:3:KDO:O1A	1.77	0.82
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:902:FTT:H112	5:B:903:FTT:H111	1.67	0.76
5:B:901:FTT:C14	5:B:903:FTT:H131	2.15	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:O	1:B:680:VAL:HG12	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:O1A	3:F:4:KDO:C1	2.34	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
1:B:57:GLU:O	1:B:60:LEU:HB3	1.87	0.74
1:A:370:ILE:H	1:A:370:ILE:HD13	1.51	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLN:HE21	1:A:311:SER:HB2	1.51	0.73
1:A:62:GLN:HG3	1:A:167:LYS:HZ3	1.53	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:134:GLY:C	1:B:146:GLY:HA2	2.10	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: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: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
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:134:GLY:C	1:A:146:GLY:HA2	2.12	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
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:901:FTT:H143	7:A:930:DAO:H111	1.74	0.68
5:A:900:FTT:H142	5:B:900:FTT:H122	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LYS:H	1:A:442:GLN:NE2	1.91	0.68
1:B:339:HIS:O	1:B:402:LEU:HD23	1.93	0.68
6:A:910:DPO:P2	6:B:910:DPO:O6	2.51	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:B:197:LEU:HD12	1:B:197:LEU:C	2.14	0.67
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:A:197:LEU:HD12	1:A:197:LEU:C	2.15	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: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
1:B:70:LEU:CD1	1:B:90:LEU:HD21	2.25	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:299:ASN:N	1:A:299:ASN:HD22	1.92	0.67
1:A:678:ALA:CB	1:A:683:ALA:HA	2.22	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:11:VAL:CB	2:C:228:ILE:HG22	2.25	0.66
1:B:401:ASN:C	1:B:402:LEU:HD22	2.14	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
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:284:TYR:CE1	1:A:298:GLN:HG2	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLN:NE2	1:A:713:ALA:HA	2.08	0.65
1:A:353:GLN:HE21	1:A:384:ARG:CD	2.07	0.65
1:A:401:ASN:C	1:A:402:LEU:HD22	2.16	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
1:B:392:GLY:HA3	1:B:396:SER:OG	1.97	0.64
8:A:980:EAP:H11	3:E:5:GMH:H6	1.79	0.64
6:B:910:DPO:O3	3:F:1:GCN:C1	2.46	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:A:189:VAL:HG13	1:A:190:TYR:CD2	2.33	0.63
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:B:523:ILE:HD13	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:105:TYR:CE2	1:A:110:LYS:HB2	2.35	0.62
1:A:33:SER:OG	1:A:34:ALA:N	2.32	0.62
1:A:315:TYR:O	1:A:316:GLY:O	2.18	0.62
1:A:46:VAL:HG12	1:A:48:GLN:H	1.65	0.62
1:A:676:ASP:OD2	2:C:200:ASN:HB2	2.00	0.62
1:A:401:ASN:CG	1:A:402:LEU:H	2.03	0.62
1:B:46:VAL:HG12	1:B:48:GLN:H	1.64	0.62
1:A:148:LEU:HD23	1:A:148:LEU:C	2.21	0.62
1:A:50:ILE:CG2	1:A:51:SER:N	2.63	0.62
1:B:516:GLN:NE2	1:B:516:GLN:HA	2.07	0.62
5:A:901:FTT:H71	5:B:900:FTT:H72	1.82	0.62
1:A:104:ASN:ND2	1:A:149:LEU:HD23	2.15	0.61
1:A:42:PRO:HB2	1:A:44:GLN:OE1	2.00	0.61
1:B:107:ASN:ND2	1:B:153:SER:H	1.97	0.61
1:A:352:LEU:C	1:A:352:LEU:HD12	2.20	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: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
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
1:B:197:LEU:O	1:B:197:LEU:HD12	2.02	0.60
1:B:284:TYR:CE1	1:B:298:GLN:HG2	2.33	0.60
1:B:42:PRO:HB2	1:B:44:GLN:OE1	2.02	0.60
1:B:380:PHE:CE1	5:B:900:FTT:H51	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:352:LEU:HD12	1:B:352:LEU:C	2.22	0.59
1:B:549:GLY:HA2	1:B:583:ILE:HG22	1.84	0.59
1:B:62:GLN:HG3	1:B:167:LYS:HZ3	1.67	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:NE2	1:A:516:GLN:HA	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:A:401:ASN:CG	1:A:402:LEU:N	2.53	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:B:401:ASN:CG	1:B:402:LEU:N	2.56	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:148:LEU:HD23	1:A:148:LEU:O	2.03	0.58
1:A:44:GLN:HG2	1:A:45:LYS:N	2.18	0.58
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:401:ASN:CG	1:B:402:LEU:H	2.06	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:H	2:C:232:ILE:HD12	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:LYS:HB2	1:B:175:GLN:HB3	1.85	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:453:TRP:O	1:B:455:LYS:N	2.36	0.57
1:B:95:PHE:HE1	1:B:578:ALA:HB2	1.68	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
1:A:108:GLY:H	1:A:150:ASN:HD21	1.50	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
1:A:93:ARG:HH21	1:A:582:GLU:CD	2.09	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:148:LEU:HD23	1:B:148:LEU:C	2.26	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:549:GLY:HA2	1:A:583:ILE:HG22	1.85	0.56
1:A:163:GLU:HB2	1:A:724:ARG:HG2	1.87	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
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:71:SER:HB3	1:A:648:ARG:HD2	1.88	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:11:VAL:HG12	1:A:12:THR:H	1.71	0.55
1:B:476:ALA:C	1:B:478:THR:H	2.10	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
2:C:232:ILE:O	2:C:233:ASN:C	2.44	0.55
1:A:163:GLU:HA	1:A:723:PHE:O	2.07	0.55
1:A:62:GLN:HG3	1:A:167:LYS:NZ	2.20	0.55
1:B:62:GLN:HG3	1:B:167:LYS:NZ	2.21	0.55
2:C:167:ALA:C	2:C:169:ALA:H	2.10	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: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:A:476:ALA:C	1:A:478:THR:H	2.09	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
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
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:295:THR:O	1:B:361:LEU:HD12	2.06	0.54
1:B:72:TYR:CE2	1:B:628:TRP:HB2	2.42	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:N	1:B:523:ILE:HD13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:4:KDO:H32	3:F:5:GMH:H71	1.89	0.54
1:A:197:LEU:O	1:A:197:LEU:HD12	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:HG12	1:B:546:VAL:O	2.07	0.53
2:D:177:LYS:HB3	2:D:194:LEU:HD12	1.90	0.53
1:B:93:ARG:HH21	1:B:582:GLU:CD	2.11	0.53
2:D:178:VAL:HG11	2:D:210:MET:SD	2.48	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:576:Ile:HD11	1:B:606:TYR:CE1	2.43	0.53
1:B:163:GLU:HB2	1:B:724:ARG:HG2	1.90	0.53
1:A:113:GLY:O	1:A:114:ASN:HB2	2.08	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
1:B:291:ASN:O	1:B:293:THR:N	2.42	0.53
2:D:167:ALA:C	2:D:169:ALA:H	2.13	0.53
1:A:102:GLN:HG2	1:A:118:ASP:OD2	2.09	0.53
1:A:628:TRP:CD1	1:A:646:GLY:HA3	2.44	0.53
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:426:LYS:O	1:B:428:PRO:HD3	2.09	0.52
1:B:298:GLN:HE22	5:B:900:FTT:H142	1.73	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ASP:OD1	3:F:4:KDO:H7	2.10	0.52
1:B:312:VAL:HG23	1:B:423:PHE:CZ	2.45	0.52
1:A:523:ILE:N	1:A:523:ILE:HD13	2.25	0.52
1:B:563:ASP:HA	1:B:571:VAL:CG2	2.40	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: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
1:A:390:TRP:CZ3	1:A:433:PRO:HB3	2.45	0.51
2:C:183:THR:O	2:C:185:ASP:N	2.44	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:352:LEU:HB2	1:A:384:ARG:O	2.11	0.51
1:A:58:MET:O	1:A:60:LEU:N	2.37	0.51
1:B:343:ARG:HH11	1:B:400:LEU:CD2	2.20	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:HH11	1:B:543:ARG:HG3	1.75	0.51
1:B:591:ALA:O	2:D:166:ARG:NH2	2.43	0.51
1:B:591:ALA:C	2:D:166:ARG:HH22	2.14	0.51
1:B:217:PRO:HD2	1:B:233:SER:OG	2.10	0.51
1:B:71:SER:HB3	1:B:648:ARG:HD2	1.91	0.51
1:B:608:THR:HG22	1:B:608:THR:O	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
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
1:B:354:ASN:C	1:B:354:ASN:ND2	2.65	0.51
5:B:900:FTT:O2	7:B:930:DAO:C2	2.57	0.51
2:C:167:ALA:C	2:C:169:ALA:N	2.64	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:O	1:A:687:VAL:HG23	2.10	0.50
1:B:185:ASP:CG	1:B:189:VAL:HG12	2.32	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:A:503:PRO:CA	1:A:536:VAL:HG12	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:GLY:HA2	1:B:214:ALA:O	2.12	0.50
1:B:592:SER:O	1:B:631:TYR:HA	2.11	0.50
1:B:163:GLU:HA	1:B:723:PHE:O	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: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:B:106:LEU:HD12	1:B:151:MET:O	2.12	0.49
1:B:19:GLU:HG2	1:B:20:SER:H	1.74	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:354:ASN:C	1:A:354:ASN:ND2	2.64	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:A:110:LYS:HG3	1:A:111:LEU:N	2.27	0.49
1:A:185:ASP:CG	1:A:189:VAL:HG12	2.33	0.49
1:A:500:GLY:O	1:A:501:VAL:C	2.50	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: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:CD1	1:A:523:ILE:H	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:CB	2:D:214:ARG:HH11	2.26	0.49
5:A:901:FTT:C1	3:E:1:GCN:H32	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:PHE:C	1:B:499:ASN:H	2.17	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: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:110:LYS:HG3	1:B:111:LEU:N	2.29	0.48
1:B:262:LEU:HD23	1:B:266:PHE:CG	2.48	0.48
1:B:500:GLY:O	1:B:501:VAL:C	2.51	0.48
1:B:628:TRP:CH2	1:B:630:ASP:HB3	2.48	0.48
1:B:81:ARG:CG	1:B:84:SER:HB3	2.33	0.48
1:A:60:LEU:HD21	1:A:628:TRP:CZ2	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
1:B:95:PHE:CE1	1:B:578:ALA:HB2	2.48	0.48
1:B:240:GLU:OE1	1:B:240:GLU:HA	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:354:ASN:HD22	1:B:354:ASN:C	2.17	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:354:ASN:HD22	1:A:354:ASN:C	2.17	0.48
1:A:142:LYS:N	1:A:442:GLN:HE22	2.04	0.48
1:A:72:TYR:CE1	1:A:648:ARG:HD3	2.48	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: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
2:D:227:ASN:C	2:D:227:ASN:HD22	2.16	0.47
1:A:106:LEU:HD12	1:A:151:MET:O	2.14	0.47
1:A:483:ASP:OD1	3:F:4:KDO:O8	2.30	0.47
1:B:339:HIS:C	1:B:402:LEU:HD23	2.33	0.47
1:B:37:THR:HB	1:B:448:GLN:HE22	1.78	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:58:MET:O	1:B:60:LEU:N	2.38	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:PHE:C	1:A:499:ASN:H	2.18	0.47
1:B:277:ARG:HG3	1:B:277:ARG:HH11	1.79	0.47
1:B:516:GLN:NE2	1:B:516:GLN:CA	2.73	0.47
2:C:227:ASN:HD22	2:C:227:ASN:C	2.16	0.47
2:D:176:VAL:O	2:D:227:ASN:HA	2.15	0.47
2:D:197:LYS:NZ	2:D:197:LYS:HB2	2.29	0.47
1:A:228:ASN:OD1	1:A:229:PHE:N	2.48	0.47
1:B:520:ASP:OD1	1:B:520:ASP:N	2.46	0.47
2:C:229:LEU:HD12	2:C:229:LEU:N	2.29	0.47
1:A:15:PRO:O	1:A:16:ALA:CB	2.63	0.47
1:B:241:THR:OG1	1:B:275:TYR:HB3	2.15	0.47
5:B:901:FTT:H122	5:B:903:FTT:C10	2.44	0.47
2:D:167:ALA:C	2:D:169:ALA:N	2.67	0.47
3:F:4:KDO:H1B	3:F:4:KDO:C1	2.13	0.47
1:A:10:THR:HG22	1:A:11:VAL:N	2.30	0.47
1:A:182:ASP:CG	1:A:183:SER:H	2.18	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: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:CB	2:C:214:ARG:HH11	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
5:A:903:FTT:C1	3:E:2:GCN:H32	2.42	0.47
1:B:267:ASN:C	1:B:267:ASN:HD22	2.19	0.47
5:B:901:FTT:H122	5:B:903:FTT:H111	1.93	0.47
1:A:339:HIS:C	1:A:402:LEU:HD23	2.36	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:60:LEU:C	1:B:60:LEU:HD23	2.35	0.46
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:NZ	2:C:197:LYS:HB2	2.30	0.46
1:A:219:PHE:CD2	1:A:220:THR:N	2.84	0.46
1:A:331:ALA:C	1:A:332:LEU:HD23	2.35	0.46
1:A:115:PHE:CD2	1:A:387:ILE:HD13	2.50	0.46
1:A:344:LYS:HE2	1:A:394:ASP:H	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:TYR:HD1	1:A:667:THR:OG1	1.98	0.46
1:B:530:LYS:N	1:B:530:LYS:HD2	2.30	0.46
1:B:133:ARG:NH2	1:B:582:GLU:OE2	2.47	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:CD1	1:B:370:ILE:H	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:190:TYR:HD2	1:B:190:TYR:N	2.12	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
5:B:901:FTT:H91	7:B:930:DAO:H72	1.96	0.46
5:B:901:FTT:H122	5:B:903:FTT:H101	1.98	0.46
5:B:901:FTT:O2	3:F:1:GCN:C3	2.61	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
1:B:72:TYR:CE1	1:B:648:ARG:HD3	2.51	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
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
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
1:B:313:TYR:HD1	1:B:313:TYR:H	1.64	0.46
5:A:901:FTT:O2	3:E:1:GCN:C3	2.64	0.46
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:A:92:ILE:N	1:A:92:ILE:HD12	2.31	0.45
1:B:182:ASP:CG	1:B:183:SER:H	2.19	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:HD2	1:A:190:TYR:N	2.13	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:LYS:O	1:B:556:LYS:HA	2.16	0.45
1:A:357:VAL:HG22	1:A:358:ASP:N	2.32	0.45
1:B:576:ILE:HG22	1:B:577:ARG:N	2.32	0.45
1:B:687:VAL:O	1:B:687:VAL:HG23	2.16	0.45
1:A:161:LEU:O	1:A:180:PHE:HA	2.16	0.45
1:A:182:ASP:CG	1:A:183:SER:N	2.70	0.45
1:A:616:THR:N	1:A:659:ASN:HD21	2.10	0.45
1:A:695:PHE:O	1:A:696:ASP:C	2.55	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
1:A:323:ASN:O	1:A:326:SER:HB3	2.17	0.45
1:A:511:PHE:C	1:A:511:PHE:CD1	2.90	0.45
1:A:60:LEU:C	1:A:60:LEU:HD23	2.36	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
1:B:331:ALA:C	1:B:332:LEU:HD23	2.38	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:530:LYS:N	1:A:530:LYS:HD2	2.32	0.44
1:B:493:VAL:O	1:B:504:TYR:HB2	2.17	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
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:B:270:ALA:O	1:B:272:ASN:N	2.51	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:A:381:MET:SD	1:A:381:MET:C	2.95	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:92:ILE:N	1:B:92:ILE:HD12	2.32	0.44
1:A:111:LEU:HD23	1:A:301:ARG:HH12	1.83	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:381:MET:C	1:B:381:MET:SD	2.96	0.44
1:B:449:ASP:OD2	1:B:451:ALA:HB2	2.18	0.44
1:B:724:ARG:HH11	1:B:724:ARG:HG3	1.82	0.44
5:A:901:FTT:O2	3:E:1:GCN:H32	2.17	0.44
1:A:317:VAL:HA	1:A:341:LEU:HA	1.99	0.44
1:B:695:PHE:O	1:B:696:ASP:C	2.56	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
1:A:273:ASN:HD21	1:A:312:VAL:N	1.99	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:OD2	1:A:468:ASP:N	2.50	0.43
1:A:470:GLU:HG3	1:A:481:LYS:HB3	2.00	0.43
1:B:182:ASP:CG	1:B:183:SER:N	2.71	0.43
1:B:543:ARG:NH1	1:B:543:ARG:HG3	2.33	0.43
1:A:628:TRP:CH2	1:A:630:ASP:HB3	2.53	0.43
1:B:357:VAL:HG22	1:B:358:ASP:N	2.33	0.43
1:B:523:ILE:CD1	1:B:523:ILE:H	2.22	0.43
1:B:94:GLY:HA2	1:B:620:VAL:HB	1.99	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:529:GLY:C	1:B:530:LYS:HD2	2.38	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:GLY:C	1:A:530:LYS:HD2	2.39	0.43
1:A:81:ARG:CG	1:A:84:SER:HB3	2.31	0.43
1:B:112:GLN:CA	1:B:112:GLN:NE2	2.82	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
1:A:520:ASP:N	1:A:520:ASP:OD1	2.48	0.43
1:A:579:ARG:CG	1:A:603:ASP:HB3	2.34	0.43
1:A:94:GLY:HA2	1:A:620:VAL:HB	2.00	0.43
1:A:672:LEU:HD12	1:A:673:VAL:H	1.84	0.43
1:B:677:LEU:HB2	1:B:685:SER:O	2.19	0.43
1:B:591:ALA:HA	2:D:166:ARG:NH2	2.33	0.43
1:A:112:GLN:CA	1:A:112:GLN:NE2	2.81	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: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:255:PRO:HA	1:B:261:ARG:HG2	2.01	0.43
1:B:206:LYS:HE3	1:B:265:ASP:OD1	2.19	0.43
2:C:232:ILE:CD1	2:C:232:ILE:H	2.29	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:192:TYR:CD1	1:B:192:TYR:C	2.92	0.43
1:B:268:GLU:OE1	1:B:268:GLU:N	2.52	0.43
1:B:365:PHE:CE1	1:B:372:HIS:CG	3.07	0.43
1:B:365:PHE:CD1	1:B:372:HIS:HB2	2.54	0.43
1:A:555:THR:HG22	1:A:577:ARG:HA	2.01	0.42
1:A:678:ALA:C	1:A:680:VAL:H	2.23	0.42
1:A:93:ARG:O	1:A:95:PHE:CD1	2.72	0.42
1:B:511:PHE:C	1:B:511:PHE:CD1	2.92	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:B:678:ALA:C	1:B:680:VAL:H	2.23	0.42
2:C:215:TYR:CD1	2:C:216:GLU:N	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:PRO:HA	1:A:261:ARG:HG2	2.02	0.42
1:A:37:THR:HB	1:A:448:GLN:HE22	1.85	0.42
1:A:543:ARG:HG3	1:A:543:ARG:NH1	2.33	0.42
1:B:142:LYS:O	1:B:143:SER:HB3	2.19	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: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: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:A:93:ARG:O	1:A:95:PHE:HD1	2.02	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
1:B:135:PRO:HD3	1:B:554:LEU:HD13	1.99	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:436:ILE:CG2	1:B:438:ASN:HD21	2.33	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
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:277:ARG:HH11	1:A:277:ARG:HG3	1.83	0.42
1:B:267:ASN:HD22	1:B:269:GLY:H	1.67	0.42
1:B:531:GLN:HB2	1:B:554:LEU:HD12	2.00	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
1:B:93:ARG:O	1:B:95:PHE:HD1	2.02	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:A:206:LYS:HE3	1:A:265:ASP:OD1	2.20	0.41
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:C:178:VAL:HG11	2:C:210:MET:CE	2.49	0.41
2:D:173:GLU:OE2	2:D:232:ILE:HG22	2.20	0.41
2:D:178:VAL:HG11	2:D:210:MET:CE	2.50	0.41
1:B:122:ASP:CG	1:B:123:PRO:HD2	2.40	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:181:ASP:OD1	2:C:190:ASN:CG	2.58	0.41
1:A:256:LEU:HD11	1:A:262:LEU:CD1	2.51	0.41
1:A:58:MET:C	1:A:60:LEU:H	2.22	0.41
1:B:132:MET:SD	1:B:136:VAL:HG11	2.60	0.41
1:B:44:GLN:OE1	1:B:44:GLN:N	2.49	0.41
1:A:27:THR:HG22	2:C:166:ARG:HD2	2.02	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: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
1:A:433:PRO:CG	1:A:475:VAL:HG21	2.51	0.41
1:A:619:GLN:NE2	1:A:702:SER:OG	2.53	0.41
1:B:60:LEU:O	1:B:60:LEU:HD23	2.20	0.41
1:B:204:GLN:NE2	1:B:714:GLU:H	2.19	0.41
1:A:481:LYS:NZ	8:B:980:EAP:H21	2.36	0.41
2:D:227:ASN:C	2:D:227:ASN:ND2	2.73	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:B:185:ASP:OD1	1:B:189:VAL:HG12	2.21	0.41
1:B:197:LEU:CD1	1:B:197:LEU:C	2.84	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:352:LEU:HD12	1:B:353:GLN:C	2.41	0.41
1:A:136:VAL:C	1:A:138:VAL:N	2.73	0.41
1:A:81:ARG:HD3	1:A:81:ARG:HA	1.93	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:B:111:LEU:HD23	1:B:301:ARG:HH12	1.85	0.41
1:B:589:LEU:HA	1:B:589:LEU:HD12	1.86	0.41
5:B:902:FTT:H51	7:B:930:DAO:C1	2.51	0.41
2:C:172:ILE:HD11	2:C:201:MET:SD	2.61	0.41
2:C:227:ASN:C	2:C:227:ASN:ND2	2.73	0.41
1:A:284:TYR:HD2	5:A:902:FTT:C14	2.20	0.41
1:B:199:ARG:NH2	1:B:212:ARG:NH1	2.68	0.41
1:B:674:ARG:CB	1:B:688:ALA:HB2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:164:PRO:HG2	2:C:202:PHE:CD2	2.55	0.41
2:C:165:ALA:O	2:C:166:ARG:C	2.58	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: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: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:A:9:ILE:CG1	1:A:10:THR:N	2.82	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:903:FTT:C2	10:B:940:MYR:C1	2.99	0.40
5:B:901:FTT:C14	5:B:903:FTT:H111	2.02	0.40
1:A:476:ALA:C	1:A:478:THR:N	2.74	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:HD12	2:C:232:ILE:O	2.21	0.40
1:A:117:ASN:CG	1:A:352:LEU:HD23	2.41	0.40
1:A:555:THR:CG2	1:A:577:ARG:HG3	2.51	0.40
5:A:902:FTT:H51	7:A:930:DAO:C1	2.51	0.40
1:B:475:VAL:CG2	1:B:475:VAL:O	2.66	0.40
5:A:900:FTT:H112	5:B:900:FTT:H102	2.02	0.40
1:A:19:GLU:HG3	1:A:20:SER:N	2.36	0.40
1:A:316:GLY:C	1:A:341:LEU:HD12	2.41	0.40
1:A:641:LEU:HD12	1:A:642:THR:H	1.86	0.40
1:B:433:PRO:CG	1:B:475:VAL:HG21	2.51	0.40
1:B:476:ALA:C	1:B:478:THR:N	2.74	0.40
1:B:72:TYR:HE2	1:B:628:TRP:HB2	1.87	0.40
2:C:188:VAL:HG22	2:C:189:ASP:H	1.86	0.40
2:D:181:ASP:OD1	2:D:190:ASN:CG	2.60	0.40
2:D:183:THR:HG23	2:D:189:ASP:HB2	2.04	0.40
1:A:313:TYR:HD1	1:A:313:TYR:H	1.64	0.40
1:A:365:PHE:C	1:A:365:PHE:CD1	2.95	0.40
1:A:531:GLN:HB2	1:A:554:LEU:HD12	2.04	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 [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	698/725 (96%)	590 (84%)	77 (11%)	31 (4%)	2	16
1	B	687/725 (95%)	582 (85%)	79 (12%)	26 (4%)	3	19
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%)	2	14

All (77) Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	518 (90%)	61 (10%)	7	25
1	B	572/601 (95%)	516 (90%)	56 (10%)	8	29
2	C	66/200 (33%)	60 (91%)	6 (9%)	9	31
2	D	66/200 (33%)	61 (92%)	5 (8%)	13	39
All	All	1283/1602 (80%)	1155 (90%)	128 (10%)	7	27

All (128) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	64	LYS
1	A	80	THR
1	A	81	ARG
1	A	110	LYS
1	A	112	GLN
1	A	118	ASP
1	A	185	ASP
1	A	191	SER
1	A	192	TYR
1	A	205	GLN
1	A	211	GLN
1	A	258	ASN
1	A	267	ASN
1	A	268	GLU
1	A	272	ASN
1	A	275	TYR
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	354	ASN
1	A	356	SER
1	A	359	THR
1	A	367	THR
1	A	370	ILE
1	A	383	MET
1	A	387	ILE
1	A	388	ASN
1	A	393	TYR
1	A	397	VAL
1	A	457	LEU
1	A	460	LEU
1	A	480	ASP
1	A	486	GLN
1	A	493	VAL
1	A	499	ASN
1	A	510	SER
1	A	511	PHE
1	A	516	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	520	ASP
1	A	523	ILE
1	A	530	LYS
1	A	531	GLN
1	A	557	THR
1	A	565	GLU
1	A	583	ILE
1	A	589	LEU
1	A	611	THR
1	A	620	VAL
1	A	675	TYR
1	A	679	ARG
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	110	LYS
1	B	112	GLN
1	B	118	ASP
1	B	191	SER
1	B	192	TYR
1	B	205	GLN
1	B	211	GLN
1	B	258	ASN
1	B	267	ASN
1	B	268	GLU
1	B	272	ASN
1	B	275	TYR
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	354	ASN
1	B	356	SER
1	B	359	THR
1	B	367	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	370	ILE
1	B	383	MET
1	B	388	ASN
1	B	393	TYR
1	B	397	VAL
1	B	440	GLN
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	510	SER
1	B	511	PHE
1	B	516	GLN
1	B	520	ASP
1	B	523	ILE
1	B	530	LYS
1	B	531	GLN
1	B	557	THR
1	B	565	GLU
1	B	589	LEU
1	B	611	THR
1	B	620	VAL
1	B	675	TYR
1	B	679	ARG
1	B	694	LEU
2	C	163	TYR
2	C	168	GLN
2	C	201	MET
2	C	215	TYR
2	C	227	ASN
2	C	232	ILE
2	D	163	TYR
2	D	168	GLN
2	D	201	MET
2	D	215	TYR
2	D	227	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) 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	107	ASN
1	A	112	GLN
1	A	204	GLN
1	A	205	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	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	486	GLN
1	A	516	GLN
1	A	558	ASN
1	A	615	ASN
1	A	619	GLN
1	A	659	ASN
1	A	692	ASN
1	B	32	GLN
1	B	62	GLN
1	B	100	GLN
1	B	107	ASN
1	B	112	GLN
1	B	204	GLN
1	B	205	GLN
1	B	211	GLN
1	B	267	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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	558	ASN
1	B	615	ASN
1	B	619	GLN
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
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	3,5	10,10,11	0.81	0	13,13,15	0.76	0
3	GCN	E	2	3,5,4	10,10,11	1.03	1 (10%)	13,13,15	2.64	2 (15%)
3	KDO	E	3	3	12,15,16	0.73	0	16,21,24	0.86	0
3	KDO	E	4	3	12,15,16	0.47	0	16,21,24	0.89	0
3	GMH	E	5	8,3	13,13,14	0.80	0	17,18,20	0.67	0
3	GCN	F	1	3,5	10,10,11	0.81	0	13,13,15	0.76	0
3	GCN	F	2	3,5,4	10,10,11	1.04	1 (10%)	13,13,15	2.63	2 (15%)
3	KDO	F	3	3	12,15,16	0.74	0	16,21,24	0.85	0
3	KDO	F	4	3	12,15,16	0.46	0	16,21,24	0.89	0
3	GMH	F	5	8,3	13,13,14	0.80	0	17,18,20	0.68	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	3,5	-	2/2/15/18	0/1/1/1
3	GCN	E	2	3,5,4	-	0/2/15/18	0/1/1/1
3	KDO	E	3	3	-	0/6/26/30	0/1/1/1
3	KDO	E	4	3	-	6/6/26/30	0/1/1/1
3	GMH	E	5	8,3	-	2/6/23/26	0/1/1/1
3	GCN	F	1	3,5	-	2/2/15/18	0/1/1/1
3	GCN	F	2	3,5,4	-	0/2/15/18	0/1/1/1
3	KDO	F	3	3	-	0/6/26/30	0/1/1/1
3	KDO	F	4	3	-	6/6/26/30	0/1/1/1
3	GMH	F	5	8,3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	GCN	C1-C2	2.72	1.55	1.52
3	E	2	GCN	C1-C2	2.68	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	GCN	C3-C2-C1	8.75	116.92	109.82
3	F	2	GCN	C3-C2-C1	8.71	116.90	109.82
3	E	2	GCN	C1-O5-C5	2.55	115.65	112.19
3	F	2	GCN	C1-O5-C5	2.52	115.61	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	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	E	5	GMH	O6-C6-C7-O7
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	E	4	KDO	C6-C7-C8-O8
3	F	4	KDO	C6-C7-C8-O8

There are no ring outliers.

10 monomers are involved in 42 short contacts:

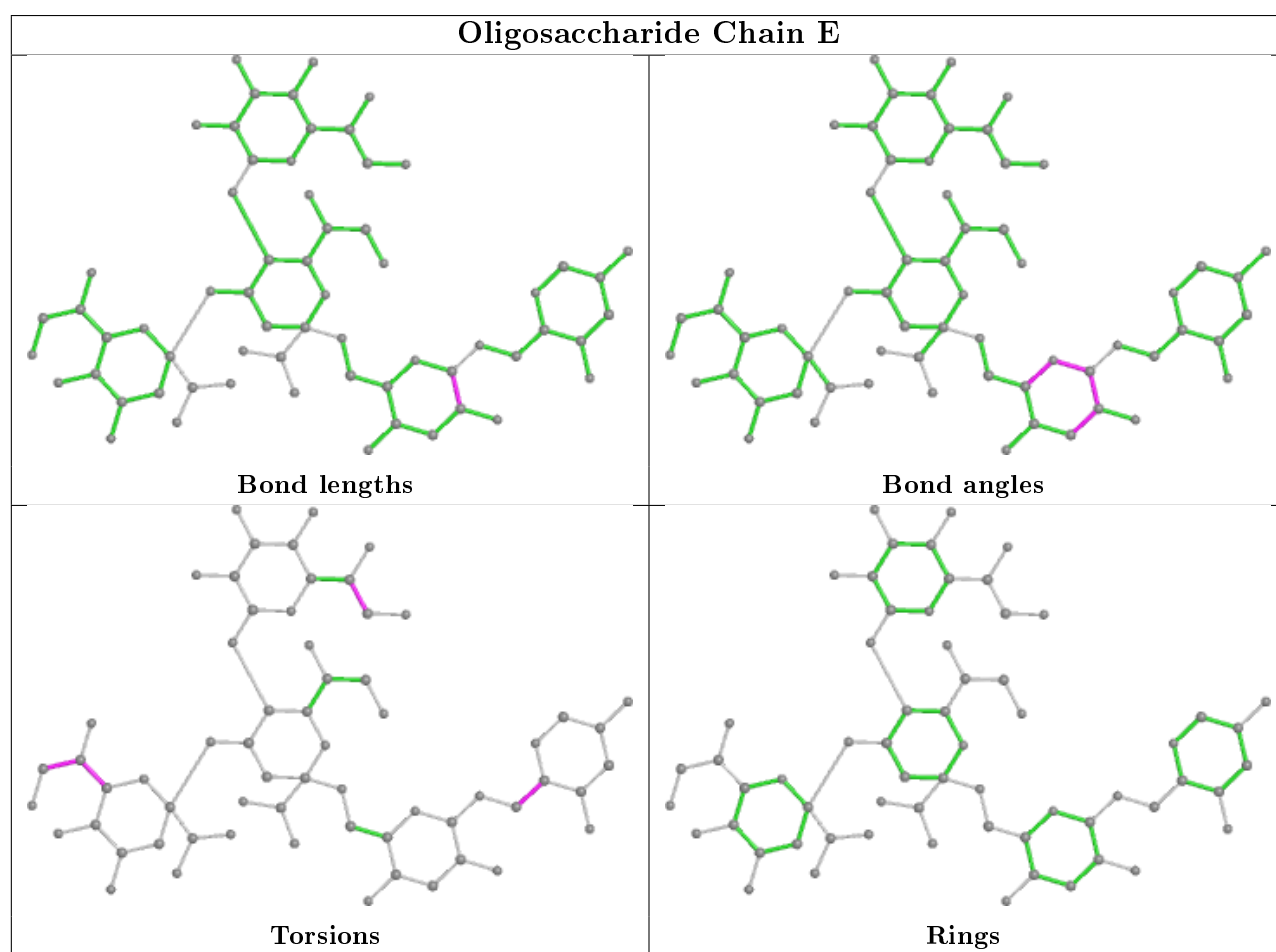
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	4	KDO	3	0
3	F	2	GCN	7	0

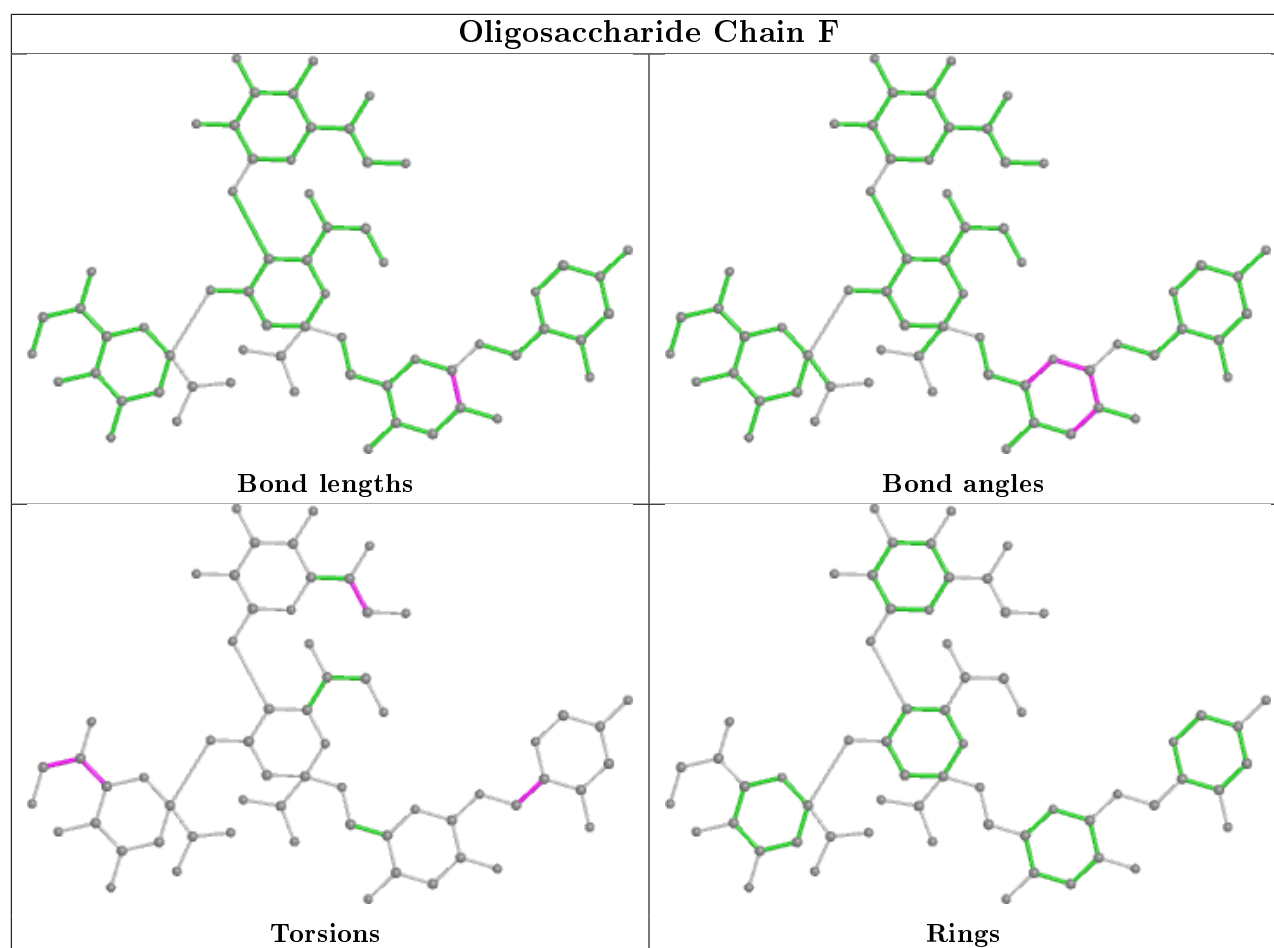
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	GCN	5	0
3	E	3	KDO	3	0
3	E	1	GCN	7	0
3	F	4	KDO	7	0
3	F	3	KDO	3	0
3	E	5	GMH	4	0
3	F	5	GMH	4	0
3	F	1	GCN	7	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
9	FCI	A	1050	-	45,51,56	1.43	4 (8%)	51,78,87	1.15	4 (7%)
10	MYR	B	940	5	14,14,15	0.99	1 (7%)	13,13,15	0.81	1 (7%)
8	EAP	B	980	3	3,6,7	2.86	1 (33%)	0,6,9	0.00	-
5	FTT	B	901	-	15,15,16	0.33	0	15,15,17	0.80	0
5	FTT	B	900	3	15,15,16	4.13	1 (6%)	15,15,17	2.26	3 (20%)
4	PO4	B	950	3	0,3,4	0.00	-	0,3,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FTT	A	900	3	15,15,16	0.43	0	15,15,17	0.70	1 (6%)
4	PO4	A	950	3	0,3,4	0.00	-	0,3,6	0.00	-
6	DPO	A	910	-	4,7,8	2.44	1 (25%)	5,10,13	0.96	0
7	DAO	A	930	5	12,12,13	1.05	1 (8%)	11,11,13	0.80	1 (9%)
9	FCI	B	1050	-	45,51,56	1.44	4 (8%)	51,78,87	1.15	4 (7%)
5	FTT	B	903	10	15,15,16	0.51	0	15,15,17	0.51	0
5	FTT	A	901	-	15,15,16	0.33	0	15,15,17	0.80	0
8	EAP	A	980	3	3,6,7	2.87	1 (33%)	0,6,9	0.00	-
6	DPO	B	910	-	4,7,8	2.44	1 (25%)	5,10,13	0.96	0
5	FTT	A	902	3,7	15,15,16	0.33	0	15,15,17	0.80	0
5	FTT	B	902	3,7	15,15,16	0.33	0	15,15,17	0.80	0
7	DAO	B	930	5	12,12,13	1.05	1 (8%)	11,11,13	0.80	1 (9%)
5	FTT	A	903	-	15,15,16	0.51	0	15,15,17	0.51	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
9	FCI	A	1050	-	-	11/57/102/116	0/3/6/6
10	MYR	B	940	5	-	2/12/12/13	-
8	EAP	B	980	3	-	0/0/4/5	-
5	FTT	B	901	-	-	5/14/14/15	-
5	FTT	B	900	3	-	2/14/14/15	-
5	FTT	A	900	3	-	0/14/14/15	-
6	DPO	A	910	-	-	0/2/5/6	-
7	DAO	A	930	5	-	1/10/10/11	-
9	FCI	B	1050	-	-	11/57/102/116	0/3/6/6
5	FTT	B	903	10	-	2/14/14/15	-
5	FTT	A	901	-	-	2/14/14/15	-
8	EAP	A	980	3	-	0/0/4/5	-
6	DPO	B	910	-	-	0/2/5/6	-
5	FTT	A	902	3,7	-	3/14/14/15	-
5	FTT	B	902	3,7	-	3/14/14/15	-
7	DAO	B	930	5	-	1/10/10/11	-
5	FTT	A	903	-	-	2/14/14/15	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	900	FTT	C9-C8	15.93	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	5.15	2.19	2.04
9	A	1050	FCI	O3-FE	5.10	2.19	2.04
8	A	980	EAP	P-O4	-4.58	1.49	1.63
8	B	980	EAP	P-O4	-4.57	1.49	1.63
6	B	910	DPO	P1-O4	-4.36	1.50	1.63
6	A	910	DPO	P1-O4	-4.35	1.50	1.63
10	B	940	MYR	O2-C1	-3.67	1.23	1.42
7	A	930	DAO	O2-C1	-3.58	1.23	1.42
7	B	930	DAO	O2-C1	-3.57	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

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	900	FTT	C9-C8-C7	7.96	154.83	114.42
9	A	1050	FCI	C1-C10-N1	3.46	120.58	111.16
9	B	1050	FCI	C1-C10-N1	3.46	120.57	111.16
9	A	1050	FCI	C34-N8-C9	2.20	130.56	125.65
9	B	1050	FCI	C34-N8-C9	2.20	130.56	125.65
9	A	1050	FCI	O17-C8-N4	-2.15	119.33	122.95
9	B	1050	FCI	O17-C8-N4	-2.13	119.36	122.95
5	B	900	FTT	O2-C1-C2	-2.12	119.26	125.43
5	A	900	FTT	O2-C1-C2	-2.12	119.26	125.43
9	B	1050	FCI	C30-N5-C3	2.10	130.35	125.65
9	A	1050	FCI	C30-N5-C3	2.10	130.34	125.65
7	B	930	DAO	O2-C1-C2	2.08	125.34	111.66
7	A	930	DAO	O2-C1-C2	2.08	125.34	111.66
10	B	940	MYR	O2-C1-C2	2.06	125.23	111.66
5	B	900	FTT	C10-C9-C8	2.05	124.82	114.42

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	901	FTT	C1-C2-C3-O3
5	A	901	FTT	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	1050	FCI	C25-C30-N5-C3
9	B	1050	FCI	C25-C30-N5-C3
5	A	901	FTT	O3-C3-C4-C5
5	A	902	FTT	O3-C3-C4-C5
5	B	902	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	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
5	B	901	FTT	O3-C3-C4-C5
9	A	1050	FCI	N4-C16-C7-O7
9	B	1050	FCI	N4-C16-C7-O7
9	A	1050	FCI	N2-C11-C2-N9
9	B	1050	FCI	N2-C11-C2-N9
9	A	1050	FCI	N4-C16-C7-N3
9	B	1050	FCI	N4-C16-C7-N3
5	B	901	FTT	C1-C2-C3-C4
9	A	1050	FCI	C29-C34-N8-C9
9	B	1050	FCI	C29-C34-N8-C9
5	B	901	FTT	C2-C3-C4-C5
9	A	1050	FCI	N2-C11-C2-O2
9	B	1050	FCI	N2-C11-C2-O2
5	A	902	FTT	O2-C1-C2-C3
5	B	902	FTT	O2-C1-C2-C3
9	A	1050	FCI	C2-C11-N2-C5
9	B	1050	FCI	C2-C11-N2-C5
10	B	940	MYR	C2-C3-C4-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
5	B	903	FTT	C1-C2-C3-O3
5	A	903	FTT	C1-C2-C3-O3
9	A	1050	FCI	O1-C1-C10-C18
9	B	1050	FCI	O1-C1-C10-C18

Continued on next page...

Continued from previous page...

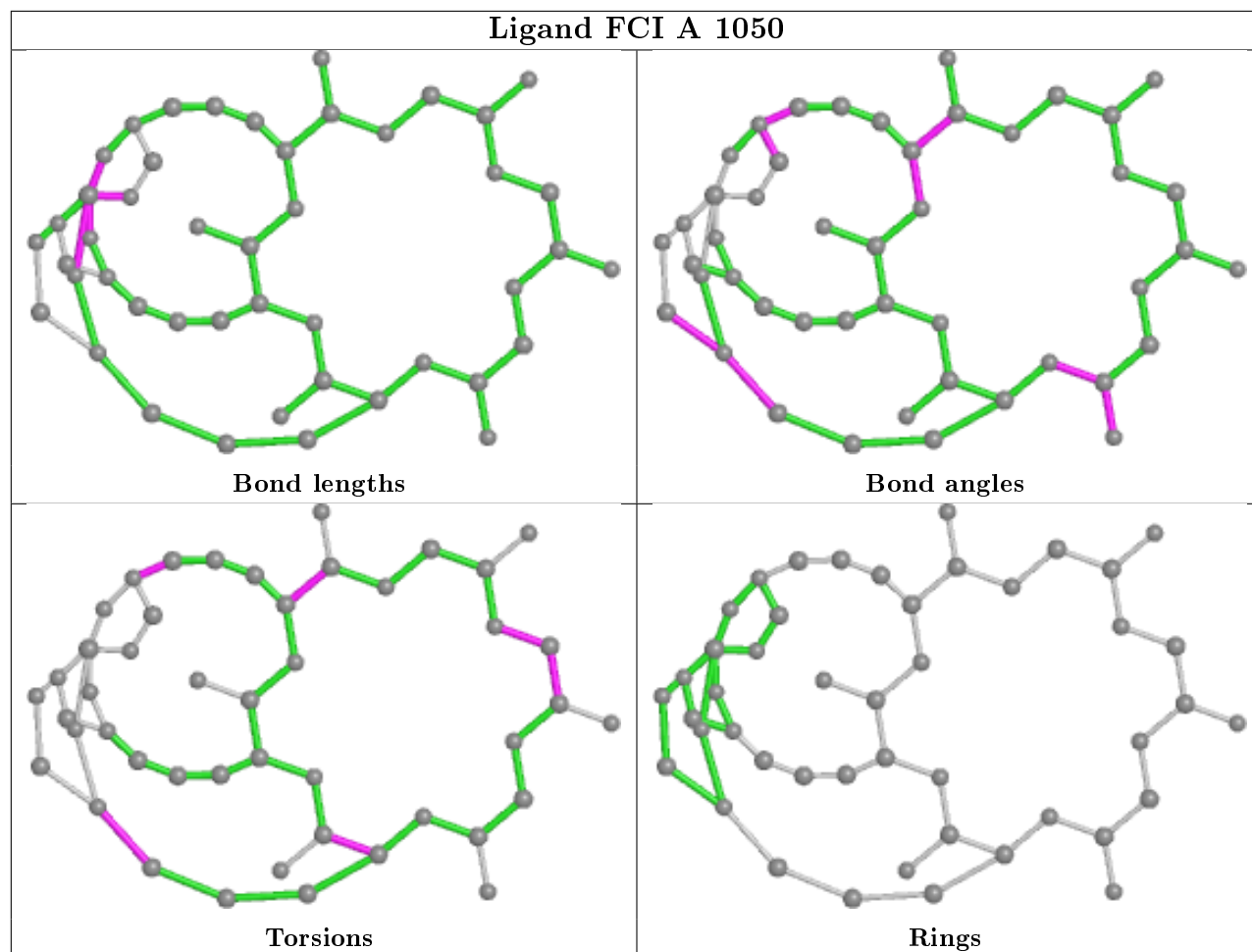
Mol	Chain	Res	Type	Atoms
10	B	940	MYR	O2-C1-C2-C3

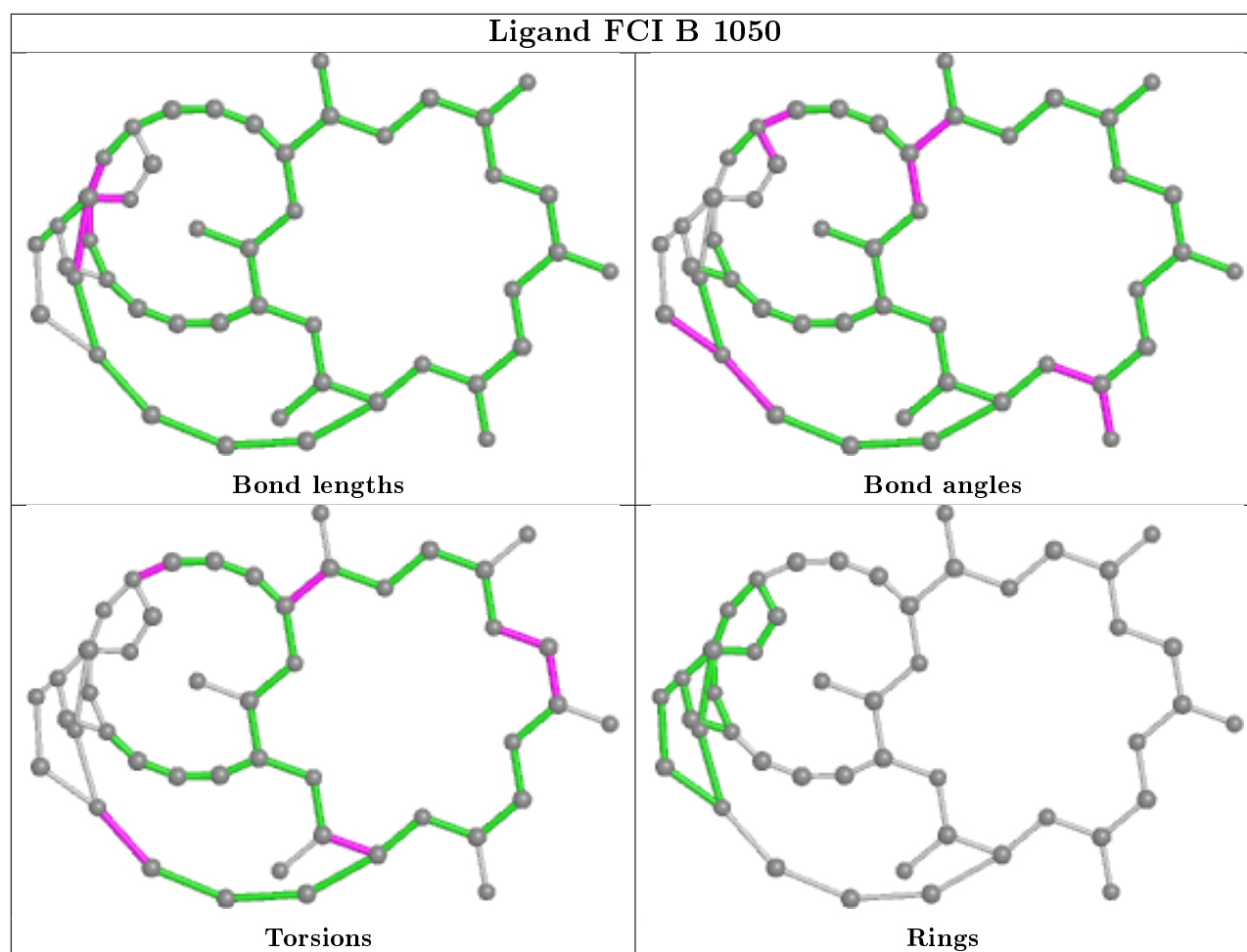
There are no ring outliers.

17 monomers are involved in 138 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1050	FCI	2	0
10	B	940	MYR	4	0
8	B	980	EAP	3	0
5	B	901	FTT	39	0
5	B	900	FTT	17	0
5	A	900	FTT	12	0
6	A	910	DPO	8	0
7	A	930	DAO	5	0
9	B	1050	FCI	1	0
5	B	903	FTT	64	0
5	A	901	FTT	9	0
8	A	980	EAP	2	0
6	B	910	DPO	8	0
5	A	902	FTT	6	0
5	B	902	FTT	39	0
7	B	930	DAO	7	0
5	A	903	FTT	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%)	-0.16	3 (0%) 92 93	24, 61, 110, 177	0
1	B	691/725 (95%)	0.45	66 (9%) 8 8	44, 115, 186, 210	0
2	C	78/229 (34%)	0.76	11 (14%) 2 2	43, 112, 179, 209	0
2	D	78/229 (34%)	2.38	38 (48%) 0 0	102, 187, 210, 210	0
All	All	1549/1908 (81%)	0.29	118 (7%) 13 13	24, 88, 186, 210	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	178	VAL	7.9
1	B	255	PRO	7.8
2	D	225	VAL	7.6
2	D	159	ASN	7.3
1	B	250	GLU	6.8
2	D	213	TRP	6.7
2	D	223	GLY	6.4
2	D	176	VAL	6.3
2	D	224	ILE	6.1
2	D	222	SER	6.0
1	B	249	LYS	5.9
2	D	193	ILE	5.9
2	D	226	VAL	5.9
2	D	195	SER	5.9
2	D	177	LYS	5.9
1	B	315	TYR	5.6
2	D	158	ARG	5.3
2	D	227	ASN	5.3
1	B	638	LEU	5.3
2	D	212	ARG	5.2
1	B	260	LYS	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	262	LEU	4.8
2	D	180	PHE	4.7
1	B	256	LEU	4.7
2	D	194	LEU	4.6
1	B	251	GLY	4.5
1	B	100	GLN	4.5
2	D	214	ARG	4.3
2	D	219	LYS	4.3
1	B	631	TYR	4.3
1	B	252	THR	4.2
2	D	218	GLY	4.2
1	B	261	ARG	4.0
1	B	694	LEU	4.0
1	B	248	PRO	3.9
2	D	182	VAL	3.8
2	D	216	GLU	3.8
2	D	217	PRO	3.8
1	B	266	PHE	3.8
2	D	191	VAL	3.7
2	C	211	ARG	3.6
2	D	215	TYR	3.6
1	B	385	ASN	3.6
2	D	188	VAL	3.5
1	B	394	ASP	3.4
2	D	210	MET	3.4
1	B	19	GLU	3.3
2	D	235	THR	3.3
1	B	725	PHE	3.3
1	B	419	THR	3.3
2	C	221	GLY	3.2
1	B	85	ASN	3.2
1	B	254	GLU	3.2
1	B	101	SER	3.1
2	D	201	MET	3.1
1	B	508	SER	3.1
2	D	181	ASP	3.1
1	B	606	TYR	3.1
1	B	80	THR	3.0
2	D	160	GLN	3.0
1	B	184	LEU	2.9
1	B	664	GLY	2.9
1	B	190	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	84	SER	2.9
2	C	212	ARG	2.9
1	B	663	VAL	2.9
1	B	132	MET	2.9
1	A	391	PHE	2.9
1	B	342	ALA	2.8
1	B	633	PHE	2.8
1	B	605	GLU	2.8
1	B	623	HIS	2.8
2	D	200	ASN	2.8
2	D	179	LYS	2.8
2	D	228	ILE	2.7
1	B	452	GLN	2.7
1	B	332	LEU	2.6
1	B	102	GLN	2.6
1	B	103	ASN	2.6
1	B	715	ARG	2.5
2	D	196	ALA	2.5
1	B	340	TYR	2.5
1	B	698	GLU	2.5
1	B	661	PHE	2.5
2	C	183	THR	2.5
2	D	220	PRO	2.4
1	B	79	GLY	2.4
1	B	345	TYR	2.4
2	C	197	LYS	2.4
2	C	186	GLY	2.4
1	B	336	ASP	2.4
2	D	185	ASP	2.4
1	B	147	GLY	2.3
1	B	353	GLN	2.3
1	B	711	TRP	2.3
2	C	185	ASP	2.3
1	B	99	GLY	2.2
1	B	343	ARG	2.2
1	B	104	ASN	2.2
1	B	322	ALA	2.2
1	A	400	LEU	2.2
1	B	69	ALA	2.2
1	B	73	THR	2.2
1	B	347	VAL	2.2
2	C	188	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	696	ASP	2.2
1	B	330	ALA	2.1
1	B	391	PHE	2.1
1	B	614	GLY	2.1
2	C	161	PRO	2.1
1	B	637	PRO	2.1
2	C	206	VAL	2.1
2	C	210	MET	2.1
1	A	344	LYS	2.1
1	B	319	SER	2.1
1	B	323	ASN	2.0
2	D	186	GLY	2.0
1	B	341	LEU	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 ⓘ

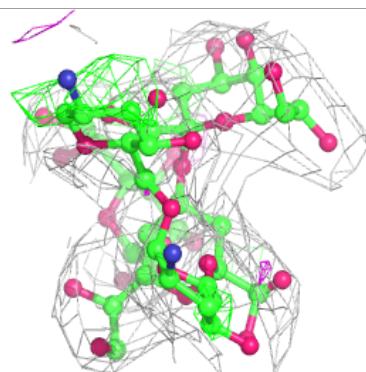
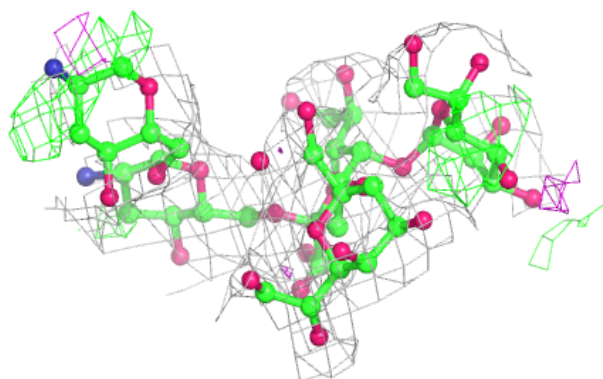
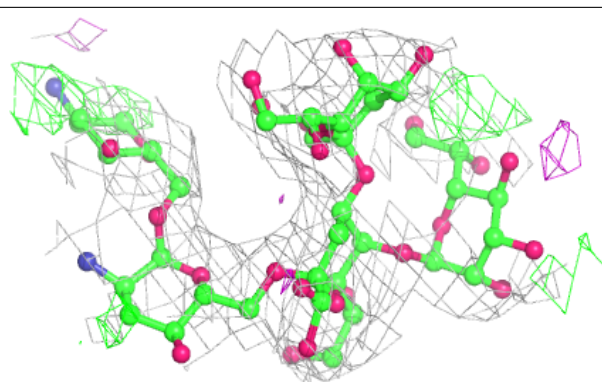
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.77	0.24	73,80,98,98	0
3	GMH	F	5	13/14	0.87	0.19	62,67,79,81	0
3	KDO	E	4	15/16	0.88	0.20	73,80,98,98	0
3	GMH	E	5	13/14	0.88	0.14	62,67,79,81	0
3	GCN	E	1	10/11	0.88	0.23	62,74,79,87	0
3	GCN	F	2	10/11	0.89	0.08	49,60,64,74	0
3	GCN	E	2	10/11	0.91	0.14	49,60,64,74	0
3	KDO	E	3	15/16	0.92	0.17	65,72,98,98	0
3	KDO	F	3	15/16	0.93	0.21	65,72,98,98	0
3	GCN	F	1	10/11	0.94	0.11	62,74,79,87	0

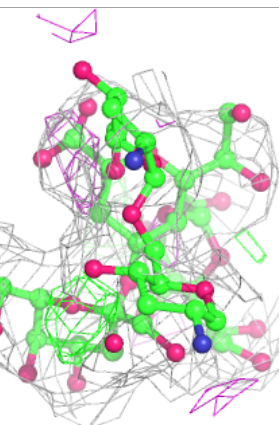
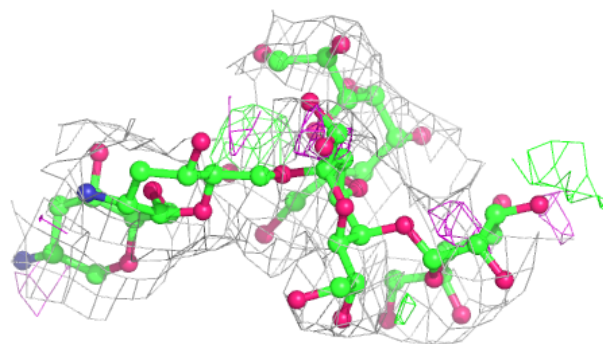
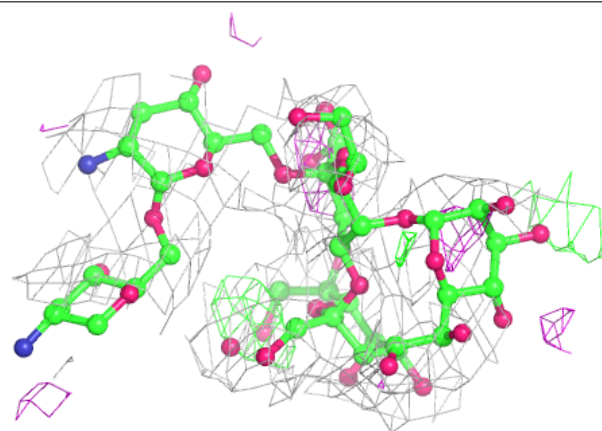
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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 ⓘ

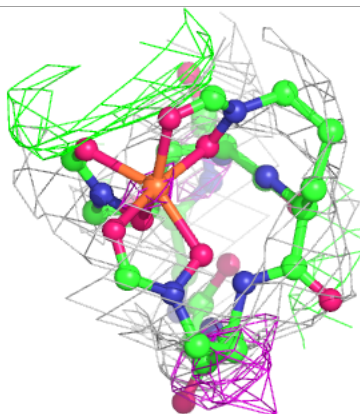
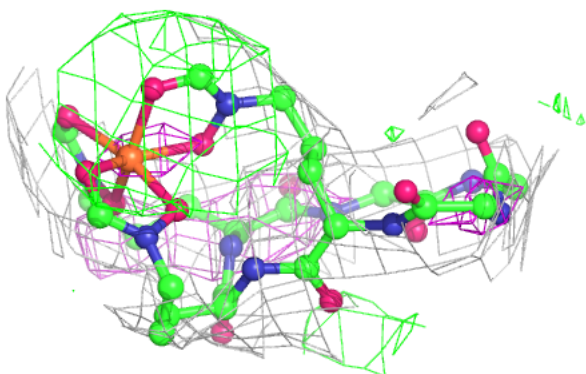
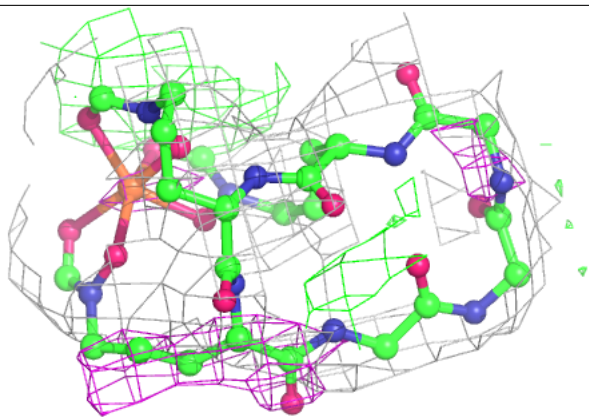
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	0.42	0.88	75,88,92,97	0
5	FTT	B	901	16/17	0.63	0.73	63,70,78,79	0
6	DPO	B	910	8/9	0.69	0.22	62,80,93,95	0
6	DPO	A	910	8/9	0.70	0.22	62,80,93,95	0
10	MYR	B	940	15/16	0.73	1.04	69,86,94,95	0
5	FTT	A	903	16/17	0.74	0.47	75,88,92,97	0
7	DAO	A	930	13/14	0.78	0.60	69,75,82,86	0
5	FTT	A	901	16/17	0.79	0.43	63,70,78,79	0
5	FTT	A	900	16/17	0.80	0.46	76,87,96,102	0
9	FCI	B	1050	46/51	0.81	0.25	44,57,70,81	0
7	DAO	B	930	13/14	0.82	0.40	69,75,82,86	0
5	FTT	B	900	16/17	0.83	0.41	84,95,98,102	0
5	FTT	B	902	16/17	0.83	0.57	63,70,78,79	0
9	FCI	A	1050	46/51	0.87	0.28	44,57,70,81	0
5	FTT	A	902	16/17	0.88	0.47	63,70,78,79	0
8	EAP	A	980	7/8	0.89	0.14	81,87,93,95	0
8	EAP	B	980	7/8	0.89	0.16	81,87,93,95	0
4	PO4	A	950	4/5	0.94	0.10	71,74,76,81	0
4	PO4	B	950	4/5	0.95	0.13	71,74,76,81	0

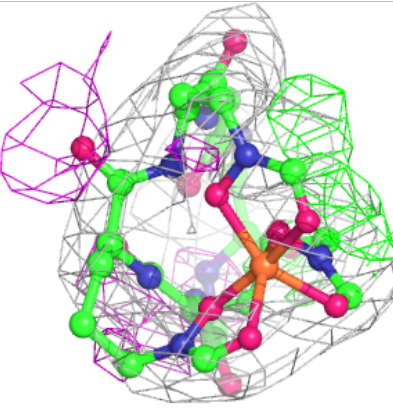
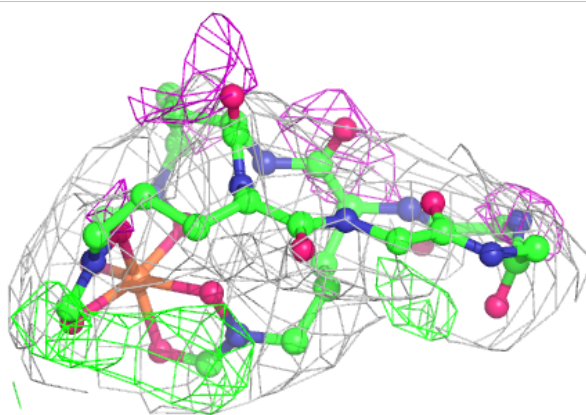
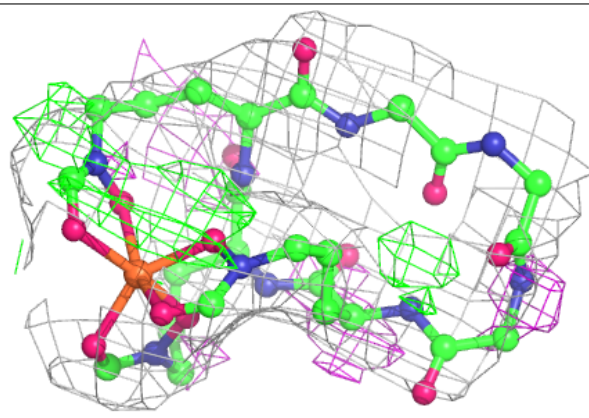
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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