wwPDB X-ray Structure Validation Summary Report (i)

Dec 15, 2016 – 04:34 PM EST

PDB ID	:	5EBZ
Title	:	Crystal structure of human IKK1
Authors	:	Polley, S.; Passos, D.; Huang, D.; Biswas, T.; Verma, I.; Lyumkis, D.; Ghosh, G.
Deposited on	:	2015-10-20
Resolution	:	4.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

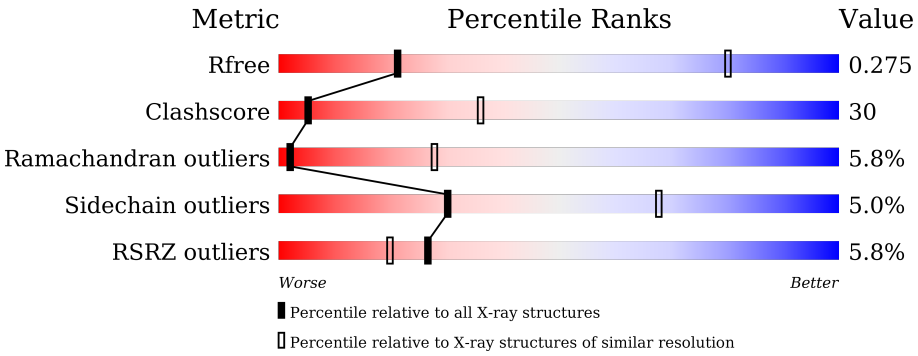
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 4.50 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}	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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. 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	655	4% 46% 47% 6%
1	B	655	6% 44% 49% 6%
1	C	655	3% 44% 50% 5%
1	D	655	7% 44% 51% 5%
1	E	655	4% 43% 51% 6%
1	F	655	7% 44% 51%

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Mol	Chain	Length	Quality of chain
1	G	655	3% 44% 50% 5%
1	H	655	8% 44% 50% 6%
1	I	655	6% 43% 51% 5%
1	J	655	8% 44% 50% 5%
1	K	655	7% 42% 52% 5%
1	L	655	6% 43% 52% 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	Z4K	C	709	-	-	-	X
2	5TL	A	701	-	-	-	X
2	5TL	B	701	-	-	-	X
2	5TL	C	701	-	-	-	X
2	5TL	D	701	-	-	-	X
2	5TL	E	701	-	-	-	X
2	5TL	F	701	-	-	-	X
2	5TL	H	701	-	-	-	X
2	5TL	I	701	-	-	-	X
2	5TL	J	701	-	-	-	X
2	5TL	K	701	-	-	-	X
2	5TL	L	701	-	-	-	X
3	5LS	B	707	-	-	-	X
3	5LS	D	702	-	-	-	X
3	5LS	G	702	-	-	-	X
3	5LS	K	702	-	-	-	X
3	5LS	L	704	-	-	-	X
4	GLC	J	705	-	-	X	-
4	GLC	K	703	-	-	-	X
5	PDX	G	704	-	-	-	X
5	PDX	K	707	-	-	-	X
5	PDX	L	709	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 65132 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 Inhibitor of nuclear factor kappa-B kinase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	B	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	C	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	D	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	E	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	F	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	G	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	H	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	I	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	J	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	K	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	L	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ASP	-	expression tag	UNP O15111
A	7	PRO	-	expression tag	UNP O15111
A	8	GLU	-	expression tag	UNP O15111
A	9	PHE	-	expression tag	UNP O15111
A	176	GLU	SER	engineered mutation	UNP O15111

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Chain	Residue	Modelled	Actual	Comment	Reference
A	180	GLU	SER	engineered mutation	UNP O15111
A	268	ILE	VAL	variant	UNP O15111
B	6	ASP	-	expression tag	UNP O15111
B	7	PRO	-	expression tag	UNP O15111
B	8	GLU	-	expression tag	UNP O15111
B	9	PHE	-	expression tag	UNP O15111
B	176	GLU	SER	engineered mutation	UNP O15111
B	180	GLU	SER	engineered mutation	UNP O15111
B	268	ILE	VAL	variant	UNP O15111
C	6	ASP	-	expression tag	UNP O15111
C	7	PRO	-	expression tag	UNP O15111
C	8	GLU	-	expression tag	UNP O15111
C	9	PHE	-	expression tag	UNP O15111
C	176	GLU	SER	engineered mutation	UNP O15111
C	180	GLU	SER	engineered mutation	UNP O15111
C	268	ILE	VAL	variant	UNP O15111
D	6	ASP	-	expression tag	UNP O15111
D	7	PRO	-	expression tag	UNP O15111
D	8	GLU	-	expression tag	UNP O15111
D	9	PHE	-	expression tag	UNP O15111
D	176	GLU	SER	engineered mutation	UNP O15111
D	180	GLU	SER	engineered mutation	UNP O15111
D	268	ILE	VAL	variant	UNP O15111
E	6	ASP	-	expression tag	UNP O15111
E	7	PRO	-	expression tag	UNP O15111
E	8	GLU	-	expression tag	UNP O15111
E	9	PHE	-	expression tag	UNP O15111
E	176	GLU	SER	engineered mutation	UNP O15111
E	180	GLU	SER	engineered mutation	UNP O15111
E	268	ILE	VAL	variant	UNP O15111
F	6	ASP	-	expression tag	UNP O15111
F	7	PRO	-	expression tag	UNP O15111
F	8	GLU	-	expression tag	UNP O15111
F	9	PHE	-	expression tag	UNP O15111
F	176	GLU	SER	engineered mutation	UNP O15111
F	180	GLU	SER	engineered mutation	UNP O15111
F	268	ILE	VAL	variant	UNP O15111
G	6	ASP	-	expression tag	UNP O15111
G	7	PRO	-	expression tag	UNP O15111
G	8	GLU	-	expression tag	UNP O15111
G	9	PHE	-	expression tag	UNP O15111
G	176	GLU	SER	engineered mutation	UNP O15111

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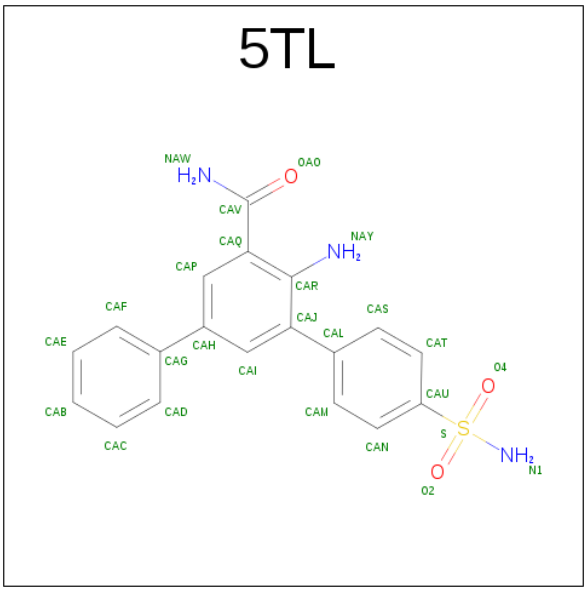
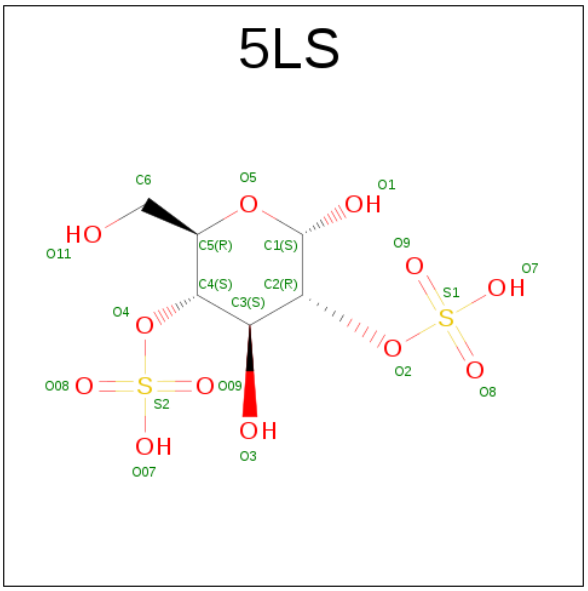
Chain	Residue	Modelled	Actual	Comment	Reference
G	180	GLU	SER	engineered mutation	UNP O15111
G	268	ILE	VAL	variant	UNP O15111
H	6	ASP	-	expression tag	UNP O15111
H	7	PRO	-	expression tag	UNP O15111
H	8	GLU	-	expression tag	UNP O15111
H	9	PHE	-	expression tag	UNP O15111
H	176	GLU	SER	engineered mutation	UNP O15111
H	180	GLU	SER	engineered mutation	UNP O15111
H	268	ILE	VAL	variant	UNP O15111
I	6	ASP	-	expression tag	UNP O15111
I	7	PRO	-	expression tag	UNP O15111
I	8	GLU	-	expression tag	UNP O15111
I	9	PHE	-	expression tag	UNP O15111
I	176	GLU	SER	engineered mutation	UNP O15111
I	180	GLU	SER	engineered mutation	UNP O15111
I	268	ILE	VAL	variant	UNP O15111
J	6	ASP	-	expression tag	UNP O15111
J	7	PRO	-	expression tag	UNP O15111
J	8	GLU	-	expression tag	UNP O15111
J	9	PHE	-	expression tag	UNP O15111
J	176	GLU	SER	engineered mutation	UNP O15111
J	180	GLU	SER	engineered mutation	UNP O15111
J	268	ILE	VAL	variant	UNP O15111
K	6	ASP	-	expression tag	UNP O15111
K	7	PRO	-	expression tag	UNP O15111
K	8	GLU	-	expression tag	UNP O15111
K	9	PHE	-	expression tag	UNP O15111
K	176	GLU	SER	engineered mutation	UNP O15111
K	180	GLU	SER	engineered mutation	UNP O15111
K	268	ILE	VAL	variant	UNP O15111
L	6	ASP	-	expression tag	UNP O15111
L	7	PRO	-	expression tag	UNP O15111
L	8	GLU	-	expression tag	UNP O15111
L	9	PHE	-	expression tag	UNP O15111
L	176	GLU	SER	engineered mutation	UNP O15111
L	180	GLU	SER	engineered mutation	UNP O15111
L	268	ILE	VAL	variant	UNP O15111

- Molecule 2 is 2-azanyl-5-phenyl-3-(4-sulfamoylphenyl)benzamide (three-letter code: 5TL) (formula: $C_{19}H_{17}N_3O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	B	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	C	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	D	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	E	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	F	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	G	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	H	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	I	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	J	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	K	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
2	L	1	Total	C	N	O	S	0	0
			26	19	3	3	1		

- Molecule 3 is [(2 {R},3 {S},4 {S},5 {R},6 {S})-2-(hydroxymethyl)-4,6-bis(oxidanyl)-5-sulfooxy-oxan-3-yl] hydrogen sulfate (three-letter code: 5LS) (formula: $C_6H_{12}O_{12}S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			20	6	12	2		
3	A	1	Total	C	O	S	0	0
			20	6	12	2		
3	B	1	Total	C	O	S	0	0
			20	6	12	2		
3	B	1	Total	C	O	S	0	0
			20	6	12	2		
3	C	1	Total	C	O	S	0	0
			20	6	12	2		
3	C	1	Total	C	O	S	0	0
			20	6	12	2		
3	D	1	Total	C	O	S	0	0
			20	6	12	2		
3	D	1	Total	C	O	S	0	0
			20	6	12	2		
3	D	1	Total	C	O	S	0	0
			20	6	12	2		
3	D	1	Total	C	O	S	0	0
			20	6	12	2		
3	E	1	Total	C	O	S	0	0
			20	6	12	2		
3	E	1	Total	C	O	S	0	0
			20	6	12	2		
3	F	1	Total	C	O	S	0	0
			20	6	12	2		
3	F	1	Total	C	O	S	0	0
			20	6	12	2		

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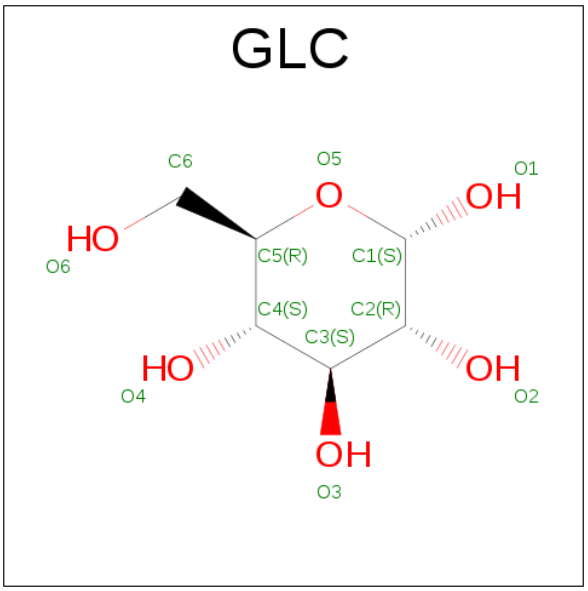
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	O	S	0	0
			20	6	12	2		
3	G	1	Total	C	O	S	0	0
			20	6	12	2		
3	H	1	Total	C	O	S	0	0
			20	6	12	2		
3	H	1	Total	C	O	S	0	0
			20	6	12	2		
3	H	1	Total	C	O	S	0	0
			20	6	12	2		
3	I	1	Total	C	O	S	0	0
			20	6	12	2		
3	I	1	Total	C	O	S	0	0
			20	6	12	2		
3	J	1	Total	C	O	S	0	0
			20	6	12	2		
3	J	1	Total	C	O	S	0	0
			20	6	12	2		
3	K	1	Total	C	O	S	0	0
			20	6	12	2		
3	K	1	Total	C	O	S	0	0
			20	6	12	2		
3	L	1	Total	C	O	S	0	0
			20	6	12	2		
3	L	1	Total	C	O	S	0	0
			20	6	12	2		
3	L	1	Total	C	O	S	0	0
			20	6	12	2		

- Molecule 4 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0
4	C	1	Total C O 11 6 5	0	0
4	C	1	Total C O 11 6 5	0	0
4	D	1	Total C O 11 6 5	0	0
4	D	1	Total C O 11 6 5	0	0
4	E	1	Total C O 11 6 5	0	0
4	E	1	Total C O 11 6 5	0	0
4	F	1	Total C O 11 6 5	0	0
4	F	1	Total C O 11 6 5	0	0
4	G	1	Total C O 11 6 5	0	0
4	G	1	Total C O 11 6 5	0	0

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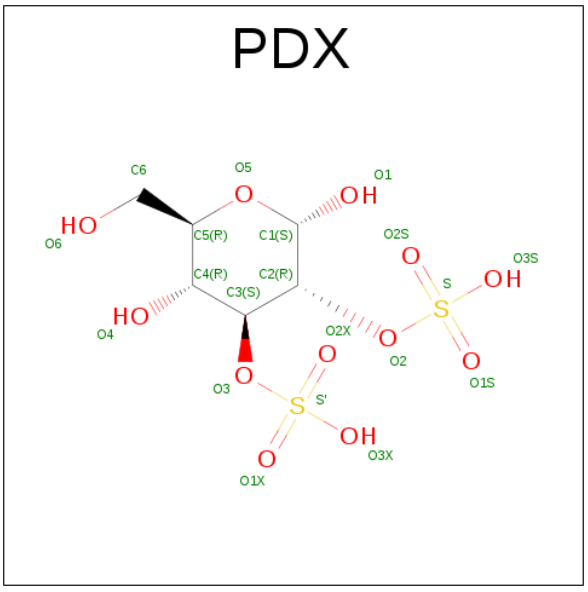
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 11 6 5	0	0
4	H	1	Total C O 11 6 5	0	0
4	I	1	Total C O 11 6 5	0	0
4	I	1	Total C O 11 6 5	0	0
4	J	1	Total C O 11 6 5	0	0
4	J	1	Total C O 11 6 5	0	0
4	K	1	Total C O 11 6 5	0	0
4	K	1	Total C O 11 6 5	0	0
4	L	1	Total C O 11 6 5	0	0
4	L	1	Total C O 11 6 5	0	0

- Molecule 5 is 2,3-DI-O-SULFO-ALPHA-D-GLUCOPYRANOSE (three-letter code: PDX) (formula: $C_6H_{12}O_{12}S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O S 19 6 11 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			19	6	11	2		
5	B	1	Total	C	O	S	0	0
			19	6	11	2		
5	B	1	Total	C	O	S	0	0
			19	6	11	2		
5	C	1	Total	C	O	S	0	0
			19	6	11	2		
5	C	1	Total	C	O	S	0	0
			19	6	11	2		
5	D	1	Total	C	O	S	0	0
			19	6	11	2		
5	D	1	Total	C	O	S	0	0
			19	6	11	2		
5	E	1	Total	C	O	S	0	0
			19	6	11	2		
5	E	1	Total	C	O	S	0	0
			19	6	11	2		
5	F	1	Total	C	O	S	0	0
			19	6	11	2		
5	F	1	Total	C	O	S	0	0
			19	6	11	2		
5	G	1	Total	C	O	S	0	0
			19	6	11	2		
5	G	1	Total	C	O	S	0	0
			19	6	11	2		
5	H	1	Total	C	O	S	0	0
			19	6	11	2		
5	I	1	Total	C	O	S	0	0
			19	6	11	2		
5	I	1	Total	C	O	S	0	0
			19	6	11	2		
5	J	1	Total	C	O	S	0	0
			19	6	11	2		
5	J	1	Total	C	O	S	0	0
			19	6	11	2		
5	K	1	Total	C	O	S	0	0
			19	6	11	2		
5	K	1	Total	C	O	S	0	0
			19	6	11	2		
5	L	1	Total	C	O	S	0	0
			19	6	11	2		

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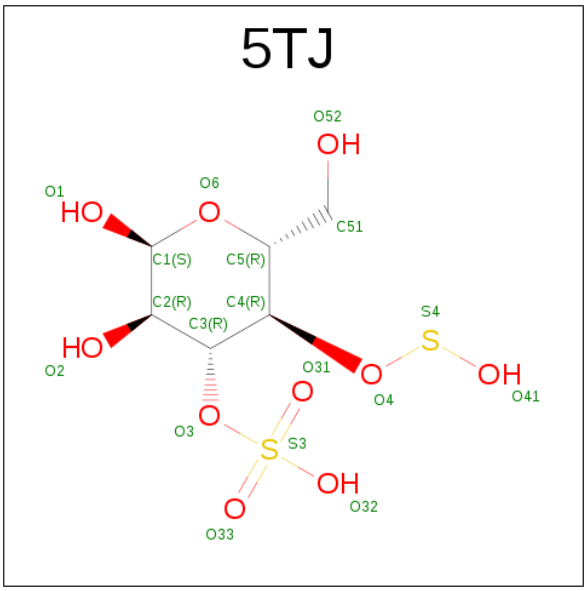
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C O S 19 6 11 2	0	0
5	L	1	Total C O S 19 6 11 2	0	0

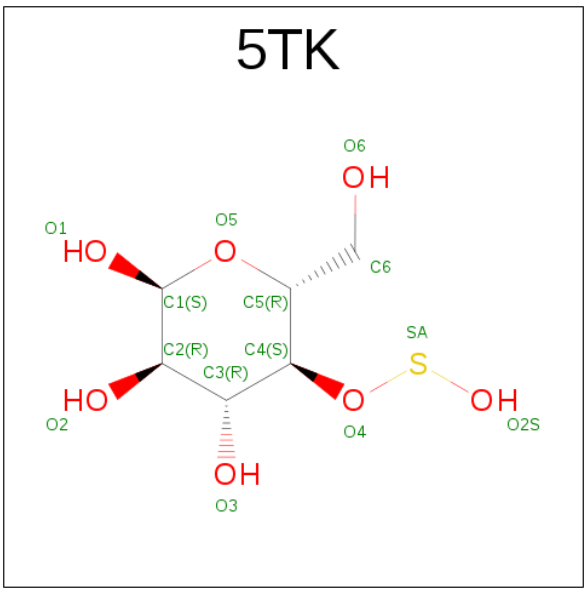
- Molecule 6 is [(2 {R},3 {R},4 {R},5 {R},6 {S})-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate (three-letter code: 5TJ) (formula: $C_6H_{12}O_{10}S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O S 17 6 9 2	0	0
6	A	1	Total C O S 17 6 9 2	0	0
6	D	1	Total C O S 17 6 9 2	0	0
6	D	1	Total C O S 17 6 9 2	0	0
6	H	1	Total C O S 17 6 9 2	0	0
6	H	1	Total C O S 17 6 9 2	0	0
6	I	1	Total C O S 17 6 9 2	0	0
6	I	1	Total C O S 17 6 9 2	0	0

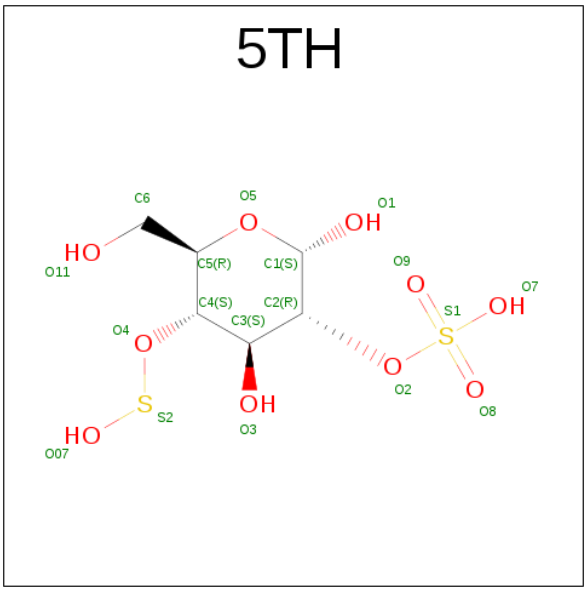
- Molecule 7 is (2 {S},3 {R},4 {R},5 {S},6 {R})-6-(hydroxymethyl)-5-oxidanylsulfanyloxy-ox

ane-2,3,4-triol (three-letter code: 5TK) (formula: $C_6H_{12}O_7S$).



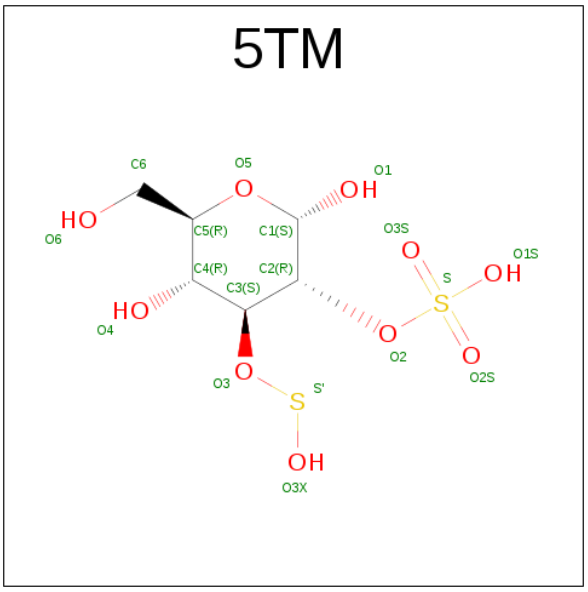
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			13	6	6	1		
7	C	1	Total	C	O	S	0	0
			13	6	6	1		
7	G	1	Total	C	O	S	0	0
			13	6	6	1		
7	I	1	Total	C	O	S	0	0
			13	6	6	1		

- Molecule 8 is [(2 {S},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-2,4-bis(oxidanyl)-5-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate (three-letter code: 5TH) (formula: $C_6H_{12}O_{10}S_2$).



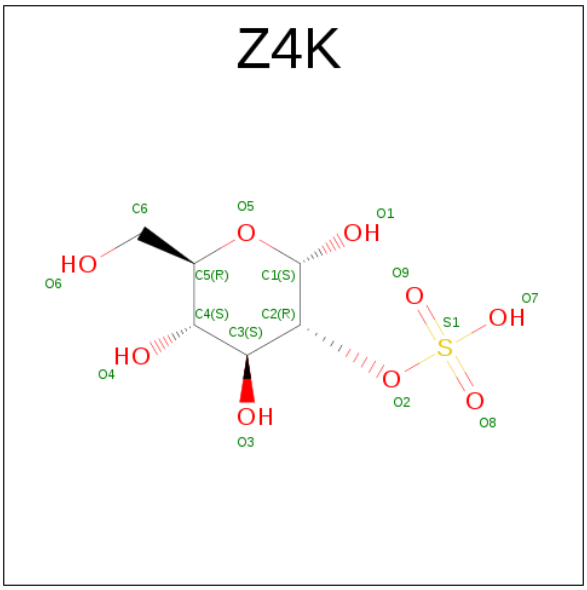
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O S 17 6 9 2	0	0
8	C	1	Total C O S 17 6 9 2	0	0
8	G	1	Total C O S 17 6 9 2	0	0
8	I	1	Total C O S 17 6 9 2	0	0

- Molecule 9 is [(2 {S},3 {R},4 {S},5 {R},6 {R})-6-(hydroxymethyl)-2,5-bis(oxidanyl)-4-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate (three-letter code: 5TM) (formula: $C_6H_{12}O_{10}S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O S 17 6 9 2	0	0
9	C	1	Total C O S 17 6 9 2	0	0
9	G	1	Total C O S 17 6 9 2	0	0
9	J	1	Total C O S 17 6 9 2	0	0

- Molecule 10 is 2-O-sulfo-alpha-D-glucopyranose (three-letter code: Z4K) (formula: $C_6H_{12}O_9S$).



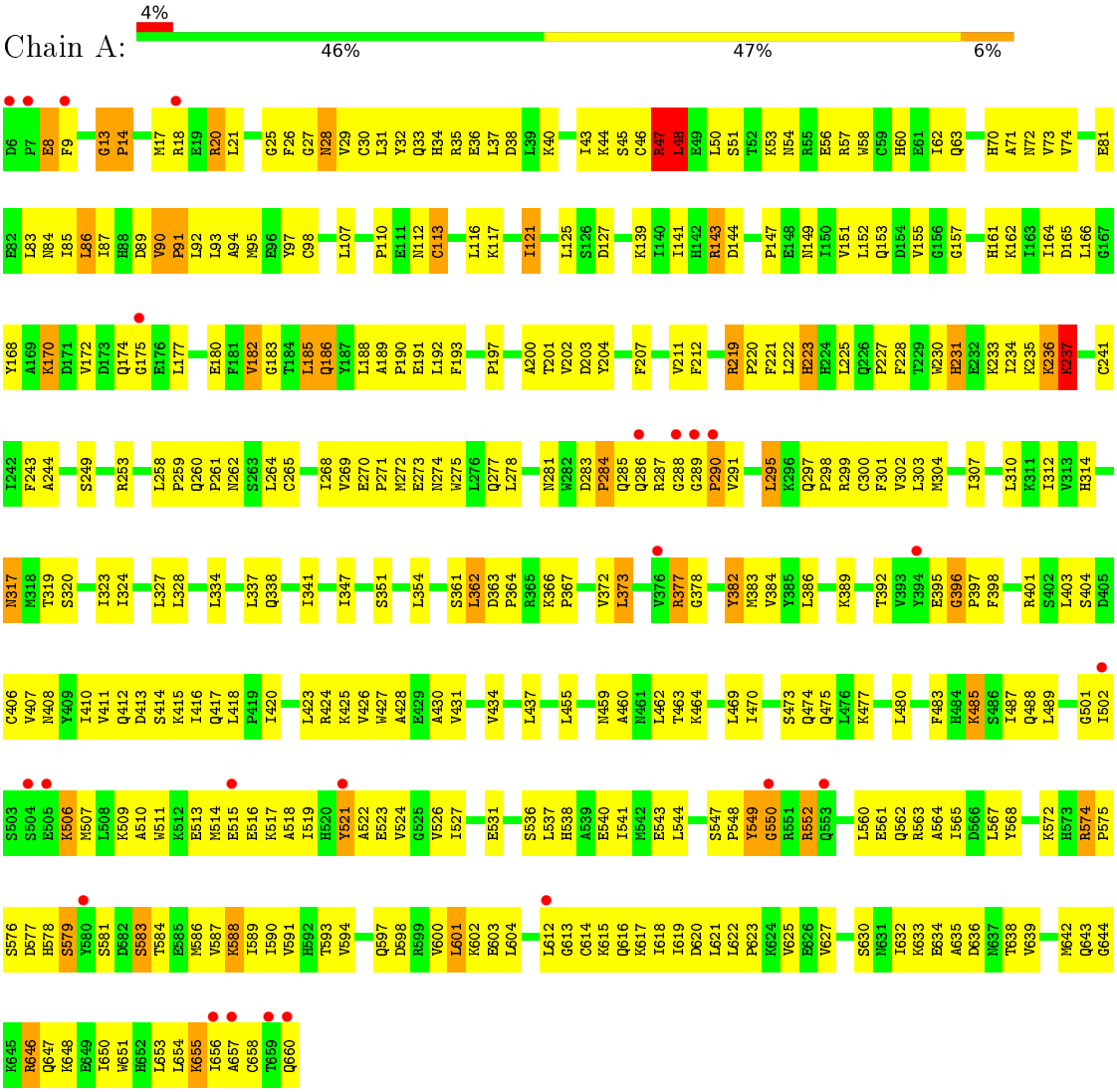
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O S 15 6 8 1	0	0
10	C	1	Total C O S 15 6 8 1	0	0
10	H	1	Total C O S 15 6 8 1	0	0
10	J	1	Total C O S 15 6 8 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

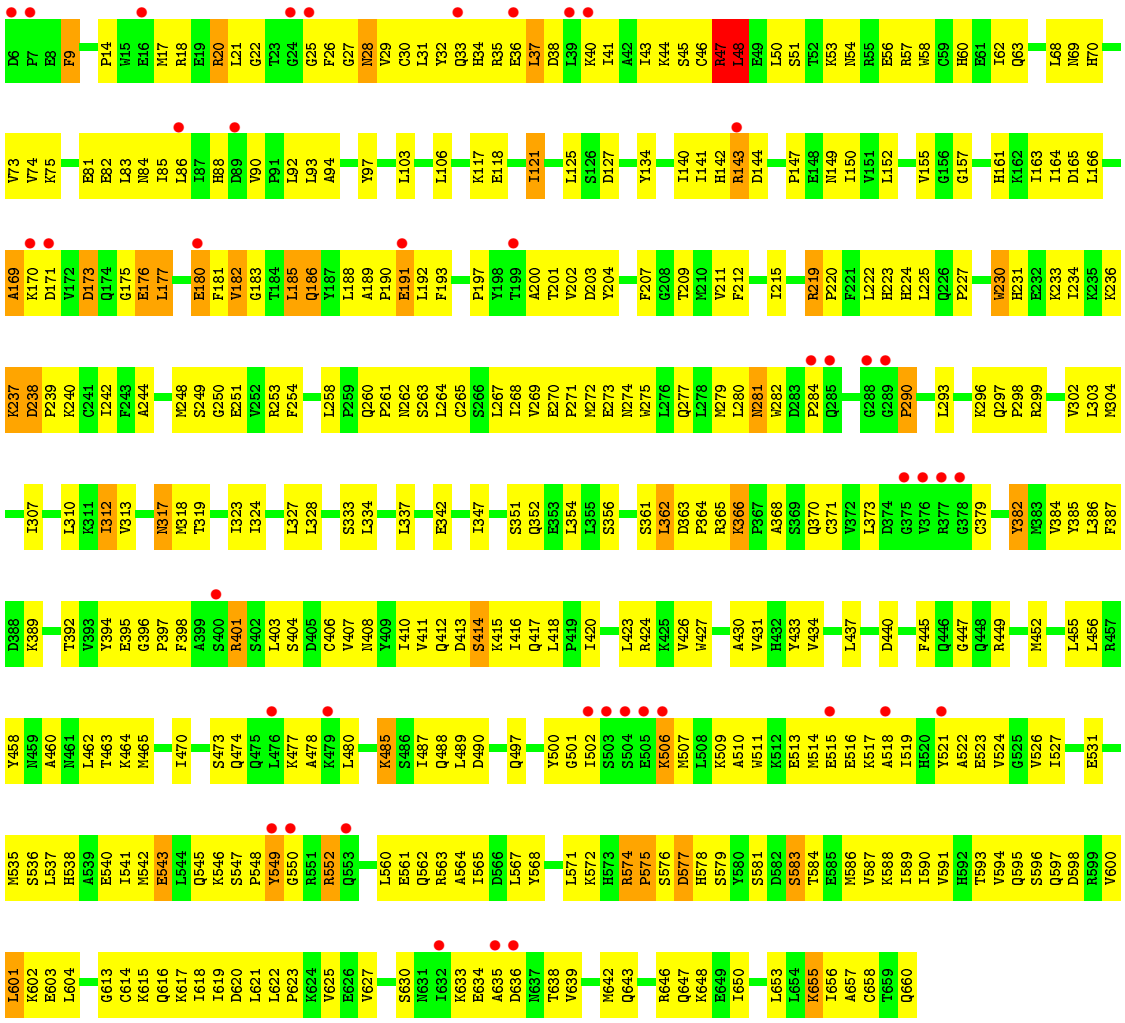
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain A:



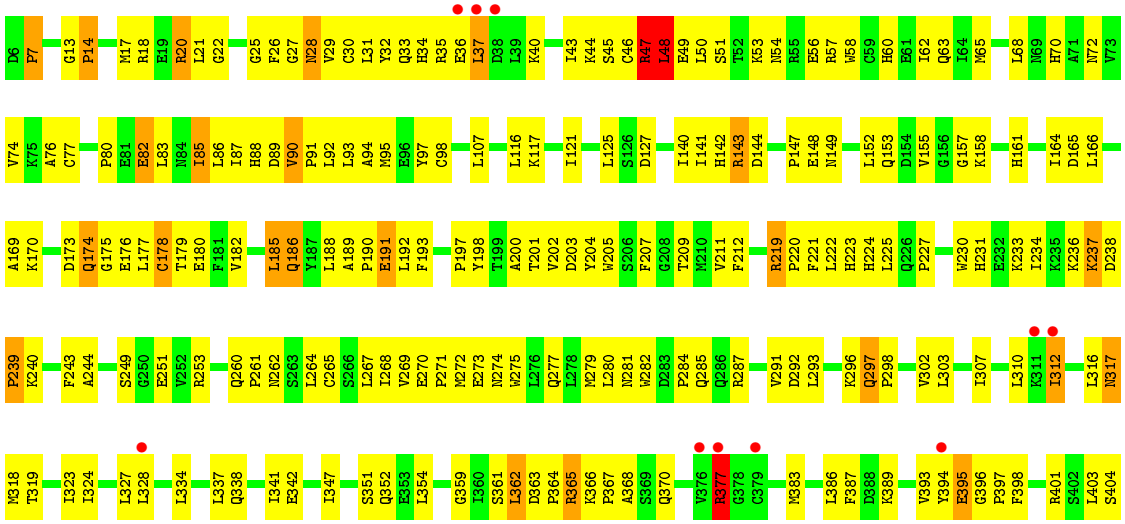
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

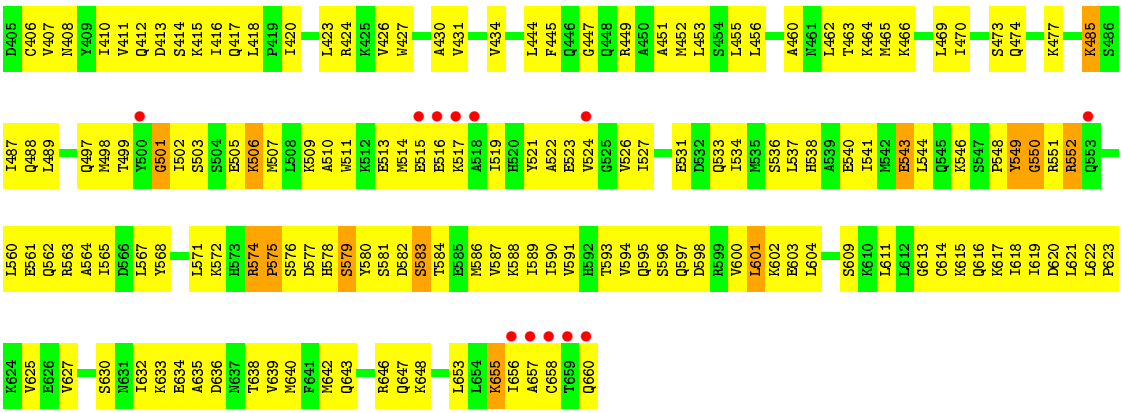
Chain B:



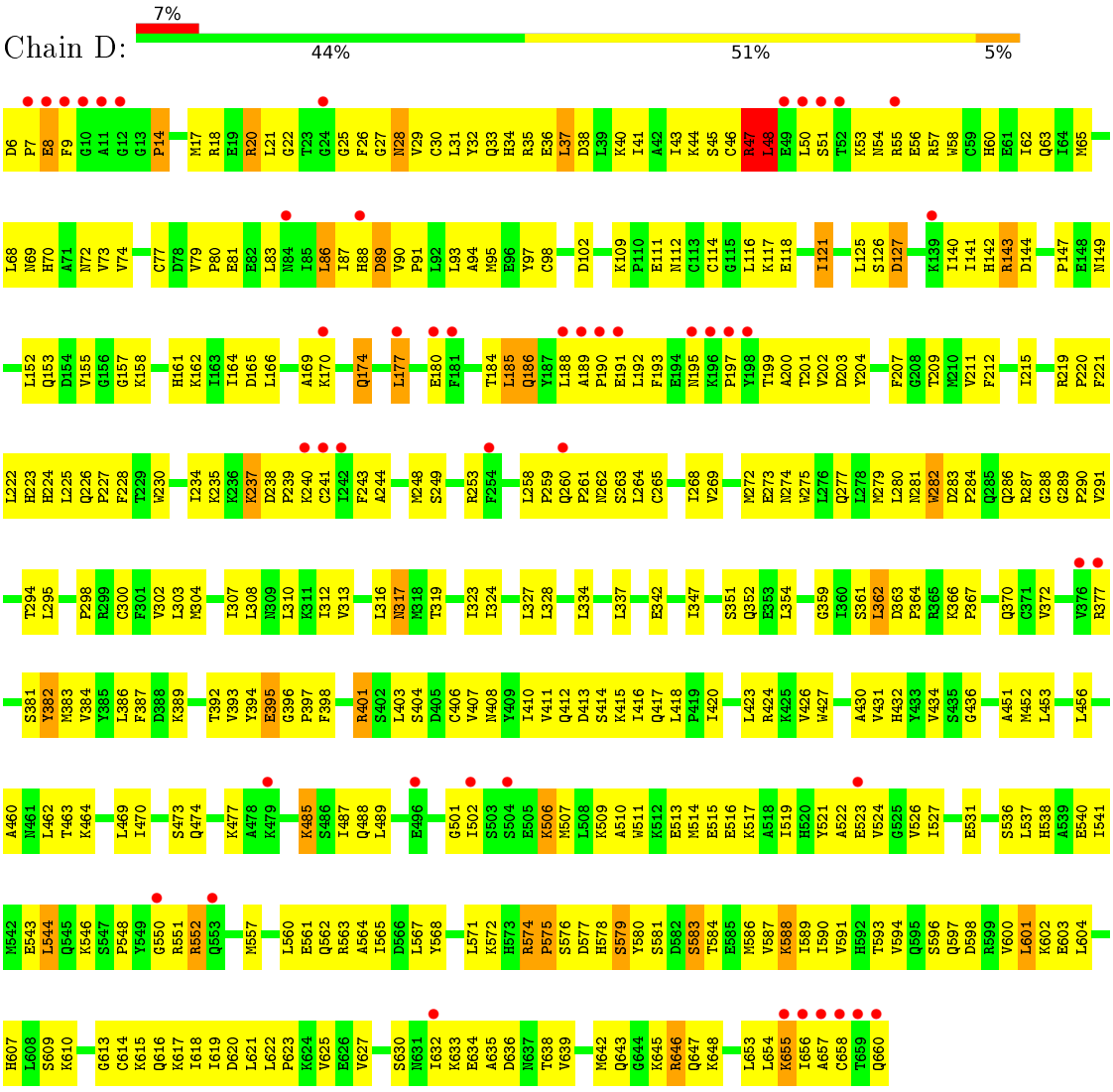
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain C:

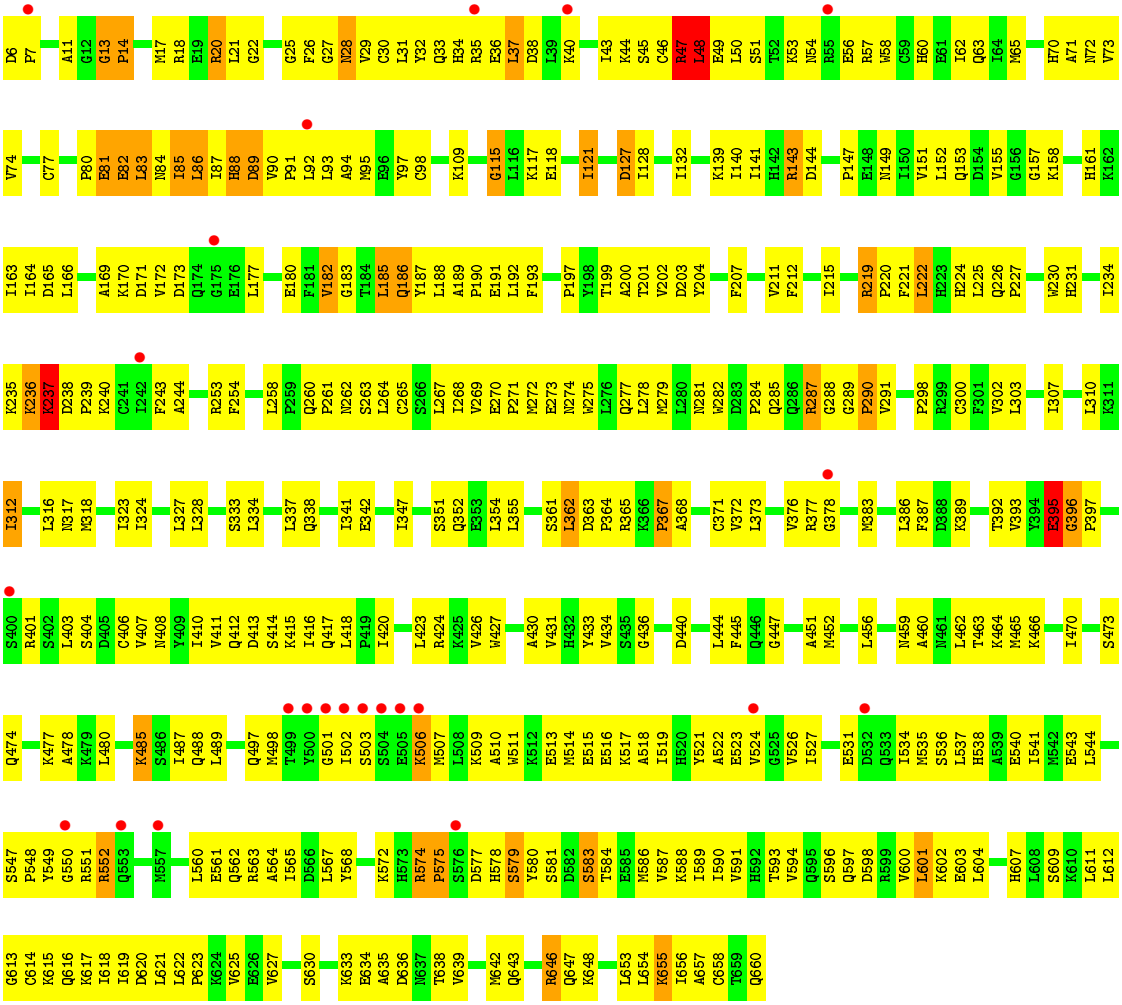




• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

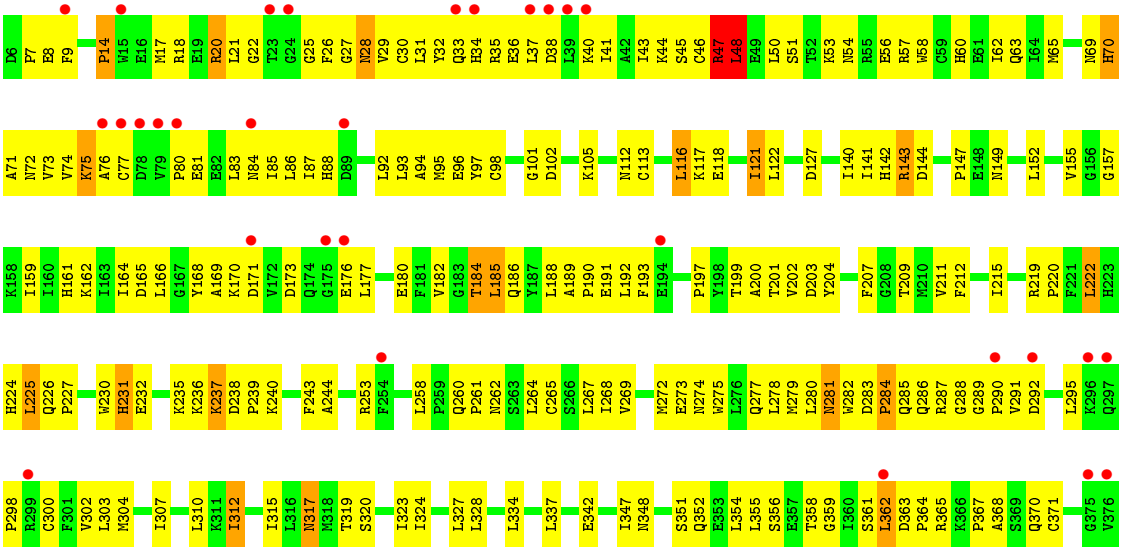


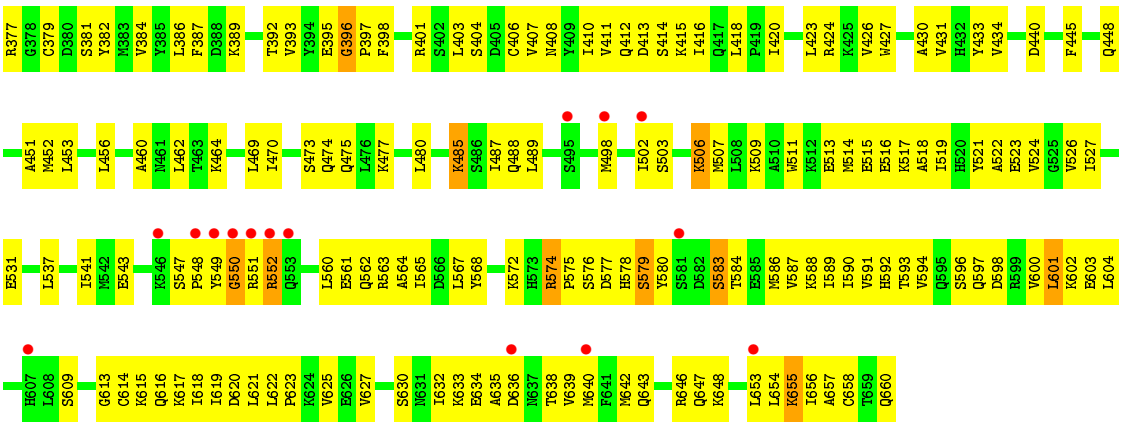
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha



• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

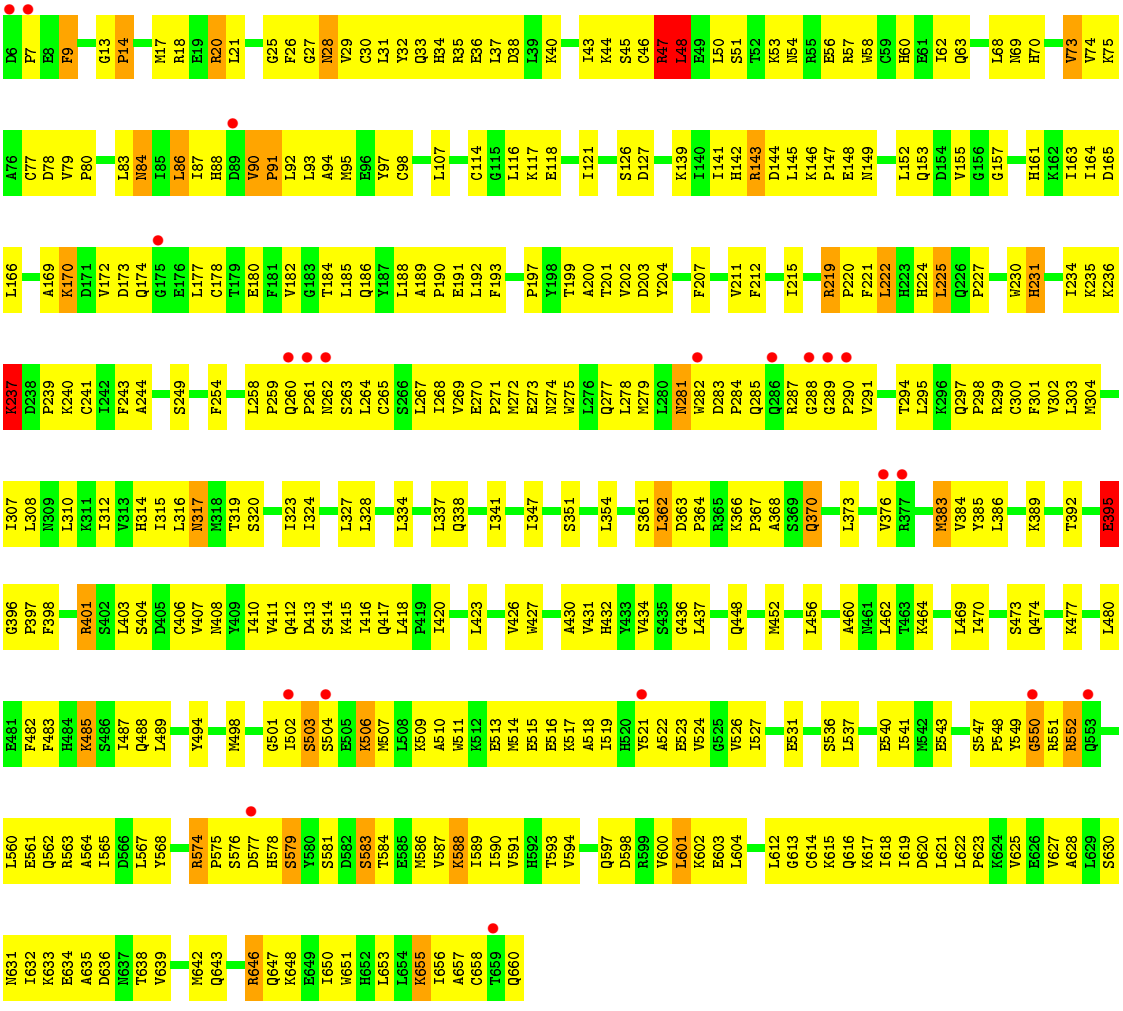
Chain F:





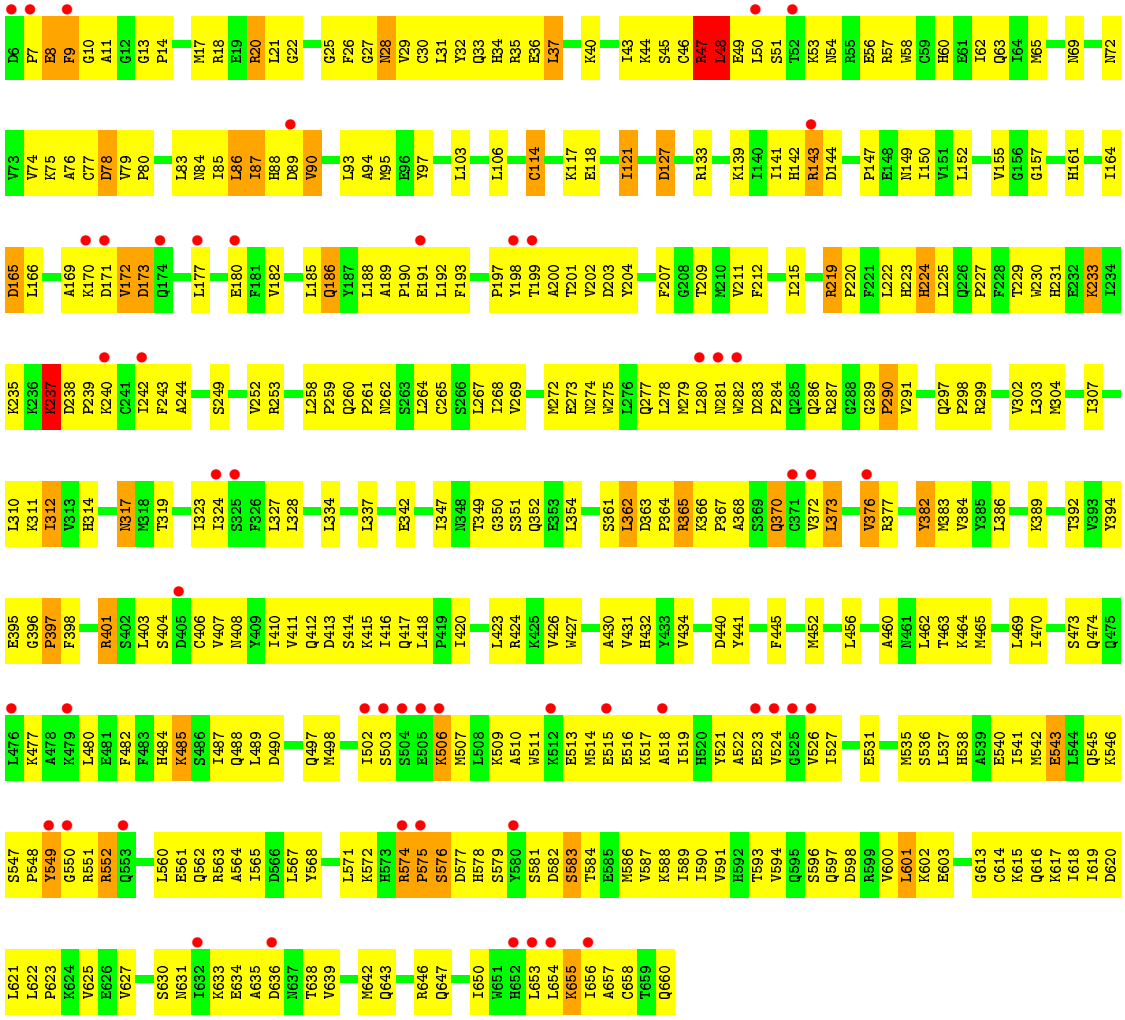
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain G:



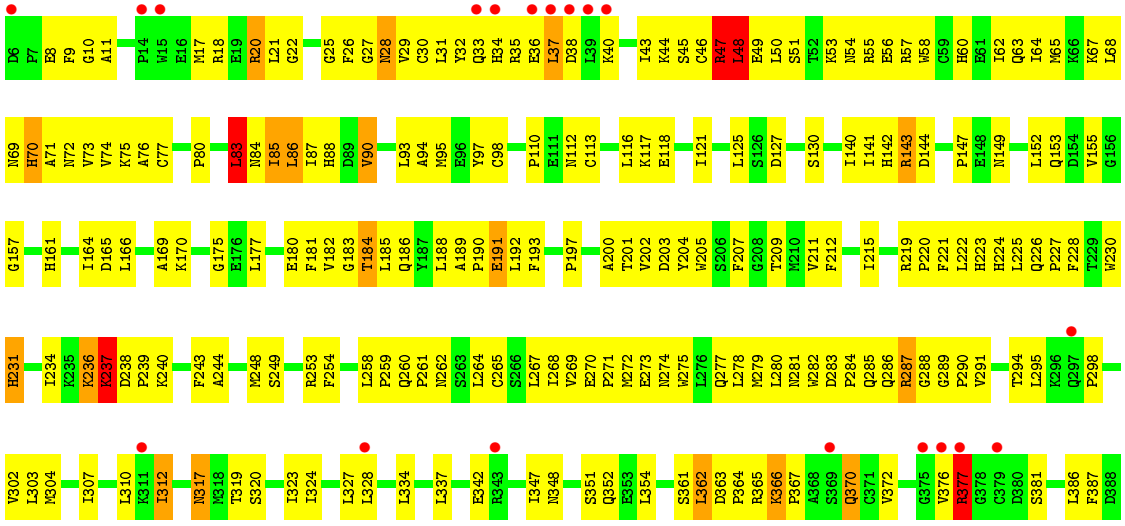
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

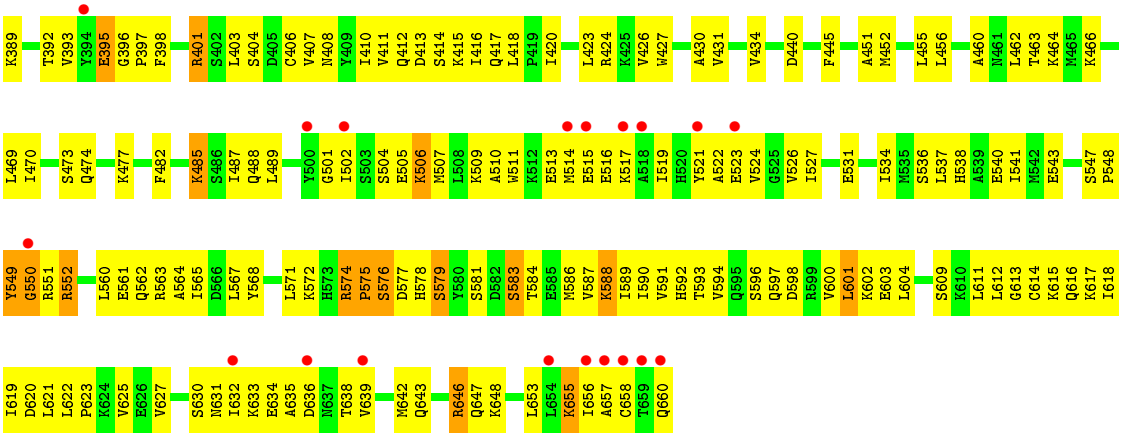
Chain H:



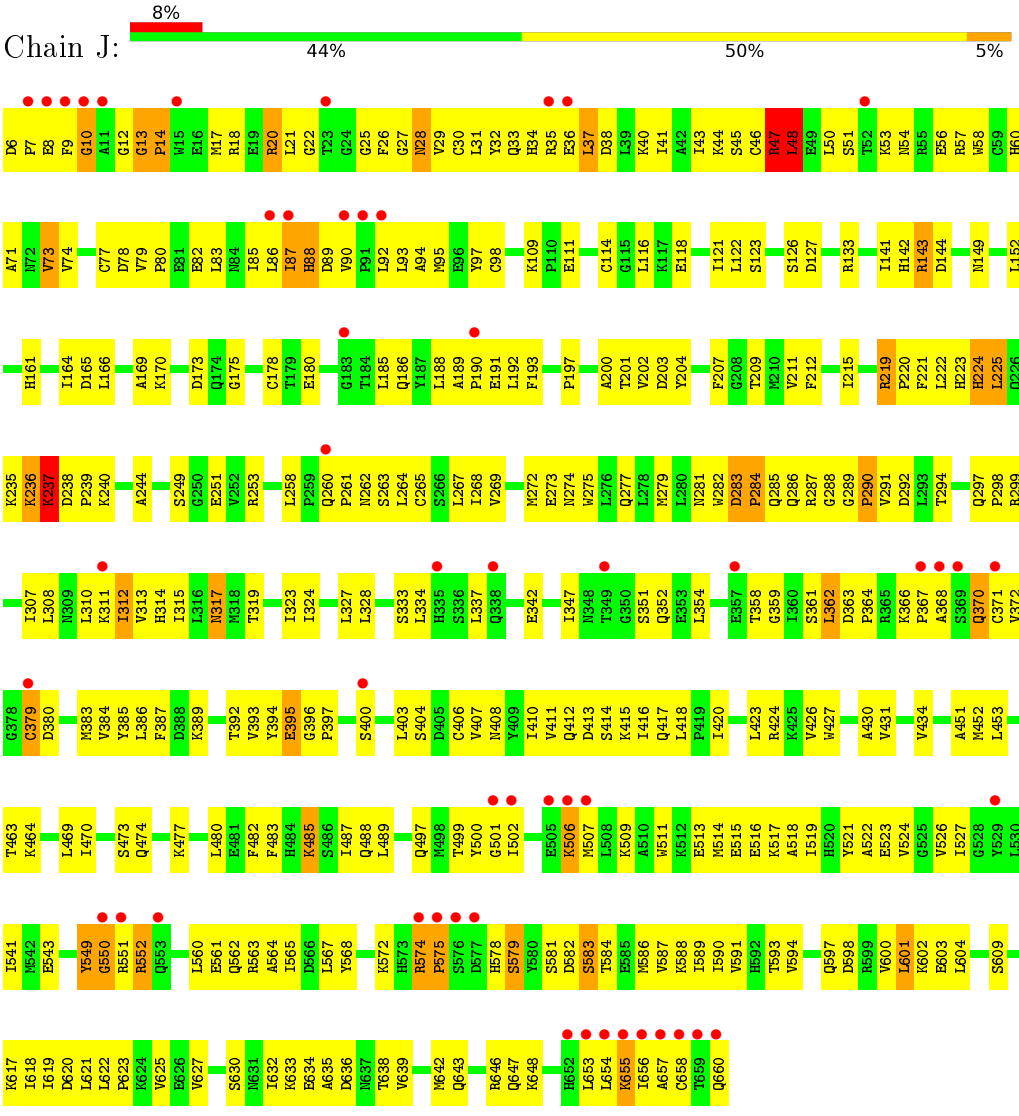
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain I:

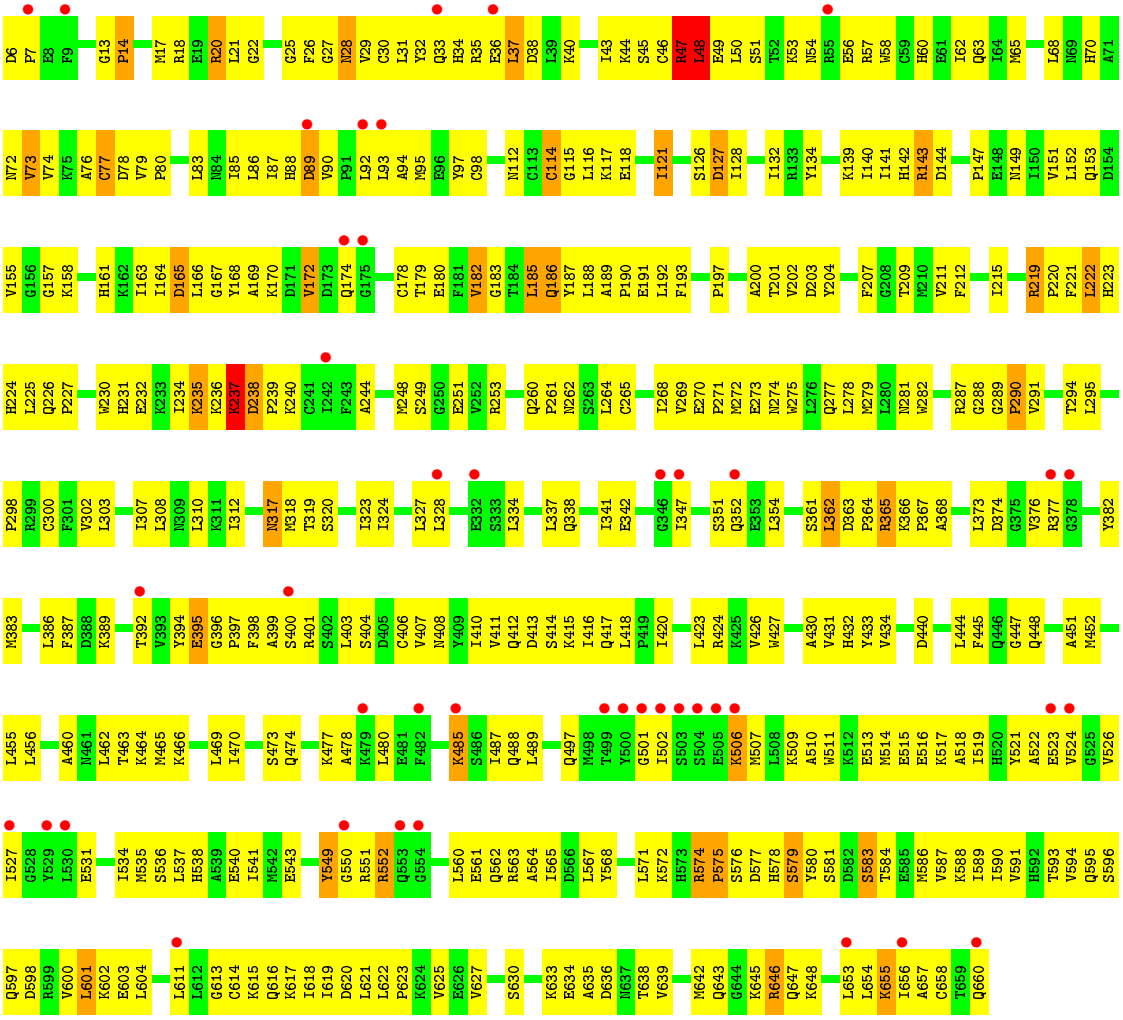




• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

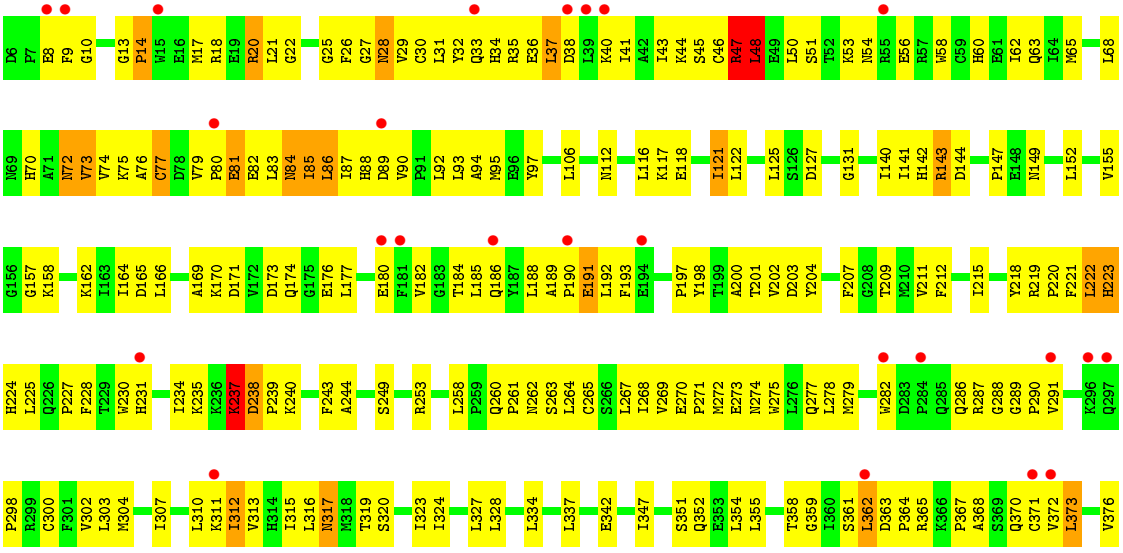


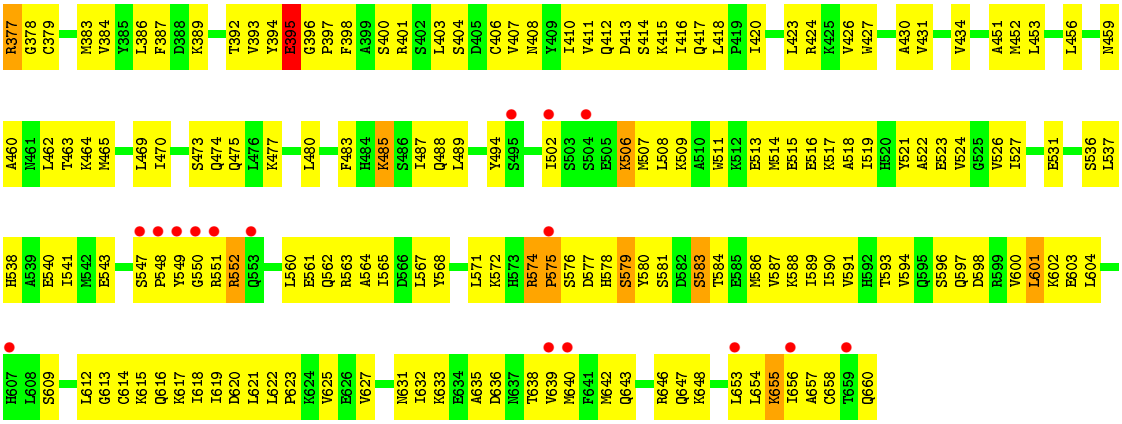
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha



• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

Chain L:




R377 G378 C379 M383 V384 Y385 L386 F387 D388 K389 T392 V393 Y394 E395 G396 P397 F398 A399 S400 R401 S402 L403 S404 D405 C406 V407 N408 Y409 I410 V411 Q412 D413 S414 K415 I416 Q417 L418 P419 I420 L423 R424 K425 V426 W427 A430 V431 V434 A451 M452 L453 L456 N459
A460 N461 L462 T463 K464 M465 L469 I470 S473 Q474 Q475 L476 K477 L480 F483 H484 K485 S486 I487 Q488 L489 Y494 S495 I502 S503 S504 E505 K506 M507 L508 K509 A510 W511 K512 E513 M514 E515 E516 K517 A518 I519 H520 Y521 A522 E523 V524 G525 V526 I527 E531 S536 L537
H538 A539 E540 I541 M542 E543 S547 P548 Y549 G550 R551 R552 Q553 L560 E561 Q562 R563 A564 I565 D566 L567 Y568 L571 K572 H573 R574 P575 S576 D577 H578 S579 Y580 S581 D582 S583 T584 E585 M586 V587 K588 I589 I590 V591 H592 T593 V594 Q595 S596 Q597 D598 R599 V600 L601 K602 E603 L604
H607 L608 S609 L612 G613 C614 K615 Q616 K617 I618 I619 D620 L621 L622 P623 K624 V625 E626 V627 N631 I632 K633 E634 A635 D636 N637 T638 V639 M640 F641 W642 Q643 R646 Q647 K648 L653 L654 K655 I656 A657 C658 I659 Q660

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	174.51Å 186.94Å 275.83Å 90.00° 98.84° 90.00°	Depositor
Resolution (Å)	29.94 – 4.50 44.79 – 4.44	Depositor EDS
% Data completeness (in resolution range)	68.1 (29.94-4.50) 80.6 (44.79-4.44)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 4.45Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.238 , 0.276 0.241 , 0.275	Depositor DCC
R_{free} test set	3450 reflections (4.02%)	DCC
Wilson B-factor (Å^2)	178.9	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 311.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	65132	wwPDB-VP
Average B, all atoms (Å^2)	267.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.78 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.5998e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Z4K, PDX, 5TJ, 5LS, 5TH, GLC, 5TL, 5TM, 5TK

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	0.29	0/5370	0.43	0/7239
1	B	0.27	0/5370	0.42	0/7239
1	C	0.27	0/5370	0.43	0/7239
1	D	0.27	0/5370	0.43	0/7239
1	E	0.28	0/5370	0.43	0/7239
1	F	0.27	0/5370	0.43	0/7239
1	G	0.31	0/5370	0.44	0/7239
1	H	0.27	0/5370	0.42	0/7239
1	I	0.27	0/5370	0.43	0/7239
1	J	0.27	0/5370	0.43	0/7239
1	K	0.28	0/5370	0.43	0/7239
1	L	0.26	0/5370	0.42	0/7239
All	All	0.28	0/64440	0.43	0/86868

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5263	0	5320	348	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5263	0	5320	349	0
1	C	5263	0	5320	334	0
1	D	5263	0	5320	341	0
1	E	5263	0	5320	343	0
1	F	5263	0	5320	325	0
1	G	5263	0	5320	362	0
1	H	5263	0	5320	325	0
1	I	5263	0	5320	326	0
1	J	5263	0	5320	325	0
1	K	5263	0	5320	344	0
1	L	5263	0	5320	346	0
2	A	26	0	0	3	0
2	B	26	0	0	2	0
2	C	26	0	0	4	0
2	D	26	0	0	2	0
2	E	26	0	0	3	0
2	F	26	0	0	6	0
2	G	26	0	0	5	0
2	H	26	0	0	2	0
2	I	26	0	0	6	0
2	J	26	0	0	2	0
2	K	26	0	0	3	0
2	L	26	0	0	2	0
3	A	40	0	0	1	0
3	B	40	0	0	2	0
3	C	40	0	0	1	0
3	D	80	0	0	1	0
3	E	40	0	0	0	0
3	F	40	0	0	0	0
3	G	40	0	0	0	0
3	H	60	0	0	1	0
3	I	40	0	0	0	0
3	J	40	0	0	2	0
3	K	40	0	0	0	0
3	L	60	0	0	0	0
4	A	22	0	18	1	0
4	B	22	0	18	3	0
4	C	22	0	18	3	0
4	D	22	0	18	0	0
4	E	22	0	18	3	0
4	F	22	0	18	2	0
4	G	22	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	22	0	18	1	0
4	I	22	0	18	4	0
4	J	22	0	18	7	0
4	K	22	0	18	0	0
4	L	22	0	18	4	0
5	A	38	0	20	0	0
5	B	38	0	20	2	0
5	C	38	0	20	1	0
5	D	38	0	20	0	0
5	E	38	0	20	0	0
5	F	38	0	20	0	0
5	G	38	0	20	0	0
5	H	19	0	10	0	0
5	I	38	0	20	0	0
5	J	38	0	20	4	0
5	K	38	0	20	1	0
5	L	57	0	30	2	0
6	A	34	0	0	0	0
6	D	34	0	0	1	0
6	H	34	0	0	0	0
6	I	34	0	0	0	0
7	A	13	0	0	0	0
7	C	13	0	0	1	0
7	G	13	0	0	0	0
7	I	13	0	0	0	0
8	A	17	0	0	0	0
8	C	17	0	0	1	0
8	G	17	0	0	0	0
8	I	17	0	0	0	0
9	B	17	0	0	0	0
9	C	17	0	0	1	0
9	G	17	0	0	0	0
9	J	17	0	0	0	0
10	B	15	0	0	0	0
10	C	15	0	0	2	0
10	H	15	0	0	0	0
10	J	15	0	0	0	0
All	All	65132	0	64296	3919	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 30.

The worst 5 of 3919 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)
2:J:701:5TL:CAS	2:J:701:5TL:NAY	1.99	1.20
2:G:701:5TL:NAY	2:G:701:5TL:CAS	2.00	1.18
2:D:701:5TL:CAS	2:D:701:5TL:NAY	1.99	1.17
2:K:701:5TL:CAS	2:K:701:5TL:NAY	2.00	1.17
2:A:701:5TL:NAY	2:A:701:5TL:CAS	2.00	1.16

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	653/655 (100%)	504 (77%)	113 (17%)	36 (6%)	2 29
1	B	653/655 (100%)	514 (79%)	106 (16%)	33 (5%)	2 31
1	C	653/655 (100%)	511 (78%)	105 (16%)	37 (6%)	2 28
1	D	653/655 (100%)	515 (79%)	104 (16%)	34 (5%)	2 30
1	E	653/655 (100%)	511 (78%)	104 (16%)	38 (6%)	2 28
1	F	653/655 (100%)	505 (77%)	111 (17%)	37 (6%)	2 28
1	G	653/655 (100%)	508 (78%)	114 (18%)	31 (5%)	3 32
1	H	653/655 (100%)	507 (78%)	99 (15%)	47 (7%)	1 22
1	I	653/655 (100%)	502 (77%)	110 (17%)	41 (6%)	2 26
1	J	653/655 (100%)	515 (79%)	98 (15%)	40 (6%)	2 27
1	K	653/655 (100%)	506 (78%)	105 (16%)	42 (6%)	2 26
1	L	653/655 (100%)	500 (77%)	113 (17%)	40 (6%)	2 27
All	All	7836/7860 (100%)	6098 (78%)	1282 (16%)	456 (6%)	2 28

5 of 456 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU

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Mol	Chain	Res	Type
1	A	521	TYR
1	A	549	TYR
1	B	48	LEU
1	B	173	ASP

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	589/589 (100%)	557 (95%)	32 (5%)	27	66
1	B	589/589 (100%)	557 (95%)	32 (5%)	27	66
1	C	589/589 (100%)	563 (96%)	26 (4%)	35	71
1	D	589/589 (100%)	567 (96%)	22 (4%)	41	75
1	E	589/589 (100%)	559 (95%)	30 (5%)	29	67
1	F	589/589 (100%)	561 (95%)	28 (5%)	31	69
1	G	589/589 (100%)	555 (94%)	34 (6%)	25	64
1	H	589/589 (100%)	559 (95%)	30 (5%)	29	67
1	I	589/589 (100%)	561 (95%)	28 (5%)	31	69
1	J	589/589 (100%)	560 (95%)	29 (5%)	31	68
1	K	589/589 (100%)	559 (95%)	30 (5%)	29	67
1	L	589/589 (100%)	557 (95%)	32 (5%)	27	66
All	All	7068/7068 (100%)	6715 (95%)	353 (5%)	30	68

5 of 353 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	281	ASN
1	G	506	LYS
1	L	72	ASN
1	F	543	GLU
1	G	170	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 276 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	317	ASN
1	G	475	GLN
1	L	72	ASN
1	F	459	ASN
1	G	112	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

112 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	$\#\|Z\| > 2$
2	5TL	A	701	-	28,28,28	2.68	11 (39%)	36,41,41	5.12	20 (55%)
3	5LS	A	702	4	19,20,20	1.09	0	26,31,31	1.04	2 (7%)
4	GLC	A	703	3,5	11,11,12	0.56	0	15,15,17	0.43	0
5	PDX	A	704	4	19,19,20	1.39	2 (10%)	24,29,31	0.80	1 (4%)
3	5LS	A	705	4	19,20,20	1.11	0	26,31,31	1.03	2 (7%)
4	GLC	A	706	3,5	11,11,12	0.85	0	15,15,17	1.15	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	PDX	A	707	4	19,19,20	1.35	2 (10%)	24,29,31	0.83	1 (4%)
6	5TJ	A	708	9,3	14,17,18	1.01	0	19,24,26	0.92	1 (5%)
6	5TJ	A	709	9,10	14,17,18	1.02	0	19,24,26	0.83	1 (5%)
7	5TK	A	710	10,8	10,13,14	0.56	0	13,17,19	0.40	0
8	5TH	A	711	7	14,17,18	1.41	2 (14%)	17,24,26	0.50	0
2	5TL	B	701	-	28,28,28	2.72	11 (39%)	36,41,41	5.06	21 (58%)
4	GLC	B	702	3,5	11,11,12	0.65	0	15,15,17	0.45	0
5	PDX	B	703	4	19,19,20	1.30	2 (10%)	24,29,31	0.62	0
3	5LS	B	704	4	19,20,20	1.14	0	26,31,31	1.06	2 (7%)
4	GLC	B	705	3,5	11,11,12	0.55	0	15,15,17	0.42	0
5	PDX	B	706	4	19,19,20	1.41	2 (10%)	24,29,31	0.91	2 (8%)
3	5LS	B	707	6	19,20,20	1.08	0	26,31,31	1.06	2 (7%)
9	5TM	B	708	6	14,17,18	1.22	1 (7%)	17,24,26	0.53	0
10	Z4K	B	709	7,6	15,15,16	1.21	1 (6%)	19,22,24	0.55	0
2	5TL	C	701	-	28,28,28	2.67	11 (39%)	36,41,41	5.15	20 (55%)
3	5LS	C	702	4	19,20,20	1.06	0	26,31,31	1.02	2 (7%)
4	GLC	C	703	3,5	11,11,12	0.52	0	15,15,17	0.37	0
5	PDX	C	704	4	19,19,20	1.41	2 (10%)	24,29,31	0.80	1 (4%)
3	5LS	C	705	4	19,20,20	1.03	0	26,31,31	0.96	1 (3%)
4	GLC	C	706	3,5	11,11,12	0.45	0	15,15,17	0.38	0
5	PDX	C	707	4	19,19,20	1.41	2 (10%)	24,29,31	0.82	1 (4%)
9	5TM	C	708	6	14,17,18	1.18	1 (7%)	17,24,26	0.63	0
10	Z4K	C	709	7,6	15,15,16	1.15	1 (6%)	19,22,24	0.54	0
7	5TK	C	710	10,8	10,13,14	0.62	0	13,17,19	0.56	0
8	5TH	C	711	7	14,17,18	1.43	2 (14%)	17,24,26	0.63	0
2	5TL	D	701	-	28,28,28	2.71	10 (35%)	36,41,41	5.18	20 (55%)
3	5LS	D	702	4	19,20,20	1.08	0	26,31,31	1.03	2 (7%)
4	GLC	D	703	3,5	11,11,12	0.54	0	15,15,17	0.39	0
5	PDX	D	704	4	19,19,20	1.38	2 (10%)	24,29,31	0.79	1 (4%)
3	5LS	D	705	4	19,20,20	1.10	0	26,31,31	1.06	2 (7%)
4	GLC	D	706	3,5	11,11,12	0.58	0	15,15,17	0.52	0
5	PDX	D	707	4	19,19,20	1.37	2 (10%)	24,29,31	0.80	1 (4%)
3	5LS	D	708	4	19,20,20	1.11	0	26,31,31	1.06	2 (7%)
3	5LS	D	709	6	19,20,20	1.10	0	26,31,31	1.04	2 (7%)
6	5TJ	D	710	9,3	14,17,18	0.99	0	19,24,26	0.86	1 (5%)
6	5TJ	D	711	9,10	14,17,18	0.98	0	19,24,26	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	5TL	E	701	-	28,28,28	2.66	10 (35%)	36,41,41	5.11	18 (50%)
3	5LS	E	702	4	19,20,20	1.11	0	26,31,31	1.04	3 (11%)
4	GLC	E	703	3,5	11,11,12	0.64	0	15,15,17	0.71	1 (6%)
5	PDX	E	704	4	19,19,20	1.41	2 (10%)	24,29,31	0.80	1 (4%)
3	5LS	E	705	4	19,20,20	1.10	0	26,31,31	1.06	2 (7%)
4	GLC	E	706	3,5	11,11,12	0.58	0	15,15,17	0.59	0
5	PDX	E	707	4	19,19,20	1.38	2 (10%)	24,29,31	0.78	1 (4%)
2	5TL	F	701	-	28,28,28	2.71	10 (35%)	36,41,41	5.09	21 (58%)
3	5LS	F	702	4	19,20,20	1.11	0	26,31,31	1.06	2 (7%)
4	GLC	F	703	3,5	11,11,12	0.59	0	15,15,17	0.56	0
5	PDX	F	704	4	19,19,20	1.47	2 (10%)	24,29,31	1.00	2 (8%)
3	5LS	F	705	4	19,20,20	1.10	0	26,31,31	1.05	2 (7%)
4	GLC	F	706	3,5	11,11,12	0.67	0	15,15,17	0.52	0
5	PDX	F	707	4	19,19,20	1.38	2 (10%)	24,29,31	0.83	1 (4%)
2	5TL	G	701	-	28,28,28	2.67	11 (39%)	36,41,41	5.17	21 (58%)
3	5LS	G	702	4	19,20,20	1.10	0	26,31,31	1.05	2 (7%)
4	GLC	G	703	3,5	11,11,12	0.56	0	15,15,17	0.34	0
5	PDX	G	704	4	19,19,20	1.39	2 (10%)	24,29,31	0.85	1 (4%)
3	5LS	G	705	4	19,20,20	1.09	0	26,31,31	1.06	2 (7%)
4	GLC	G	706	3,5	11,11,12	0.54	0	15,15,17	0.50	0
5	PDX	G	707	4	19,19,20	1.36	2 (10%)	24,29,31	0.83	1 (4%)
9	5TM	G	708	6	14,17,18	1.28	2 (14%)	17,24,26	0.54	0
7	5TK	G	709	10,8	10,13,14	0.62	0	13,17,19	0.39	0
8	5TH	G	710	7	14,17,18	1.30	2 (14%)	17,24,26	0.55	0
2	5TL	H	701	-	28,28,28	2.71	11 (39%)	36,41,41	5.08	21 (58%)
3	5LS	H	702	4	19,20,20	1.09	0	26,31,31	1.05	2 (7%)
4	GLC	H	703	3,5	11,11,12	0.79	0	15,15,17	0.51	0
5	PDX	H	704	4	19,19,20	1.42	2 (10%)	24,29,31	0.84	1 (4%)
3	5LS	H	705	4	19,20,20	1.10	0	26,31,31	1.05	2 (7%)
4	GLC	H	706	3,5	11,11,12	0.66	0	15,15,17	0.44	0
3	5LS	H	707	6	19,20,20	1.07	0	26,31,31	1.02	2 (7%)
6	5TJ	H	708	9,3	14,17,18	1.00	0	19,24,26	0.83	1 (5%)
6	5TJ	H	709	9,10	14,17,18	1.03	0	19,24,26	0.89	1 (5%)
10	Z4K	H	710	7,6	15,15,16	1.19	1 (6%)	19,22,24	0.66	0
2	5TL	I	701	-	28,28,28	2.69	10 (35%)	36,41,41	5.09	20 (55%)
3	5LS	I	702	4	19,20,20	1.12	0	26,31,31	1.10	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GLC	I	703	3,5	11,11,12	0.65	0	15,15,17	0.60	0
5	PDX	I	704	4	19,19,20	1.42	2 (10%)	24,29,31	0.90	2 (8%)
3	5LS	I	705	4	19,20,20	1.09	0	26,31,31	1.05	2 (7%)
4	GLC	I	706	3,5	11,11,12	0.57	0	15,15,17	0.56	0
5	PDX	I	707	4	19,19,20	1.37	2 (10%)	24,29,31	0.83	1 (4%)
6	5TJ	I	708	9,3	14,17,18	1.01	0	19,24,26	0.92	1 (5%)
6	5TJ	I	709	9,10	14,17,18	1.00	0	19,24,26	0.93	1 (5%)
7	5TK	I	710	10,8	10,13,14	0.52	0	13,17,19	0.36	0
8	5TH	I	711	7	14,17,18	1.37	2 (14%)	17,24,26	0.57	0
2	5TL	J	701	-	28,28,28	2.71	11 (39%)	36,41,41	5.21	20 (55%)
4	GLC	J	702	3,5	11,11,12	0.81	0	15,15,17	1.24	1 (6%)
5	PDX	J	703	4	19,19,20	1.39	2 (10%)	24,29,31	0.79	1 (4%)
3	5LS	J	704	4	19,20,20	1.10	0	26,31,31	1.10	2 (7%)
4	GLC	J	705	3,5	11,11,12	0.89	0	15,15,17	1.15	2 (13%)
5	PDX	J	706	4	19,19,20	1.43	2 (10%)	24,29,31	1.05	2 (8%)
3	5LS	J	707	6	19,20,20	1.10	0	26,31,31	1.06	2 (7%)
9	5TM	J	708	6	14,17,18	1.24	1 (7%)	17,24,26	0.60	0
10	Z4K	J	709	7,6	15,15,16	1.24	1 (6%)	19,22,24	0.55	0
2	5TL	K	701	-	28,28,28	2.63	10 (35%)	36,41,41	5.24	20 (55%)
3	5LS	K	702	4	19,20,20	1.09	0	26,31,31	1.02	2 (7%)
4	GLC	K	703	3,5	11,11,12	0.58	0	15,15,17	0.32	0
5	PDX	K	704	4	19,19,20	1.42	2 (10%)	24,29,31	0.84	1 (4%)
3	5LS	K	705	4	19,20,20	1.04	0	26,31,31	0.94	1 (3%)
4	GLC	K	706	3,5	11,11,12	0.52	0	15,15,17	0.51	0
5	PDX	K	707	4	19,19,20	1.39	2 (10%)	24,29,31	0.82	1 (4%)
2	5TL	L	701	-	28,28,28	2.71	11 (39%)	36,41,41	5.12	19 (52%)
3	5LS	L	702	4	19,20,20	1.08	0	26,31,31	1.06	2 (7%)
5	PDX	L	703	4	19,19,20	1.52	2 (10%)	24,29,31	1.02	2 (8%)
3	5LS	L	704	4	19,20,20	1.08	0	26,31,31	1.03	2 (7%)
4	GLC	L	705	3,5	11,11,12	0.60	0	15,15,17	0.51	0
5	PDX	L	706	4	19,19,20	1.46	2 (10%)	24,29,31	1.03	2 (8%)
3	5LS	L	707	4	19,20,20	1.01	0	26,31,31	1.45	2 (7%)
4	GLC	L	708	3,5	11,11,12	0.56	0	15,15,17	0.47	0
5	PDX	L	709	4	19,19,20	1.40	2 (10%)	24,29,31	0.82	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5TL	A	701	-	-	0/18/18/18	0/3/3/3
3	5LS	A	702	4	-	0/12/32/32	0/1/1/1
4	GLC	A	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	A	704	4	-	0/12/29/32	0/1/1/1
3	5LS	A	705	4	-	0/12/32/32	0/1/1/1
4	GLC	A	706	3,5	-	0/2/19/22	0/1/1/1
5	PDX	A	707	4	-	0/12/29/32	0/1/1/1
6	5TJ	A	708	9,3	-	0/9/27/30	0/1/1/1
6	5TJ	A	709	9,10	-	0/9/27/30	0/1/1/1
7	5TK	A	710	10,8	-	0/4/22/25	0/1/1/1
8	5TH	A	711	7	-	0/9/27/30	0/1/1/1
2	5TL	B	701	-	-	0/18/18/18	0/3/3/3
4	GLC	B	702	3,5	-	0/2/19/22	0/1/1/1
5	PDX	B	703	4	-	0/12/29/32	0/1/1/1
3	5LS	B	704	4	-	0/12/32/32	0/1/1/1
4	GLC	B	705	3,5	-	0/2/19/22	0/1/1/1
5	PDX	B	706	4	-	0/12/29/32	0/1/1/1
3	5LS	B	707	6	-	0/12/32/32	0/1/1/1
9	5TM	B	708	6	-	0/9/27/30	0/1/1/1
10	Z4K	B	709	7,6	-	0/7/24/27	0/1/1/1
2	5TL	C	701	-	-	0/18/18/18	0/3/3/3
3	5LS	C	702	4	-	0/12/32/32	0/1/1/1
4	GLC	C	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	C	704	4	-	0/12/29/32	0/1/1/1
3	5LS	C	705	4	-	0/12/32/32	0/1/1/1
4	GLC	C	706	3,5	-	0/2/19/22	0/1/1/1
5	PDX	C	707	4	-	0/12/29/32	0/1/1/1
9	5TM	C	708	6	-	0/9/27/30	0/1/1/1
10	Z4K	C	709	7,6	-	0/7/24/27	0/1/1/1
7	5TK	C	710	10,8	-	0/4/22/25	0/1/1/1
8	5TH	C	711	7	-	0/9/27/30	0/1/1/1
2	5TL	D	701	-	-	0/18/18/18	0/3/3/3
3	5LS	D	702	4	-	0/12/32/32	0/1/1/1
4	GLC	D	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	D	704	4	-	0/12/29/32	0/1/1/1
3	5LS	D	705	4	-	0/12/32/32	0/1/1/1
4	GLC	D	706	3,5	-	0/2/19/22	0/1/1/1
5	PDX	D	707	4	-	0/12/29/32	0/1/1/1
3	5LS	D	708	4	-	0/12/32/32	0/1/1/1
3	5LS	D	709	6	-	0/12/32/32	0/1/1/1
6	5TJ	D	710	9,3	-	0/9/27/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	5TJ	D	711	9,10	-	0/9/27/30	0/1/1/1
2	5TL	E	701	-	-	0/18/18/18	0/3/3/3
3	5LS	E	702	4	-	0/12/32/32	0/1/1/1
4	GLC	E	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	E	704	4	-	0/12/29/32	0/1/1/1
3	5LS	E	705	4	-	0/12/32/32	0/1/1/1
4	GLC	E	706	3,5	-	0/2/19/22	0/1/1/1
5	PDX	E	707	4	-	0/12/29/32	0/1/1/1
2	5TL	F	701	-	-	0/18/18/18	0/3/3/3
3	5LS	F	702	4	-	0/12/32/32	0/1/1/1
4	GLC	F	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	F	704	4	-	0/12/29/32	0/1/1/1
3	5LS	F	705	4	-	0/12/32/32	0/1/1/1
4	GLC	F	706	3,5	-	0/2/19/22	0/1/1/1
5	PDX	F	707	4	-	0/12/29/32	0/1/1/1
2	5TL	G	701	-	-	0/18/18/18	0/3/3/3
3	5LS	G	702	4	-	0/12/32/32	0/1/1/1
4	GLC	G	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	G	704	4	-	0/12/29/32	0/1/1/1
3	5LS	G	705	4	-	0/12/32/32	0/1/1/1
4	GLC	G	706	3,5	-	0/2/19/22	0/1/1/1
5	PDX	G	707	4	-	0/12/29/32	0/1/1/1
9	5TM	G	708	6	-	0/9/27/30	0/1/1/1
7	5TK	G	709	10,8	-	0/4/22/25	0/1/1/1
8	5TH	G	710	7	-	0/9/27/30	0/1/1/1
2	5TL	H	701	-	-	0/18/18/18	0/3/3/3
3	5LS	H	702	4	-	0/12/32/32	0/1/1/1
4	GLC	H	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	H	704	4	-	0/12/29/32	0/1/1/1
3	5LS	H	705	4	-	0/12/32/32	0/1/1/1
4	GLC	H	706	3,5	-	0/2/19/22	0/1/1/1
3	5LS	H	707	6	-	0/12/32/32	0/1/1/1
6	5TJ	H	708	9,3	-	0/9/27/30	0/1/1/1
6	5TJ	H	709	9,10	-	0/9/27/30	0/1/1/1
10	Z4K	H	710	7,6	-	0/7/24/27	0/1/1/1
2	5TL	I	701	-	-	0/18/18/18	0/3/3/3
3	5LS	I	702	4	-	0/12/32/32	0/1/1/1
4	GLC	I	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	I	704	4	-	0/12/29/32	0/1/1/1
3	5LS	I	705	4	-	0/12/32/32	0/1/1/1
4	GLC	I	706	3,5	-	0/2/19/22	0/1/1/1
5	PDX	I	707	4	-	0/12/29/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	5TJ	I	708	9,3	-	0/9/27/30	0/1/1/1
6	5TJ	I	709	9,10	-	0/9/27/30	0/1/1/1
7	5TK	I	710	10,8	-	0/4/22/25	0/1/1/1
8	5TH	I	711	7	-	0/9/27/30	0/1/1/1
2	5TL	J	701	-	-	0/18/18/18	0/3/3/3
4	GLC	J	702	3,5	-	0/2/19/22	0/1/1/1
5	PDX	J	703	4	-	0/12/29/32	0/1/1/1
3	5LS	J	704	4	-	0/12/32/32	0/1/1/1
4	GLC	J	705	3,5	-	0/2/19/22	0/1/1/1
5	PDX	J	706	4	-	0/12/29/32	0/1/1/1
3	5LS	J	707	6	-	0/12/32/32	0/1/1/1
9	5TM	J	708	6	-	0/9/27/30	0/1/1/1
10	Z4K	J	709	7,6	-	0/7/24/27	0/1/1/1
2	5TL	K	701	-	-	0/18/18/18	0/3/3/3
3	5LS	K	702	4	-	0/12/32/32	0/1/1/1
4	GLC	K	703	3,5	-	0/2/19/22	0/1/1/1
5	PDX	K	704	4	-	0/12/29/32	0/1/1/1
3	5LS	K	705	4	-	0/12/32/32	0/1/1/1
4	GLC	K	706	3,5	-	0/2/19/22	0/1/1/1
5	PDX	K	707	4	-	0/12/29/32	0/1/1/1
2	5TL	L	701	-	-	0/18/18/18	0/3/3/3
3	5LS	L	702	4	-	0/12/32/32	0/1/1/1
5	PDX	L	703	4	-	0/12/29/32	0/1/1/1
3	5LS	L	704	4	-	0/12/32/32	0/1/1/1
4	GLC	L	705	3,5	-	0/2/19/22	0/1/1/1
5	PDX	L	706	4	-	0/12/29/32	0/1/1/1
3	5LS	L	707	4	-	0/12/32/32	0/1/1/1
4	GLC	L	708	3,5	-	0/2/19/22	0/1/1/1
5	PDX	L	709	4	-	0/12/29/32	0/1/1/1

The worst 5 of 192 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	701	5TL	S-N1	-7.07	1.48	1.60
2	H	701	5TL	S-N1	-7.02	1.48	1.60
2	F	701	5TL	S-N1	-6.99	1.48	1.60
2	B	701	5TL	S-N1	-6.92	1.48	1.60
2	L	701	5TL	S-N1	-6.82	1.48	1.60

The worst 5 of 338 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	701	5TL	CAT-CAS-CAL	-13.49	102.19	121.15
2	J	701	5TL	CAT-CAS-CAL	-13.45	102.24	121.15
2	L	701	5TL	CAT-CAS-CAL	-13.42	102.29	121.15
2	A	701	5TL	CAT-CAS-CAL	-13.38	102.34	121.15
2	C	701	5TL	CAT-CAS-CAL	-13.34	102.40	121.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

43 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	5TL	3	0
3	A	705	5LS	1	0
4	A	706	GLC	1	0
2	B	701	5TL	2	0
5	B	703	PDX	1	0
4	B	705	GLC	3	0
5	B	706	PDX	1	0
3	B	707	5LS	2	0
2	C	701	5TL	4	0
3	C	702	5LS	1	0
5	C	704	PDX	1	0
4	C	706	GLC	3	0
9	C	708	5TM	1	0
10	C	709	Z4K	2	0
7	C	710	5TK	1	0
8	C	711	5TH	1	0
2	D	701	5TL	2	0
3	D	705	5LS	1	0
6	D	710	5TJ	1	0
2	E	701	5TL	3	0
4	E	703	GLC	1	0
4	E	706	GLC	2	0
2	F	701	5TL	6	0
4	F	703	GLC	1	0
4	F	706	GLC	1	0
2	G	701	5TL	5	0
4	G	706	GLC	1	0
2	H	701	5TL	2	0
4	H	703	GLC	1	0
3	H	705	5LS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	701	5TL	6	0
4	I	706	GLC	4	0
2	J	701	5TL	2	0
4	J	702	GLC	1	0
3	J	704	5LS	2	0
4	J	705	GLC	6	0
5	J	706	PDX	4	0
2	K	701	5TL	3	0
5	K	707	PDX	1	0
2	L	701	5TL	2	0
4	L	705	GLC	2	0
5	L	706	PDX	2	0
4	L	708	GLC	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	655/655 (100%)	0.06	24 (3%)	45	36	124, 249, 346, 440	0
1	B	655/655 (100%)	0.22	42 (6%)	23	16	166, 260, 355, 433	0
1	C	655/655 (100%)	0.07	22 (3%)	49	39	148, 254, 349, 435	0
1	D	655/655 (100%)	0.19	48 (7%)	18	14	164, 262, 366, 442	0
1	E	655/655 (100%)	0.12	23 (3%)	48	38	132, 252, 350, 465	0
1	F	655/655 (100%)	0.21	45 (6%)	20	15	164, 262, 370, 469	0
1	G	655/655 (100%)	0.04	21 (3%)	51	40	67, 249, 345, 479	0
1	H	655/655 (100%)	0.29	52 (7%)	15	12	149, 261, 356, 419	0
1	I	655/655 (100%)	0.16	38 (5%)	26	20	130, 257, 355, 440	0
1	J	655/655 (100%)	0.26	55 (8%)	14	11	162, 264, 366, 440	0
1	K	655/655 (100%)	0.21	43 (6%)	22	16	128, 252, 347, 450	0
1	L	655/655 (100%)	0.20	41 (6%)	23	17	165, 263, 370, 484	0
All	All	7860/7860 (100%)	0.17	454 (5%)	26	20	67, 257, 357, 484	0

The worst 5 of 454 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	78	ASP	12.8
1	J	7	PRO	9.7
1	K	504	SER	7.9
1	D	180	GLU	7.8
1	L	89	ASP	7.6

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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	5LS	K	702	20/20	0.11	0.99	14.18	363,425,467,471	0
4	GLC	K	703	11/12	0.47	1.14	9.56	360,413,466,537	0
3	5LS	D	702	20/20	0.50	0.65	4.49	340,440,517,518	0
2	5TL	L	701	26/26	0.51	0.77	3.52	158,266,335,350	0
5	PDX	K	707	19/20	0.68	0.50	3.02	257,458,487,488	0
3	5LS	L	704	20/20	0.48	0.49	2.92	358,404,444,460	0
2	5TL	H	701	26/26	0.65	0.51	2.50	226,257,279,282	0
2	5TL	E	701	26/26	0.55	0.59	2.34	127,197,233,277	0
3	5LS	B	707	20/20	0.13	1.10	2.12	410,470,536,552	0
2	5TL	K	701	26/26	0.59	0.57	1.91	131,202,237,288	0
5	PDX	I	704	19/20	0.76	0.32	1.75	247,401,449,453	0
10	Z4K	C	709	15/16	0.81	0.62	1.73	512,546,562,567	0
2	5TL	A	701	26/26	0.72	0.51	1.71	121,206,278,306	0
5	PDX	G	704	19/20	0.72	0.49	1.66	394,475,502,529	0
2	5TL	B	701	26/26	0.48	0.63	1.55	149,237,280,287	0
2	5TL	J	701	26/26	0.54	0.55	1.40	179,264,307,319	0
3	5LS	G	702	20/20	0.66	0.48	1.31	282,367,436,438	0
2	5TL	I	701	26/26	0.68	0.49	1.20	152,242,284,323	0
2	5TL	C	701	26/26	0.73	0.44	1.04	150,234,279,291	0
2	5TL	F	701	26/26	0.61	0.44	0.97	157,307,408,431	0
2	5TL	D	701	26/26	0.73	0.43	0.71	197,297,320,332	0
4	GLC	C	706	11/12	0.64	0.34	0.39	287,335,428,484	0
2	5TL	G	701	26/26	0.78	0.39	0.28	108,200,280,288	0
5	PDX	L	709	19/20	0.20	0.49	0.25	302,421,476,480	0
5	PDX	E	707	19/20	0.58	0.36	0.11	330,398,456,471	0
5	PDX	C	704	19/20	0.81	0.21	-2.04	382,434,463,471	0
3	5LS	K	705	20/20	0.82	0.17	-	347,522,574,579	0
3	5LS	D	705	20/20	0.59	0.18	-	368,431,456,471	0
3	5LS	F	705	20/20	0.68	0.26	-	404,467,489,501	0
5	PDX	G	707	19/20	0.70	0.29	-	241,384,434,436	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	5LS	A	702	20/20	0.77	0.56	-	337,376,407,435	0
3	5LS	E	702	20/20	0.60	0.41	-	384,414,438,442	0
3	5LS	F	702	20/20	0.70	0.34	-	348,474,507,510	0
9	5TM	J	708	17/18	0.69	0.54	-	429,491,543,555	0
4	GLC	H	703	11/12	0.69	0.28	-	220,288,388,445	0
9	5TM	G	708	17/18	0.29	0.50	-	462,507,517,524	0
10	Z4K	J	709	15/16	0.51	0.30	-	437,501,519,520	0
9	5TM	C	708	17/18	0.68	0.35	-	479,506,524,529	0
8	5TH	I	711	17/18	0.70	0.43	-	384,477,520,526	0
4	GLC	F	703	11/12	0.45	0.57	-	347,378,409,472	0
3	5LS	L	707	20/20	0.51	0.39	-	442,520,539,550	0
5	PDX	I	707	19/20	0.60	0.51	-	270,404,472,478	0
4	GLC	I	706	11/12	0.87	0.35	-	197,292,365,403	0
5	PDX	L	703	19/20	0.80	0.49	-	291,428,471,474	0
4	GLC	B	702	11/12	0.82	0.27	-	259,379,417,450	0
5	PDX	A	707	19/20	0.67	0.51	-	218,410,475,496	0
3	5LS	A	705	20/20	0.48	0.29	-	320,445,483,493	0
5	PDX	J	706	19/20	0.15	0.70	-	321,419,508,517	0
3	5LS	G	705	20/20	0.87	0.21	-	361,462,493,495	0
7	5TK	I	710	13/14	0.83	0.62	-	409,452,467,476	0
3	5LS	C	702	20/20	0.80	0.40	-	412,438,452,452	0
4	GLC	I	703	11/12	0.83	0.27	-	216,358,388,409	0
4	GLC	J	705	11/12	0.89	0.51	-	329,361,377,405	0
9	5TM	B	708	17/18	0.51	0.77	-	442,503,540,543	0
6	5TJ	A	709	17/18	0.66	0.44	-	394,528,538,539	0
3	5LS	D	708	20/20	0.52	0.41	-	406,436,450,462	0
6	5TJ	D	710	17/18	0.72	0.94	-	487,535,554,557	0
5	PDX	C	707	19/20	0.61	0.44	-	242,541,570,575	0
3	5LS	J	707	20/20	0.52	0.39	-	472,553,561,566	0
6	5TJ	H	708	17/18	0.57	0.74	-	305,465,516,533	0
3	5LS	I	705	20/20	0.82	0.16	-	255,515,567,577	0
4	GLC	C	703	11/12	0.76	0.38	-	358,404,431,439	0
3	5LS	E	705	20/20	0.76	0.17	-	275,459,474,500	0
3	5LS	H	707	20/20	0.66	1.05	-	430,502,561,583	0
5	PDX	H	704	19/20	0.80	0.62	-	266,436,468,474	0
3	5LS	C	705	20/20	0.45	0.29	-	318,398,444,472	0
4	GLC	E	703	11/12	0.76	0.42	-	335,392,442,495	0
3	5LS	B	704	20/20	0.40	0.47	-	356,421,481,498	0
3	5LS	H	705	20/20	0.77	0.38	-	402,453,485,501	0
5	PDX	J	703	19/20	0.71	0.34	-	404,488,531,532	0
3	5LS	L	702	20/20	0.72	0.34	-	414,473,550,553	0
7	5TK	C	710	13/14	0.72	0.99	-	498,545,563,567	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	PDX	L	706	19/20	0.43	0.65	-	373,474,502,503	0
5	PDX	A	704	19/20	0.51	0.96	-	294,542,568,576	0
5	PDX	D	704	19/20	0.64	0.44	-	395,433,465,466	0
4	GLC	J	702	11/12	0.74	0.33	-	394,429,498,537	0
6	5TJ	I	709	17/18	0.82	0.52	-	385,519,554,575	0
3	5LS	H	702	20/20	0.70	0.23	-	291,429,473,484	0
3	5LS	I	702	20/20	0.81	0.32	-	388,452,499,510	0
4	GLC	A	703	11/12	0.77	0.42	-	366,443,481,495	0
8	5TH	A	711	17/18	0.64	0.29	-	382,454,506,522	0
8	5TH	C	711	17/18	0.42	0.75	-	286,465,514,523	0
3	5LS	J	704	20/20	0.60	0.31	-	308,429,475,496	0
4	GLC	B	705	11/12	0.76	1.04	-	333,423,476,483	0
5	PDX	F	704	19/20	0.50	0.47	-	366,456,485,489	0
4	GLC	E	706	11/12	0.89	0.18	-	275,289,341,375	0
4	GLC	F	706	11/12	0.78	0.55	-	267,377,431,435	0
3	5LS	D	709	20/20	0.33	0.44	-	390,510,562,568	0
7	5TK	A	710	13/14	0.71	0.78	-	377,494,522,528	0
5	PDX	F	707	19/20	0.25	0.54	-	366,469,493,510	0
4	GLC	A	706	11/12	0.76	0.43	-	357,383,424,432	0
10	Z4K	H	710	15/16	0.51	0.28	-	442,503,528,534	0
5	PDX	D	707	19/20	0.44	0.30	-	373,430,480,492	0
5	PDX	K	704	19/20	0.37	0.44	-	442,555,569,571	0
6	5TJ	A	708	17/18	0.48	0.60	-	520,543,568,570	0
5	PDX	B	706	19/20	0.55	0.65	-	309,489,529,530	0
7	5TK	G	709	13/14	0.68	0.64	-	431,547,571,574	0
4	GLC	L	708	11/12	0.83	0.64	-	315,385,428,432	0
5	PDX	E	704	19/20	0.59	0.34	-	120,485,579,583	0
4	GLC	H	706	11/12	0.84	0.38	-	361,408,422,461	0
4	GLC	K	706	11/12	0.76	0.20	-	321,350,440,452	0
4	GLC	L	705	11/12	0.60	0.41	-	330,367,393,433	0
6	5TJ	I	708	17/18	0.60	0.85	-	468,554,566,566	0
4	GLC	G	703	11/12	0.58	0.37	-	370,394,435,475	0
6	5TJ	D	711	17/18	0.44	0.55	-	291,502,575,583	0
4	GLC	G	706	11/12	0.84	0.27	-	263,307,356,360	0
5	PDX	B	703	19/20	0.76	0.34	-	246,460,539,547	0
8	5TH	G	710	17/18	0.40	0.45	-	386,527,562,566	0
4	GLC	D	706	11/12	0.79	0.40	-	380,397,417,446	0
6	5TJ	H	709	17/18	0.50	0.45	-	452,494,530,541	0
4	GLC	D	703	11/12	0.23	0.80	-	419,441,472,478	0
10	Z4K	B	709	15/16	0.46	0.33	-	441,493,519,523	0

6.5 Other polymers (i)

There are no such residues in this entry.