wwPDB X-ray Structure Validation Summary Report (i)

Jan 20, 2024 – 10:02 pm GMT

PDB ID	:	7NYN
Title	:	Mutant Y526A of SH3 domain of JNK-interacting Protein 1 (JIP1)
Authors	:	Perez, L.M.; Ielasi, F.S.; Palencia, A.; Jensen, M.R.
Deposited on	:	2021-03-23
Resolution	:	1.54 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
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 (i)) were used in the production of this report:

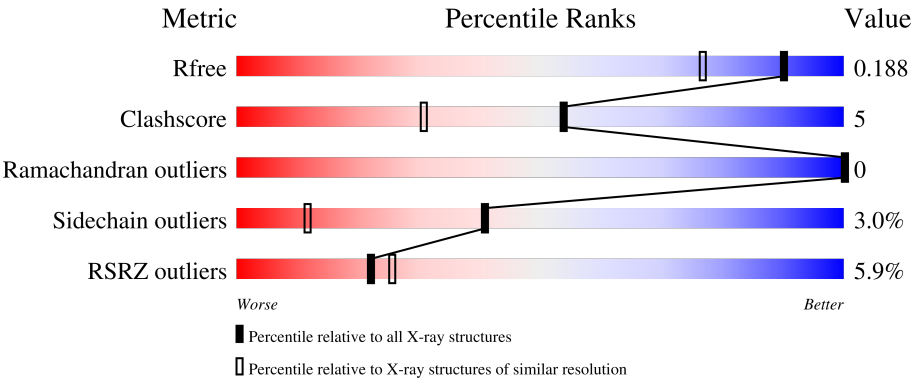
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.54 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	AAA	63	5% 83% 14%
1	BBB	63	5% 83% 14%
1	CCC	63	3% 90% 5% 5%
1	DDD	63	5% 87% 10%
1	EEE	63	5% 87% 8% 5%

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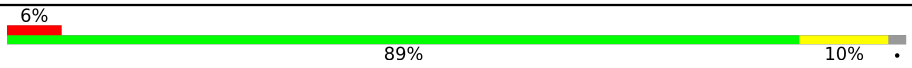
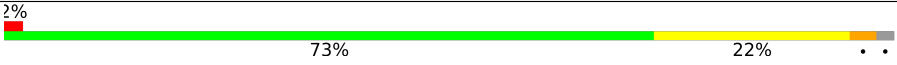
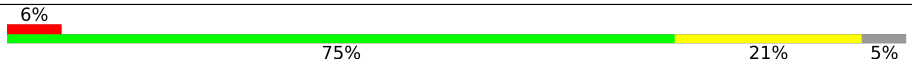
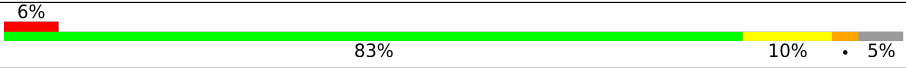
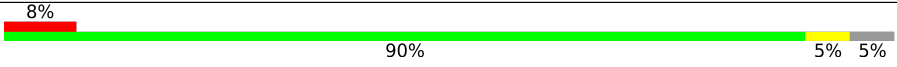
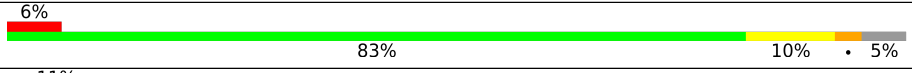
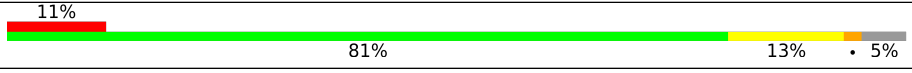
Mol	Chain	Length	Quality of chain
1	FFF	63	
1	GGG	63	
1	HHH	63	
1	III	63	
1	JJJ	63	
1	KKK	63	
1	LLL	63	

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
6	SO4	HHH	603	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7091 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 SH3 domain of JNK-interacting Protein 1 (JIP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	63	Total	C	N	O	S	0	1	0
			531	338	89	102	2			
1	BBB	61	Total	C	N	O	S	0	1	0
			516	330	85	100	1			
1	CCC	60	Total	C	N	O	S	0	0	0
			498	318	83	96	1			
1	DDD	61	Total	C	N	O	S	0	0	0
			508	324	85	98	1			
1	EEE	60	Total	C	N	O	S	0	0	0
			501	320	83	96	2			
1	FFF	62	Total	C	N	O	S	0	1	0
			525	334	87	102	2			
1	GGG	62	Total	C	N	O	S	0	0	0
			515	328	87	98	2			
1	HHH	60	Total	C	N	O	S	0	0	0
			498	318	83	96	1			
1	III	60	Total	C	N	O	S	0	0	0
			498	318	83	96	1			
1	JJJ	60	Total	C	N	O	S	0	0	0
			498	318	83	96	1			
1	KKK	60	Total	C	N	O	S	0	1	0
			507	323	84	99	1			
1	LLL	60	Total	C	N	O	S	0	2	0
			516	331	84	100	1			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	487	GLY	-	expression tag	UNP Q9UQF2
AAA	488	HIS	-	expression tag	UNP Q9UQF2
AAA	489	MET	-	expression tag	UNP Q9UQF2
AAA	526	ALA	TYR	engineered mutation	UNP Q9UQF2
BBB	487	GLY	-	expression tag	UNP Q9UQF2

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	488	HIS	-	expression tag	UNP Q9UQF2
BBB	489	MET	-	expression tag	UNP Q9UQF2
BBB	526	ALA	TYR	engineered mutation	UNP Q9UQF2
CCC	487	GLY	-	expression tag	UNP Q9UQF2
CCC	488	HIS	-	expression tag	UNP Q9UQF2
CCC	489	MET	-	expression tag	UNP Q9UQF2
CCC	526	ALA	TYR	engineered mutation	UNP Q9UQF2
DDD	487	GLY	-	expression tag	UNP Q9UQF2
DDD	488	HIS	-	expression tag	UNP Q9UQF2
DDD	489	MET	-	expression tag	UNP Q9UQF2
DDD	526	ALA	TYR	engineered mutation	UNP Q9UQF2
EEE	487	GLY	-	expression tag	UNP Q9UQF2
EEE	488	HIS	-	expression tag	UNP Q9UQF2
EEE	489	MET	-	expression tag	UNP Q9UQF2
EEE	526	ALA	TYR	engineered mutation	UNP Q9UQF2
FFF	487	GLY	-	expression tag	UNP Q9UQF2
FFF	488	HIS	-	expression tag	UNP Q9UQF2
FFF	489	MET	-	expression tag	UNP Q9UQF2
FFF	526	ALA	TYR	engineered mutation	UNP Q9UQF2
GGG	487	GLY	-	expression tag	UNP Q9UQF2
GGG	488	HIS	-	expression tag	UNP Q9UQF2
GGG	489	MET	-	expression tag	UNP Q9UQF2
GGG	526	ALA	TYR	engineered mutation	UNP Q9UQF2
HHH	487	GLY	-	expression tag	UNP Q9UQF2
HHH	488	HIS	-	expression tag	UNP Q9UQF2
HHH	489	MET	-	expression tag	UNP Q9UQF2
HHH	526	ALA	TYR	engineered mutation	UNP Q9UQF2
III	487	GLY	-	expression tag	UNP Q9UQF2
III	488	HIS	-	expression tag	UNP Q9UQF2
III	489	MET	-	expression tag	UNP Q9UQF2
III	526	ALA	TYR	engineered mutation	UNP Q9UQF2
JJJ	487	GLY	-	expression tag	UNP Q9UQF2
JJJ	488	HIS	-	expression tag	UNP Q9UQF2
JJJ	489	MET	-	expression tag	UNP Q9UQF2
JJJ	526	ALA	TYR	engineered mutation	UNP Q9UQF2
KKK	487	GLY	-	expression tag	UNP Q9UQF2
KKK	488	HIS	-	expression tag	UNP Q9UQF2
KKK	489	MET	-	expression tag	UNP Q9UQF2
KKK	526	ALA	TYR	engineered mutation	UNP Q9UQF2
LLL	487	GLY	-	expression tag	UNP Q9UQF2
LLL	488	HIS	-	expression tag	UNP Q9UQF2
LLL	489	MET	-	expression tag	UNP Q9UQF2

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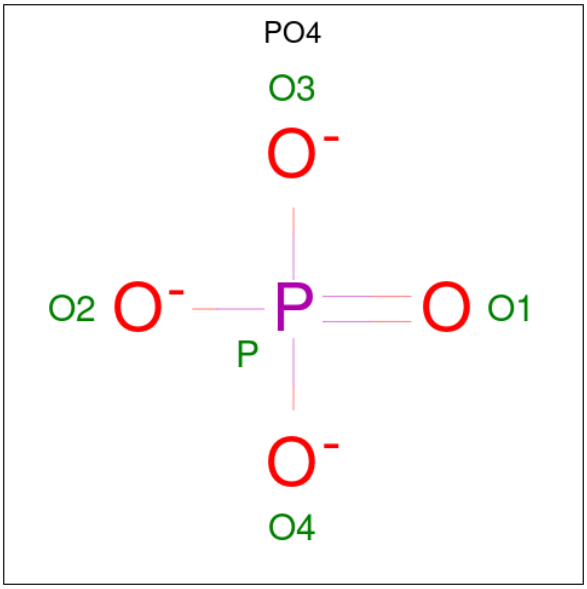
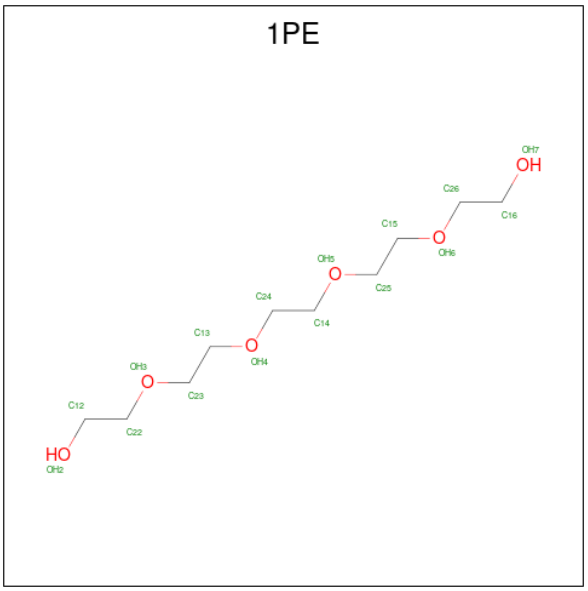
Chain	Residue	Modelled	Actual	Comment	Reference
LLL	526	ALA	TYR	engineered mutation	UNP Q9UQF2

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



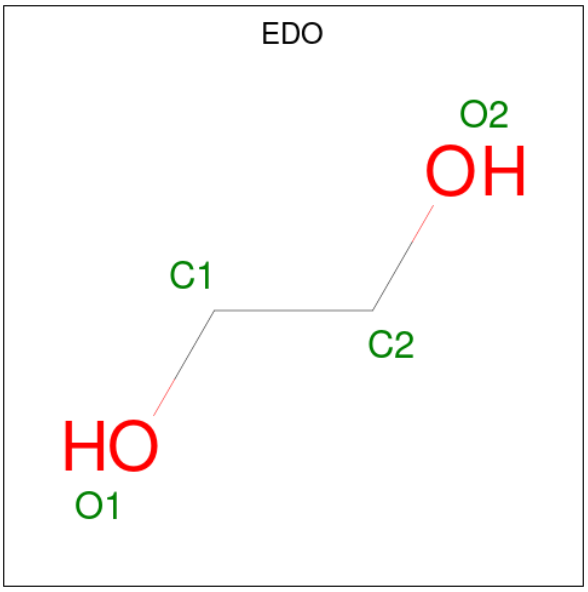
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total O P 5 4 1	0	0
2	HHH	1	Total O P 5 4 1	0	0
2	HHH	1	Total O P 5 4 1	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



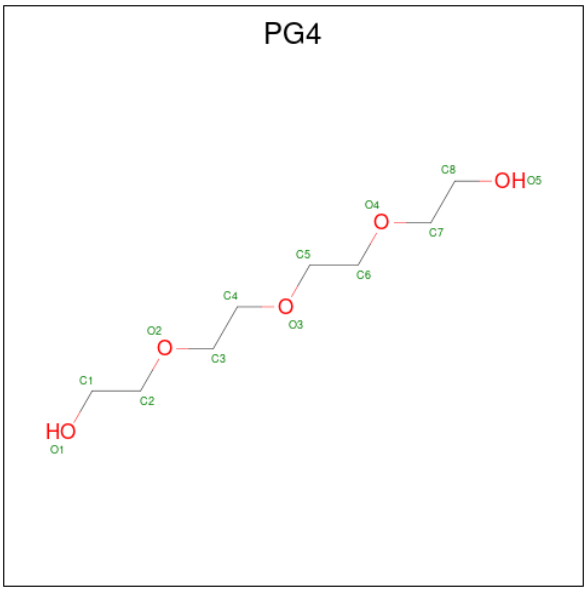
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 16 10 6	0	0
3	AAA	1	Total C O 16 10 6	0	0
3	BBB	1	Total C O 16 10 6	0	0
3	CCC	1	Total C O 16 10 6	0	0
3	DDD	1	Total C O 16 10 6	0	0
3	FFF	1	Total C O 16 10 6	0	0
3	GGG	1	Total C O 16 10 6	0	0
3	HHH	1	Total C O 16 10 6	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



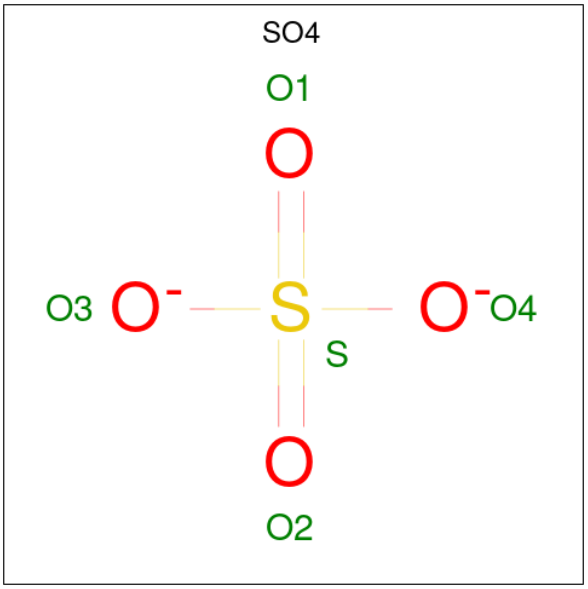
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	FFF	1	Total	C	O	0	0
			4	2	2		
4	GGG	1	Total	C	O	0	0
			4	2	2		
4	LLL	1	Total	C	O	0	0
			4	2	2		
4	LLL	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



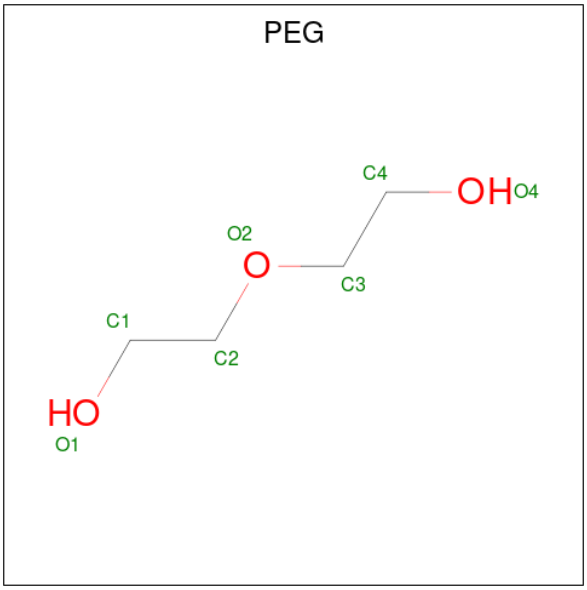
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	1	Total C O 13 8 5	0	0
5	DDD	1	Total C O 13 8 5	0	0
5	DDD	1	Total C O 13 8 5	0	0
5	GGG	1	Total C O 13 8 5	0	0
5	JJJ	1	Total C O 13 8 5	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	CCC	1	Total O S 5 4 1	0	0
6	DDD	1	Total O S 5 4 1	0	0
6	EEE	1	Total O S 5 4 1	0	0
6	HHH	1	Total O S 5 4 1	0	0
6	III	1	Total O S 5 4 1	0	0
6	KKK	1	Total O S 5 4 1	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	GGG	1	Total C O 7 4 3	0	0
7	III	1	Total C O 7 4 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	71	Total O 71 71	0	0
8	BBB	77	Total O 77 77	0	0

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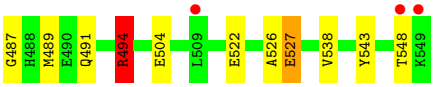
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	CCC	75	Total O 75 75	0	0
8	DDD	67	Total O 67 67	0	0
8	EEE	50	Total O 50 50	0	0
8	FFF	59	Total O 59 59	0	0
8	GGG	85	Total O 85 85	0	0
8	HHH	50	Total O 50 50	0	0
8	III	47	Total O 47 47	0	0
8	JJJ	39	Total O 39 39	0	0
8	KKK	44	Total O 44 44	0	0
8	LLL	36	Total O 36 36	0	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.

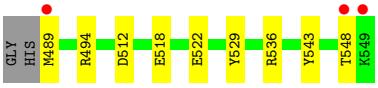
• Molecule 1: SH3 domain of JNK-interacting Protein 1 (JIP1)

Chain AAA:



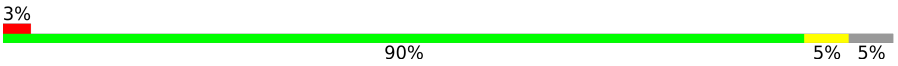
• Molecule 1: SH3 domain of JNK-interacting Protein 1 (JIP1)

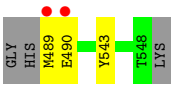
Chain BBB:



• Molecule 1: SH3 domain of JNK-interacting Protein 1 (JIP1)

Chain CCC:





• Molecule 1: SH3 domain of JNK-interacting Protein 1 (JIP1)

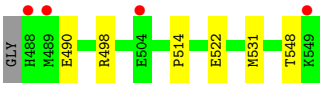
Chain DDD:

• Molecule 1: SH3 domain of JNK-interacting Protein 1 (JIP1)

Chain EEE:

• Molecule 1: SH3 domain of JNK-interacting Protein 1 (JIP1)

Chain FFF:

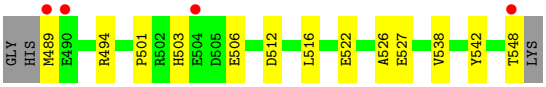


• Molecule 1: SH3 domain of JNK-interacting Protein 1 (JIP1)

Chain GGG:

• Molecule 1: SH3 domain of JNK-interacting Protein 1 (JIP1)

Chain HHH:

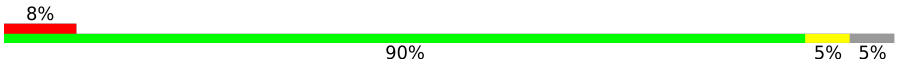


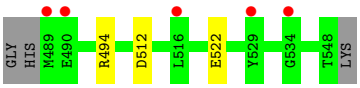
• Molecule 1: SH3 domain of JNK-interacting Protein 1 (JIP1)

Chain III:

• Molecule 1: SH3 domain of JNK-interacting Protein 1 (JIP1)

Chain JJJ:





• Molecule 1: SH3 domain of JNK-interacting Protein 1 (JIP1)

Chain KKK:

• Molecule 1: SH3 domain of JNK-interacting Protein 1 (JIP1)

Chain LLL:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	210.64Å 62.48Å 87.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.35 – 1.54 49.35 – 1.54	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.35-1.54) 99.9 (49.35-1.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 1.54Å)	Xtriage
Refinement program	REFMAC 7.1.007	Depositor
R, R_{free}	0.138 , 0.180 0.150 , 0.188	Depositor DCC
R_{free} test set	1798 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	7091	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: PG4, EDO, SO4, PEG, PO4, 1PE

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	AAA	0.98	2/548 (0.4%)	1.28	3/742 (0.4%)
1	BBB	0.91	1/530 (0.2%)	1.11	1/721 (0.1%)
1	CCC	0.89	0/511	1.08	1/696 (0.1%)
1	DDD	0.93	1/521 (0.2%)	1.01	3/707 (0.4%)
1	EEE	0.74	0/514	0.95	0/699
1	FFF	0.79	0/538	0.98	1/729 (0.1%)
1	GGG	0.91	0/529	1.09	4/719 (0.6%)
1	HHH	0.80	1/511 (0.2%)	0.90	0/696
1	III	0.83	0/511	1.01	2/696 (0.3%)
1	JJJ	0.76	0/511	1.00	1/696 (0.1%)
1	KKK	0.77	0/520	0.93	0/708
1	LLL	0.78	0/533	0.98	1/726 (0.1%)
All	All	0.84	5/6277 (0.1%)	1.03	17/8535 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	GGG	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	522	GLU	CD-OE2	-9.64	1.15	1.25
1	HHH	522	GLU	CD-OE2	-5.72	1.19	1.25
1	AAA	487	GLY	N-CA	5.57	1.54	1.46
1	BBB	522	GLU	CD-OE2	-5.49	1.19	1.25
1	AAA	527	GLU	CD-OE2	5.07	1.31	1.25

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	494	ARG	CG-CD-NE	-12.52	85.50	111.80
1	CCC	543	TYR	CB-CG-CD1	7.75	125.65	121.00
1	BBB	543	TYR	CB-CG-CD1	7.67	125.61	121.00
1	AAA	494	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	GGG	543	TYR	CB-CG-CD1	7.05	125.23	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	GGG	507	LEU	Mainchain

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	AAA	531	0	495	7	0
1	BBB	516	0	469	6	0
1	CCC	498	0	459	1	0
1	DDD	508	0	472	2	0
1	EEE	501	0	466	2	0
1	FFF	525	0	486	2	0
1	GGG	515	0	476	9	0
1	HHH	498	0	459	7	0
1	III	498	0	459	6	0
1	JJJ	498	0	459	0	0
1	KKK	507	0	464	8	0
1	LLL	516	0	473	4	0
2	AAA	5	0	0	0	0
2	HHH	10	0	0	1	0
3	AAA	32	0	44	4	0
3	BBB	16	0	22	3	0
3	CCC	16	0	22	0	0
3	DDD	16	0	22	3	0
3	FFF	16	0	22	2	0
3	GGG	16	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	HHH	16	0	22	1	0
4	AAA	4	0	6	1	0
4	CCC	8	0	12	0	0
4	FFF	4	0	6	0	0
4	GGG	4	0	6	0	0
4	LLL	8	0	12	0	0
5	BBB	13	0	18	5	0
5	DDD	26	0	36	2	0
5	GGG	13	0	18	0	0
5	JJJ	13	0	18	0	0
6	CCC	5	0	0	0	0
6	DDD	5	0	0	0	0
6	EEE	5	0	0	0	0
6	HHH	5	0	0	0	0
6	III	5	0	0	0	0
6	KKK	5	0	0	0	0
7	GGG	7	0	10	0	0
7	III	7	0	10	1	0
8	AAA	71	0	0	3	0
8	BBB	77	0	0	5	0
8	CCC	75	0	0	0	0
8	DDD	67	0	0	2	0
8	EEE	50	0	0	0	0
8	FFF	59	0	0	0	0
8	GGG	85	0	0	1	0
8	HHH	50	0	0	0	0
8	III	47	0	0	0	0
8	JJJ	39	0	0	0	0
8	KKK	44	0	0	1	0
8	LLL	36	0	0	1	0
All	All	7091	0	5965	66	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 5.

The worst 5 of 66 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BBB:601:PG4:H72	8:BBB:748:HOH:O	1.59	1.00
1:BBB:529[A]:TYR:CE1	1:BBB:536:ARG:HD3	2.09	0.87
1:BBB:518:GLU:OE2	1:BBB:529[A]:TYR:CD2	2.29	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KKK:490:GLU:HA	1:KKK:490:GLU:OE1	1.82	0.79
1:EEE:547:VAL:O	1:EEE:548:THR:HG23	1.85	0.77

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	AAA	62/63 (98%)	60 (97%)	2 (3%)	0	100	100
1	BBB	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
1	CCC	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
1	DDD	59/63 (94%)	58 (98%)	1 (2%)	0	100	100
1	EEE	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
1	FFF	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
1	GGG	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
1	HHH	58/63 (92%)	58 (100%)	0	0	100	100
1	III	58/63 (92%)	58 (100%)	0	0	100	100
1	JJJ	58/63 (92%)	58 (100%)	0	0	100	100
1	KKK	59/63 (94%)	58 (98%)	1 (2%)	0	100	100
1	LLL	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
All	All	711/756 (94%)	700 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	54/53 (102%)	52 (96%)	2 (4%)	34 7
1	BBB	51/53 (96%)	50 (98%)	1 (2%)	55 24
1	CCC	50/53 (94%)	50 (100%)	0	100 100
1	DDD	51/53 (96%)	51 (100%)	0	100 100
1	EEE	51/53 (96%)	48 (94%)	3 (6%)	19 2
1	FFF	53/53 (100%)	51 (96%)	2 (4%)	33 6
1	GGG	52/53 (98%)	51 (98%)	1 (2%)	57 26
1	HHH	50/53 (94%)	49 (98%)	1 (2%)	55 24
1	III	50/53 (94%)	49 (98%)	1 (2%)	55 24
1	JJJ	50/53 (94%)	48 (96%)	2 (4%)	31 6
1	KKK	51/53 (96%)	49 (96%)	2 (4%)	32 6
1	LLL	52/53 (98%)	49 (94%)	3 (6%)	20 2
All	All	615/636 (97%)	597 (97%)	18 (3%)	41 13

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	KKK	491	GLN
1	LLL	548	THR
1	LLL	522	GLU
1	GGG	536	ARG
1	KKK	490	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

31 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	$\#\|Z\| > 2$
3	1PE	GGG	602	-	15,15,15	0.28	0	14,14,14	0.38	0
5	PG4	JJJ	601	-	12,12,12	0.25	0	11,11,11	0.34	0
5	PG4	GGG	603	-	12,12,12	0.37	0	11,11,11	0.35	0
6	SO4	DDD	601	-	4,4,4	0.24	0	6,6,6	0.14	0
3	1PE	CCC	602	-	15,15,15	0.26	0	14,14,14	0.31	0
6	SO4	EEE	601	-	4,4,4	0.28	0	6,6,6	0.11	0
7	PEG	III	602	-	6,6,6	0.27	0	5,5,5	0.20	0
3	1PE	BBB	602	-	15,15,15	0.31	0	14,14,14	0.35	0
2	PO4	HHH	602	-	4,4,4	0.73	0	6,6,6	0.42	0
4	EDO	CCC	603	-	3,3,3	0.66	0	2,2,2	0.51	0
4	EDO	AAA	604	-	3,3,3	1.02	0	2,2,2	1.73	1 (50%)
6	SO4	CCC	601	-	4,4,4	0.26	0	6,6,6	0.09	0
7	PEG	GGG	601	-	6,6,6	0.67	0	5,5,5	0.42	0
5	PG4	BBB	601	-	12,12,12	0.25	0	11,11,11	0.43	0
6	SO4	KKK	601	-	4,4,4	0.31	0	6,6,6	0.09	0
2	PO4	HHH	601	-	4,4,4	1.23	1 (25%)	6,6,6	0.37	0
4	EDO	GGG	604	-	3,3,3	0.21	0	2,2,2	0.30	0
3	1PE	AAA	603	-	15,15,15	0.40	0	14,14,14	0.50	0
4	EDO	CCC	604	-	3,3,3	0.26	0	2,2,2	0.29	0
5	PG4	DDD	602	-	12,12,12	0.31	0	11,11,11	0.39	0
6	SO4	HHH	603	-	4,4,4	0.20	0	6,6,6	0.11	0
4	EDO	LLL	602	-	3,3,3	0.43	0	2,2,2	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	1PE	AAA	602	-	15,15,15	0.39	0	14,14,14	0.80	0
5	PG4	DDD	604	-	12,12,12	0.34	0	11,11,11	0.25	0
2	PO4	AAA	601	-	4,4,4	1.73	1 (25%)	6,6,6	0.30	0
4	EDO	FFF	602	-	3,3,3	0.23	0	2,2,2	0.49	0
3	1PE	FFF	601	-	15,15,15	0.27	0	14,14,14	0.43	0
3	1PE	HHH	604	-	15,15,15	0.50	0	14,14,14	0.27	0
4	EDO	LLL	601	-	3,3,3	0.08	0	2,2,2	0.19	0
3	1PE	DDD	603	-	15,15,15	0.21	0	14,14,14	0.44	0
6	SO4	III	601	-	4,4,4	0.29	0	6,6,6	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	GGG	602	-	-	3/13/13/13	-
5	PG4	JJJ	601	-	-	4/10/10/10	-
5	PG4	GGG	603	-	-	4/10/10/10	-
3	1PE	CCC	602	-	-	5/13/13/13	-
7	PEG	III	602	-	-	1/4/4/4	-
3	1PE	BBB	602	-	-	8/13/13/13	-
4	EDO	CCC	603	-	-	1/1/1/1	-
4	EDO	AAA	604	-	-	0/1/1/1	-
7	PEG	GGG	601	-	-	3/4/4/4	-
5	PG4	BBB	601	-	-	6/10/10/10	-
4	EDO	GGG	604	-	-	1/1/1/1	-
3	1PE	AAA	603	-	-	7/13/13/13	-
4	EDO	CCC	604	-	-	1/1/1/1	-
5	PG4	DDD	602	-	-	2/10/10/10	-
4	EDO	LLL	602	-	-	1/1/1/1	-
3	1PE	AAA	602	-	-	3/13/13/13	-
5	PG4	DDD	604	-	-	7/10/10/10	-
4	EDO	FFF	602	-	-	1/1/1/1	-
3	1PE	FFF	601	-	-	9/13/13/13	-
3	1PE	HHH	604	-	-	8/13/13/13	-
4	EDO	LLL	601	-	-	1/1/1/1	-
3	1PE	DDD	603	-	-	10/13/13/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	601	PO4	P-O3	-3.31	1.44	1.54
2	HHH	601	PO4	P-O1	2.17	1.55	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	AAA	604	EDO	O2-C2-C1	2.37	128.93	111.91

There are no chirality outliers.

5 of 86 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	602	1PE	C24-C14-OH5-C25
5	BBB	601	PG4	C1-C2-O2-C3
3	BBB	602	1PE	OH2-C12-C22-OH3
3	CCC	602	1PE	OH4-C13-C23-OH3
3	GGG	602	1PE	OH4-C13-C23-OH3

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	III	602	PEG	1	0
3	BBB	602	1PE	3	0
2	HHH	602	PO4	1	0
4	AAA	604	EDO	1	0
5	BBB	601	PG4	5	0
3	AAA	603	1PE	3	0
3	AAA	602	1PE	1	0
5	DDD	604	PG4	2	0
3	FFF	601	1PE	2	0
3	HHH	604	1PE	1	0
3	DDD	603	1PE	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	AAA	63/63 (100%)	0.52	3 (4%)	30	34	19, 22, 58, 120	0
1	BBB	61/63 (96%)	0.05	3 (4%)	29	33	21, 27, 68, 114	0
1	CCC	60/63 (95%)	0.07	2 (3%)	46	53	21, 30, 63, 128	0
1	DDD	61/63 (96%)	0.15	3 (4%)	29	33	22, 30, 58, 107	0
1	EEE	60/63 (95%)	-0.09	3 (5%)	28	32	26, 33, 70, 96	0
1	FFF	62/63 (98%)	-0.02	4 (6%)	18	21	27, 33, 70, 108	0
1	GGG	62/63 (98%)	-0.19	1 (1%)	72	77	22, 28, 51, 86	0
1	HHH	60/63 (95%)	-0.16	4 (6%)	17	20	27, 35, 69, 115	0
1	III	60/63 (95%)	0.04	4 (6%)	17	20	26, 36, 69, 110	0
1	JJJ	60/63 (95%)	0.06	5 (8%)	11	12	29, 40, 71, 93	0
1	KKK	60/63 (95%)	-0.04	4 (6%)	17	20	28, 39, 79, 106	0
1	LLL	60/63 (95%)	0.53	7 (11%)	4	4	30, 41, 77, 105	0
All	All	729/756 (96%)	0.08	43 (5%)	22	25	19, 34, 72, 128	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	LLL	529[A]	TYR	8.3
1	LLL	489	MET	8.0
1	KKK	489	MET	7.6
1	AAA	549	LYS	6.9
1	JJJ	489	MET	6.6

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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
4	EDO	AAA	604	4/4	0.62	0.22	51,52,53,58	0
6	SO4	HHH	603	5/5	0.78	0.47	134,165,185,225	0
2	PO4	HHH	602	5/5	0.83	0.46	103,104,133,134	0
5	PG4	JJJ	601	13/13	0.85	0.15	53,71,88,101	0
3	1PE	HHH	604	16/16	0.86	0.18	56,67,104,108	0
4	EDO	LLL	601	4/4	0.87	0.09	64,71,71,72	0
3	1PE	FFF	601	16/16	0.87	0.12	50,75,83,97	0
4	EDO	FFF	602	4/4	0.87	0.11	57,59,63,66	0
7	PEG	GGG	601	7/7	0.88	0.10	51,59,65,70	0
3	1PE	BBB	602	16/16	0.89	0.13	48,65,97,124	0
4	EDO	LLL	602	4/4	0.90	0.09	49,58,62,64	0
4	EDO	CCC	603	4/4	0.90	0.19	53,54,55,60	0
7	PEG	III	602	7/7	0.90	0.08	49,56,65,70	0
5	PG4	GGG	603	13/13	0.91	0.15	51,62,89,102	0
6	SO4	CCC	601	5/5	0.93	0.24	79,98,114,123	0
3	1PE	CCC	602	16/16	0.93	0.17	40,47,70,71	0
3	1PE	GGG	602	16/16	0.94	0.08	42,48,67,79	0
3	1PE	DDD	603	16/16	0.94	0.11	54,67,80,84	0
4	EDO	CCC	604	4/4	0.94	0.19	49,55,58,72	0
3	1PE	AAA	603	16/16	0.95	0.19	38,74,118,124	0
5	PG4	DDD	604	13/13	0.95	0.12	56,60,87,92	0
4	EDO	GGG	604	4/4	0.95	0.18	61,61,63,69	0
3	1PE	AAA	602	16/16	0.95	0.10	36,46,60,65	0
5	PG4	DDD	602	13/13	0.96	0.07	34,46,79,87	0
5	PG4	BBB	601	13/13	0.96	0.14	30,40,56,58	13
6	SO4	III	601	5/5	0.97	0.18	74,75,81,85	0
6	SO4	KKK	601	5/5	0.97	0.14	71,73,80,95	0
6	SO4	EEE	601	5/5	0.97	0.15	73,77,91,93	0
2	PO4	HHH	601	5/5	0.97	0.19	64,73,77,88	0
2	PO4	AAA	601	5/5	0.98	0.09	40,40,47,51	5
6	SO4	DDD	601	5/5	0.98	0.13	59,59,80,92	0

6.5 Other polymers (i)

There are no such residues in this entry.