Full wwPDB X-ray Structure Validation Report (i)

May 22, 2023 – 01:37 pm BST

PDB ID	:	7ZV9
Title	:	Crystal structure of FLT3 in complex with a monomeric FLT3 Ligand variant
Authors	:	Pannecoucke, E.; Savvides, S.N.
Deposited on	:	2022-05-14
Resolution	:	4.51 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 (i) 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 (1)) were used in the production of this report:

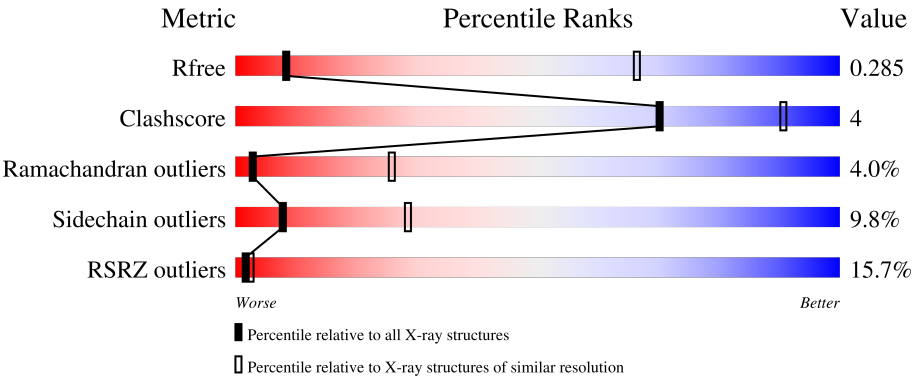
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.51 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	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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 <=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	155	8% 74% 12% • 14%
1	C	155	3% 75% 10% • 14%
1	E	155	6% 77% 7% • 14%
1	G	155	7% 74% 9% • • 14%
1	I	155	7% 78% 8% • 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	155	2% 77% 11% 12%
1	M	155	4% 79% 7% 14%
1	O	155	5% 79% 8% 14%
2	B	582	14% 62% 10% 27%
2	D	582	14% 63% 9% 27%
2	F	582	14% 63% 8% 28%
2	H	582	11% 64% 9% 27%
2	J	582	14% 63% 8% 28%
2	L	582	15% 64% 10% 26%
2	N	582	15% 64% 9% 26%
2	P	582	12% 63% 9% 27%
3	Q	2	100%
3	R	2	50% 50%
3	S	2	100%
3	T	2	50% 50%
3	U	2	100%
3	V	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26691 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 Fms-related tyrosine kinase 3 ligand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	1	0
			915	563	163	181	8			
1	C	134	Total	C	N	O	S	0	1	0
			879	532	162	178	7			
1	E	134	Total	C	N	O	S	0	1	0
			844	504	159	174	7			
1	G	134	Total	C	N	O	S	0	0	0
			884	541	161	176	6			
1	I	135	Total	C	N	O	S	0	1	0
			907	554	162	183	8			
1	K	137	Total	C	N	O	S	0	0	0
			892	544	163	177	8			
1	M	134	Total	C	N	O	S	0	0	0
			908	561	158	181	8			
1	O	134	Total	C	N	O	S	0	1	0
			919	571	160	181	7			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP P49771
A	-19	GLY	-	expression tag	UNP P49771
A	-18	SER	-	expression tag	UNP P49771
A	-17	SER	-	expression tag	UNP P49771
A	-16	HIS	-	expression tag	UNP P49771
A	-15	HIS	-	expression tag	UNP P49771
A	-14	HIS	-	expression tag	UNP P49771
A	-13	HIS	-	expression tag	UNP P49771
A	-12	HIS	-	expression tag	UNP P49771
A	-11	HIS	-	expression tag	UNP P49771
A	-10	SER	-	expression tag	UNP P49771
A	-9	SER	-	expression tag	UNP P49771
A	-8	GLY	-	expression tag	UNP P49771

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	LEU	-	expression tag	UNP P49771
A	-6	VAL	-	expression tag	UNP P49771
A	-5	PRO	-	expression tag	UNP P49771
A	-4	ARG	-	expression tag	UNP P49771
A	-3	GLY	-	expression tag	UNP P49771
A	-2	SER	-	expression tag	UNP P49771
A	-1	HIS	-	expression tag	UNP P49771
A	0	MET	-	expression tag	UNP P49771
A	27	ASP	LEU	engineered mutation	UNP P49771
C	-20	MET	-	initiating methionine	UNP P49771
C	-19	GLY	-	expression tag	UNP P49771
C	-18	SER	-	expression tag	UNP P49771
C	-17	SER	-	expression tag	UNP P49771
C	-16	HIS	-	expression tag	UNP P49771
C	-15	HIS	-	expression tag	UNP P49771
C	-14	HIS	-	expression tag	UNP P49771
C	-13	HIS	-	expression tag	UNP P49771
C	-12	HIS	-	expression tag	UNP P49771
C	-11	HIS	-	expression tag	UNP P49771
C	-10	SER	-	expression tag	UNP P49771
C	-9	SER	-	expression tag	UNP P49771
C	-8	GLY	-	expression tag	UNP P49771
C	-7	LEU	-	expression tag	UNP P49771
C	-6	VAL	-	expression tag	UNP P49771
C	-5	PRO	-	expression tag	UNP P49771
C	-4	ARG	-	expression tag	UNP P49771
C	-3	GLY	-	expression tag	UNP P49771
C	-2	SER	-	expression tag	UNP P49771
C	-1	HIS	-	expression tag	UNP P49771
C	0	MET	-	expression tag	UNP P49771
C	27	ASP	LEU	engineered mutation	UNP P49771
E	-20	MET	-	initiating methionine	UNP P49771
E	-19	GLY	-	expression tag	UNP P49771
E	-18	SER	-	expression tag	UNP P49771
E	-17	SER	-	expression tag	UNP P49771
E	-16	HIS	-	expression tag	UNP P49771
E	-15	HIS	-	expression tag	UNP P49771
E	-14	HIS	-	expression tag	UNP P49771
E	-13	HIS	-	expression tag	UNP P49771
E	-12	HIS	-	expression tag	UNP P49771
E	-11	HIS	-	expression tag	UNP P49771
E	-10	SER	-	expression tag	UNP P49771

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-9	SER	-	expression tag	UNP P49771
E	-8	GLY	-	expression tag	UNP P49771
E	-7	LEU	-	expression tag	UNP P49771
E	-6	VAL	-	expression tag	UNP P49771
E	-5	PRO	-	expression tag	UNP P49771
E	-4	ARG	-	expression tag	UNP P49771
E	-3	GLY	-	expression tag	UNP P49771
E	-2	SER	-	expression tag	UNP P49771
E	-1	HIS	-	expression tag	UNP P49771
E	0	MET	-	expression tag	UNP P49771
E	27	ASP	LEU	engineered mutation	UNP P49771
G	-20	MET	-	initiating methionine	UNP P49771
G	-19	GLY	-	expression tag	UNP P49771
G	-18	SER	-	expression tag	UNP P49771
G	-17	SER	-	expression tag	UNP P49771
G	-16	HIS	-	expression tag	UNP P49771
G	-15	HIS	-	expression tag	UNP P49771
G	-14	HIS	-	expression tag	UNP P49771
G	-13	HIS	-	expression tag	UNP P49771
G	-12	HIS	-	expression tag	UNP P49771
G	-11	HIS	-	expression tag	UNP P49771
G	-10	SER	-	expression tag	UNP P49771
G	-9	SER	-	expression tag	UNP P49771
G	-8	GLY	-	expression tag	UNP P49771
G	-7	LEU	-	expression tag	UNP P49771
G	-6	VAL	-	expression tag	UNP P49771
G	-5	PRO	-	expression tag	UNP P49771
G	-4	ARG	-	expression tag	UNP P49771
G	-3	GLY	-	expression tag	UNP P49771
G	-2	SER	-	expression tag	UNP P49771
G	-1	HIS	-	expression tag	UNP P49771
G	0	MET	-	expression tag	UNP P49771
G	27	ASP	LEU	engineered mutation	UNP P49771
I	-20	MET	-	initiating methionine	UNP P49771
I	-19	GLY	-	expression tag	UNP P49771
I	-18	SER	-	expression tag	UNP P49771
I	-17	SER	-	expression tag	UNP P49771
I	-16	HIS	-	expression tag	UNP P49771
I	-15	HIS	-	expression tag	UNP P49771
I	-14	HIS	-	expression tag	UNP P49771
I	-13	HIS	-	expression tag	UNP P49771
I	-12	HIS	-	expression tag	UNP P49771

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	-11	HIS	-	expression tag	UNP P49771
I	-10	SER	-	expression tag	UNP P49771
I	-9	SER	-	expression tag	UNP P49771
I	-8	GLY	-	expression tag	UNP P49771
I	-7	LEU	-	expression tag	UNP P49771
I	-6	VAL	-	expression tag	UNP P49771
I	-5	PRO	-	expression tag	UNP P49771
I	-4	ARG	-	expression tag	UNP P49771
I	-3	GLY	-	expression tag	UNP P49771
I	-2	SER	-	expression tag	UNP P49771
I	-1	HIS	-	expression tag	UNP P49771
I	0	MET	-	expression tag	UNP P49771
I	27	ASP	LEU	engineered mutation	UNP P49771
K	-20	MET	-	initiating methionine	UNP P49771
K	-19	GLY	-	expression tag	UNP P49771
K	-18	SER	-	expression tag	UNP P49771
K	-17	SER	-	expression tag	UNP P49771
K	-16	HIS	-	expression tag	UNP P49771
K	-15	HIS	-	expression tag	UNP P49771
K	-14	HIS	-	expression tag	UNP P49771
K	-13	HIS	-	expression tag	UNP P49771
K	-12	HIS	-	expression tag	UNP P49771
K	-11	HIS	-	expression tag	UNP P49771
K	-10	SER	-	expression tag	UNP P49771
K	-9	SER	-	expression tag	UNP P49771
K	-8	GLY	-	expression tag	UNP P49771
K	-7	LEU	-	expression tag	UNP P49771
K	-6	VAL	-	expression tag	UNP P49771
K	-5	PRO	-	expression tag	UNP P49771
K	-4	ARG	-	expression tag	UNP P49771
K	-3	GLY	-	expression tag	UNP P49771
K	-2	SER	-	expression tag	UNP P49771
K	-1	HIS	-	expression tag	UNP P49771
K	0	MET	-	expression tag	UNP P49771
K	27	ASP	LEU	engineered mutation	UNP P49771
M	-20	MET	-	initiating methionine	UNP P49771
M	-19	GLY	-	expression tag	UNP P49771
M	-18	SER	-	expression tag	UNP P49771
M	-17	SER	-	expression tag	UNP P49771
M	-16	HIS	-	expression tag	UNP P49771
M	-15	HIS	-	expression tag	UNP P49771
M	-14	HIS	-	expression tag	UNP P49771

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	-13	HIS	-	expression tag	UNP P49771
M	-12	HIS	-	expression tag	UNP P49771
M	-11	HIS	-	expression tag	UNP P49771
M	-10	SER	-	expression tag	UNP P49771
M	-9	SER	-	expression tag	UNP P49771
M	-8	GLY	-	expression tag	UNP P49771
M	-7	LEU	-	expression tag	UNP P49771
M	-6	VAL	-	expression tag	UNP P49771
M	-5	PRO	-	expression tag	UNP P49771
M	-4	ARG	-	expression tag	UNP P49771
M	-3	GLY	-	expression tag	UNP P49771
M	-2	SER	-	expression tag	UNP P49771
M	-1	HIS	-	expression tag	UNP P49771
M	0	MET	-	expression tag	UNP P49771
M	27	ASP	LEU	engineered mutation	UNP P49771
O	-20	MET	-	initiating methionine	UNP P49771
O	-19	GLY	-	expression tag	UNP P49771
O	-18	SER	-	expression tag	UNP P49771
O	-17	SER	-	expression tag	UNP P49771
O	-16	HIS	-	expression tag	UNP P49771
O	-15	HIS	-	expression tag	UNP P49771
O	-14	HIS	-	expression tag	UNP P49771
O	-13	HIS	-	expression tag	UNP P49771
O	-12	HIS	-	expression tag	UNP P49771
O	-11	HIS	-	expression tag	UNP P49771
O	-10	SER	-	expression tag	UNP P49771
O	-9	SER	-	expression tag	UNP P49771
O	-8	GLY	-	expression tag	UNP P49771
O	-7	LEU	-	expression tag	UNP P49771
O	-6	VAL	-	expression tag	UNP P49771
O	-5	PRO	-	expression tag	UNP P49771
O	-4	ARG	-	expression tag	UNP P49771
O	-3	GLY	-	expression tag	UNP P49771
O	-2	SER	-	expression tag	UNP P49771
O	-1	HIS	-	expression tag	UNP P49771
O	0	MET	-	expression tag	UNP P49771
O	27	ASP	LEU	engineered mutation	UNP P49771

- Molecule 2 is a protein called Receptor-type tyrosine-protein kinase FLT3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			2440	1517	445	467	11			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	422	Total	C	N	O	S	0	0	0
			2400	1494	446	449	11			
2	F	420	Total	C	N	O	S	0	0	0
			2430	1520	445	453	12			
2	H	423	Total	C	N	O	S	0	0	0
			2389	1474	449	454	12			
2	J	417	Total	C	N	O	S	0	0	0
			2372	1473	441	446	12			
2	L	430	Total	C	N	O	S	0	0	0
			2453	1527	451	464	11			
2	N	428	Total	C	N	O	S	0	0	0
			2418	1504	448	456	10			
2	P	427	Total	C	N	O	S	0	0	0
			2417	1500	445	459	13			

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	227	MET	THR	conflict	UNP P36888
B	542	GLY	-	expression tag	UNP P36888
B	543	SER	-	expression tag	UNP P36888
B	544	SER	-	expression tag	UNP P36888
B	545	GLY	-	expression tag	UNP P36888
B	546	LEU	-	expression tag	UNP P36888
B	547	VAL	-	expression tag	UNP P36888
B	548	PRO	-	expression tag	UNP P36888
B	549	ARG	-	expression tag	UNP P36888
B	550	GLY	-	expression tag	UNP P36888
B	551	SER	-	expression tag	UNP P36888
B	552	GLY	-	expression tag	UNP P36888
B	553	GLY	-	expression tag	UNP P36888
B	554	SER	-	expression tag	UNP P36888
B	555	GLY	-	expression tag	UNP P36888
B	556	GLY	-	expression tag	UNP P36888
B	557	SER	-	expression tag	UNP P36888
B	558	GLY	-	expression tag	UNP P36888
B	559	LEU	-	expression tag	UNP P36888
B	560	ASN	-	expression tag	UNP P36888
B	561	ASP	-	expression tag	UNP P36888
B	562	ILE	-	expression tag	UNP P36888
B	563	PHE	-	expression tag	UNP P36888
B	564	GLU	-	expression tag	UNP P36888
B	565	ALA	-	expression tag	UNP P36888

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	566	GLN	-	expression tag	UNP P36888
B	567	LYS	-	expression tag	UNP P36888
B	568	ILE	-	expression tag	UNP P36888
B	569	GLU	-	expression tag	UNP P36888
B	570	TRP	-	expression tag	UNP P36888
B	571	HIS	-	expression tag	UNP P36888
B	572	GLU	-	expression tag	UNP P36888
B	573	GLY	-	expression tag	UNP P36888
B	574	ARG	-	expression tag	UNP P36888
B	575	THR	-	expression tag	UNP P36888
B	576	LYS	-	expression tag	UNP P36888
B	577	HIS	-	expression tag	UNP P36888
B	578	HIS	-	expression tag	UNP P36888
B	579	HIS	-	expression tag	UNP P36888
B	580	HIS	-	expression tag	UNP P36888
B	581	HIS	-	expression tag	UNP P36888
B	582	HIS	-	expression tag	UNP P36888
D	227	MET	THR	conflict	UNP P36888
D	542	GLY	-	expression tag	UNP P36888
D	543	SER	-	expression tag	UNP P36888
D	544	SER	-	expression tag	UNP P36888
D	545	GLY	-	expression tag	UNP P36888
D	546	LEU	-	expression tag	UNP P36888
D	547	VAL	-	expression tag	UNP P36888
D	548	PRO	-	expression tag	UNP P36888
D	549	ARG	-	expression tag	UNP P36888
D	550	GLY	-	expression tag	UNP P36888
D	551	SER	-	expression tag	UNP P36888
D	552	GLY	-	expression tag	UNP P36888
D	553	GLY	-	expression tag	UNP P36888
D	554	SER	-	expression tag	UNP P36888
D	555	GLY	-	expression tag	UNP P36888
D	556	GLY	-	expression tag	UNP P36888
D	557	SER	-	expression tag	UNP P36888
D	558	GLY	-	expression tag	UNP P36888
D	559	LEU	-	expression tag	UNP P36888
D	560	ASN	-	expression tag	UNP P36888
D	561	ASP	-	expression tag	UNP P36888
D	562	ILE	-	expression tag	UNP P36888
D	563	PHE	-	expression tag	UNP P36888
D	564	GLU	-	expression tag	UNP P36888
D	565	ALA	-	expression tag	UNP P36888

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	566	GLN	-	expression tag	UNP P36888
D	567	LYS	-	expression tag	UNP P36888
D	568	ILE	-	expression tag	UNP P36888
D	569	GLU	-	expression tag	UNP P36888
D	570	TRP	-	expression tag	UNP P36888
D	571	HIS	-	expression tag	UNP P36888
D	572	GLU	-	expression tag	UNP P36888
D	573	GLY	-	expression tag	UNP P36888
D	574	ARG	-	expression tag	UNP P36888
D	575	THR	-	expression tag	UNP P36888
D	576	LYS	-	expression tag	UNP P36888
D	577	HIS	-	expression tag	UNP P36888
D	578	HIS	-	expression tag	UNP P36888
D	579	HIS	-	expression tag	UNP P36888
D	580	HIS	-	expression tag	UNP P36888
D	581	HIS	-	expression tag	UNP P36888
D	582	HIS	-	expression tag	UNP P36888
F	227	MET	THR	conflict	UNP P36888
F	542	GLY	-	expression tag	UNP P36888
F	543	SER	-	expression tag	UNP P36888
F	544	SER	-	expression tag	UNP P36888
F	545	GLY	-	expression tag	UNP P36888
F	546	LEU	-	expression tag	UNP P36888
F	547	VAL	-	expression tag	UNP P36888
F	548	PRO	-	expression tag	UNP P36888
F	549	ARG	-	expression tag	UNP P36888
F	550	GLY	-	expression tag	UNP P36888
F	551	SER	-	expression tag	UNP P36888
F	552	GLY	-	expression tag	UNP P36888
F	553	GLY	-	expression tag	UNP P36888
F	554	SER	-	expression tag	UNP P36888
F	555	GLY	-	expression tag	UNP P36888
F	556	GLY	-	expression tag	UNP P36888
F	557	SER	-	expression tag	UNP P36888
F	558	GLY	-	expression tag	UNP P36888
F	559	LEU	-	expression tag	UNP P36888
F	560	ASN	-	expression tag	UNP P36888
F	561	ASP	-	expression tag	UNP P36888
F	562	ILE	-	expression tag	UNP P36888
F	563	PHE	-	expression tag	UNP P36888
F	564	GLU	-	expression tag	UNP P36888
F	565	ALA	-	expression tag	UNP P36888

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	566	GLN	-	expression tag	UNP P36888
F	567	LYS	-	expression tag	UNP P36888
F	568	ILE	-	expression tag	UNP P36888
F	569	GLU	-	expression tag	UNP P36888
F	570	TRP	-	expression tag	UNP P36888
F	571	HIS	-	expression tag	UNP P36888
F	572	GLU	-	expression tag	UNP P36888
F	573	GLY	-	expression tag	UNP P36888
F	574	ARG	-	expression tag	UNP P36888
F	575	THR	-	expression tag	UNP P36888
F	576	LYS	-	expression tag	UNP P36888
F	577	HIS	-	expression tag	UNP P36888
F	578	HIS	-	expression tag	UNP P36888
F	579	HIS	-	expression tag	UNP P36888
F	580	HIS	-	expression tag	UNP P36888
F	581	HIS	-	expression tag	UNP P36888
F	582	HIS	-	expression tag	UNP P36888
H	227	MET	THR	conflict	UNP P36888
H	542	GLY	-	expression tag	UNP P36888
H	543	SER	-	expression tag	UNP P36888
H	544	SER	-	expression tag	UNP P36888
H	545	GLY	-	expression tag	UNP P36888
H	546	LEU	-	expression tag	UNP P36888
H	547	VAL	-	expression tag	UNP P36888
H	548	PRO	-	expression tag	UNP P36888
H	549	ARG	-	expression tag	UNP P36888
H	550	GLY	-	expression tag	UNP P36888
H	551	SER	-	expression tag	UNP P36888
H	552	GLY	-	expression tag	UNP P36888
H	553	GLY	-	expression tag	UNP P36888
H	554	SER	-	expression tag	UNP P36888
H	555	GLY	-	expression tag	UNP P36888
H	556	GLY	-	expression tag	UNP P36888
H	557	SER	-	expression tag	UNP P36888
H	558	GLY	-	expression tag	UNP P36888
H	559	LEU	-	expression tag	UNP P36888
H	560	ASN	-	expression tag	UNP P36888
H	561	ASP	-	expression tag	UNP P36888
H	562	ILE	-	expression tag	UNP P36888
H	563	PHE	-	expression tag	UNP P36888
H	564	GLU	-	expression tag	UNP P36888
H	565	ALA	-	expression tag	UNP P36888

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	566	GLN	-	expression tag	UNP P36888
H	567	LYS	-	expression tag	UNP P36888
H	568	ILE	-	expression tag	UNP P36888
H	569	GLU	-	expression tag	UNP P36888
H	570	TRP	-	expression tag	UNP P36888
H	571	HIS	-	expression tag	UNP P36888
H	572	GLU	-	expression tag	UNP P36888
H	573	GLY	-	expression tag	UNP P36888
H	574	ARG	-	expression tag	UNP P36888
H	575	THR	-	expression tag	UNP P36888
H	576	LYS	-	expression tag	UNP P36888
H	577	HIS	-	expression tag	UNP P36888
H	578	HIS	-	expression tag	UNP P36888
H	579	HIS	-	expression tag	UNP P36888
H	580	HIS	-	expression tag	UNP P36888
H	581	HIS	-	expression tag	UNP P36888
H	582	HIS	-	expression tag	UNP P36888
J	227	MET	THR	conflict	UNP P36888
J	542	GLY	-	expression tag	UNP P36888
J	543	SER	-	expression tag	UNP P36888
J	544	SER	-	expression tag	UNP P36888
J	545	GLY	-	expression tag	UNP P36888
J	546	LEU	-	expression tag	UNP P36888
J	547	VAL	-	expression tag	UNP P36888
J	548	PRO	-	expression tag	UNP P36888
J	549	ARG	-	expression tag	UNP P36888
J	550	GLY	-	expression tag	UNP P36888
J	551	SER	-	expression tag	UNP P36888
J	552	GLY	-	expression tag	UNP P36888
J	553	GLY	-	expression tag	UNP P36888
J	554	SER	-	expression tag	UNP P36888
J	555	GLY	-	expression tag	UNP P36888
J	556	GLY	-	expression tag	UNP P36888
J	557	SER	-	expression tag	UNP P36888
J	558	GLY	-	expression tag	UNP P36888
J	559	LEU	-	expression tag	UNP P36888
J	560	ASN	-	expression tag	UNP P36888
J	561	ASP	-	expression tag	UNP P36888
J	562	ILE	-	expression tag	UNP P36888
J	563	PHE	-	expression tag	UNP P36888
J	564	GLU	-	expression tag	UNP P36888
J	565	ALA	-	expression tag	UNP P36888

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	566	GLN	-	expression tag	UNP P36888
J	567	LYS	-	expression tag	UNP P36888
J	568	ILE	-	expression tag	UNP P36888
J	569	GLU	-	expression tag	UNP P36888
J	570	TRP	-	expression tag	UNP P36888
J	571	HIS	-	expression tag	UNP P36888
J	572	GLU	-	expression tag	UNP P36888
J	573	GLY	-	expression tag	UNP P36888
J	574	ARG	-	expression tag	UNP P36888
J	575	THR	-	expression tag	UNP P36888
J	576	LYS	-	expression tag	UNP P36888
J	577	HIS	-	expression tag	UNP P36888
J	578	HIS	-	expression tag	UNP P36888
J	579	HIS	-	expression tag	UNP P36888
J	580	HIS	-	expression tag	UNP P36888
J	581	HIS	-	expression tag	UNP P36888
J	582	HIS	-	expression tag	UNP P36888
L	227	MET	THR	conflict	UNP P36888
L	542	GLY	-	expression tag	UNP P36888
L	543	SER	-	expression tag	UNP P36888
L	544	SER	-	expression tag	UNP P36888
L	545	GLY	-	expression tag	UNP P36888
L	546	LEU	-	expression tag	UNP P36888
L	547	VAL	-	expression tag	UNP P36888
L	548	PRO	-	expression tag	UNP P36888
L	549	ARG	-	expression tag	UNP P36888
L	550	GLY	-	expression tag	UNP P36888
L	551	SER	-	expression tag	UNP P36888
L	552	GLY	-	expression tag	UNP P36888
L	553	GLY	-	expression tag	UNP P36888
L	554	SER	-	expression tag	UNP P36888
L	555	GLY	-	expression tag	UNP P36888
L	556	GLY	-	expression tag	UNP P36888
L	557	SER	-	expression tag	UNP P36888
L	558	GLY	-	expression tag	UNP P36888
L	559	LEU	-	expression tag	UNP P36888
L	560	ASN	-	expression tag	UNP P36888
L	561	ASP	-	expression tag	UNP P36888
L	562	ILE	-	expression tag	UNP P36888
L	563	PHE	-	expression tag	UNP P36888
L	564	GLU	-	expression tag	UNP P36888
L	565	ALA	-	expression tag	UNP P36888

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	566	GLN	-	expression tag	UNP P36888
L	567	LYS	-	expression tag	UNP P36888
L	568	ILE	-	expression tag	UNP P36888
L	569	GLU	-	expression tag	UNP P36888
L	570	TRP	-	expression tag	UNP P36888
L	571	HIS	-	expression tag	UNP P36888
L	572	GLU	-	expression tag	UNP P36888
L	573	GLY	-	expression tag	UNP P36888
L	574	ARG	-	expression tag	UNP P36888
L	575	THR	-	expression tag	UNP P36888
L	576	LYS	-	expression tag	UNP P36888
L	577	HIS	-	expression tag	UNP P36888
L	578	HIS	-	expression tag	UNP P36888
L	579	HIS	-	expression tag	UNP P36888
L	580	HIS	-	expression tag	UNP P36888
L	581	HIS	-	expression tag	UNP P36888
L	582	HIS	-	expression tag	UNP P36888
N	227	MET	THR	conflict	UNP P36888
N	542	GLY	-	expression tag	UNP P36888
N	543	SER	-	expression tag	UNP P36888
N	544	SER	-	expression tag	UNP P36888
N	545	GLY	-	expression tag	UNP P36888
N	546	LEU	-	expression tag	UNP P36888
N	547	VAL	-	expression tag	UNP P36888
N	548	PRO	-	expression tag	UNP P36888
N	549	ARG	-	expression tag	UNP P36888
N	550	GLY	-	expression tag	UNP P36888
N	551	SER	-	expression tag	UNP P36888
N	552	GLY	-	expression tag	UNP P36888
N	553	GLY	-	expression tag	UNP P36888
N	554	SER	-	expression tag	UNP P36888
N	555	GLY	-	expression tag	UNP P36888
N	556	GLY	-	expression tag	UNP P36888
N	557	SER	-	expression tag	UNP P36888
N	558	GLY	-	expression tag	UNP P36888
N	559	LEU	-	expression tag	UNP P36888
N	560	ASN	-	expression tag	UNP P36888
N	561	ASP	-	expression tag	UNP P36888
N	562	ILE	-	expression tag	UNP P36888
N	563	PHE	-	expression tag	UNP P36888
N	564	GLU	-	expression tag	UNP P36888
N	565	ALA	-	expression tag	UNP P36888

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	566	GLN	-	expression tag	UNP P36888
N	567	LYS	-	expression tag	UNP P36888
N	568	ILE	-	expression tag	UNP P36888
N	569	GLU	-	expression tag	UNP P36888
N	570	TRP	-	expression tag	UNP P36888
N	571	HIS	-	expression tag	UNP P36888
N	572	GLU	-	expression tag	UNP P36888
N	573	GLY	-	expression tag	UNP P36888
N	574	ARG	-	expression tag	UNP P36888
N	575	THR	-	expression tag	UNP P36888
N	576	LYS	-	expression tag	UNP P36888
N	577	HIS	-	expression tag	UNP P36888
N	578	HIS	-	expression tag	UNP P36888
N	579	HIS	-	expression tag	UNP P36888
N	580	HIS	-	expression tag	UNP P36888
N	581	HIS	-	expression tag	UNP P36888
N	582	HIS	-	expression tag	UNP P36888
P	227	MET	THR	conflict	UNP P36888
P	542	GLY	-	expression tag	UNP P36888
P	543	SER	-	expression tag	UNP P36888
P	544	SER	-	expression tag	UNP P36888
P	545	GLY	-	expression tag	UNP P36888
P	546	LEU	-	expression tag	UNP P36888
P	547	VAL	-	expression tag	UNP P36888
P	548	PRO	-	expression tag	UNP P36888
P	549	ARG	-	expression tag	UNP P36888
P	550	GLY	-	expression tag	UNP P36888
P	551	SER	-	expression tag	UNP P36888
P	552	GLY	-	expression tag	UNP P36888
P	553	GLY	-	expression tag	UNP P36888
P	554	SER	-	expression tag	UNP P36888
P	555	GLY	-	expression tag	UNP P36888
P	556	GLY	-	expression tag	UNP P36888
P	557	SER	-	expression tag	UNP P36888
P	558	GLY	-	expression tag	UNP P36888
P	559	LEU	-	expression tag	UNP P36888
P	560	ASN	-	expression tag	UNP P36888
P	561	ASP	-	expression tag	UNP P36888
P	562	ILE	-	expression tag	UNP P36888
P	563	PHE	-	expression tag	UNP P36888
P	564	GLU	-	expression tag	UNP P36888
P	565	ALA	-	expression tag	UNP P36888

Continued on next page...

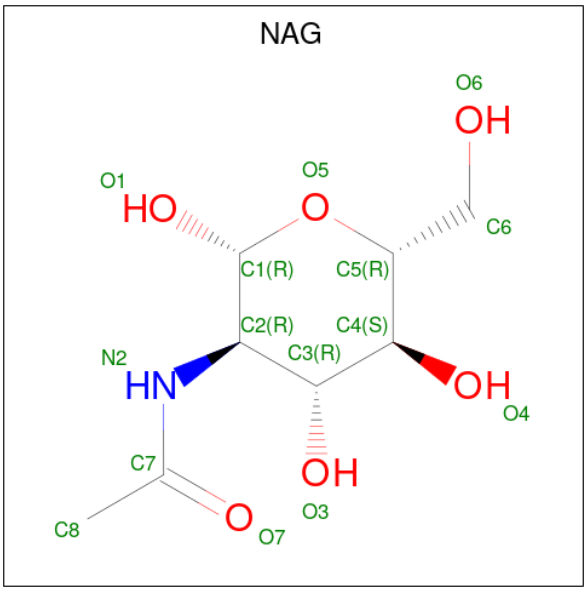
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	566	GLN	-	expression tag	UNP P36888
P	567	LYS	-	expression tag	UNP P36888
P	568	ILE	-	expression tag	UNP P36888
P	569	GLU	-	expression tag	UNP P36888
P	570	TRP	-	expression tag	UNP P36888
P	571	HIS	-	expression tag	UNP P36888
P	572	GLU	-	expression tag	UNP P36888
P	573	GLY	-	expression tag	UNP P36888
P	574	ARG	-	expression tag	UNP P36888
P	575	THR	-	expression tag	UNP P36888
P	576	LYS	-	expression tag	UNP P36888
P	577	HIS	-	expression tag	UNP P36888
P	578	HIS	-	expression tag	UNP P36888
P	579	HIS	-	expression tag	UNP P36888
P	580	HIS	-	expression tag	UNP P36888
P	581	HIS	-	expression tag	UNP P36888
P	582	HIS	-	expression tag	UNP P36888

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	2	Total	C	N	O	28	0	0
			28	16	2	10			
3	R	2	Total	C	N	O	28	0	0
			28	16	2	10			
3	S	2	Total	C	N	O	28	0	0
			28	16	2	10			
3	T	2	Total	C	N	O	28	0	0
			28	16	2	10			
3	U	2	Total	C	N	O	28	0	0
			28	16	2	10			
3	V	2	Total	C	N	O	28	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



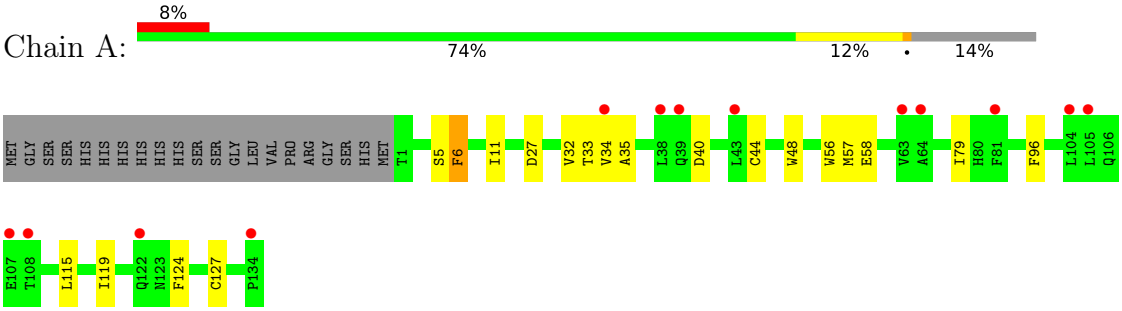
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 8 1 5	14	0
4	B	1	Total C N O 14 8 1 5	14	0
4	H	1	Total C N O 14 8 1 5	14	0
4	P	1	Total C N O 14 8 1 5	14	0

3 Residue-property plots (i)

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

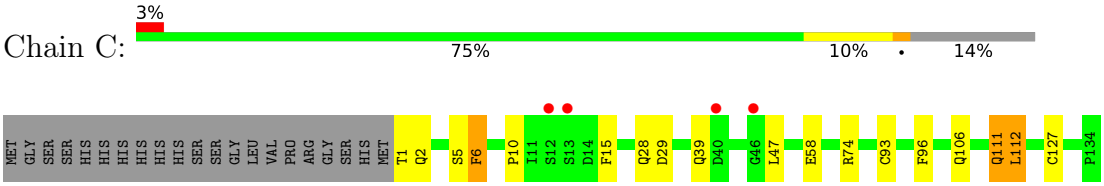
• Molecule 1: Fms-related tyrosine kinase 3 ligand

Chain A:



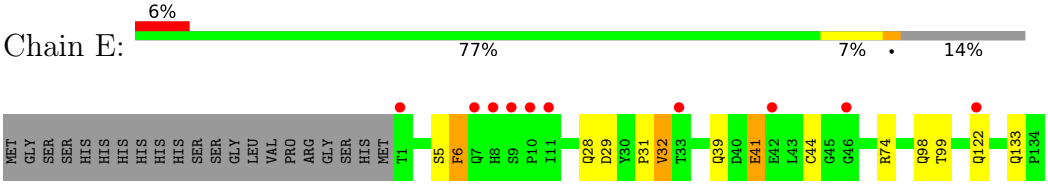
• Molecule 1: Fms-related tyrosine kinase 3 ligand

Chain C:



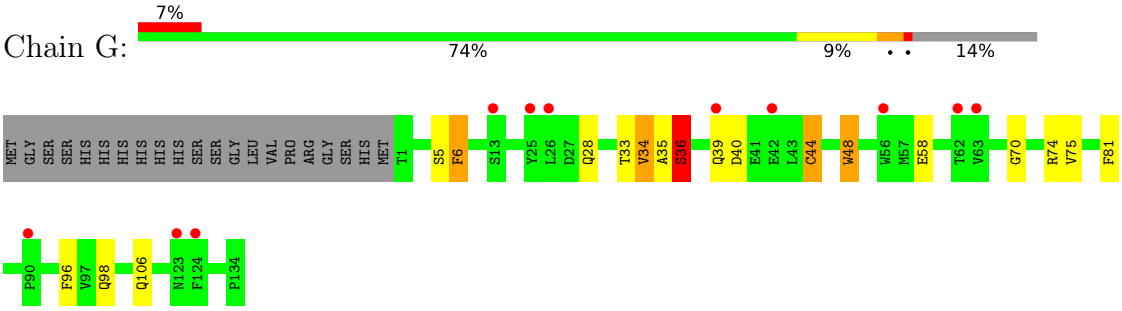
• Molecule 1: Fms-related tyrosine kinase 3 ligand

Chain E:

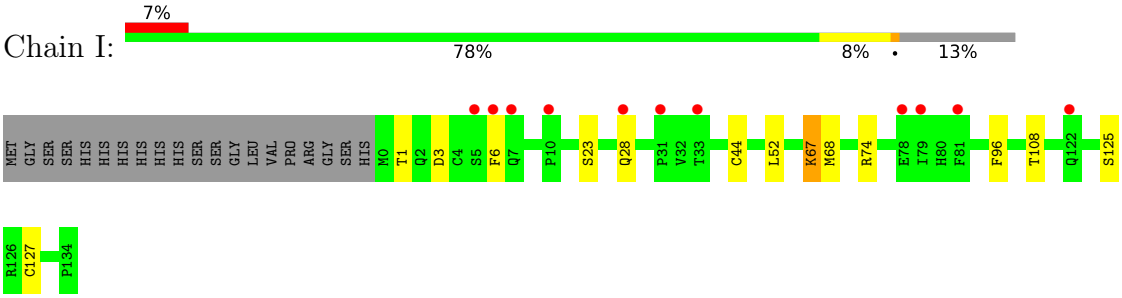


• Molecule 1: Fms-related tyrosine kinase 3 ligand

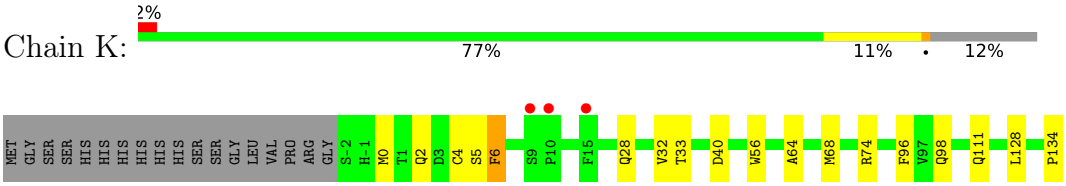
Chain G:



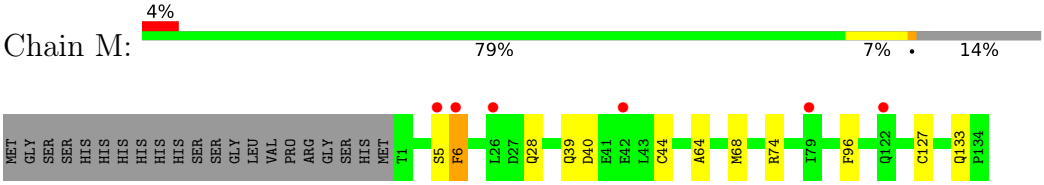
• Molecule 1: Fms-related tyrosine kinase 3 ligand



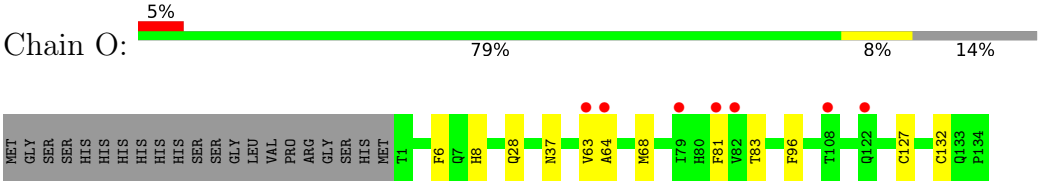
• Molecule 1: Fms-related tyrosine kinase 3 ligand



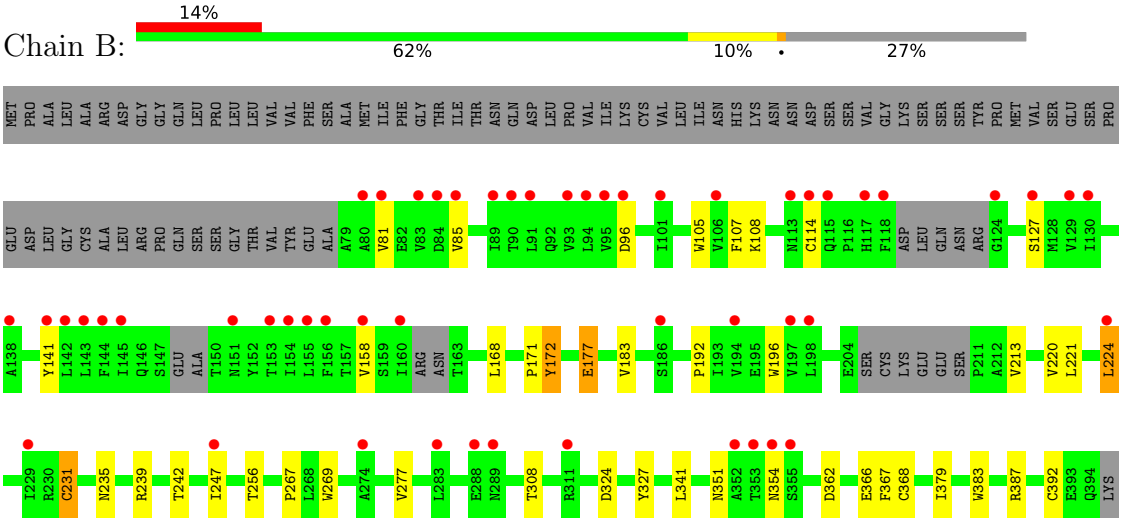
• Molecule 1: Fms-related tyrosine kinase 3 ligand

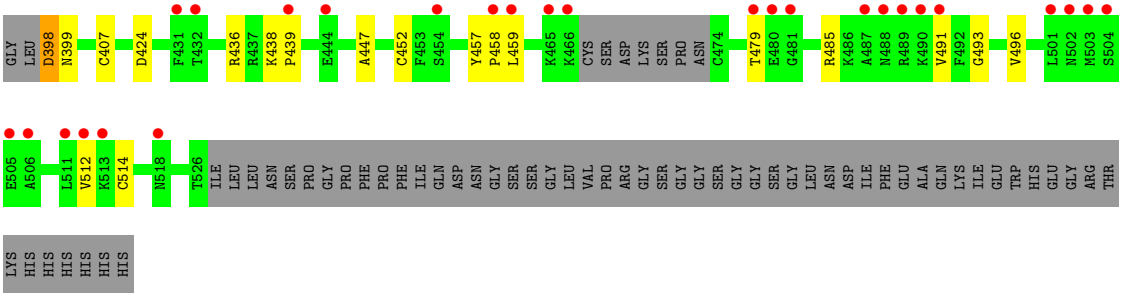


• Molecule 1: Fms-related tyrosine kinase 3 ligand

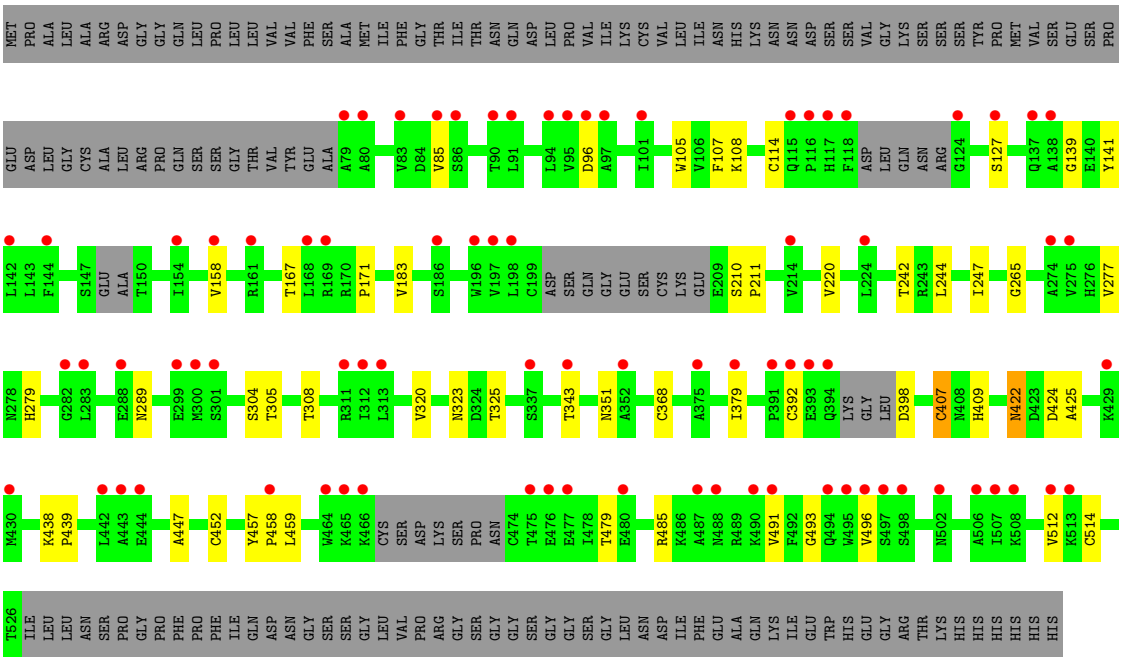


• Molecule 2: Receptor-type tyrosine-protein kinase FLT3

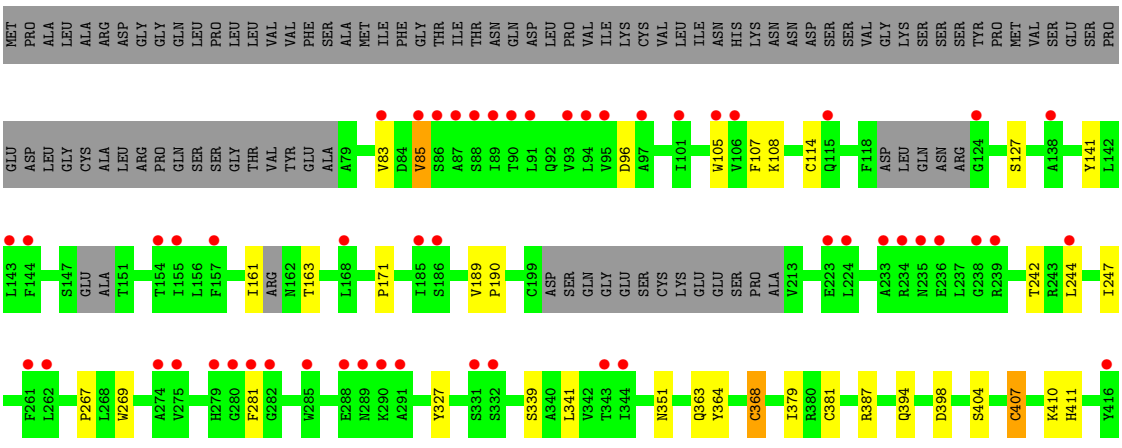


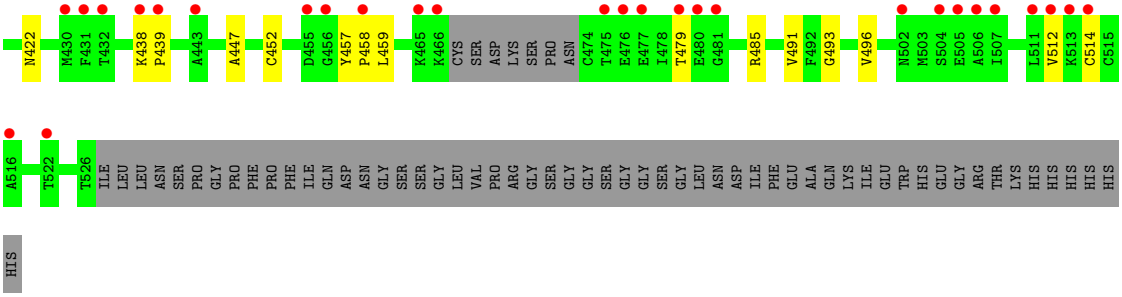


• Molecule 2: Receptor-type tyrosine-protein kinase FLT3



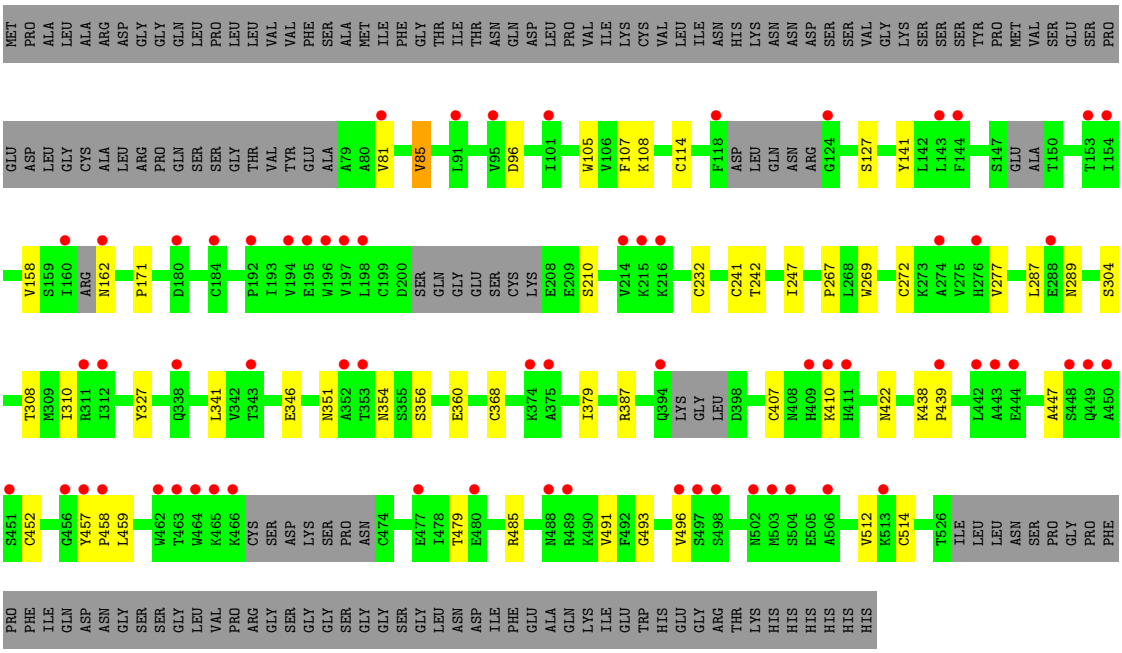
• Molecule 2: Receptor-type tyrosine-protein kinase FLT3





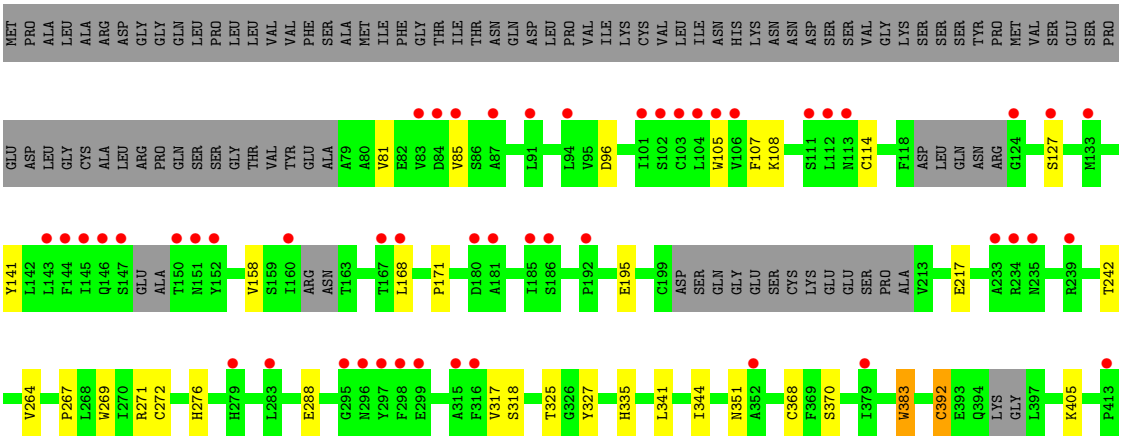
• Molecule 2: Receptor-type tyrosine-protein kinase FLT3

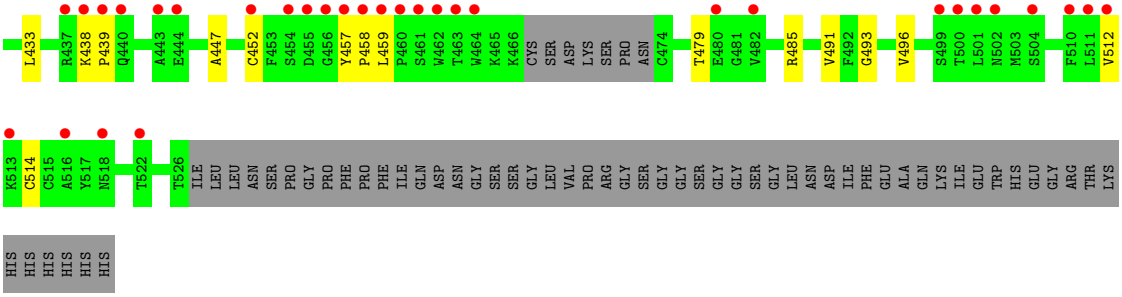
Chain H:

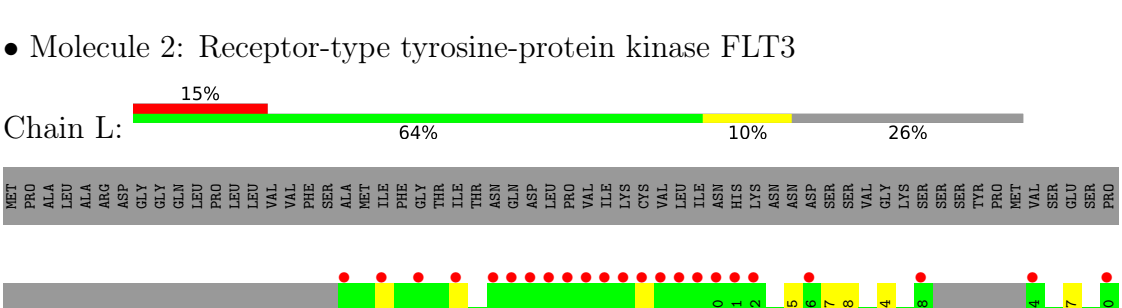


• Molecule 2: Receptor-type tyrosine-protein kinase FLT3

Chain J:

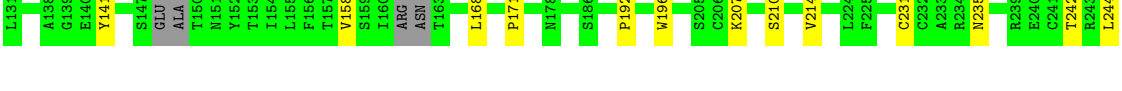


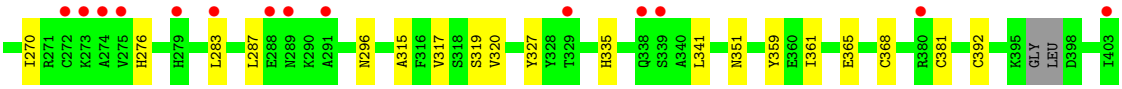


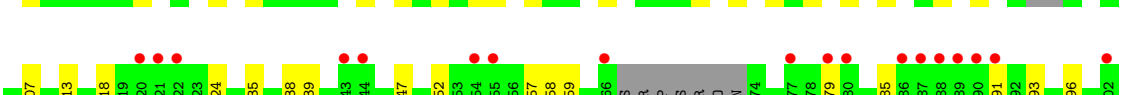


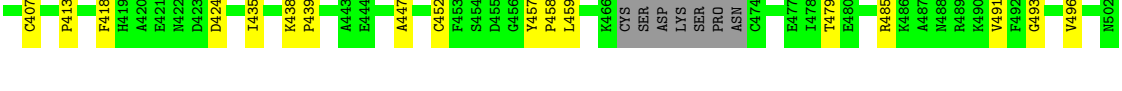
• Molecule 2: Receptor-type tyrosine-protein kinase FLT3

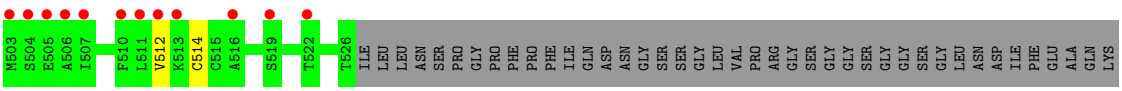
Chain L:

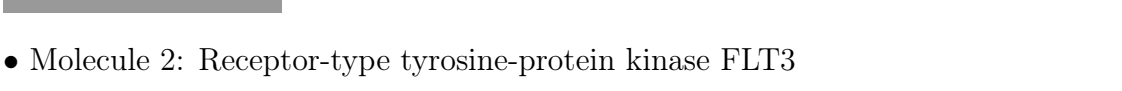


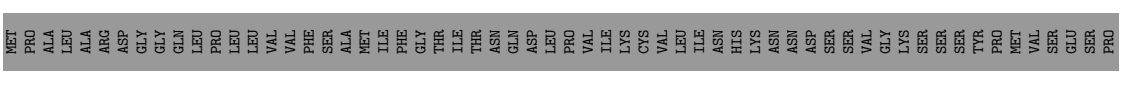


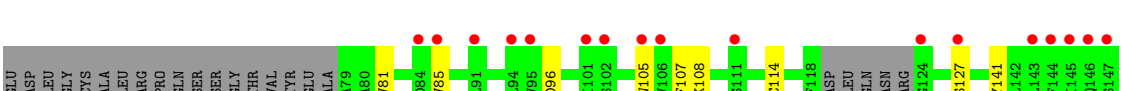


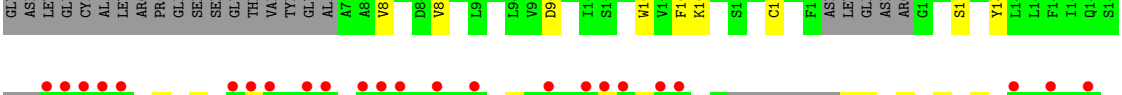


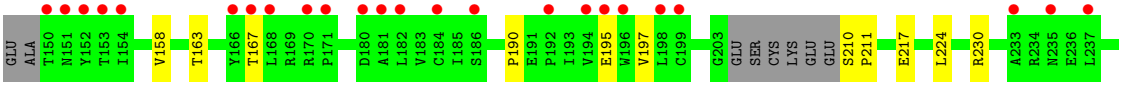






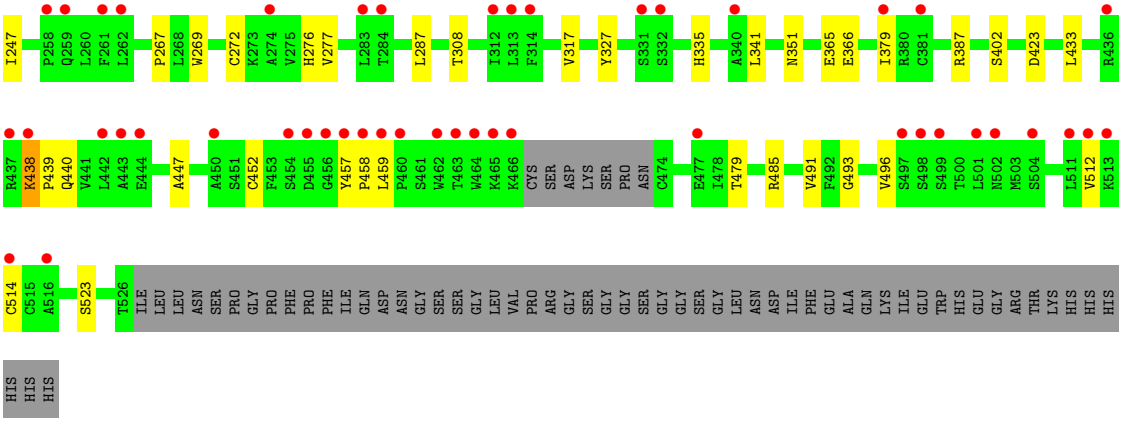






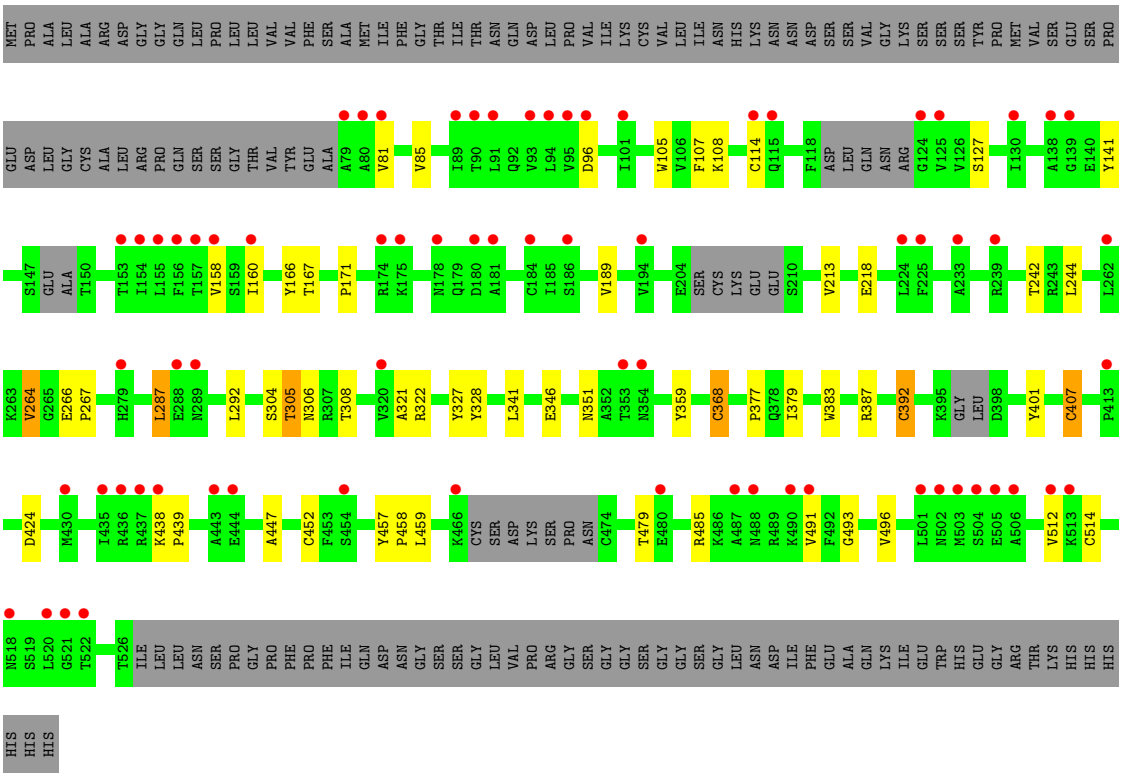
• Molecule 2: Receptor-type tyrosine-protein kinase FLT3

Chain N:



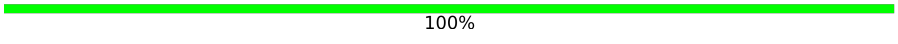
• Molecule 2: Receptor-type tyrosine-protein kinase FLT3

Chain P:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

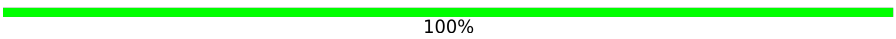
Chain S:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

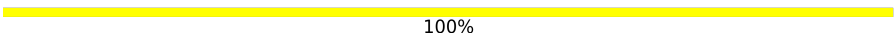
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	139.21Å 139.22Å 143.69Å 90.02° 90.03° 89.99°	Depositor
Resolution (Å)	47.90 – 4.51 47.90 – 4.51	Depositor EDS
% Data completeness (in resolution range)	66.2 (47.90-4.51) 66.0 (47.90-4.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 4.45Å)	Xtriage
Refinement program	BUSTER 2.10.3, PHENIX 1.20-4459, PDB-REDO	Depositor
R, R_{free}	0.278 , 0.291 0.299 , 0.285	Depositor DCC
R_{free} test set	2027 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	214.3	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 462.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage

Continued on next page...

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

Continued from previous page...

Property	Value	Source
Estimated twinning fraction	0.027 for h,-l,k 0.027 for h,l,-k 0.027 for l,k,-h 0.027 for -l,k,h 0.387 for k,-h,l 0.387 for -k,h,l 0.029 for k,-l,-h 0.029 for -l,h,-k 0.026 for -l,-h,k 0.026 for -k,l,-h 0.025 for l,-h,-k 0.025 for -k,-l,h 0.028 for k,l,h 0.028 for l,h,k 0.390 for h,-k,-l 0.390 for -h,k,-l 0.387 for -h,-k,l 0.389 for k,h,-l 0.389 for -k,-h,-l 0.035 for -l,-k,-h 0.037 for l,-k,h 0.030 for -h,-l,-k 0.033 for -h,l,k	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	26691	wwPDB-VP
Average B, all atoms (Å^2)	200.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

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

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	0.24	0/933	0.45	0/1277
1	C	0.27	0/896	0.50	0/1235
1	E	0.24	0/858	0.48	0/1183
1	G	0.26	0/903	0.50	0/1247
1	I	0.55	1/926 (0.1%)	0.77	3/1273 (0.2%)
1	K	0.26	0/911	0.47	0/1256
1	M	0.23	0/930	0.47	0/1281
1	O	0.24	0/941	0.46	0/1294
2	B	0.26	0/2470	0.48	2/3425 (0.1%)
2	D	0.25	0/2429	0.46	0/3369
2	F	0.25	0/2464	0.46	0/3408
2	H	0.26	0/2415	0.44	0/3347
2	J	0.25	0/2401	0.44	0/3331
2	L	0.26	0/2483	0.45	0/3447
2	N	0.26	0/2449	0.46	0/3398
2	P	0.26	0/2444	0.46	0/3391
All	All	0.27	1/26853 (0.0%)	0.47	5/37162 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3
2	D	0	4
2	F	0	4
2	H	0	3
2	J	0	3
2	L	0	4
2	N	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	3
All	All	0	28

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	23[A]	SER	C-N	-15.00	0.99	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	23[A]	SER	C-N-CA	-13.96	86.79	121.70
1	I	23[A]	SER	O-C-N	12.12	142.09	122.70
1	I	23[A]	SER	CA-C-N	-10.11	94.97	117.20
2	B	172	TYR	CA-CB-CG	5.43	123.73	113.40
2	B	398	ASP	CB-CG-OD2	5.17	122.95	118.30

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	438	LYS	Peptide
2	B	457	TYR	Peptide
2	B	459	LEU	Peptide
2	D	210	SER	Peptide
2	D	438	LYS	Peptide
2	D	457	TYR	Peptide
2	D	459	LEU	Peptide
2	F	438	LYS	Peptide,Mainchain
2	F	457	TYR	Peptide
2	F	459	LEU	Peptide
2	H	438	LYS	Peptide
2	H	457	TYR	Peptide
2	H	459	LEU	Peptide
2	J	438	LYS	Peptide
2	J	457	TYR	Peptide
2	J	459	LEU	Peptide
2	L	438	LYS	Peptide,Mainchain
2	L	457	TYR	Peptide
2	L	459	LEU	Peptide
2	N	210	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	N	438	LYS	Peptide
2	N	457	TYR	Peptide
2	N	459	LEU	Peptide
2	P	438	LYS	Peptide
2	P	457	TYR	Peptide
2	P	459	LEU	Peptide

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	915	0	715	11	0
1	C	879	0	656	4	0
1	E	844	0	578	5	0
1	G	884	0	661	5	0
1	I	907	0	697	2	0
1	K	892	0	649	10	0
1	M	908	0	684	3	0
1	O	919	0	723	3	0
2	B	2440	0	1569	18	0
2	D	2400	0	1501	15	0
2	F	2430	0	1573	15	0
2	H	2389	0	1489	12	0
2	J	2372	0	1484	14	0
2	L	2453	0	1562	18	0
2	N	2418	0	1505	12	0
2	P	2417	0	1534	16	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
4	B	28	0	26	0	0
4	H	14	0	13	0	0
4	P	14	0	13	0	0
All	All	26691	0	17782	160	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 4.

All (160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:32:VAL:HG13	1:K:56:TRP:CD2	2.06	0.90
1:A:32:VAL:HG13	1:A:56:TRP:CD2	2.09	0.87
1:A:33:THR:N	1:A:34:VAL:N	2.26	0.84
2:B:398:ASP:OD1	2:B:399:ASN:N	2.12	0.81
2:B:399:ASN:O	2:B:399:ASN:OD1	1.98	0.81
2:B:256:THR:HG21	2:B:399:ASN:HB3	1.61	0.81
2:F:83:VAL:HB	2:F:161:ILE:CB	2.11	0.81
1:A:32:VAL:HG13	1:A:56:TRP:CE2	2.18	0.79
1:C:10:PRO:HA	2:D:279:HIS:NE2	2.00	0.77
2:J:267:PRO:HB2	2:J:269:TRP:HE1	1.54	0.72
2:D:265:GLY:H	2:D:320:VAL:CB	2.01	0.71
2:J:267:PRO:HB2	2:J:269:TRP:NE1	2.08	0.68
1:A:115:LEU:O	1:A:119:ILE:HG12	1.94	0.67
2:H:327:TYR:HA	2:H:341:LEU:HA	1.79	0.64
2:J:327:TYR:HA	2:J:341:LEU:HA	1.79	0.64
1:K:32:VAL:HG13	1:K:56:TRP:CG	2.31	0.63
2:F:394:GLN:HA	2:F:404:SER:HB2	1.83	0.60
1:K:32:VAL:HG13	1:K:56:TRP:CE2	2.36	0.59
1:A:32:VAL:HG13	1:A:56:TRP:CG	2.38	0.58
1:G:35:ALA:O	1:G:36:SER:HB2	2.03	0.58
1:A:35:ALA:HA	1:A:96:PHE:HB3	1.86	0.57
2:L:413:PRO:HG2	2:L:435:ILE:CB	2.35	0.56
2:N:440:GLN:HA	2:N:523:SER:CB	2.35	0.56
2:D:422:ASN:ND2	2:D:425:ALA:H	2.04	0.56
2:N:327:TYR:HA	2:N:341:LEU:HA	1.88	0.56
2:F:327:TYR:HA	2:F:341:LEU:HA	1.88	0.55
1:G:44:CYS:HB3	1:G:48:TRP:CZ2	2.41	0.55
2:L:327:TYR:HA	2:L:341:LEU:HA	1.88	0.55
2:B:221:LEU:HD23	2:B:224:LEU:HD23	1.89	0.54
2:P:327:TYR:HA	2:P:341:LEU:HA	1.88	0.54
2:D:422:ASN:HD21	2:D:425:ALA:H	1.55	0.54
2:D:277:VAL:HA	2:D:308:THR:HG22	1.90	0.53
2:F:339:SER:HB2	1:O:63:VAL:HG23	1.90	0.53
1:O:37:ASN:ND2	1:O:132:CYS:SG	2.82	0.53
2:B:327:TYR:HA	2:B:341:LEU:HA	1.88	0.53
2:P:304:SER:O	2:P:305:THR:O	2.27	0.53
2:N:197:VAL:HG21	2:N:230:ARG:H	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:81:VAL:HB	2:P:158:VAL:HA	1.92	0.52
2:B:81:VAL:HB	2:B:158:VAL:HA	1.92	0.52
2:H:81:VAL:HB	2:H:158:VAL:HA	1.92	0.52
2:J:81:VAL:HB	2:J:158:VAL:HA	1.92	0.52
2:L:81:VAL:HB	2:L:158:VAL:HA	1.92	0.51
2:D:368:CYS:HA	2:D:409:HIS:NE2	2.26	0.51
1:K:32:VAL:HG12	1:K:33:THR:H	1.74	0.51
2:N:81:VAL:HB	2:N:158:VAL:HA	1.92	0.51
1:E:31:PRO:O	1:E:32:VAL:O	2.29	0.51
1:A:11:ILE:CD1	1:A:119:ILE:HG13	2.40	0.51
1:E:31:PRO:O	1:E:99:THR:O	2.28	0.51
2:L:196:TRP:CD2	2:L:231:CYS:SG	3.04	0.50
2:N:277:VAL:HA	2:N:308:THR:HG23	1.94	0.50
2:F:189:VAL:HB	2:F:190:PRO:HD2	1.91	0.50
1:K:32:VAL:CG1	1:K:56:TRP:CG	2.95	0.50
2:J:267:PRO:HB3	2:J:318:SER:HA	1.93	0.50
2:P:304:SER:O	2:P:308:THR:OG1	2.27	0.49
2:J:325:THR:CB	2:J:344:ILE:HA	2.42	0.49
1:I:3:ASP:O	1:I:125:SER:OG	2.30	0.49
1:K:4:CYS:SG	1:K:128:LEU:HD21	2.53	0.49
2:L:270:ILE:HG23	2:L:315:ALA:HB3	1.95	0.49
2:P:264:VAL:HG13	2:P:321:ALA:HA	1.95	0.48
2:L:317:VAL:HG11	2:L:320:VAL:HG12	1.96	0.48
1:I:67:LYS:HD2	1:I:68:MET:HG2	1.95	0.48
1:A:44:CYS:SG	1:A:48:TRP:CH2	3.07	0.47
2:B:383:TRP:HE1	2:B:392:CYS:HB3	1.79	0.47
1:E:39:GLN:HA	1:E:133:GLN:CB	2.45	0.47
1:K:5:SER:O	1:K:6:PHE:O	2.33	0.47
2:L:196:TRP:CE3	2:L:231:CYS:SG	3.07	0.47
2:N:287:LEU:O	2:N:327:TYR:O	2.33	0.47
2:H:85:VAL:H	2:H:162:ASN:N	2.11	0.47
2:P:166:TYR:HA	2:P:189:VAL:HB	1.97	0.47
2:B:105:TRP:HD1	2:B:114:CYS:HG	1.62	0.47
2:D:139:GLY:H	2:D:158:VAL:HB	1.80	0.47
2:H:171:PRO:HD2	2:H:242:THR:CB	2.45	0.46
1:M:5:SER:O	1:M:6:PHE:O	2.34	0.46
2:L:107:PHE:HA	2:L:141:TYR:HD1	1.80	0.46
1:C:5:SER:O	1:C:6:PHE:O	2.34	0.46
1:G:33:THR:O	1:G:34:VAL:HB	2.16	0.46
2:D:304:SER:O	2:D:308:THR:OG1	2.34	0.46
2:J:370:SER:HA	2:J:405:LYS:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:107:PHE:HA	2:N:141:TYR:HD1	1.80	0.46
2:B:107:PHE:HA	2:B:141:TYR:HD1	1.80	0.46
2:F:85:VAL:H	2:F:163:THR:CB	2.28	0.46
2:D:325:THR:HG23	2:D:343:THR:HA	1.98	0.46
2:J:107:PHE:HA	2:J:141:TYR:HD1	1.80	0.46
1:C:111:GLN:HE21	1:C:111:GLN:HB3	1.60	0.46
2:B:196:TRP:CE3	2:B:231:CYS:SG	3.08	0.45
1:E:5:SER:O	1:E:6:PHE:O	2.35	0.45
2:F:107:PHE:HA	2:F:141:TYR:HD1	1.81	0.45
2:H:107:PHE:HA	2:H:141:TYR:HD1	1.80	0.45
1:A:5:SER:O	1:A:6:PHE:O	2.34	0.45
2:B:277:VAL:HA	2:B:308:THR:HG23	1.98	0.45
2:J:383:TRP:CE3	2:J:392:CYS:SG	3.09	0.45
1:M:64:ALA:HB1	1:M:68:MET:HB2	1.97	0.45
2:P:107:PHE:HA	2:P:141:TYR:HD1	1.80	0.45
2:B:177:GLU:H	2:B:177:GLU:CD	2.19	0.45
2:P:171:PRO:HD2	2:P:242:THR:CB	2.47	0.45
2:P:383:TRP:NE1	2:P:392:CYS:SG	2.89	0.45
1:M:39:GLN:HA	1:M:133:GLN:CB	2.47	0.45
2:H:277:VAL:HA	2:H:308:THR:HG23	1.97	0.45
2:P:287:LEU:O	2:P:327:TYR:O	2.34	0.45
1:G:5:SER:O	1:G:6:PHE:O	2.35	0.44
1:K:32:VAL:HG12	1:K:33:THR:N	2.31	0.44
2:L:196:TRP:CE2	2:L:231:CYS:SG	3.11	0.44
2:P:383:TRP:HE1	2:P:392:CYS:HB3	1.83	0.44
2:D:171:PRO:HD2	2:D:242:THR:CB	2.47	0.44
1:A:57:MET:HG3	1:A:79:ILE:HD11	2.00	0.44
2:B:362:ASP:HA	2:B:436:ARG:CB	2.47	0.44
2:F:410:LYS:CE	2:H:410:LYS:HA	2.48	0.44
2:L:171:PRO:HD2	2:L:242:THR:CB	2.48	0.44
2:N:447:ALA:HB3	2:N:452:CYS:HA	2.00	0.44
2:B:171:PRO:HD2	2:B:242:THR:CB	2.48	0.43
2:F:447:ALA:HB3	2:F:452:CYS:HA	2.00	0.43
2:H:447:ALA:HB3	2:H:452:CYS:HA	2.00	0.43
1:A:119:ILE:HA	1:A:124:PHE:HE2	1.83	0.43
2:D:447:ALA:HB3	2:D:452:CYS:HA	2.00	0.43
2:L:381:CYS:HB2	2:L:418:PHE:CE1	2.53	0.43
2:P:105:TRP:HD1	2:P:114:CYS:HG	1.65	0.43
2:F:171:PRO:HD2	2:F:242:THR:CB	2.48	0.43
2:B:192:PRO:HB3	2:B:235:ASN:HB3	2.00	0.43
2:D:105:TRP:HD1	2:D:114:CYS:HG	1.63	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:447:ALA:HB3	2:L:452:CYS:HA	2.01	0.43
2:B:183:VAL:HG22	2:B:220:VAL:HG13	2.00	0.43
2:F:105:TRP:HD1	2:F:114:CYS:HG	1.64	0.43
2:H:105:TRP:HD1	2:H:114:CYS:HG	1.62	0.43
2:H:287:LEU:O	2:H:327:TYR:O	2.36	0.43
2:N:105:TRP:HD1	2:N:114:CYS:HG	1.65	0.43
2:J:447:ALA:HB3	2:J:452:CYS:HA	2.01	0.43
1:G:39:GLN:HB2	1:G:48:TRP:HH2	1.84	0.42
2:P:447:ALA:HB3	2:P:452:CYS:HA	2.01	0.42
2:D:183:VAL:HG12	2:D:220:VAL:HA	2.01	0.42
2:L:105:TRP:HD1	2:L:114:CYS:HG	1.66	0.42
2:P:368:CYS:HB3	2:P:407:CYS:SG	2.59	0.42
2:J:105:TRP:HD1	2:J:114:CYS:HG	1.65	0.42
2:L:359:TYR:HB3	2:L:361:ILE:HG23	2.01	0.42
2:N:267:PRO:HB2	2:N:269:TRP:HE1	1.84	0.42
2:B:447:ALA:HB3	2:B:452:CYS:HA	2.00	0.42
2:L:381:CYS:HB2	2:L:418:PHE:HE1	1.83	0.42
1:C:15:PHE:CG	1:C:112:LEU:HD11	2.54	0.42
2:J:171:PRO:HD2	2:J:242:THR:CB	2.49	0.42
2:F:83:VAL:H	2:F:161:ILE:HA	1.85	0.42
2:H:267:PRO:HB2	2:H:269:TRP:HE1	1.85	0.41
1:K:64:ALA:HB1	1:K:68:MET:HB2	2.02	0.41
2:N:195:GLU:HA	2:N:217:GLU:HA	2.02	0.41
2:L:381:CYS:SG	2:L:392:CYS:O	2.78	0.41
2:B:267:PRO:HB2	2:B:269:TRP:HE1	1.85	0.41
2:F:379:ILE:HA	2:F:422:ASN:HB3	2.02	0.41
2:L:192:PRO:HB3	2:L:235:ASN:HB3	2.01	0.41
1:O:64:ALA:HB1	1:O:68:MET:HB2	2.01	0.41
1:E:41:GLU:HB3	1:E:44:CYS:HB3	2.02	0.41
2:F:267:PRO:HB2	2:F:269:TRP:HE1	1.85	0.41
2:F:368:CYS:HB3	2:F:407:CYS:SG	2.61	0.41
2:D:407:CYS:HA	2:D:409:HIS:CD2	2.56	0.41
2:J:195:GLU:HA	2:J:217:GLU:HA	2.03	0.41
2:L:276:HIS:HD2	2:L:335:HIS:CE1	2.38	0.41
1:K:32:VAL:CG1	1:K:56:TRP:CD1	3.04	0.41
2:P:287:LEU:HB3	2:P:328:TYR:CE1	2.56	0.41
2:J:276:HIS:HD2	2:J:335:HIS:CE1	2.39	0.40
2:D:107:PHE:HA	2:D:141:TYR:HD1	1.87	0.40
2:N:276:HIS:HD2	2:N:335:HIS:CE1	2.40	0.40
2:H:304:SER:HB3	2:H:310:ILE:HD13	2.03	0.40
2:P:266:GLU:HA	2:P:267:PRO:HD3	1.96	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	129/155 (83%)	126 (98%)	1 (1%)	2 (2%)	9	45
1	C	132/155 (85%)	126 (96%)	4 (3%)	2 (2%)	10	46
1	E	132/155 (85%)	126 (96%)	3 (2%)	3 (2%)	6	37
1	G	132/155 (85%)	124 (94%)	4 (3%)	4 (3%)	4	31
1	I	133/155 (86%)	124 (93%)	7 (5%)	2 (2%)	10	46
1	K	135/155 (87%)	128 (95%)	5 (4%)	2 (2%)	10	46
1	M	132/155 (85%)	126 (96%)	4 (3%)	2 (2%)	10	46
1	O	132/155 (85%)	129 (98%)	3 (2%)	0	100	100
2	B	409/582 (70%)	351 (86%)	39 (10%)	19 (5%)	2	24
2	D	410/582 (70%)	345 (84%)	47 (12%)	18 (4%)	2	25
2	F	410/582 (70%)	339 (83%)	54 (13%)	17 (4%)	3	25
2	H	409/582 (70%)	347 (85%)	43 (10%)	19 (5%)	2	24
2	J	403/582 (69%)	336 (83%)	52 (13%)	15 (4%)	3	28
2	L	418/582 (72%)	352 (84%)	46 (11%)	20 (5%)	2	23
2	N	418/582 (72%)	350 (84%)	45 (11%)	23 (6%)	2	21
2	P	415/582 (71%)	348 (84%)	43 (10%)	24 (6%)	1	20
All	All	4349/5896 (74%)	3777 (87%)	400 (9%)	172 (4%)	3	26

All (172) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	PHE
2	B	85	VAL
2	B	367	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	439	PRO
2	B	458	PRO
2	B	491	VAL
1	C	6	PHE
2	D	85	VAL
2	D	211	PRO
2	D	439	PRO
2	D	458	PRO
2	D	491	VAL
1	E	6	PHE
1	E	32	VAL
2	F	85	VAL
2	F	411	HIS
2	F	458	PRO
2	F	491	VAL
1	G	6	PHE
2	H	85	VAL
2	H	439	PRO
2	H	458	PRO
2	H	491	VAL
1	I	6	PHE
2	J	85	VAL
2	J	439	PRO
2	J	458	PRO
2	J	491	VAL
2	J	496	VAL
1	K	6	PHE
2	L	85	VAL
2	L	210	SER
2	L	214	VAL
2	L	439	PRO
2	L	458	PRO
2	L	491	VAL
1	M	6	PHE
2	N	85	VAL
2	N	438	LYS
2	N	439	PRO
2	N	458	PRO
2	N	491	VAL
2	P	85	VAL
2	P	292	LEU
2	P	305	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	377	PRO
2	P	439	PRO
2	P	458	PRO
2	P	491	VAL
1	A	40	ASP
2	B	96	ASP
2	B	213	VAL
2	B	387	ARG
2	B	485	ARG
2	B	496	VAL
2	B	512	VAL
1	C	47	LEU
2	D	96	ASP
2	D	167	THR
2	D	485	ARG
2	D	496	VAL
2	D	512	VAL
1	E	41	GLU
2	F	96	ASP
2	F	387	ARG
2	F	439	PRO
2	F	485	ARG
2	F	496	VAL
2	F	512	VAL
1	G	34	VAL
1	G	36	SER
1	G	70	GLY
2	H	96	ASP
2	H	354	ASN
2	H	356	SER
2	H	387	ARG
2	H	485	ARG
2	H	496	VAL
2	H	512	VAL
2	J	96	ASP
2	J	485	ARG
2	J	512	VAL
1	K	40	ASP
2	L	96	ASP
2	L	485	ARG
2	L	496	VAL
2	L	512	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	40	ASP
2	N	96	ASP
2	N	167	THR
2	N	365	GLU
2	N	387	ARG
2	N	485	ARG
2	N	496	VAL
2	N	512	VAL
2	P	96	ASP
2	P	306	ASN
2	P	387	ARG
2	P	485	ARG
2	P	496	VAL
2	P	512	VAL
2	B	479	THR
2	B	514	CYS
2	D	479	THR
2	D	514	CYS
2	F	479	THR
2	F	514	CYS
2	H	210	SER
2	H	479	THR
2	H	514	CYS
1	I	1	THR
2	J	288	GLU
2	J	479	THR
2	J	514	CYS
2	L	319	SER
2	L	479	THR
2	L	514	CYS
2	N	163	THR
2	N	402	SER
2	N	479	THR
2	N	514	CYS
2	P	479	THR
2	P	514	CYS
2	D	108	LYS
2	D	289	ASN
2	D	424	ASP
2	F	108	LYS
2	F	127	SER
2	F	364	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	422	ASN
2	L	424	ASP
2	N	190	PRO
2	N	423	ASP
2	B	108	LYS
2	B	127	SER
2	B	354	ASN
2	B	366	GLU
2	D	127	SER
2	F	363	GLN
2	H	108	LYS
2	H	127	SER
2	H	289	ASN
2	J	108	LYS
2	J	127	SER
2	L	108	LYS
2	L	127	SER
2	L	207	LYS
2	L	296	ASN
2	L	365	GLU
2	N	108	LYS
2	N	127	SER
2	P	108	LYS
2	P	127	SER
2	P	167	THR
2	P	213	VAL
2	P	322	ARG
2	P	401	TYR
2	P	424	ASP
2	B	424	ASP
2	D	305	THR
2	B	493	GLY
2	F	493	GLY
2	H	493	GLY
2	J	493	GLY
2	L	493	GLY
2	N	317	VAL
2	N	493	GLY
2	P	493	GLY
2	D	493	GLY
2	J	264	VAL
2	P	264	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	211	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	77/142 (54%)	74 (96%)	3 (4%)	32 57
1	C	69/142 (49%)	56 (81%)	13 (19%)	1 10
1	E	57/142 (40%)	52 (91%)	5 (9%)	10 33
1	G	70/142 (49%)	58 (83%)	12 (17%)	2 13
1	I	76/142 (54%)	68 (90%)	8 (10%)	7 26
1	K	67/142 (47%)	59 (88%)	8 (12%)	5 23
1	M	75/142 (53%)	70 (93%)	5 (7%)	16 43
1	O	79/142 (56%)	72 (91%)	7 (9%)	9 33
2	B	109/515 (21%)	97 (89%)	12 (11%)	6 25
2	D	94/515 (18%)	85 (90%)	9 (10%)	8 29
2	F	107/515 (21%)	99 (92%)	8 (8%)	13 40
2	H	95/515 (18%)	85 (90%)	10 (10%)	7 26
2	J	96/515 (19%)	87 (91%)	9 (9%)	8 30
2	L	103/515 (20%)	96 (93%)	7 (7%)	16 42
2	N	95/515 (18%)	88 (93%)	7 (7%)	13 40
2	P	101/515 (20%)	90 (89%)	11 (11%)	6 25
All	All	1370/5256 (26%)	1236 (90%)	134 (10%)	8 28

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	58	GLU
1	A	127	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	168	LEU
2	B	172	TYR
2	B	177	GLU
2	B	224	LEU
2	B	231	CYS
2	B	239	ARG
2	B	247	ILE
2	B	324	ASP
2	B	351	ASN
2	B	368	CYS
2	B	379	ILE
2	B	407	CYS
1	C	1	THR
1	C	2	GLN
1	C	28	GLN
1	C	29	ASP
1	C	39	GLN
1	C	58	GLU
1	C	74	ARG
1	C	93	CYS
1	C	96	PHE
1	C	106	GLN
1	C	111	GLN
1	C	112	LEU
1	C	127	CYS
2	D	244	LEU
2	D	247	ILE
2	D	323	ASN
2	D	351	ASN
2	D	379	ILE
2	D	392	CYS
2	D	398	ASP
2	D	407	CYS
2	D	422	ASN
1	E	28	GLN
1	E	29	ASP
1	E	74	ARG
1	E	98	GLN
1	E	122	GLN
2	F	244	LEU
2	F	247	ILE
2	F	281	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	351	ASN
2	F	368	CYS
2	F	381	CYS
2	F	398	ASP
2	F	407	CYS
1	G	28	GLN
1	G	36	SER
1	G	40	ASP
1	G	44	CYS
1	G	48	TRP
1	G	58	GLU
1	G	74	ARG
1	G	75	VAL
1	G	81	PHE
1	G	96	PHE
1	G	98	GLN
1	G	106	GLN
2	H	232	CYS
2	H	241	CYS
2	H	247	ILE
2	H	272	CYS
2	H	346	GLU
2	H	351	ASN
2	H	360	GLU
2	H	368	CYS
2	H	379	ILE
2	H	407	CYS
1	I	28	GLN
1	I	44	CYS
1	I	52	LEU
1	I	67	LYS
1	I	74	ARG
1	I	96	PHE
1	I	108	THR
1	I	127	CYS
2	J	168	LEU
2	J	271	ARG
2	J	272	CYS
2	J	317	VAL
2	J	351	ASN
2	J	368	CYS
2	J	383	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	392	CYS
2	J	433	LEU
1	K	0	MET
1	K	2	GLN
1	K	28	GLN
1	K	74	ARG
1	K	96	PHE
1	K	98	GLN
1	K	111	GLN
1	K	134	PRO
2	L	168	LEU
2	L	244	LEU
2	L	283	LEU
2	L	287	LEU
2	L	351	ASN
2	L	368	CYS
2	L	407	CYS
1	M	28	GLN
1	M	44	CYS
1	M	74	ARG
1	M	96	PHE
1	M	127	CYS
2	N	224	LEU
2	N	247	ILE
2	N	272	CYS
2	N	351	ASN
2	N	366	GLU
2	N	379	ILE
2	N	433	LEU
1	O	6	PHE
1	O	8	HIS
1	O	28	GLN
1	O	81	PHE
1	O	83	THR
1	O	96	PHE
1	O	127	CYS
2	P	160	ILE
2	P	218	GLU
2	P	244	LEU
2	P	287	LEU
2	P	346	GLU
2	P	351	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	359	TYR
2	P	368	CYS
2	P	379	ILE
2	P	392	CYS
2	P	407	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	399	ASN
2	D	323	ASN
2	D	422	ASN
1	E	98	GLN
2	F	351	ASN
2	J	335	HIS
2	L	335	HIS
2	N	335	HIS

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

12 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	NAG	Q	1	2,3	14,14,15	0.33	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	Q	2	3	14,14,15	0.31	0	17,19,21	0.54	0
3	NAG	R	1	2,3	14,14,15	0.33	0	17,19,21	0.69	1 (5%)
3	NAG	R	2	3	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	S	1	2,3	14,14,15	0.33	0	17,19,21	0.65	0
3	NAG	S	2	3	14,14,15	0.27	0	17,19,21	0.54	0
3	NAG	T	1	2,3	14,14,15	0.33	0	17,19,21	0.64	0
3	NAG	T	2	3	14,14,15	0.29	0	17,19,21	0.57	1 (5%)
3	NAG	U	1	2,3	14,14,15	0.33	0	17,19,21	0.65	0
3	NAG	U	2	3	14,14,15	0.32	0	17,19,21	0.50	0
3	NAG	V	1	2,3	14,14,15	0.31	0	17,19,21	0.80	1 (5%)
3	NAG	V	2	3	14,14,15	0.28	0	17,19,21	0.57	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Q	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	R	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	NAG	S	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	NAG	T	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
3	NAG	U	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	NAG	V	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	V	1	NAG	O5-C1-C2	-2.71	107.01	111.29
3	R	1	NAG	O5-C1-C2	-2.07	108.02	111.29
3	V	2	NAG	C1-O5-C5	2.02	114.93	112.19
3	T	2	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

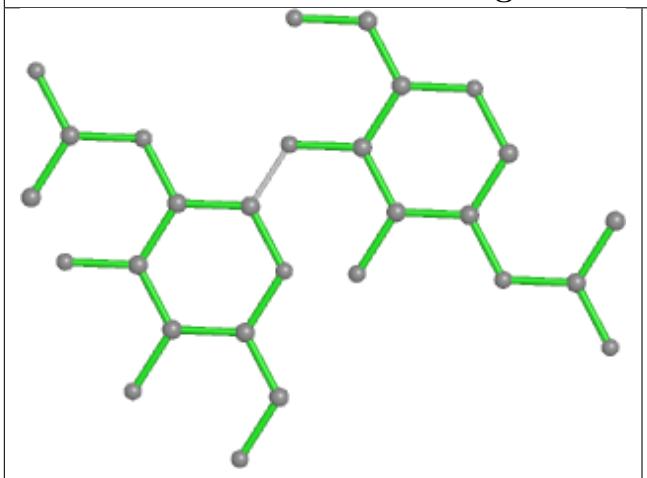
There are no torsion outliers.

There are no ring outliers.

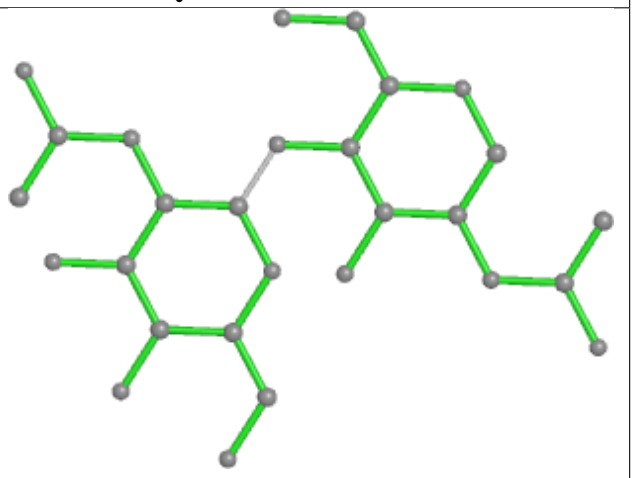
No monomer is involved in short contacts.

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

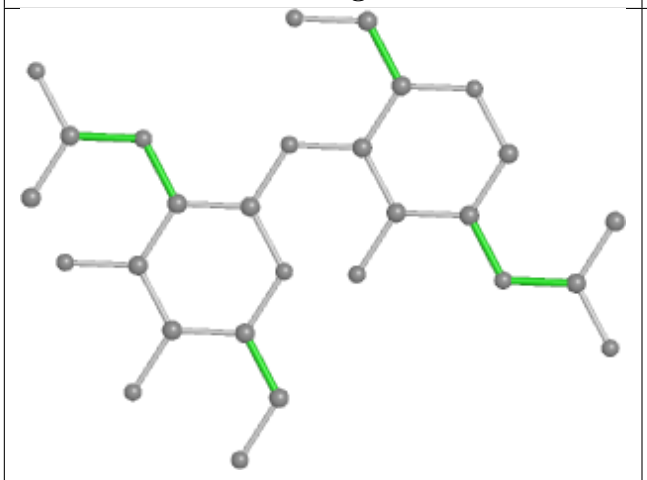
Oligosaccharide Chain Q



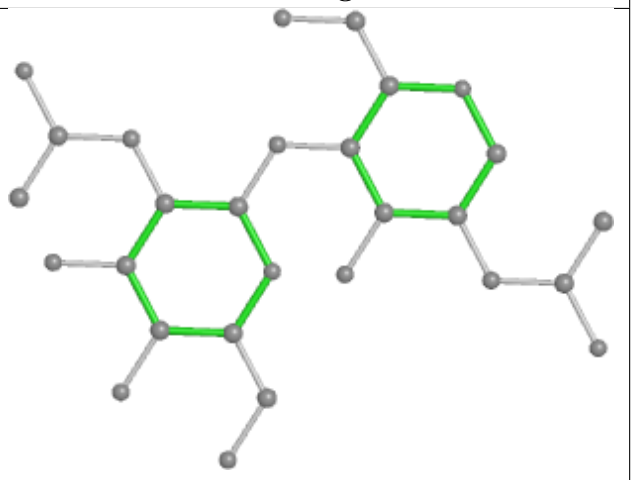
Bond lengths



Bond angles

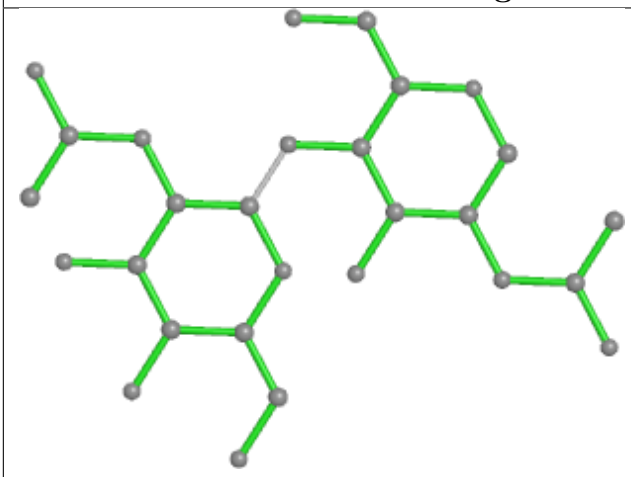


Torsions

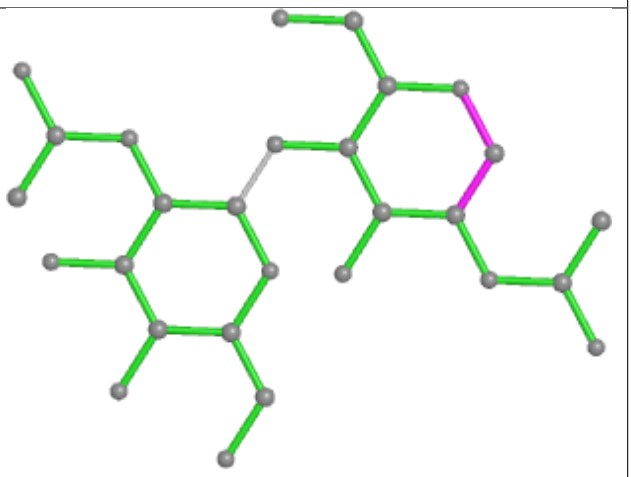


Rings

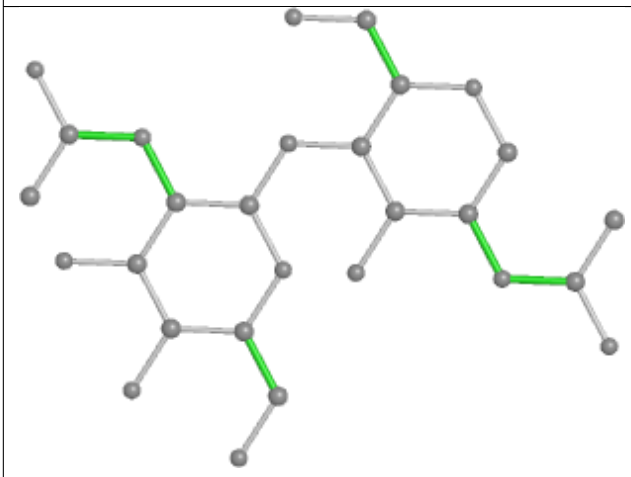
Oligosaccharide Chain R



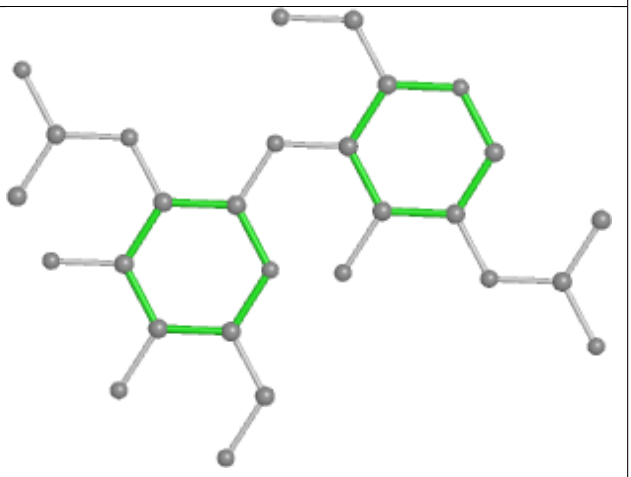
Bond lengths



Bond angles

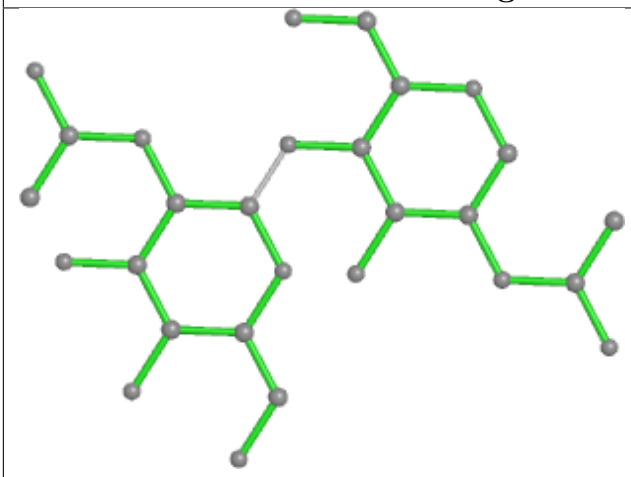


Torsions

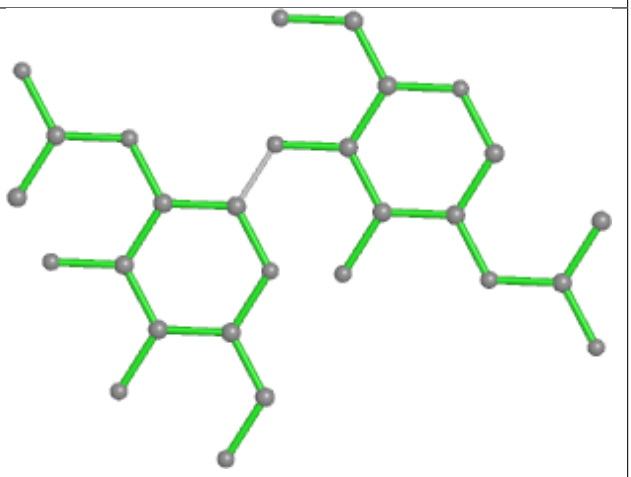


Rings

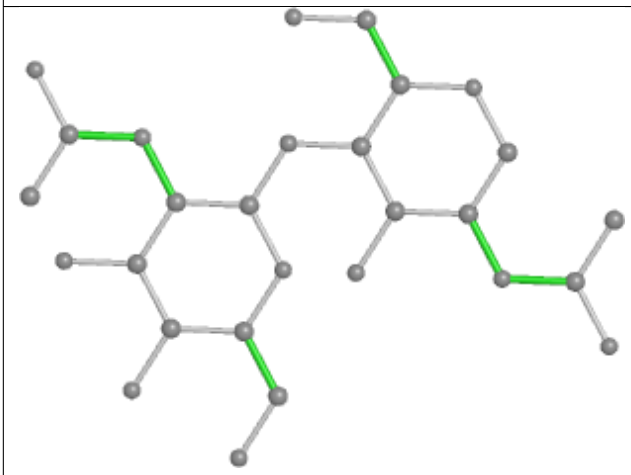
Oligosaccharide Chain S



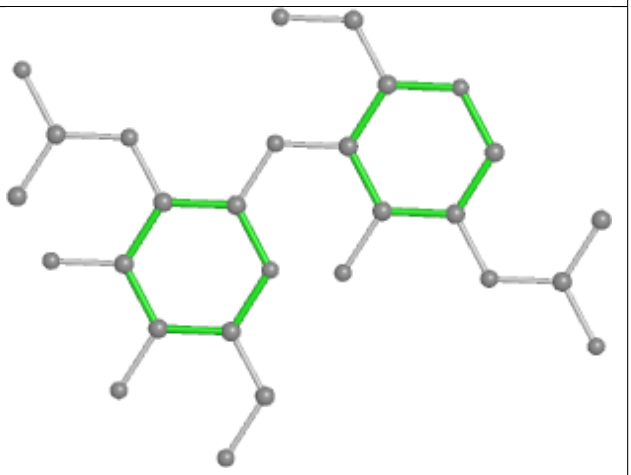
Bond lengths



Bond angles

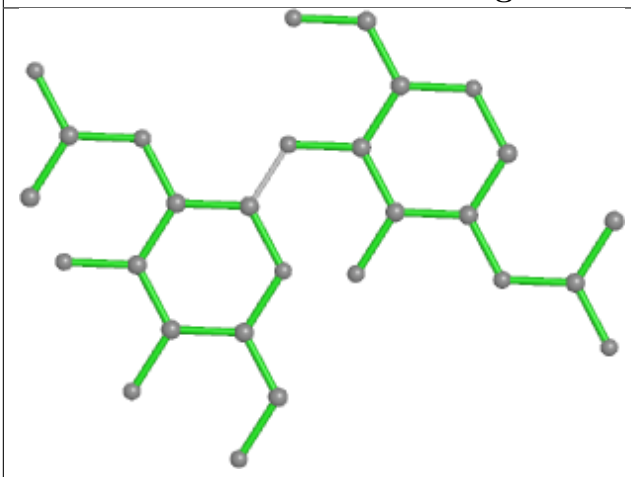


Torsions

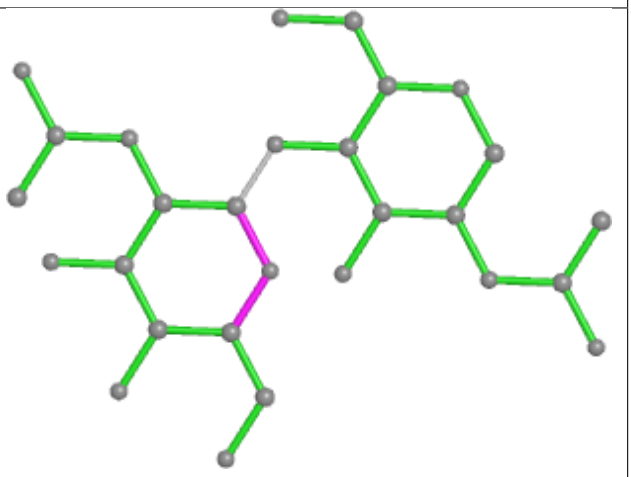


Rings

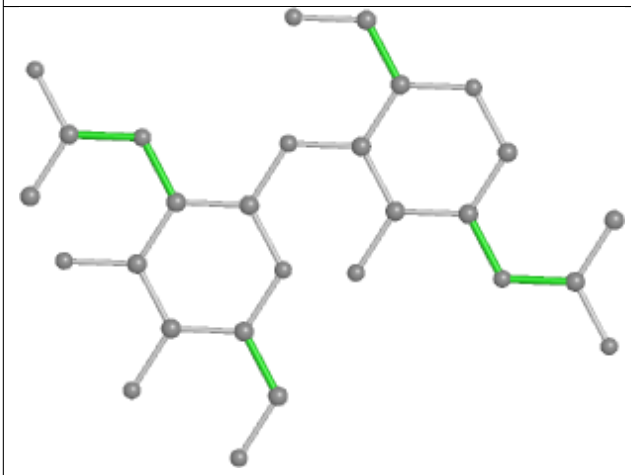
Oligosaccharide Chain T



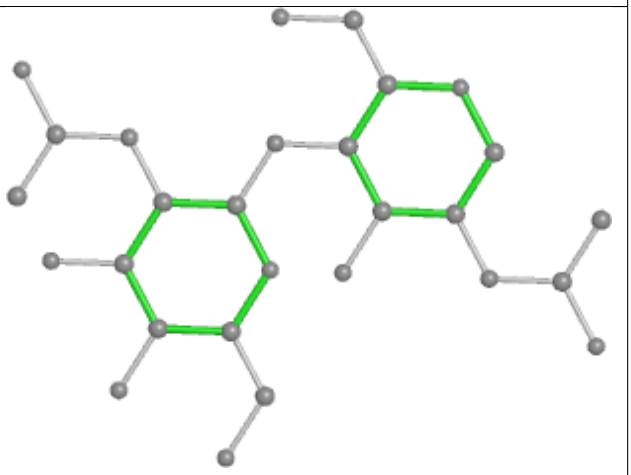
Bond lengths



Bond angles

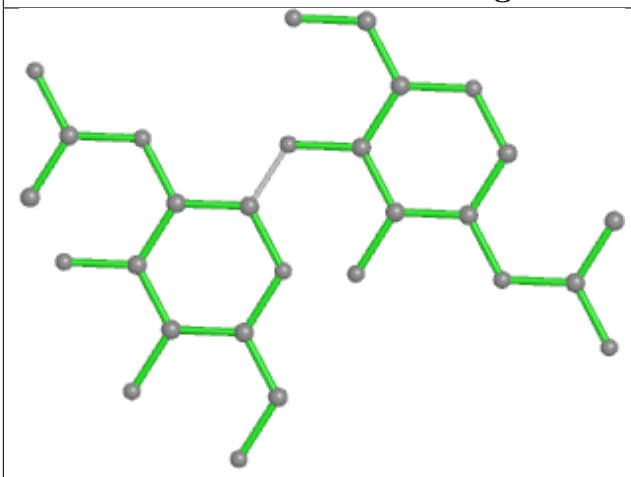


Torsions

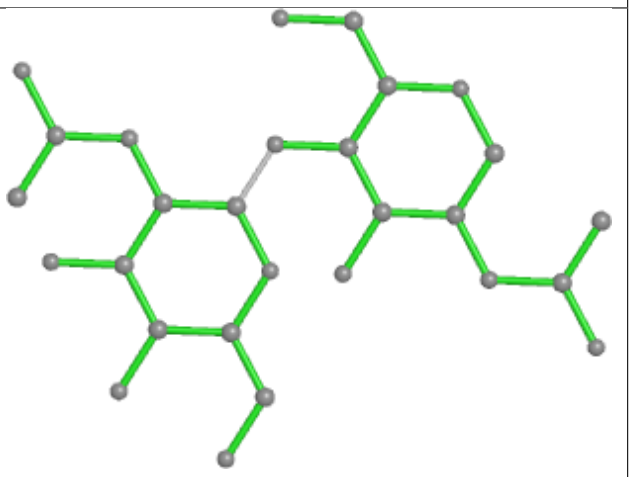


Rings

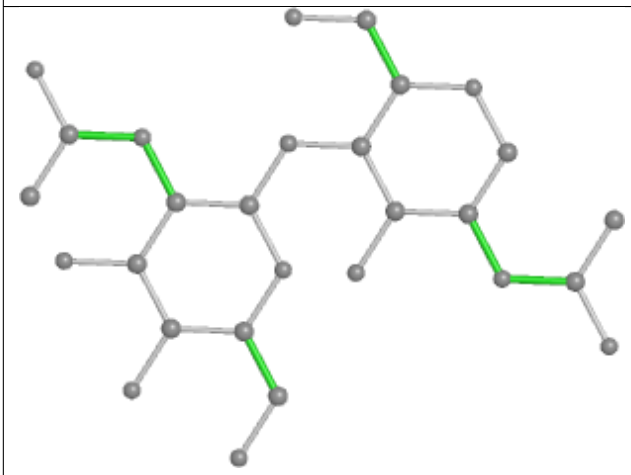
Oligosaccharide Chain U



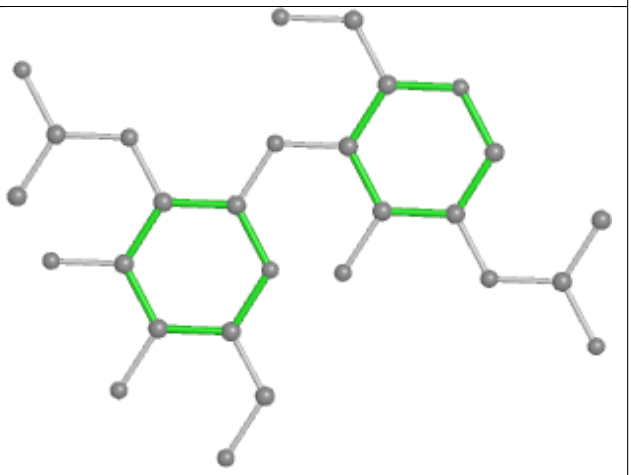
Bond lengths



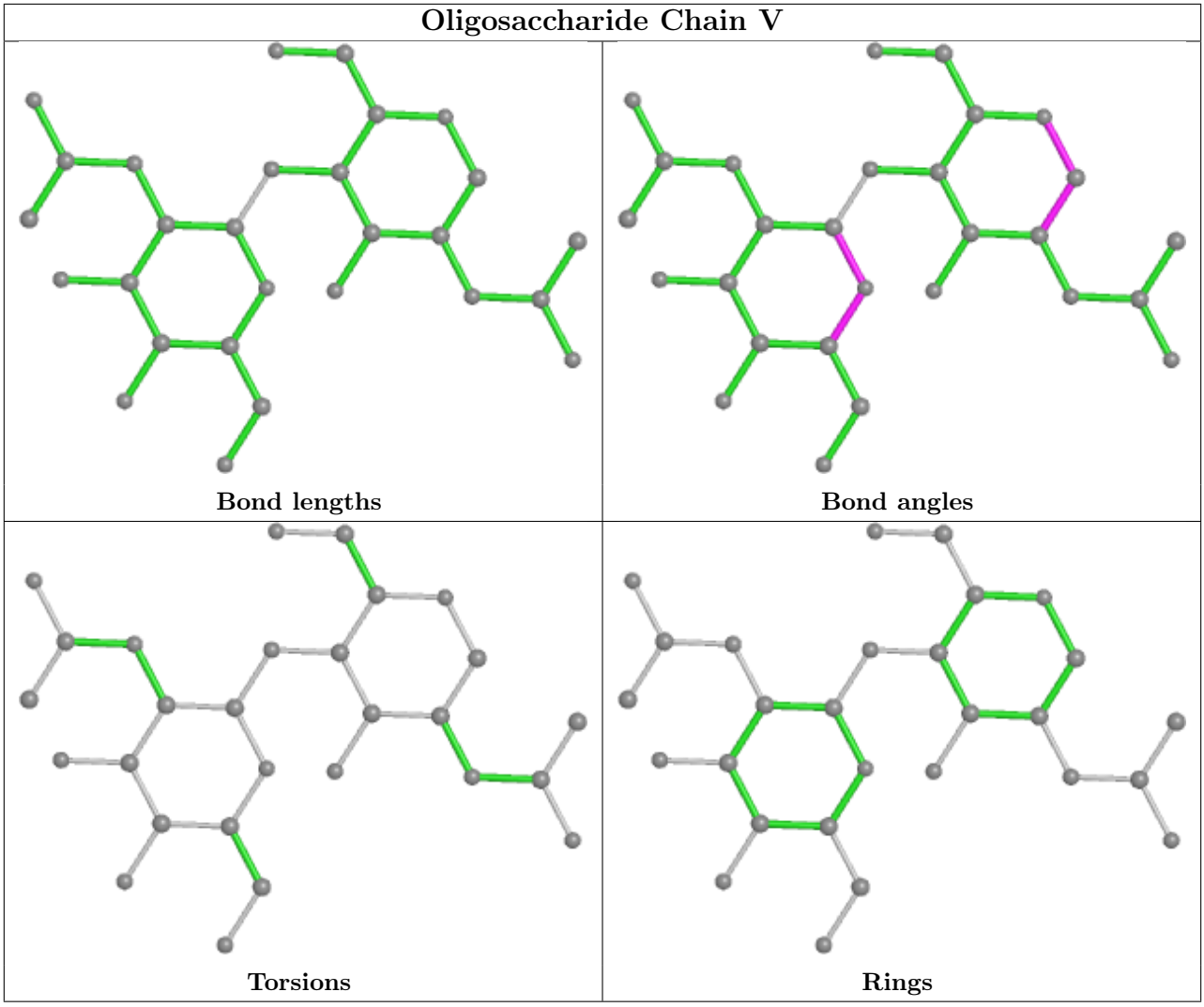
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	P	601	2	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	B	602	2	14,14,15	0.29	0	17,19,21	0.53	0
4	NAG	H	601	2	14,14,15	0.28	0	17,19,21	0.55	0
4	NAG	B	601	2	14,14,15	0.33	0	17,19,21	0.47	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
4	NAG	P	601	2	-	1/6/23/26	0/1/1/1
4	NAG	B	602	2	-	0/6/23/26	0/1/1/1
4	NAG	H	601	2	-	0/6/23/26	0/1/1/1
4	NAG	B	601	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	601	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	33:THR	C	34:VAL	N	3.81
1	A	32:VAL	C	33:THR	N	3.60
1	I	23[A]:SER	C	24:ASP	N	0.99

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, 95^{th} 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	134/155 (86%)	0.45	13 (9%) 7 7	93, 178, 196, 198	0
1	C	134/155 (86%)	0.09	4 (2%) 50 39	97, 173, 194, 196	0
1	E	134/155 (86%)	0.40	10 (7%) 14 12	138, 180, 195, 206	0
1	G	134/155 (86%)	0.25	11 (8%) 11 10	139, 177, 189, 192	0
1	I	135/155 (87%)	0.34	11 (8%) 12 11	146, 179, 188, 192	0
1	K	137/155 (88%)	0.16	3 (2%) 62 52	100, 177, 195, 203	0
1	M	134/155 (86%)	0.21	6 (4%) 33 28	139, 170, 182, 186	0
1	O	134/155 (86%)	0.30	7 (5%) 27 24	145, 175, 191, 193	0
2	B	423/582 (72%)	0.91	79 (18%) 1 2	98, 188, 289, 298	0
2	D	422/582 (72%)	0.81	81 (19%) 1 2	98, 197, 294, 299	0
2	F	420/582 (72%)	0.90	81 (19%) 1 1	145, 197, 290, 299	0
2	H	423/582 (72%)	0.78	66 (15%) 2 2	122, 201, 292, 299	0
2	J	417/582 (71%)	0.96	82 (19%) 1 1	126, 188, 289, 299	0
2	L	430/582 (73%)	1.06	87 (20%) 1 1	146, 207, 293, 299	0
2	N	428/582 (73%)	1.09	87 (20%) 1 1	136, 191, 294, 299	0
2	P	427/582 (73%)	0.82	71 (16%) 1 2	145, 209, 285, 297	0
All	All	4466/5896 (75%)	0.76	699 (15%) 2 2	93, 183, 289, 299	0

All (699) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	458	PRO	19.7
2	L	94	LEU	16.8
2	J	457	TYR	16.7
2	N	457	TYR	16.6
2	L	96	ASP	16.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	458	PRO	15.8
2	L	504	SER	14.8
2	P	124	GLY	14.1
2	B	124	GLY	13.8
2	N	513	LYS	13.5
2	N	512	VAL	13.4
2	N	456	GLY	13.4
2	P	95	VAL	13.3
2	L	95	VAL	13.0
2	H	497	SER	13.0
2	L	124	GLY	12.3
2	H	449	GLN	11.4
2	B	480	GLU	10.8
2	H	196	TRP	10.7
2	L	490	LYS	10.4
2	D	95	VAL	10.3
2	L	491	VAL	10.1
2	N	171	PRO	10.0
2	J	186	SER	9.7
2	D	496	VAL	9.6
2	B	502	ASN	9.6
2	B	95	VAL	9.6
2	L	505	GLU	9.6
2	N	466	LYS	9.6
2	P	491	VAL	9.5
2	H	466	LYS	9.5
2	D	466	LYS	9.4
2	P	79	ALA	9.4
2	B	466	LYS	9.2
2	P	94	LEU	9.2
2	B	489	ARG	9.1
2	D	497	SER	9.0
2	J	455	ASP	9.0
2	H	450	ALA	9.0
2	J	456	GLY	8.9
2	N	511	LEU	8.8
2	L	487	ALA	8.5
2	B	94	LEU	8.5
2	L	101	ILE	8.4
2	N	497	SER	8.4
2	F	480	GLU	8.4
2	F	466	LYS	8.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	439	PRO	8.2
2	J	443	ALA	8.2
2	B	488	ASN	8.1
2	J	144	PHE	8.1
2	J	504	SER	8.1
2	N	102	SER	7.9
2	J	85	VAL	7.8
2	N	462	TRP	7.8
2	P	80	ALA	7.8
2	J	145	ILE	7.7
2	B	90	THR	7.7
2	N	145	ILE	7.6
2	P	490	LYS	7.6
2	H	195	GLU	7.5
2	F	513	LYS	7.5
2	F	186	SER	7.5
2	J	84	ASP	7.4
2	L	506	ALA	7.4
2	N	498	SER	7.4
2	B	91	LEU	7.3
2	L	93	VAL	7.3
2	L	97	ALA	7.2
2	J	459	LEU	7.2
2	L	100	ASN	7.2
2	H	197	VAL	7.1
2	F	289	ASN	7.1
2	B	513	LYS	7.1
2	J	513	LYS	7.1
2	F	95	VAL	7.0
2	F	124	GLY	7.0
2	N	124	GLY	6.9
2	F	506	ALA	6.9
2	H	215	LYS	6.9
2	N	146	GLN	6.9
2	H	456	GLY	6.9
2	D	513	LYS	6.8
2	J	512	VAL	6.8
2	P	96	ASP	6.8
2	D	124	GLY	6.6
2	L	480	GLU	6.5
1	E	8	HIS	6.5
2	L	240	GLU	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	504	SER	6.5
1	M	122	GLN	6.5
2	B	512	VAL	6.5
2	L	90	THR	6.5
2	F	504	SER	6.4
2	H	465	LYS	6.4
2	B	154	ILE	6.4
2	H	458	PRO	6.4
2	L	233	ALA	6.4
2	H	214	VAL	6.4
2	B	93	VAL	6.3
2	J	102	SER	6.3
2	P	153	THR	6.3
2	H	443	ALA	6.3
2	H	448	SER	6.2
2	N	186	SER	6.2
2	B	354	ASN	6.2
2	F	279	HIS	6.1
2	B	490	LYS	6.1
2	L	502	ASN	6.1
2	J	454	SER	6.1
2	D	197	VAL	6.0
2	P	90	THR	6.0
2	P	156	PHE	5.9
2	D	443	ALA	5.9
2	N	502	ASN	5.9
2	J	150	THR	5.8
2	L	118	PHE	5.8
2	J	502	ASN	5.8
2	F	94	LEU	5.8
2	B	118	PHE	5.8
2	H	457	TYR	5.7
1	I	10	PRO	5.7
2	H	513	LYS	5.7
2	N	283	LEU	5.7
2	B	115	GLN	5.7
2	H	451	SER	5.6
2	D	312	ILE	5.6
2	D	288	GLU	5.6
2	F	288	GLU	5.6
2	B	458	PRO	5.6
2	P	502	ASN	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	103	CYS	5.5
2	J	105	TRP	5.5
2	P	513	LYS	5.5
2	L	466	LYS	5.5
2	D	491	VAL	5.5
2	L	513	LYS	5.5
2	L	421	GLU	5.5
2	B	481	GLY	5.5
2	D	138	ALA	5.5
2	N	194	VAL	5.5
2	P	505	GLU	5.4
2	D	488	ASN	5.4
2	P	504	SER	5.4
2	N	150	THR	5.4
2	L	91	LEU	5.4
2	H	498	SER	5.4
2	F	281	PHE	5.4
2	D	494	GLN	5.3
2	J	146	GLN	5.3
2	F	512	VAL	5.3
2	P	487	ALA	5.3
2	F	235	ASN	5.3
2	H	442	LEU	5.3
2	D	214	VAL	5.3
2	J	234	ARG	5.2
2	N	463	THR	5.2
2	D	79	ALA	5.2
2	D	506	ALA	5.2
2	P	93	VAL	5.2
2	D	94	LEU	5.1
2	B	144	PHE	5.1
2	L	512	VAL	5.1
2	J	501	LEU	5.1
2	L	131	LEU	5.1
2	D	480	GLU	5.1
2	H	198	LEU	5.1
2	J	462	TRP	5.1
2	L	488	ASN	5.0
2	J	296	ASN	5.0
2	N	95	VAL	5.0
1	A	122	GLN	5.0
2	N	151	ASN	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	443	ALA	5.0
2	F	291	ALA	5.0
1	E	42	GLU	4.9
2	P	354	ASN	4.9
1	O	122	GLN	4.9
2	P	91	LEU	4.9
2	P	506	ALA	4.9
2	L	98	PRO	4.8
2	L	479	THR	4.8
1	I	5	SER	4.8
2	N	455	ASP	4.8
2	J	444	GLU	4.8
2	F	479	THR	4.8
2	F	290	LYS	4.8
1	E	9	SER	4.8
2	P	157	THR	4.8
2	F	458	PRO	4.7
2	P	520	LEU	4.7
2	F	280	GLY	4.7
2	N	437	ARG	4.7
2	L	503	MET	4.7
2	P	155	LEU	4.7
2	N	459	LEU	4.7
2	J	151	ASN	4.7
2	N	195	GLU	4.7
2	P	466	LYS	4.6
2	F	505	GLU	4.6
1	M	26	LEU	4.6
2	D	487	ALA	4.6
2	L	489	ARG	4.6
2	N	331	SER	4.6
2	J	180	ASP	4.6
2	H	194	VAL	4.5
2	J	233	ALA	4.5
2	D	154	ILE	4.5
2	N	438	LYS	4.5
1	I	28	GLN	4.5
2	J	235	ASN	4.5
2	B	479	THR	4.5
2	D	477	GLU	4.4
2	J	111	SER	4.4
2	P	125	VAL	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	438	LYS	4.4
2	B	145	ILE	4.4
2	N	504	SER	4.4
1	I	33	THR	4.4
2	D	169	ARG	4.4
2	N	454	SER	4.4
2	N	274	ALA	4.4
2	N	514	CYS	4.3
2	F	93	VAL	4.3
2	D	476	GLU	4.3
2	L	205	SER	4.3
2	D	465	LYS	4.3
2	N	464	TRP	4.3
2	J	522	THR	4.3
2	J	124	GLY	4.3
2	N	168	LEU	4.3
2	B	113	ASN	4.3
2	D	115	GLN	4.3
2	H	462	TRP	4.2
1	G	39	GLN	4.2
2	N	284	THR	4.2
2	L	239	ARG	4.2
2	F	343	THR	4.2
2	H	374	LYS	4.2
2	J	295	GLY	4.2
2	J	112	LEU	4.2
2	B	501	LEU	4.2
2	L	279	HIS	4.2
2	B	491	VAL	4.2
2	B	283	LEU	4.2
2	N	167	THR	4.1
2	D	96	ASP	4.1
1	I	6	PHE	4.1
2	J	279	HIS	4.1
2	H	504	SER	4.1
2	D	186	SER	4.1
2	H	496	VAL	4.1
2	H	124	GLY	4.1
2	N	332	SER	4.1
1	K	9	SER	4.0
2	B	353	THR	4.0
2	L	275	VAL	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	455	ASP	4.0
2	L	443	ALA	4.0
2	P	288	GLU	4.0
2	P	174	ARG	4.0
2	B	156	PHE	4.0
2	D	283	LEU	4.0
2	H	488	ASN	4.0
2	L	158	VAL	4.0
2	P	512	VAL	4.0
2	J	181	ALA	4.0
2	F	511	LEU	4.0
2	F	262	LEU	4.0
2	H	95	VAL	3.9
2	H	502	ASN	3.9
2	J	316	PHE	3.9
2	L	147	SER	3.9
2	B	503	MET	3.9
2	B	101	ILE	3.9
2	P	435	ILE	3.9
2	P	160	ILE	3.9
2	J	83	VAL	3.9
2	J	500	THR	3.9
2	B	114	CYS	3.9
2	P	521	GLY	3.9
2	D	101	ILE	3.8
2	B	439	PRO	3.8
2	F	431	PHE	3.8
2	D	495	TRP	3.8
2	B	355	SER	3.8
2	J	480	GLU	3.8
2	J	379	ILE	3.8
2	N	499	SER	3.8
2	B	155	LEU	3.8
2	H	480	GLU	3.8
2	H	463	THR	3.8
2	D	464	TRP	3.8
2	J	438	LYS	3.8
1	E	33	THR	3.8
2	D	430	MET	3.8
2	H	154	ILE	3.8
1	O	63	VAL	3.8
2	F	477	GLU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	90	PRO	3.7
1	I	7	GLN	3.7
2	D	393	GLU	3.7
2	F	88	SER	3.7
2	B	511	LEU	3.7
2	N	501	LEU	3.7
2	H	143	LEU	3.7
2	L	89	ILE	3.7
2	L	225	PHE	3.7
2	N	101	ILE	3.7
2	F	85	VAL	3.7
2	P	437	ARG	3.7
2	H	288	GLU	3.6
1	A	63	VAL	3.6
1	G	26	LEU	3.6
2	B	487	ALA	3.6
2	P	518	ASN	3.6
2	J	104	LEU	3.6
2	L	99	GLY	3.6
2	N	381	CYS	3.6
2	D	198	LEU	3.6
2	F	87	ALA	3.6
2	N	312	ILE	3.6
2	P	503	MET	3.6
2	H	274	ALA	3.6
1	C	13	SER	3.6
2	J	239	ARG	3.6
2	H	216	LYS	3.6
2	J	143	LEU	3.5
2	F	91	LEU	3.5
2	D	311	ARG	3.5
2	N	465	LYS	3.5
2	J	87	ALA	3.5
2	D	117	HIS	3.5
2	N	166	TYR	3.5
2	F	443	ALA	3.5
2	L	289	ASN	3.5
2	P	154	ILE	3.5
2	L	283	LEU	3.5
2	P	194	VAL	3.5
2	N	181	ALA	3.5
2	N	436	ARG	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	158	VAL	3.4
2	B	80	ALA	3.4
2	P	130	ILE	3.4
2	N	152	TYR	3.4
2	H	162	ASN	3.4
2	B	506	ALA	3.4
2	N	442	LEU	3.4
2	N	170	ARG	3.4
2	D	507	ILE	3.4
2	B	138	ALA	3.4
2	D	83	VAL	3.4
2	D	85	VAL	3.3
2	L	274	ALA	3.3
2	P	480	GLU	3.3
2	P	444	GLU	3.3
2	F	154	THR	3.3
2	H	312	ILE	3.3
2	P	443	ALA	3.3
2	N	444	GLU	3.3
2	D	301	SER	3.3
2	J	152	TYR	3.3
2	J	160	ILE	3.3
1	A	81	PHE	3.3
2	B	96	ASP	3.3
2	B	198	LEU	3.3
2	B	194	VAL	3.2
2	D	224	LEU	3.2
1	I	31	PRO	3.2
2	F	155	ILE	3.2
2	L	160	ILE	3.2
2	N	184	CYS	3.2
1	I	122	GLN	3.2
2	D	392	CYS	3.2
2	F	261	PHE	3.2
1	O	81	PHE	3.2
2	P	181	ALA	3.2
2	L	130	ILE	3.2
2	L	507	ILE	3.2
2	L	85	VAL	3.2
2	H	506	ALA	3.2
1	A	104	LEU	3.2
2	L	154	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	233	ALA	3.2
2	F	115	GLN	3.2
2	L	224	LEU	3.2
2	N	313	LEU	3.2
2	B	352	ALA	3.2
2	H	477	GLU	3.1
2	F	234	ARG	3.1
2	L	339	SER	3.1
2	D	498	SER	3.1
2	F	502	ASN	3.1
2	N	105	TRP	3.1
2	L	511	LEU	3.1
2	N	127	SER	3.1
1	A	107	GLU	3.1
2	B	289	ASN	3.1
2	D	391	PRO	3.1
2	F	236	GLU	3.1
2	P	175	LYS	3.1
2	H	144	PHE	3.1
2	D	300	MET	3.1
2	J	518	ASN	3.1
1	I	81	PHE	3.1
2	L	140	GLU	3.1
2	D	442	LEU	3.1
1	M	42	GLU	3.1
1	O	64	ALA	3.1
2	B	288	GLU	3.0
2	B	141	TYR	3.0
2	P	320	VAL	3.0
2	L	88	SER	3.0
2	F	239	ARG	3.0
1	C	40	ASP	3.0
2	P	81	VAL	3.0
1	A	43	LEU	3.0
2	L	141	TYR	3.0
2	J	511	LEU	3.0
2	J	147	SER	3.0
2	J	352	ALA	3.0
2	H	101	ILE	2.9
2	H	464	TRP	2.9
2	F	331	SER	2.9
2	P	180	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	91	LEU	2.9
2	H	343	THR	2.9
2	N	235	ASN	2.9
1	M	5	SER	2.9
2	P	138	ALA	2.9
2	N	147	SER	2.9
2	N	237	LEU	2.9
2	J	437	ARG	2.9
1	O	108	THR	2.9
2	D	137	GLN	2.9
2	J	101	ILE	2.9
2	P	522	THR	2.9
2	B	454	SER	2.9
2	J	106	VAL	2.9
2	J	460	PRO	2.9
2	D	394	GLN	2.9
2	J	91	LEU	2.9
2	P	139	GLY	2.9
2	B	153	THR	2.9
2	P	186	SER	2.9
2	N	182	LEU	2.9
2	F	223	GLU	2.8
1	E	10	PRO	2.8
2	F	83	VAL	2.8
2	B	89	ILE	2.8
2	J	185	ILE	2.8
2	D	475	THR	2.8
2	N	180	ASP	2.8
2	L	516	ALA	2.8
2	B	505	GLU	2.8
2	F	101	ILE	2.8
2	N	153	THR	2.8
2	D	444	GLU	2.8
2	D	508	LYS	2.8
1	M	79	ILE	2.8
2	J	113	ASN	2.8
2	P	224	LEU	2.8
2	F	275	VAL	2.8
2	D	168	LEU	2.8
2	P	289	ASN	2.8
2	D	275	VAL	2.8
2	J	464	TRP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	64	ALA	2.8
2	L	92	GLN	2.8
2	B	85	VAL	2.8
2	D	161	ARG	2.8
2	L	102	SER	2.8
2	L	422	ASN	2.8
2	P	488	ASN	2.8
1	M	6	PHE	2.8
2	B	197	VAL	2.8
2	B	130	ILE	2.8
2	D	97	ALA	2.8
2	H	311	ARG	2.8
2	F	185	ILE	2.8
2	N	85	VAL	2.7
2	F	476	GLU	2.7
2	L	139	GLY	2.7
2	F	86	SER	2.7
2	H	489	ARG	2.7
2	D	116	PRO	2.7
2	N	143	LEU	2.7
2	N	144	PHE	2.7
2	J	315	ALA	2.7
2	B	117	HIS	2.7
2	B	127	SER	2.7
2	D	90	THR	2.7
2	F	157	PHE	2.6
2	H	410	LYS	2.6
2	P	436	ARG	2.6
2	H	180	ASP	2.6
2	H	409	HIS	2.6
2	D	127	SER	2.6
2	B	518	ASN	2.6
1	E	11	ILE	2.6
2	D	313	LEU	2.6
2	H	439	PRO	2.6
2	P	353	THR	2.6
2	D	375	ALA	2.6
1	G	25	TYR	2.6
2	L	522	THR	2.6
2	L	186	SER	2.6
2	L	519	SER	2.6
2	L	291	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	91	LEU	2.6
2	F	344	ILE	2.6
2	N	450	ALA	2.6
2	B	444	GLU	2.6
2	L	153	THR	2.6
1	G	124	PHE	2.6
2	D	144	PHE	2.6
1	I	79	ILE	2.6
2	N	460	PRO	2.6
2	F	138	ALA	2.6
1	K	15	PHE	2.6
2	J	440	GLN	2.6
1	A	105	LEU	2.6
2	N	84	ASP	2.6
2	L	338	GLN	2.5
2	F	430	MET	2.5
2	L	156	PHE	2.5
2	D	86	SER	2.5
2	F	456	GLY	2.5
2	F	285	TRP	2.5
2	F	332	SER	2.5
2	J	463	THR	2.5
2	H	352	ALA	2.5
1	G	123	ASN	2.5
2	H	192	PRO	2.5
2	N	379	ILE	2.5
2	H	375	ALA	2.5
1	K	10	PRO	2.5
2	B	83	VAL	2.5
2	D	142	LEU	2.5
2	L	420	ALA	2.5
2	N	94	LEU	2.5
2	F	244	LEU	2.5
2	P	279	HIS	2.5
2	D	118	PHE	2.5
2	D	502	ASN	2.5
2	N	477	GLU	2.5
2	B	84	ASP	2.5
2	B	143	LEU	2.5
2	B	432	THR	2.5
1	E	7	GLN	2.5
2	P	184	CYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	160	ILE	2.4
2	L	288	GLU	2.4
2	F	432	THR	2.4
1	O	82	VAL	2.4
2	L	455	ASP	2.4
2	P	501	LEU	2.4
2	F	416	TYR	2.4
2	H	338	GLN	2.4
2	J	167	THR	2.4
2	D	512	VAL	2.4
2	J	127	SER	2.4
1	C	46	GLY	2.4
2	B	106	VAL	2.4
1	G	62	THR	2.4
2	N	196	TRP	2.4
2	F	106	VAL	2.4
2	B	274	ALA	2.4
1	C	12	SER	2.4
1	O	79	ILE	2.4
2	H	118	PHE	2.4
2	N	516	ALA	2.4
1	A	108	THR	2.4
2	F	90	THR	2.4
2	B	129	VAL	2.4
1	E	122	GLN	2.4
2	P	430	MET	2.4
2	F	168	LEU	2.4
2	F	224	LEU	2.4
2	L	273	LYS	2.4
2	L	486	LYS	2.3
2	P	413	PRO	2.3
2	F	274	ALA	2.3
2	P	225	PHE	2.3
2	L	138	ALA	2.3
2	J	283	LEU	2.3
2	J	510	PHE	2.3
2	N	340	ALA	2.3
2	F	89	ILE	2.3
2	J	192	PRO	2.3
2	L	444	GLU	2.3
2	J	168	LEU	2.3
2	L	380	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	452	CYS	2.3
2	J	499	SER	2.3
1	G	13	SER	2.3
2	N	199	CYS	2.3
2	H	411	HIS	2.3
2	H	503	MET	2.3
2	F	144	PHE	2.3
2	N	261	PHE	2.3
2	D	343	THR	2.3
2	P	89	ILE	2.3
2	B	247	ILE	2.3
2	J	516	ALA	2.3
1	A	134	PRO	2.3
2	F	465	LYS	2.3
2	F	475	THR	2.2
2	D	490	LYS	2.2
2	H	81	VAL	2.2
1	A	34	VAL	2.2
2	J	461	SER	2.2
2	L	79	ALA	2.2
2	J	298	PHE	2.2
2	L	329	THR	2.2
2	N	198	LEU	2.2
1	G	56	TRP	2.2
2	N	259	GLN	2.2
2	F	481	GLY	2.2
2	L	454	SER	2.2
2	H	153	THR	2.2
2	N	192	PRO	2.2
2	B	431	PHE	2.2
2	D	337	SER	2.2
2	L	272	CYS	2.2
2	H	444	GLU	2.2
2	P	239	ARG	2.2
1	E	46	GLY	2.2
2	H	394	GLN	2.2
1	G	63	VAL	2.2
2	J	482	VAL	2.2
2	N	314	PHE	2.2
2	D	196	TRP	2.2
2	P	101	ILE	2.2
2	F	507	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	299	GLU	2.2
2	N	233	ALA	2.2
2	F	105	TRP	2.2
1	A	38	LEU	2.1
2	H	184	CYS	2.1
2	F	439	PRO	2.1
2	B	465	LYS	2.1
2	B	311	ARG	2.1
2	F	97	ALA	2.1
1	A	39	GLN	2.1
2	F	522	THR	2.1
2	D	429	LYS	2.1
2	P	454	SER	2.1
2	F	438	LYS	2.1
2	B	229	ILE	2.1
2	D	282	GLY	2.1
2	N	262	LEU	2.1
2	L	106	VAL	2.1
2	L	81	VAL	2.1
2	B	224	LEU	2.1
2	B	81	VAL	2.1
2	F	233	ALA	2.1
2	F	516	ALA	2.1
2	D	352	ALA	2.1
2	D	379	ILE	2.1
1	G	42	GLU	2.1
2	B	459	LEU	2.1
2	B	158	VAL	2.1
2	D	158	VAL	2.1
2	J	413	PRO	2.1
2	D	299	GLU	2.1
2	L	477	GLU	2.1
2	P	262	LEU	2.1
2	L	510	PHE	2.1
2	N	154	ILE	2.1
2	H	353	THR	2.1
2	D	274	ALA	2.1
2	F	143	LEU	2.0
2	B	151	ASN	2.0
2	L	178	ASN	2.0
1	E	1	THR	2.0
2	B	142	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	186	SER	2.0
2	N	111	SER	2.0
2	H	91	LEU	2.0
2	F	238	GLY	2.0
2	N	258	PRO	2.0
2	J	94	LEU	2.0
2	F	514	CYS	2.0
2	H	276	HIS	2.0
2	D	80	ALA	2.0
2	D	458	PRO	2.0
2	L	152	TYR	2.0
2	L	83	VAL	2.0
1	I	78	GLU	2.0
2	P	178	ASN	2.0
2	L	403	ILE	2.0
2	P	114	CYS	2.0
2	P	115	GLN	2.0
2	J	133	MET	2.0
2	N	106	VAL	2.0
2	B	160	ILE	2.0
2	F	282	GLY	2.0
2	J	297	TYR	2.0

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

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

6.3 Carbohydrates (i)

SUGAR-RSR INFOmissingINFO

6.4 Ligands (i)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.