wwPDB X-ray Structure Validation Summary Report (i)

Nov 15, 2023 – 12:49 AM JST

PDB ID	:	6IKM
Title	:	Crystal structure of SpuE-Spermidine in complex with ScFv5
Authors	:	Wu, D.; Sun, X.
Deposited on	:	2018-10-16
Resolution	:	3.40 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 (1)) were used in the production of this report:

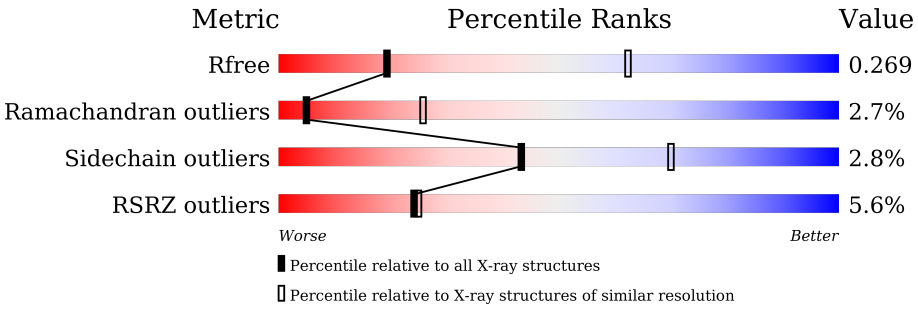
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.40 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	1026 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	340	96%
1	B	340	95%
1	C	340	96%
1	D	340	96%
1	E	340	96%
1	F	340	94%
1	G	340	96%

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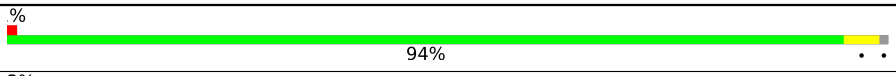
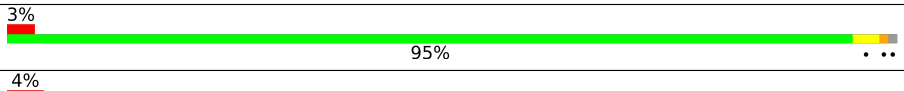
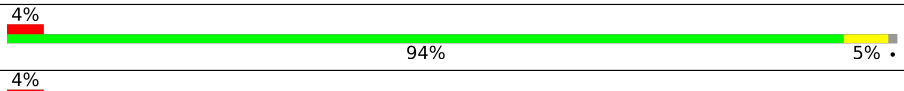
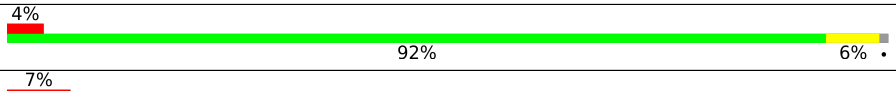
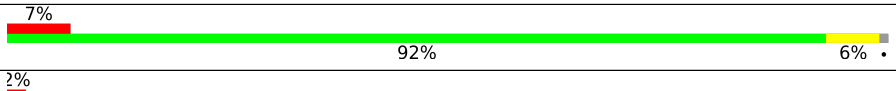
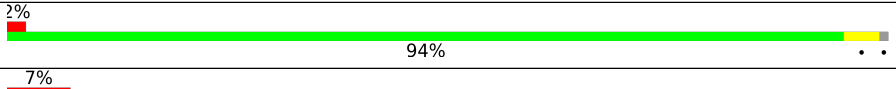
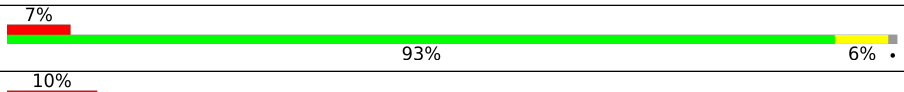
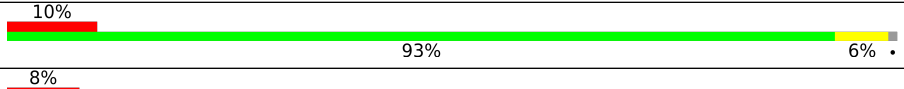
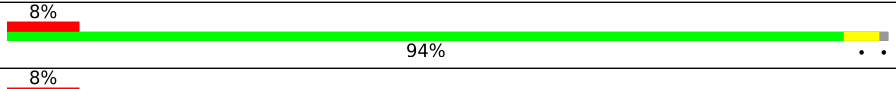
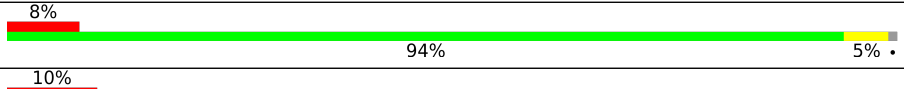
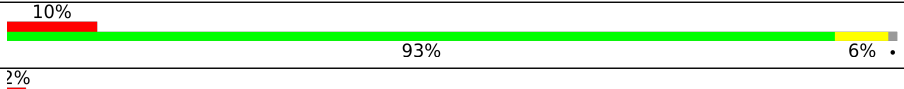
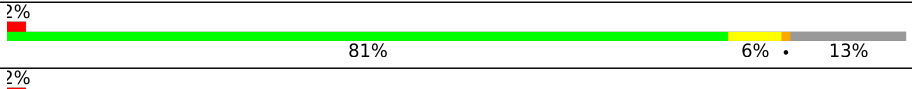
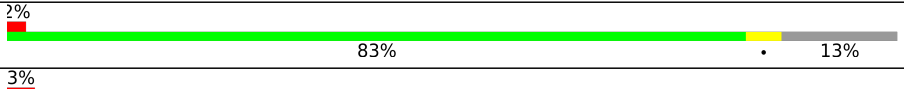
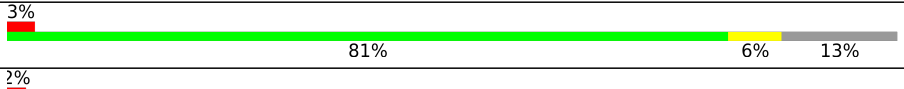
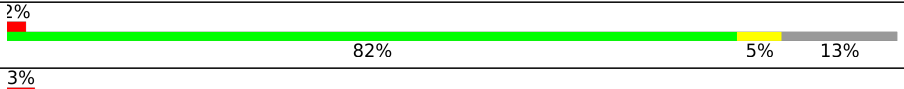
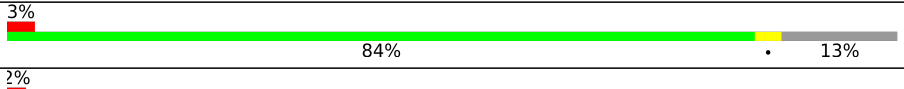
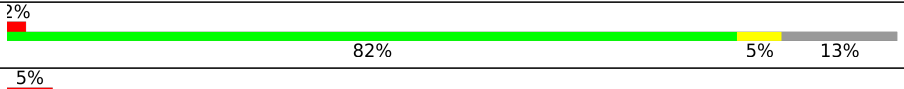
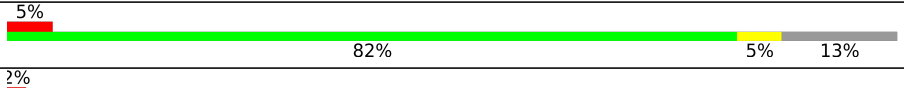
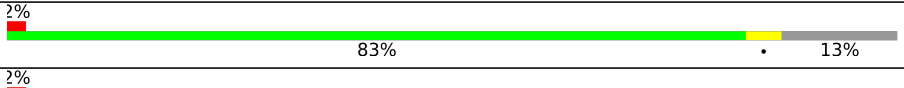
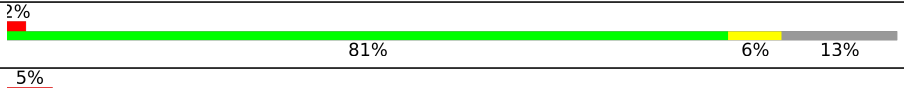
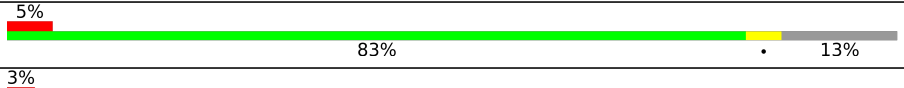
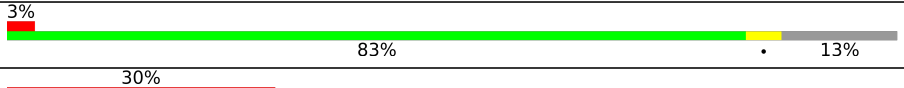
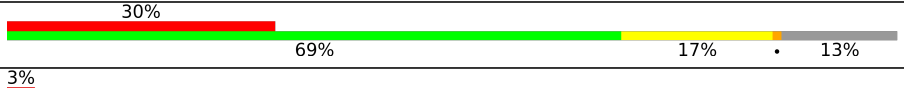
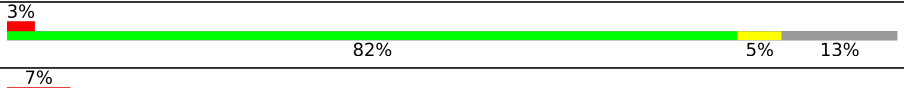
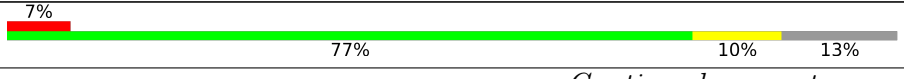
Mol	Chain	Length	Quality of chain
1	H	340	
1	I	340	
1	J	340	
1	K	340	
1	L	340	
1	M	340	
1	N	340	
1	O	340	
1	P	340	
1	Q	340	
1	R	340	
2	a	258	
2	b	258	
2	c	258	
2	d	258	
2	e	258	
2	f	258	
2	g	258	
2	h	258	
2	i	258	
2	j	258	
2	k	258	
2	l	258	
2	m	258	
2	n	258	

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Mol	Chain	Length	Quality of chain
2	o	258	18% 80% 6% • 13%
2	p	258	17% 81% 6% • 13%
2	q	258	9% 77% 9% • 13%
2	r	258	11% 79% 8% 13%

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
4	SPD	L	404	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 78156 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 Polyamine transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	B	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	C	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	D	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	E	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	F	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	G	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	H	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	I	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	J	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	K	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	L	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	M	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	N	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	O	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	P	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	R	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP A0A069QID4
A	24	PRO	-	expression tag	UNP A0A069QID4
A	25	LEU	-	expression tag	UNP A0A069QID4
A	26	GLY	-	expression tag	UNP A0A069QID4
A	27	SER	-	expression tag	UNP A0A069QID4
B	23	GLY	-	expression tag	UNP A0A069QID4
B	24	PRO	-	expression tag	UNP A0A069QID4
B	25	LEU	-	expression tag	UNP A0A069QID4
B	26	GLY	-	expression tag	UNP A0A069QID4
B	27	SER	-	expression tag	UNP A0A069QID4
C	23	GLY	-	expression tag	UNP A0A069QID4
C	24	PRO	-	expression tag	UNP A0A069QID4
C	25	LEU	-	expression tag	UNP A0A069QID4
C	26	GLY	-	expression tag	UNP A0A069QID4
C	27	SER	-	expression tag	UNP A0A069QID4
D	23	GLY	-	expression tag	UNP A0A069QID4
D	24	PRO	-	expression tag	UNP A0A069QID4
D	25	LEU	-	expression tag	UNP A0A069QID4
D	26	GLY	-	expression tag	UNP A0A069QID4
D	27	SER	-	expression tag	UNP A0A069QID4
E	23	GLY	-	expression tag	UNP A0A069QID4
E	24	PRO	-	expression tag	UNP A0A069QID4
E	25	LEU	-	expression tag	UNP A0A069QID4
E	26	GLY	-	expression tag	UNP A0A069QID4
E	27	SER	-	expression tag	UNP A0A069QID4
F	23	GLY	-	expression tag	UNP A0A069QID4
F	24	PRO	-	expression tag	UNP A0A069QID4
F	25	LEU	-	expression tag	UNP A0A069QID4
F	26	GLY	-	expression tag	UNP A0A069QID4
F	27	SER	-	expression tag	UNP A0A069QID4
G	23	GLY	-	expression tag	UNP A0A069QID4
G	24	PRO	-	expression tag	UNP A0A069QID4
G	25	LEU	-	expression tag	UNP A0A069QID4
G	26	GLY	-	expression tag	UNP A0A069QID4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	27	SER	-	expression tag	UNP A0A069QID4
H	23	GLY	-	expression tag	UNP A0A069QID4
H	24	PRO	-	expression tag	UNP A0A069QID4
H	25	LEU	-	expression tag	UNP A0A069QID4
H	26	GLY	-	expression tag	UNP A0A069QID4
H	27	SER	-	expression tag	UNP A0A069QID4
I	23	GLY	-	expression tag	UNP A0A069QID4
I	24	PRO	-	expression tag	UNP A0A069QID4
I	25	LEU	-	expression tag	UNP A0A069QID4
I	26	GLY	-	expression tag	UNP A0A069QID4
I	27	SER	-	expression tag	UNP A0A069QID4
J	23	GLY	-	expression tag	UNP A0A069QID4
J	24	PRO	-	expression tag	UNP A0A069QID4
J	25	LEU	-	expression tag	UNP A0A069QID4
J	26	GLY	-	expression tag	UNP A0A069QID4
J	27	SER	-	expression tag	UNP A0A069QID4
K	23	GLY	-	expression tag	UNP A0A069QID4
K	24	PRO	-	expression tag	UNP A0A069QID4
K	25	LEU	-	expression tag	UNP A0A069QID4
K	26	GLY	-	expression tag	UNP A0A069QID4
K	27	SER	-	expression tag	UNP A0A069QID4
L	23	GLY	-	expression tag	UNP A0A069QID4
L	24	PRO	-	expression tag	UNP A0A069QID4
L	25	LEU	-	expression tag	UNP A0A069QID4
L	26	GLY	-	expression tag	UNP A0A069QID4
L	27	SER	-	expression tag	UNP A0A069QID4
M	23	GLY	-	expression tag	UNP A0A069QID4
M	24	PRO	-	expression tag	UNP A0A069QID4
M	25	LEU	-	expression tag	UNP A0A069QID4
M	26	GLY	-	expression tag	UNP A0A069QID4
M	27	SER	-	expression tag	UNP A0A069QID4
N	23	GLY	-	expression tag	UNP A0A069QID4
N	24	PRO	-	expression tag	UNP A0A069QID4
N	25	LEU	-	expression tag	UNP A0A069QID4
N	26	GLY	-	expression tag	UNP A0A069QID4
N	27	SER	-	expression tag	UNP A0A069QID4
O	23	GLY	-	expression tag	UNP A0A069QID4
O	24	PRO	-	expression tag	UNP A0A069QID4
O	25	LEU	-	expression tag	UNP A0A069QID4
O	26	GLY	-	expression tag	UNP A0A069QID4
O	27	SER	-	expression tag	UNP A0A069QID4
P	23	GLY	-	expression tag	UNP A0A069QID4

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Chain	Residue	Modelled	Actual	Comment	Reference
P	24	PRO	-	expression tag	UNP A0A069QID4
P	25	LEU	-	expression tag	UNP A0A069QID4
P	26	GLY	-	expression tag	UNP A0A069QID4
P	27	SER	-	expression tag	UNP A0A069QID4
Q	23	GLY	-	expression tag	UNP A0A069QID4
Q	24	PRO	-	expression tag	UNP A0A069QID4
Q	25	LEU	-	expression tag	UNP A0A069QID4
Q	26	GLY	-	expression tag	UNP A0A069QID4
Q	27	SER	-	expression tag	UNP A0A069QID4
R	23	GLY	-	expression tag	UNP A0A069QID4
R	24	PRO	-	expression tag	UNP A0A069QID4
R	25	LEU	-	expression tag	UNP A0A069QID4
R	26	GLY	-	expression tag	UNP A0A069QID4
R	27	SER	-	expression tag	UNP A0A069QID4

- Molecule 2 is a protein called ScFv5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	b	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	c	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	d	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	e	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	f	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	g	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	h	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	i	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	j	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	k	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	l	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			

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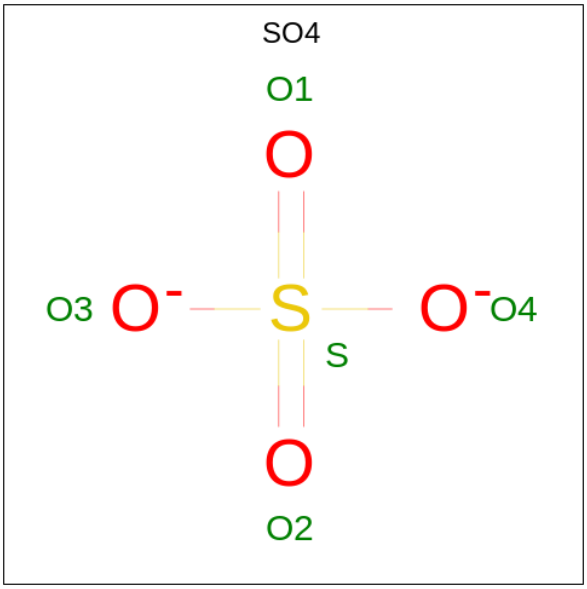
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	m	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	n	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	o	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	p	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	q	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	r	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	M	1	Total O S 5 4 1	0	0
3	M	1	Total O S 5 4 1	0	0
3	M	1	Total O S 5 4 1	0	0
3	N	1	Total O S 5 4 1	0	0
3	N	1	Total O S 5 4 1	0	0
3	N	1	Total O S 5 4 1	0	0
3	N	1	Total O S 5 4 1	0	0
3	N	1	Total O S 5 4 1	0	0
3	N	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0

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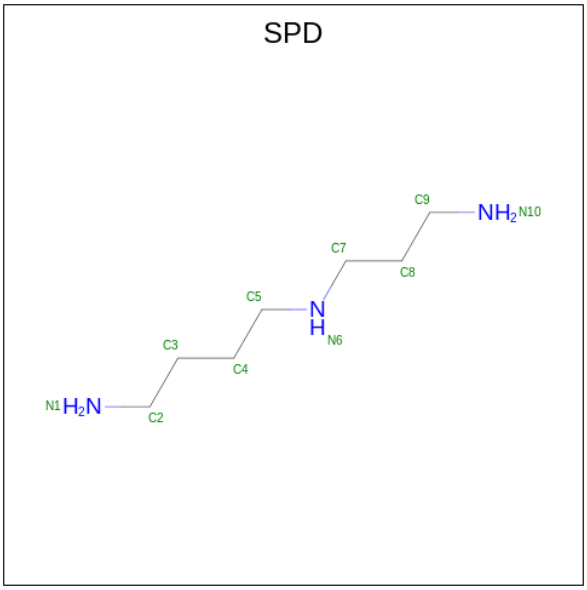
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0
3	R	1	Total O S 5 4 1	0	0
3	R	1	Total O S 5 4 1	0	0
3	R	1	Total O S 5 4 1	0	0

- Molecule 4 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 10 7 3	0	0
4	B	1	Total C N 10 7 3	0	0
4	C	1	Total C N 10 7 3	0	0
4	D	1	Total C N 10 7 3	0	0

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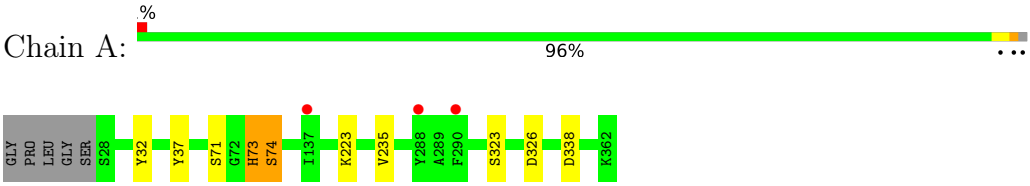
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C N 10 7 3	0	0
4	F	1	Total C N 10 7 3	0	0
4	G	1	Total C N 10 7 3	0	0
4	H	1	Total C N 10 7 3	0	0
4	I	1	Total C N 10 7 3	0	0
4	J	1	Total C N 10 7 3	0	0
4	K	1	Total C N 10 7 3	0	0
4	L	1	Total C N 10 7 3	0	0
4	M	1	Total C N 10 7 3	0	0
4	N	1	Total C N 10 7 3	0	0
4	O	1	Total C N 10 7 3	0	0
4	P	1	Total C N 10 7 3	0	0
4	Q	1	Total C N 10 7 3	0	0
4	R	1	Total C N 10 7 3	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.

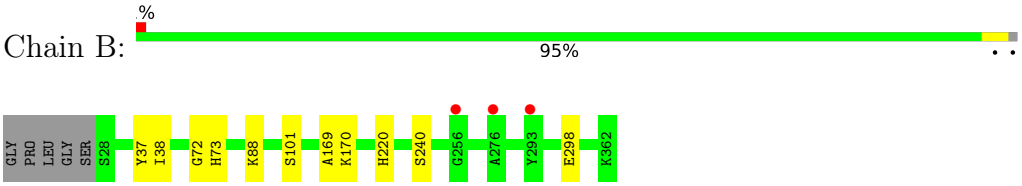
• Molecule 1: Polyamine transport protein

Chain A:



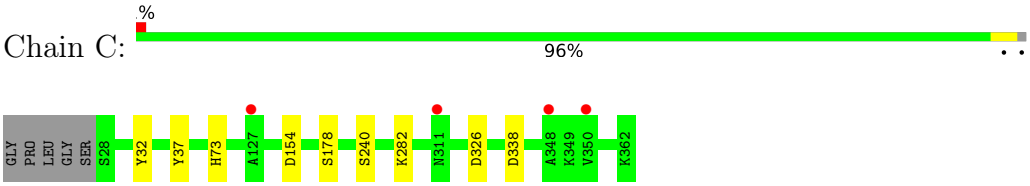
• Molecule 1: Polyamine transport protein

Chain B:



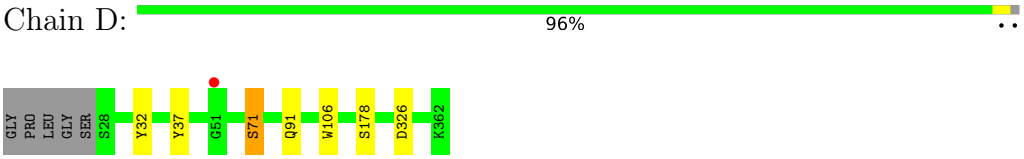
• Molecule 1: Polyamine transport protein

Chain C:



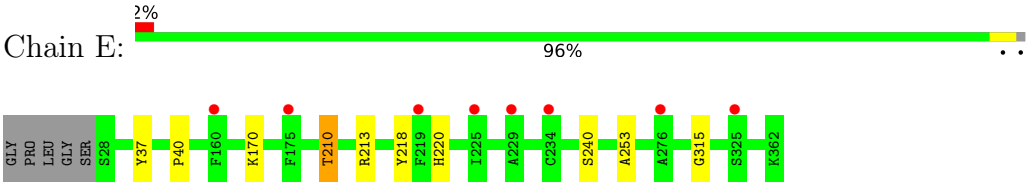
• Molecule 1: Polyamine transport protein

Chain D:



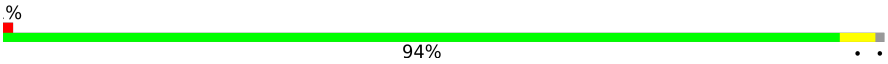
• Molecule 1: Polyamine transport protein

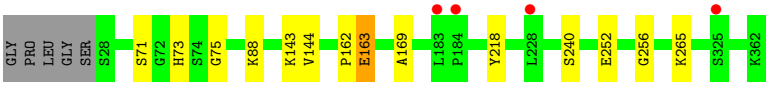
Chain E:



• Molecule 1: Polyamine transport protein

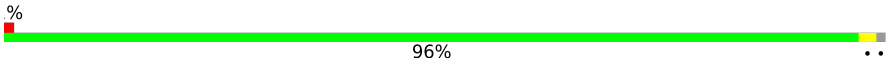
Chain F:





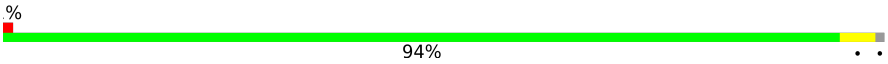
• Molecule 1: Polyamine transport protein

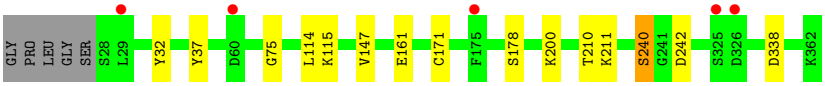
Chain G:



• Molecule 1: Polyamine transport protein

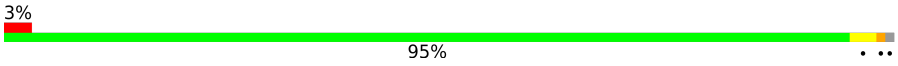
Chain H:

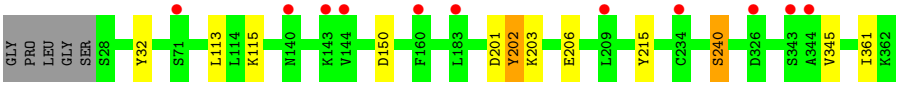




• Molecule 1: Polyamine transport protein

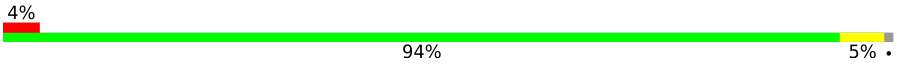
Chain I:

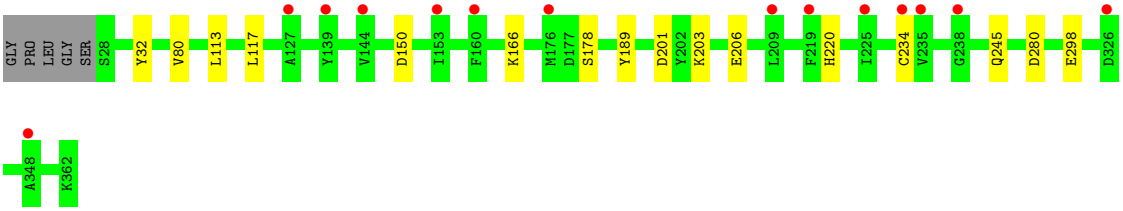




• Molecule 1: Polyamine transport protein

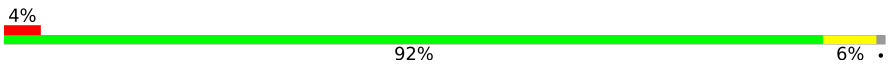
Chain J:

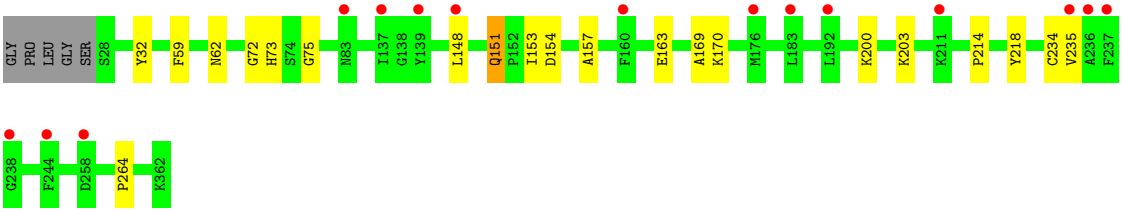




• Molecule 1: Polyamine transport protein

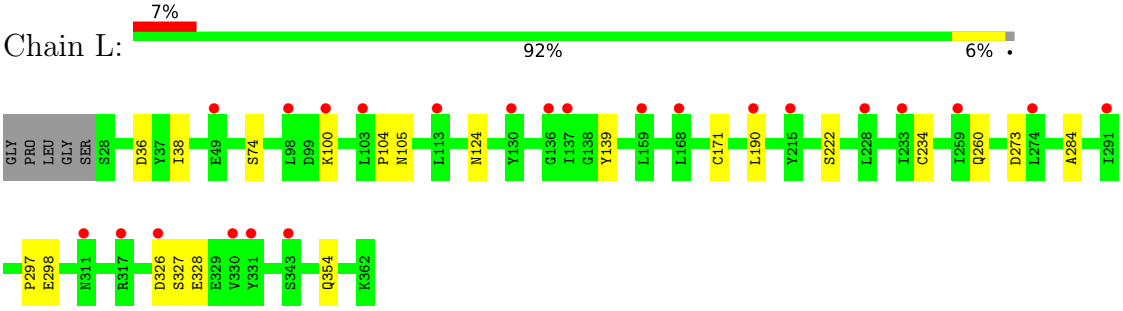
Chain K:





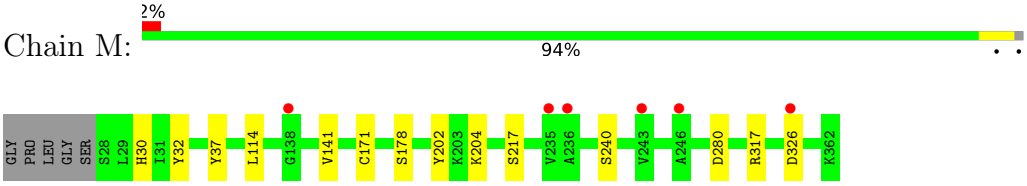
• Molecule 1: Polyamine transport protein

Chain L:



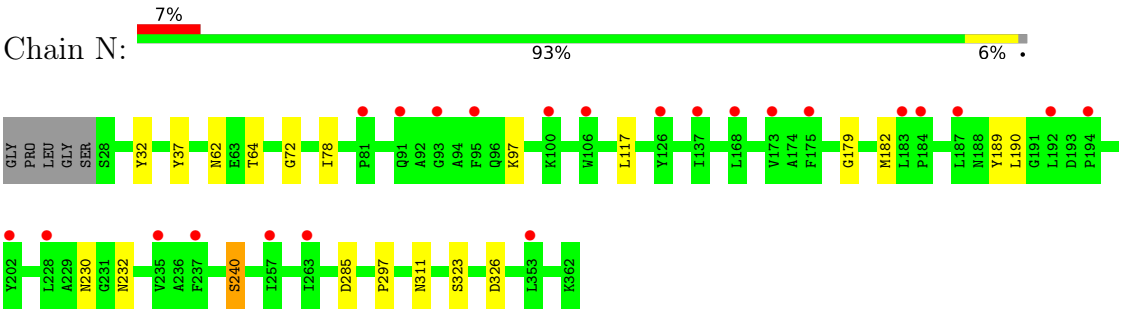
• Molecule 1: Polyamine transport protein

Chain M:



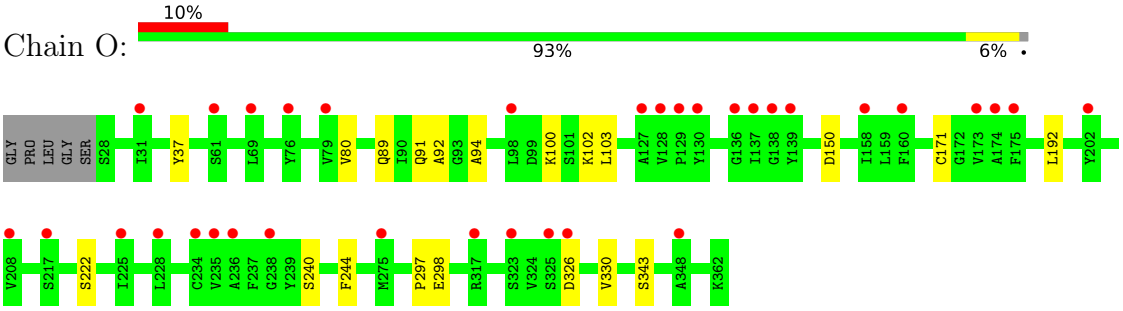
• Molecule 1: Polyamine transport protein

Chain N:



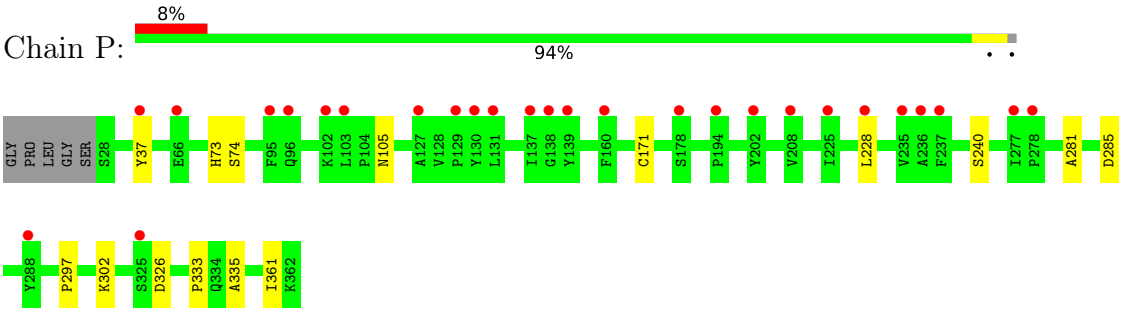
• Molecule 1: Polyamine transport protein

Chain O:



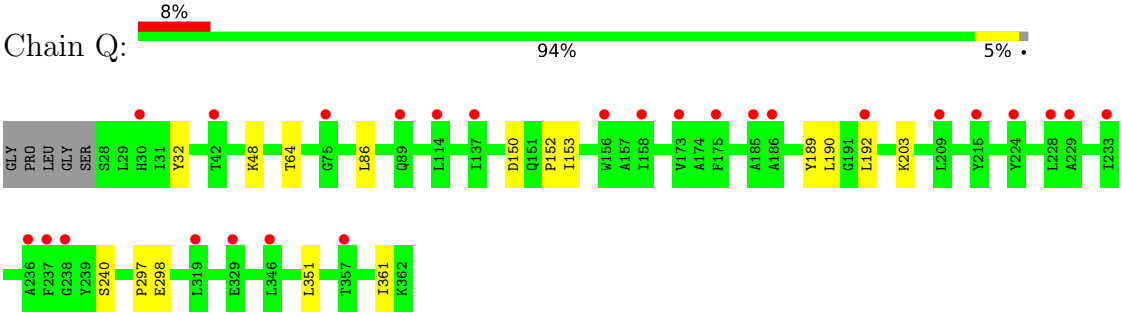
• Molecule 1: Polyamine transport protein

Chain P:



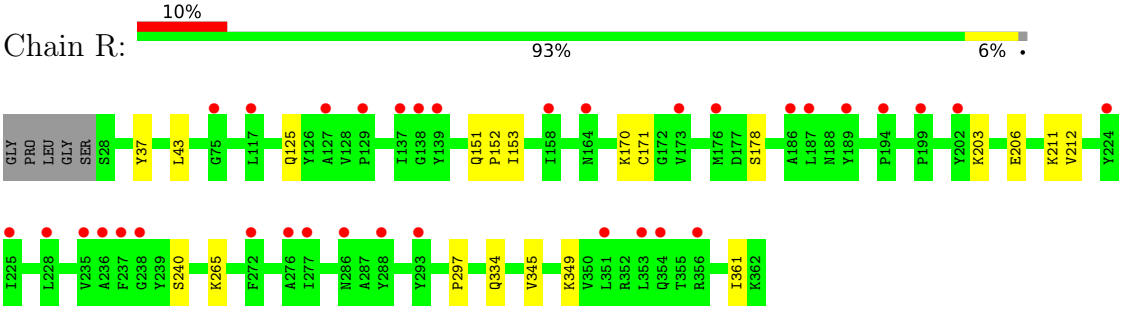
• Molecule 1: Polyamine transport protein

Chain Q:



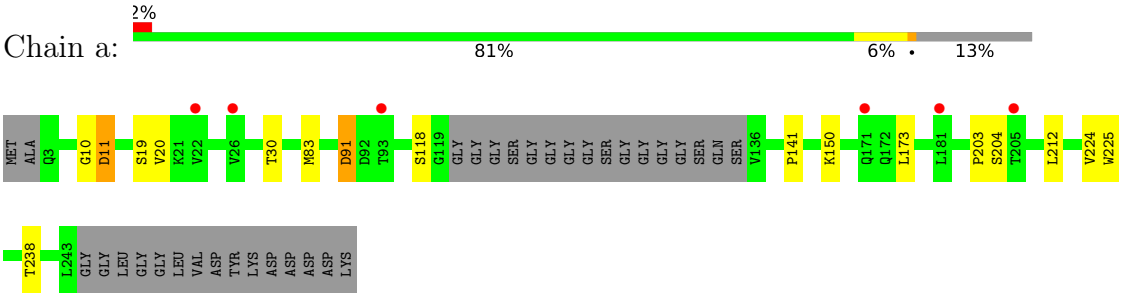
• Molecule 1: Polyamine transport protein

Chain R:



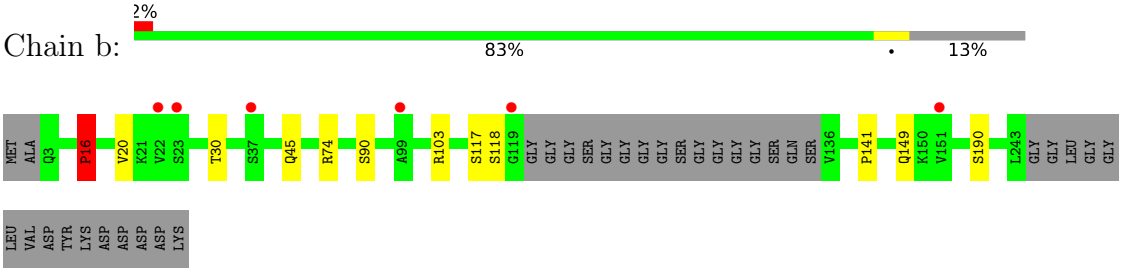
• Molecule 2: ScFv5

Chain a:



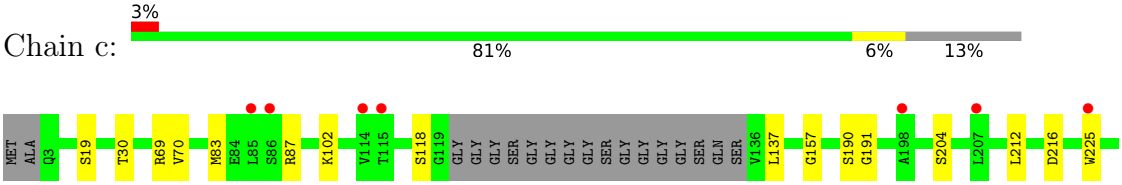
• Molecule 2: ScFv5

Chain b:



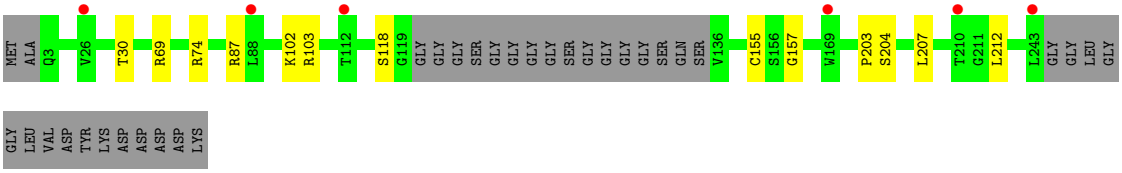
• Molecule 2: ScFv5

Chain c:



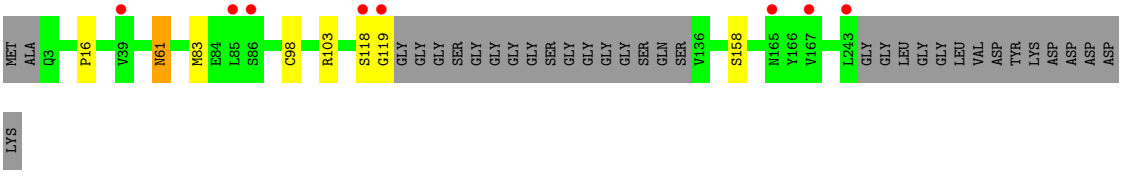
• Molecule 2: ScFv5

Chain d:



• Molecule 2: ScFv5

Chain e:

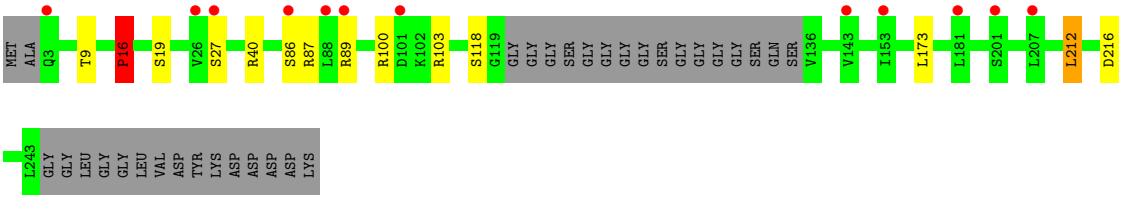


• Molecule 2: ScFv5

Chain f:

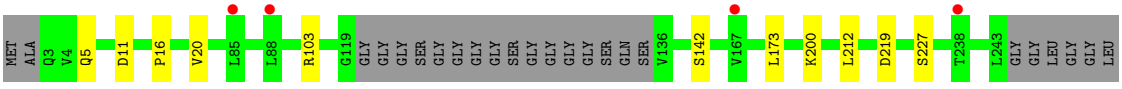
• Molecule 2: ScFv5

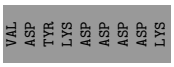
Chain g:



• Molecule 2: ScFv5

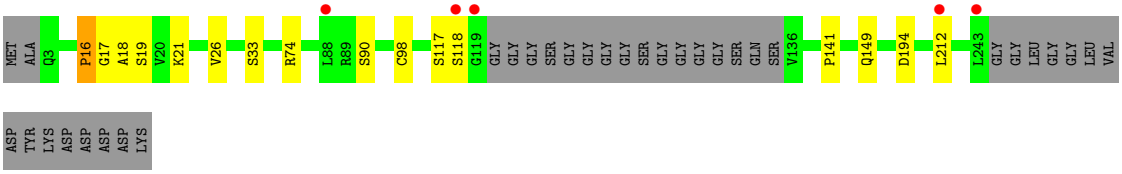
Chain h:





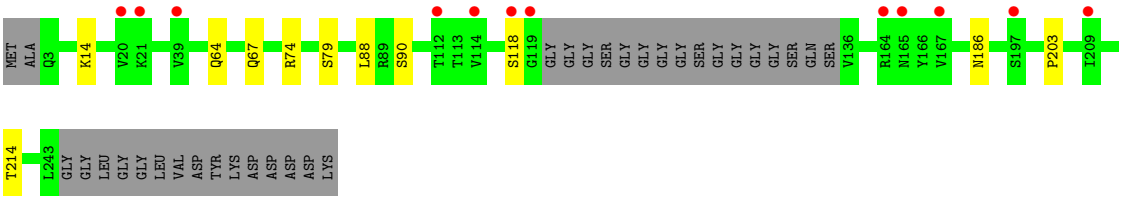
• Molecule 2: ScFv5

Chain i:



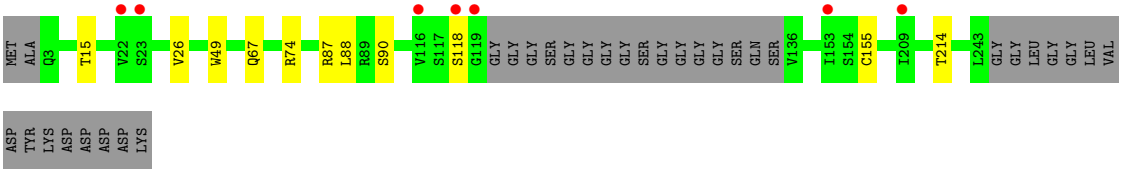
• Molecule 2: ScFv5

Chain j:



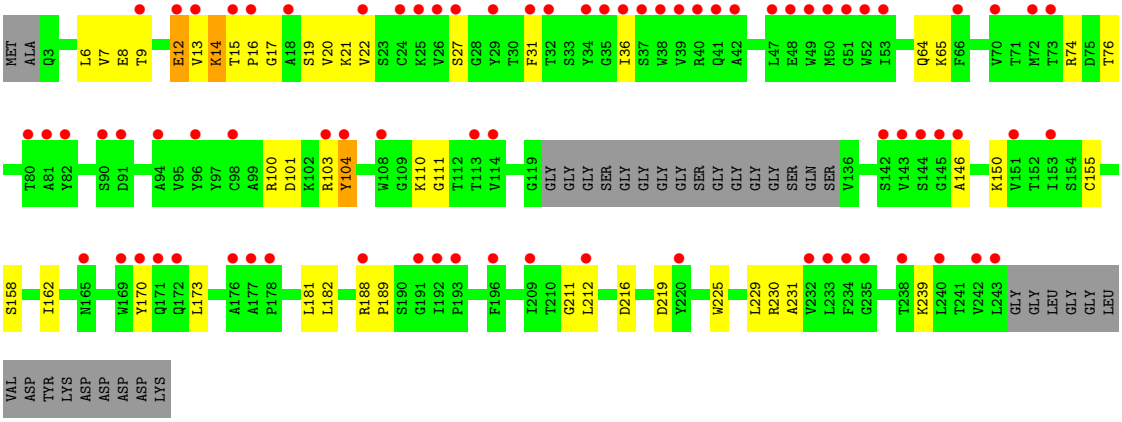
• Molecule 2: ScFv5

Chain k:



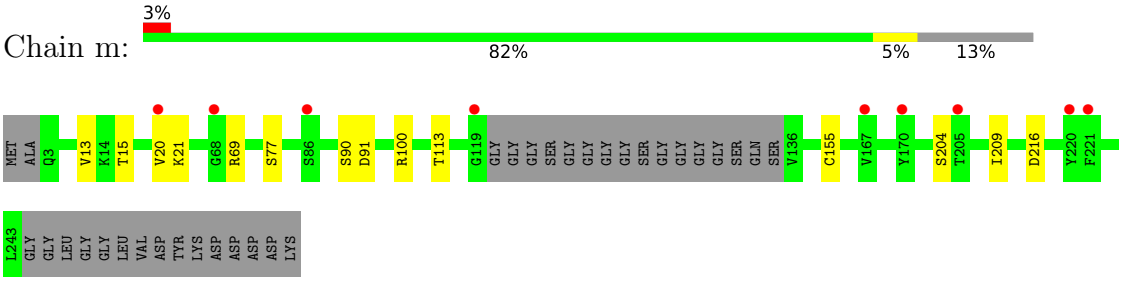
• Molecule 2: ScFv5

Chain l:



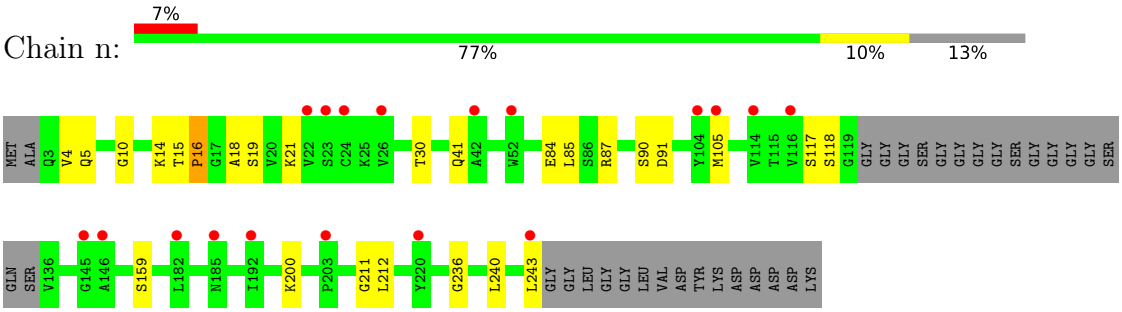
• Molecule 2: ScFv5

Chain m:



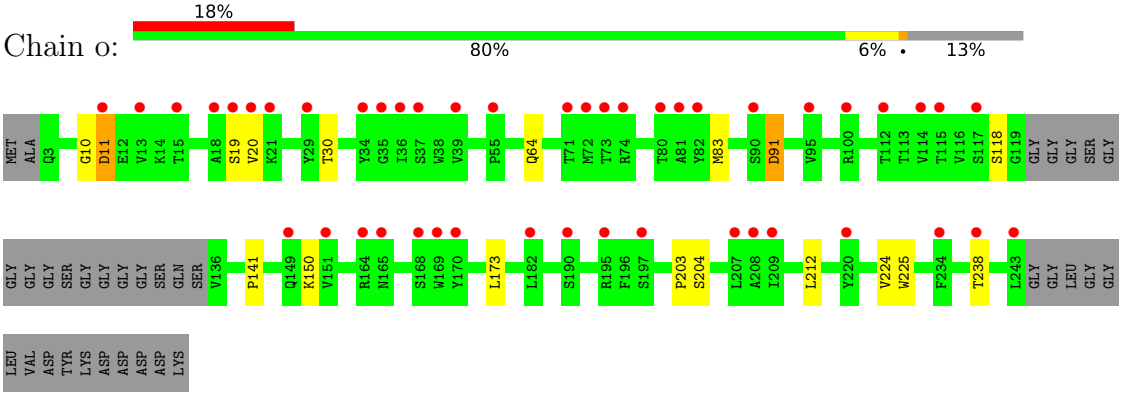
• Molecule 2: ScFv5

Chain n:



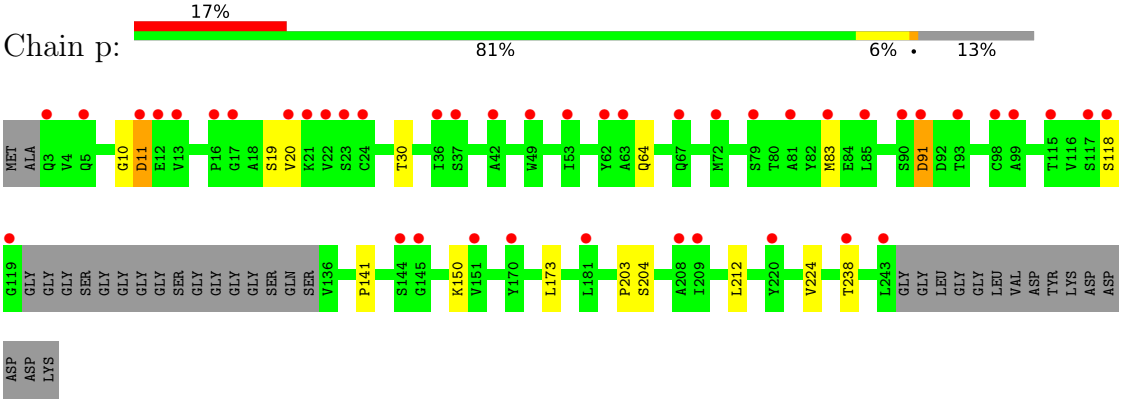
• Molecule 2: ScFv5

Chain o:



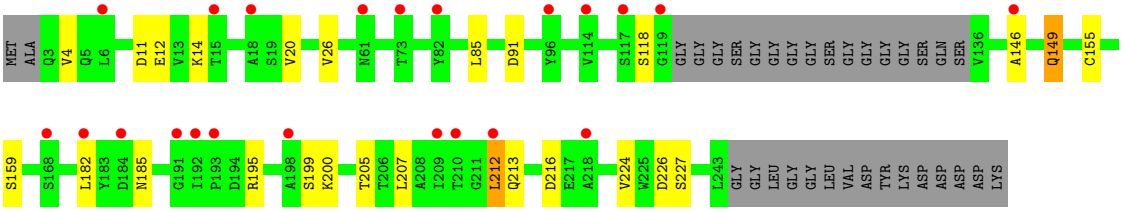
• Molecule 2: ScFv5

Chain p:

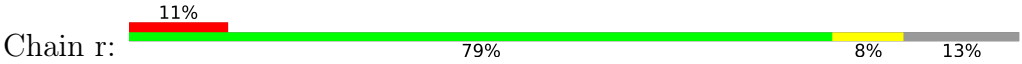


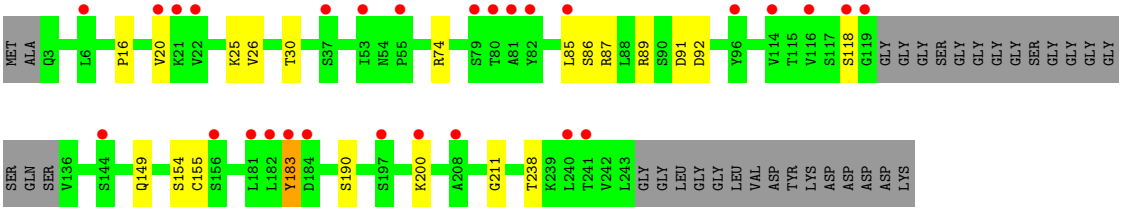
• Molecule 2: ScFv5

Chain q:



- Molecule 2: ScFv5





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	146.24Å 481.80Å 146.13Å 90.00° 120.08° 90.00°	Depositor
Resolution (Å)	46.47 – 3.40 49.70 – 3.40	Depositor EDS
% Data completeness (in resolution range)	89.5 (46.47-3.40) 89.4 (49.70-3.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.228 , 0.268 0.230 , 0.269	Depositor DCC
R_{free} test set	10758 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	63.4	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 9.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.418 for l,k,-h-l 0.418 for -h-l,k,h 0.196 for l,-k,h 0.190 for -h-l,-k,l 0.196 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	78156	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, SPD

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	0.30	0/2684	0.50	0/3653
1	B	0.31	0/2684	0.54	0/3653
1	C	0.32	0/2684	0.51	0/3653
1	D	0.30	0/2684	0.52	0/3653
1	E	0.34	0/2684	0.59	3/3653 (0.1%)
1	F	0.33	1/2684 (0.0%)	0.54	0/3653
1	G	0.34	1/2684 (0.0%)	0.54	1/3653 (0.0%)
1	H	0.32	0/2684	0.58	1/3653 (0.0%)
1	I	0.46	3/2684 (0.1%)	0.67	3/3653 (0.1%)
1	J	0.35	1/2684 (0.0%)	0.59	0/3653
1	K	0.36	1/2684 (0.0%)	0.60	1/3653 (0.0%)
1	L	0.36	0/2684	0.59	0/3653
1	M	0.32	0/2684	0.58	1/3653 (0.0%)
1	N	0.33	0/2684	0.56	0/3653
1	O	0.42	2/2684 (0.1%)	0.66	3/3653 (0.1%)
1	P	0.35	0/2684	0.60	1/3653 (0.0%)
1	Q	0.38	1/2684 (0.0%)	0.61	0/3653
1	R	0.35	0/2684	0.63	0/3653
2	a	0.44	2/1736 (0.1%)	0.75	3/2358 (0.1%)
2	b	0.37	0/1736	0.65	1/2358 (0.0%)
2	c	0.43	2/1736 (0.1%)	0.69	2/2358 (0.1%)
2	d	0.36	0/1736	0.64	1/2358 (0.0%)
2	e	0.35	0/1736	0.60	0/2358
2	f	0.42	1/1736 (0.1%)	0.65	1/2358 (0.0%)
2	g	0.39	0/1736	0.79	2/2358 (0.1%)
2	h	0.40	0/1736	0.65	0/2358
2	i	0.49	2/1736 (0.1%)	0.67	1/2358 (0.0%)
2	j	0.37	0/1736	0.64	1/2358 (0.0%)
2	k	0.54	2/1736 (0.1%)	0.69	1/2358 (0.0%)
2	l	0.47	1/1736 (0.1%)	0.90	4/2358 (0.2%)
2	m	0.38	0/1736	0.65	1/2358 (0.0%)
2	n	0.42	0/1736	0.84	5/2358 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	o	0.44	2/1736 (0.1%)	0.75	3/2358 (0.1%)
2	p	0.44	2/1736 (0.1%)	0.75	3/2358 (0.1%)
2	q	0.42	1/1736 (0.1%)	0.78	5/2358 (0.2%)
2	r	0.49	1/1736 (0.1%)	0.77	4/2358 (0.2%)
All	All	0.38	26/79560 (0.0%)	0.64	52/108198 (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
1	A	0	1
1	I	0	2
1	K	0	1
1	L	0	1
1	M	0	1
1	P	0	2
1	R	0	1
2	a	0	2
2	b	0	1
2	c	0	1
2	d	0	1
2	g	0	1
2	l	0	3
2	m	0	2
2	n	0	2
2	o	0	2
2	p	0	2
2	q	0	1
All	All	0	27

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	k	26	VAL	CB-CG2	12.30	1.78	1.52
2	i	26	VAL	CB-CG2	11.43	1.76	1.52
2	r	238	THR	CB-CG2	10.80	1.88	1.52
1	O	80	VAL	CB-CG1	8.43	1.70	1.52
2	k	26	VAL	CB-CG1	8.12	1.69	1.52

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	g	212	LEU	CB-CG-CD2	18.91	143.15	111.00
2	n	85	LEU	CA-CB-CG	15.69	151.39	115.30
2	a	91	ASP	CB-CG-OD1	-13.35	106.28	118.30
2	o	91	ASP	CB-CG-OD1	-13.33	106.30	118.30
2	p	91	ASP	CB-CG-OD1	-13.33	106.30	118.30

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	73	HIS	Peptide
2	a	10	GLY	Peptide
2	a	11	ASP	Peptide
2	b	117	SER	Peptide
2	c	157	GLY	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	333/340 (98%)	301 (90%)	28 (8%)	4 (1%)	13 41
1	B	333/340 (98%)	300 (90%)	28 (8%)	5 (2%)	10 36
1	C	333/340 (98%)	301 (90%)	28 (8%)	4 (1%)	13 41
1	D	333/340 (98%)	305 (92%)	24 (7%)	4 (1%)	13 41
1	E	333/340 (98%)	298 (90%)	30 (9%)	5 (2%)	10 36
1	F	333/340 (98%)	297 (89%)	28 (8%)	8 (2%)	6 28
1	G	333/340 (98%)	304 (91%)	26 (8%)	3 (1%)	17 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	333/340 (98%)	305 (92%)	21 (6%)	7 (2%)	7 30
1	I	333/340 (98%)	291 (87%)	39 (12%)	3 (1%)	17 49
1	J	333/340 (98%)	281 (84%)	44 (13%)	8 (2%)	6 28
1	K	333/340 (98%)	293 (88%)	31 (9%)	9 (3%)	5 26
1	L	333/340 (98%)	284 (85%)	34 (10%)	15 (4%)	2 16
1	M	333/340 (98%)	293 (88%)	35 (10%)	5 (2%)	10 36
1	N	333/340 (98%)	282 (85%)	40 (12%)	11 (3%)	4 22
1	O	333/340 (98%)	285 (86%)	39 (12%)	9 (3%)	5 26
1	P	333/340 (98%)	281 (84%)	46 (14%)	6 (2%)	8 32
1	Q	333/340 (98%)	275 (83%)	49 (15%)	9 (3%)	5 26
1	R	333/340 (98%)	274 (82%)	49 (15%)	10 (3%)	4 23
2	a	221/258 (86%)	187 (85%)	28 (13%)	6 (3%)	5 26
2	b	221/258 (86%)	197 (89%)	18 (8%)	6 (3%)	5 26
2	c	221/258 (86%)	193 (87%)	21 (10%)	7 (3%)	4 22
2	d	221/258 (86%)	187 (85%)	26 (12%)	8 (4%)	3 21
2	e	221/258 (86%)	202 (91%)	16 (7%)	3 (1%)	11 37
2	f	221/258 (86%)	196 (89%)	24 (11%)	1 (0%)	29 61
2	g	221/258 (86%)	187 (85%)	29 (13%)	5 (2%)	6 28
2	h	221/258 (86%)	190 (86%)	25 (11%)	6 (3%)	5 26
2	i	221/258 (86%)	189 (86%)	24 (11%)	8 (4%)	3 21
2	j	221/258 (86%)	185 (84%)	29 (13%)	7 (3%)	4 22
2	k	221/258 (86%)	189 (86%)	25 (11%)	7 (3%)	4 22
2	l	221/258 (86%)	146 (66%)	46 (21%)	29 (13%)	0 1
2	m	221/258 (86%)	181 (82%)	37 (17%)	3 (1%)	11 37
2	n	221/258 (86%)	173 (78%)	32 (14%)	16 (7%)	1 7
2	o	221/258 (86%)	186 (84%)	29 (13%)	6 (3%)	5 26
2	p	221/258 (86%)	186 (84%)	29 (13%)	6 (3%)	5 26
2	q	221/258 (86%)	171 (77%)	36 (16%)	14 (6%)	1 9
2	r	221/258 (86%)	179 (81%)	32 (14%)	10 (4%)	2 16
All	All	9972/10764 (93%)	8574 (86%)	1125 (11%)	273 (3%)	5 26

5 of 273 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	ASP
2	a	118	SER
2	b	16	PRO
2	b	90	SER
2	b	118	SER

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	279/282 (99%)	272 (98%)	7 (2%)	47	72
1	B	279/282 (99%)	273 (98%)	6 (2%)	52	75
1	C	279/282 (99%)	274 (98%)	5 (2%)	59	79
1	D	279/282 (99%)	275 (99%)	4 (1%)	67	83
1	E	279/282 (99%)	275 (99%)	4 (1%)	67	83
1	F	279/282 (99%)	274 (98%)	5 (2%)	59	79
1	G	279/282 (99%)	275 (99%)	4 (1%)	67	83
1	H	279/282 (99%)	272 (98%)	7 (2%)	47	72
1	I	279/282 (99%)	273 (98%)	6 (2%)	52	75
1	J	279/282 (99%)	272 (98%)	7 (2%)	47	72
1	K	279/282 (99%)	268 (96%)	11 (4%)	32	61
1	L	279/282 (99%)	274 (98%)	5 (2%)	59	79
1	M	279/282 (99%)	272 (98%)	7 (2%)	47	72
1	N	279/282 (99%)	269 (96%)	10 (4%)	35	63
1	O	279/282 (99%)	272 (98%)	7 (2%)	47	72
1	P	279/282 (99%)	273 (98%)	6 (2%)	52	75
1	Q	279/282 (99%)	273 (98%)	6 (2%)	52	75
1	R	279/282 (99%)	270 (97%)	9 (3%)	39	67
2	a	186/203 (92%)	178 (96%)	8 (4%)	29	59
2	b	186/203 (92%)	180 (97%)	6 (3%)	39	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	c	186/203 (92%)	181 (97%)	5 (3%)	44	70
2	d	186/203 (92%)	183 (98%)	3 (2%)	62	81
2	e	186/203 (92%)	181 (97%)	5 (3%)	44	70
2	f	186/203 (92%)	177 (95%)	9 (5%)	25	56
2	g	186/203 (92%)	177 (95%)	9 (5%)	25	56
2	h	186/203 (92%)	182 (98%)	4 (2%)	52	75
2	i	186/203 (92%)	178 (96%)	8 (4%)	29	59
2	j	186/203 (92%)	183 (98%)	3 (2%)	62	81
2	k	186/203 (92%)	183 (98%)	3 (2%)	62	81
2	l	186/203 (92%)	172 (92%)	14 (8%)	13	41
2	m	186/203 (92%)	178 (96%)	8 (4%)	29	59
2	n	186/203 (92%)	181 (97%)	5 (3%)	44	70
2	o	186/203 (92%)	178 (96%)	8 (4%)	29	59
2	p	186/203 (92%)	179 (96%)	7 (4%)	33	61
2	q	186/203 (92%)	178 (96%)	8 (4%)	29	59
2	r	186/203 (92%)	178 (96%)	8 (4%)	29	59
All	All	8370/8730 (96%)	8133 (97%)	237 (3%)	43	70

5 of 237 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	32	TYR
1	R	125	GLN
2	l	158	SER
2	q	216	ASP
2	r	200	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	m	64	GLN
2	n	41	GLN
2	r	149	GLN
2	n	5	GLN
2	n	54	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

72 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	SO4	O	402	-	4,4,4	0.80	0	6,6,6	0.57	0
4	SPD	G	403	-	9,9,9	0.41	0	8,8,8	0.93	0
3	SO4	N	401	-	4,4,4	0.79	0	6,6,6	0.54	0
3	SO4	M	402	-	4,4,4	0.80	0	6,6,6	0.58	0
3	SO4	H	402	-	4,4,4	0.81	0	6,6,6	0.55	0
3	SO4	B	404	-	4,4,4	0.78	0	6,6,6	0.59	0
3	SO4	B	402	-	4,4,4	0.80	0	6,6,6	0.52	0
3	SO4	E	403	-	4,4,4	0.78	0	6,6,6	0.52	0
3	SO4	L	403	-	4,4,4	0.79	0	6,6,6	0.59	0
3	SO4	N	406	-	4,4,4	0.80	0	6,6,6	0.61	0
4	SPD	A	404	-	9,9,9	0.43	0	8,8,8	0.72	0
3	SO4	E	402	-	4,4,4	0.80	0	6,6,6	0.54	0
4	SPD	C	404	-	9,9,9	0.41	0	8,8,8	1.08	0
3	SO4	D	402	-	4,4,4	0.82	0	6,6,6	0.58	0
3	SO4	A	403	-	4,4,4	0.80	0	6,6,6	0.59	0
3	SO4	N	403	-	4,4,4	0.79	0	6,6,6	0.55	0
4	SPD	F	404	-	9,9,9	0.41	0	8,8,8	1.01	0
4	SPD	I	404	-	9,9,9	0.44	0	8,8,8	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	F	401	-	4,4,4	0.77	0	6,6,6	0.59	0
3	SO4	K	403	-	4,4,4	0.79	0	6,6,6	0.52	0
3	SO4	R	403	-	4,4,4	0.79	0	6,6,6	0.52	0
3	SO4	M	401	-	4,4,4	0.77	0	6,6,6	0.57	0
4	SPD	O	407	-	9,9,9	0.41	0	8,8,8	0.97	0
3	SO4	J	401	-	4,4,4	0.81	0	6,6,6	0.55	0
3	SO4	C	401	-	4,4,4	0.80	0	6,6,6	0.57	0
3	SO4	F	402	-	4,4,4	0.79	0	6,6,6	0.60	0
4	SPD	Q	401	-	9,9,9	0.43	0	8,8,8	0.91	0
3	SO4	C	402	-	4,4,4	0.81	0	6,6,6	0.56	0
3	SO4	H	401	-	4,4,4	0.79	0	6,6,6	0.56	0
3	SO4	C	403	-	4,4,4	0.80	0	6,6,6	0.55	0
3	SO4	J	403	-	4,4,4	0.78	0	6,6,6	0.53	0
3	SO4	O	403	-	4,4,4	0.79	0	6,6,6	0.60	0
3	SO4	M	403	-	4,4,4	0.80	0	6,6,6	0.55	0
3	SO4	O	405	-	4,4,4	0.76	0	6,6,6	0.51	0
4	SPD	E	405	-	9,9,9	0.41	0	8,8,8	0.90	0
4	SPD	K	404	-	9,9,9	0.40	0	8,8,8	0.83	0
4	SPD	N	407	-	9,9,9	0.41	0	8,8,8	1.07	0
3	SO4	D	403	-	4,4,4	0.80	0	6,6,6	0.55	0
3	SO4	N	405	-	4,4,4	0.79	0	6,6,6	0.57	0
3	SO4	G	402	-	4,4,4	0.81	0	6,6,6	0.58	0
3	SO4	J	402	-	4,4,4	0.79	0	6,6,6	0.52	0
3	SO4	L	401	-	4,4,4	0.77	0	6,6,6	0.54	0
4	SPD	P	401	-	9,9,9	0.42	0	8,8,8	1.23	2 (25%)
4	SPD	L	404	-	9,9,9	0.41	0	8,8,8	1.33	2 (25%)
3	SO4	K	401	-	4,4,4	0.77	0	6,6,6	0.58	0
3	SO4	F	403	-	4,4,4	0.79	0	6,6,6	0.57	0
3	SO4	L	402	-	4,4,4	0.82	0	6,6,6	0.65	0
4	SPD	D	404	-	9,9,9	0.42	0	8,8,8	1.09	1 (12%)
3	SO4	E	404	-	4,4,4	0.79	0	6,6,6	0.60	0
3	SO4	I	401	-	4,4,4	0.79	0	6,6,6	0.57	0
3	SO4	O	404	-	4,4,4	0.79	0	6,6,6	0.56	0
3	SO4	A	402	-	4,4,4	0.80	0	6,6,6	0.61	0
3	SO4	R	402	-	4,4,4	0.79	0	6,6,6	0.56	0
4	SPD	H	403	-	9,9,9	0.42	0	8,8,8	1.01	0
3	SO4	B	401	-	4,4,4	0.78	0	6,6,6	0.58	0
3	SO4	I	402	-	4,4,4	0.79	0	6,6,6	0.54	0
3	SO4	N	402	-	4,4,4	0.79	0	6,6,6	0.56	0
3	SO4	O	401	-	4,4,4	0.76	0	6,6,6	0.64	0
3	SO4	O	406	-	4,4,4	0.78	0	6,6,6	0.56	0
3	SO4	B	403	-	4,4,4	0.80	0	6,6,6	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	E	401	-	4,4,4	0.80	0	6,6,6	0.60	0
3	SO4	G	401	-	4,4,4	0.80	0	6,6,6	0.54	0
3	SO4	K	402	-	4,4,4	0.75	0	6,6,6	0.57	0
3	SO4	N	404	-	4,4,4	0.80	0	6,6,6	0.55	0
3	SO4	D	401	-	4,4,4	0.78	0	6,6,6	0.57	0
3	SO4	A	401	-	4,4,4	0.79	0	6,6,6	0.57	0
3	SO4	R	401	-	4,4,4	0.76	0	6,6,6	0.59	0
4	SPD	B	405	-	9,9,9	0.41	0	8,8,8	0.85	0
4	SPD	M	404	-	9,9,9	0.42	0	8,8,8	0.89	0
4	SPD	R	404	-	9,9,9	0.40	0	8,8,8	1.13	1 (12%)
4	SPD	J	404	-	9,9,9	0.42	0	8,8,8	1.04	0
3	SO4	I	403	-	4,4,4	0.75	0	6,6,6	0.58	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	SPD	G	403	-	-	5/7/7/7	-
4	SPD	A	404	-	-	4/7/7/7	-
4	SPD	O	407	-	-	3/7/7/7	-
4	SPD	H	403	-	-	3/7/7/7	-
4	SPD	C	404	-	-	3/7/7/7	-
4	SPD	Q	401	-	-	3/7/7/7	-
4	SPD	N	407	-	-	5/7/7/7	-
4	SPD	P	401	-	-	3/7/7/7	-
4	SPD	R	404	-	-	4/7/7/7	-
4	SPD	B	405	-	-	5/7/7/7	-
4	SPD	E	405	-	-	6/7/7/7	-
4	SPD	L	404	-	-	4/7/7/7	-
4	SPD	M	404	-	-	4/7/7/7	-
4	SPD	J	404	-	-	6/7/7/7	-
4	SPD	K	404	-	-	5/7/7/7	-
4	SPD	D	404	-	-	3/7/7/7	-
4	SPD	F	404	-	-	3/7/7/7	-
4	SPD	I	404	-	-	3/7/7/7	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	404	SPD	C7-C8-C9	-2.39	105.54	114.28
4	R	404	SPD	C4-C5-N6	-2.33	105.84	112.14
4	P	401	SPD	C4-C5-N6	-2.22	106.14	112.14
4	L	404	SPD	C4-C5-N6	-2.22	106.15	112.14
4	P	401	SPD	C8-C7-N6	-2.18	106.26	112.14

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	405	SPD	N6-C7-C8-C9
4	P	401	SPD	N6-C7-C8-C9
4	J	404	SPD	C3-C4-C5-N6
4	O	407	SPD	C3-C4-C5-N6
4	D	404	SPD	C3-C4-C5-N6

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)

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	335/340 (98%)	0.34	3 (0%) 84 83	35, 45, 60, 64	0
1	B	335/340 (98%)	0.33	3 (0%) 84 83	33, 47, 62, 71	0
1	C	335/340 (98%)	0.39	4 (1%) 79 77	34, 45, 58, 62	0
1	D	335/340 (98%)	0.36	1 (0%) 94 93	33, 45, 58, 65	0
1	E	335/340 (98%)	0.38	8 (2%) 59 57	35, 47, 60, 65	0
1	F	335/340 (98%)	0.33	4 (1%) 79 77	35, 47, 61, 71	0
1	G	335/340 (98%)	0.38	2 (0%) 89 89	34, 43, 51, 59	0
1	H	335/340 (98%)	0.35	5 (1%) 73 72	34, 44, 52, 59	0
1	I	335/340 (98%)	0.48	11 (3%) 46 45	37, 50, 72, 78	0
1	J	335/340 (98%)	0.46	14 (4%) 36 35	38, 52, 73, 77	0
1	K	335/340 (98%)	0.49	15 (4%) 33 33	36, 52, 72, 78	0
1	L	335/340 (98%)	0.64	23 (6%) 16 18	63, 73, 84, 87	0
1	M	335/340 (98%)	0.36	6 (1%) 68 67	34, 44, 52, 63	0
1	N	335/340 (98%)	0.59	23 (6%) 16 18	62, 74, 82, 86	0
1	O	335/340 (98%)	0.67	34 (10%) 7 8	62, 72, 82, 86	0
1	P	335/340 (98%)	0.59	27 (8%) 12 13	62, 72, 82, 88	0
1	Q	335/340 (98%)	0.66	26 (7%) 13 14	62, 74, 84, 89	0
1	R	335/340 (98%)	0.66	34 (10%) 7 8	61, 73, 84, 90	0
2	a	225/258 (87%)	0.49	6 (2%) 54 53	44, 56, 64, 75	0
2	b	225/258 (87%)	0.43	6 (2%) 54 53	38, 45, 59, 89	0
2	c	225/258 (87%)	0.53	7 (3%) 49 48	42, 52, 61, 82	0
2	d	225/258 (87%)	0.46	6 (2%) 54 53	42, 52, 61, 74	0
2	e	225/258 (87%)	0.53	8 (3%) 42 42	38, 45, 59, 102	0
2	f	225/258 (87%)	0.42	4 (1%) 68 67	39, 46, 61, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	g	225/258 (87%)	0.50	12 (5%) 26 27	46, 53, 66, 79	0
2	h	225/258 (87%)	0.39	4 (1%) 68 67	46, 55, 67, 85	0
2	i	225/258 (87%)	0.50	5 (2%) 62 60	40, 49, 68, 102	0
2	j	225/258 (87%)	0.52	12 (5%) 26 27	43, 50, 70, 106	0
2	k	225/258 (87%)	0.49	7 (3%) 49 48	42, 49, 69, 103	0
2	l	225/258 (87%)	1.72	78 (34%) 0 0	80, 102, 121, 126	0
2	m	225/258 (87%)	0.45	9 (4%) 38 37	46, 53, 65, 79	0
2	n	225/258 (87%)	0.76	18 (8%) 12 13	59, 72, 84, 102	0
2	o	225/258 (87%)	1.08	46 (20%) 1 1	44, 56, 64, 75	0
2	p	225/258 (87%)	1.06	44 (19%) 1 1	44, 56, 64, 75	0
2	q	225/258 (87%)	0.81	22 (9%) 7 9	58, 73, 85, 102	0
2	r	225/258 (87%)	0.88	28 (12%) 4 5	56, 72, 83, 103	0
All	All	10080/10764 (93%)	0.55	565 (5%) 24 25	33, 53, 81, 126	0

The worst 5 of 565 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	l	38	TRP	9.2
2	l	36	ILE	5.6
2	l	16	PRO	5.6
2	l	243	LEU	5.6
2	o	73	THR	5.5

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)

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
3	SO4	O	405	5/5	0.80	0.37	85,85,85,85	0
4	SPD	L	404	10/10	0.80	0.60	67,67,67,68	0
4	SPD	R	404	10/10	0.80	0.51	67,68,68,68	0
3	SO4	R	403	5/5	0.83	0.28	85,86,86,86	0
3	SO4	O	403	5/5	0.83	0.27	88,88,88,88	0
3	SO4	O	402	5/5	0.83	0.19	92,92,93,93	0
3	SO4	R	402	5/5	0.84	0.20	90,90,90,91	0
4	SPD	N	407	10/10	0.84	0.40	67,67,67,67	0
4	SPD	Q	401	10/10	0.84	0.45	64,65,66,66	0
3	SO4	L	401	5/5	0.84	0.20	83,83,83,84	0
3	SO4	N	404	5/5	0.85	0.27	93,93,94,94	0
3	SO4	N	403	5/5	0.86	0.21	83,83,83,83	0
3	SO4	O	406	5/5	0.87	0.22	85,85,86,86	0
4	SPD	D	404	10/10	0.88	0.30	38,38,39,39	0
4	SPD	P	401	10/10	0.88	0.41	65,65,65,65	0
4	SPD	O	407	10/10	0.89	0.30	67,67,67,67	0
3	SO4	I	401	5/5	0.89	0.28	76,76,76,76	0
3	SO4	F	402	5/5	0.90	0.32	65,65,66,66	0
4	SPD	F	404	10/10	0.90	0.41	39,39,39,39	0
3	SO4	N	406	5/5	0.90	0.15	90,90,90,90	0
4	SPD	A	404	10/10	0.90	0.35	38,38,38,38	0
3	SO4	N	405	5/5	0.91	0.17	86,86,86,86	0
3	SO4	N	402	5/5	0.91	0.21	87,87,87,87	0
3	SO4	O	401	5/5	0.91	0.26	95,95,95,95	0
4	SPD	J	404	10/10	0.92	0.37	45,45,46,46	0
3	SO4	N	401	5/5	0.92	0.25	88,88,88,88	0
3	SO4	K	401	5/5	0.92	0.19	79,79,80,80	0
3	SO4	J	401	5/5	0.92	0.18	76,76,76,76	0
4	SPD	E	405	10/10	0.92	0.34	39,39,39,39	0
3	SO4	L	402	5/5	0.92	0.17	93,93,93,93	0
4	SPD	H	403	10/10	0.92	0.41	37,37,37,37	0
4	SPD	M	404	10/10	0.93	0.46	36,36,36,37	0
3	SO4	L	403	5/5	0.93	0.18	84,84,84,84	0
3	SO4	G	401	5/5	0.93	0.19	50,50,50,50	0
3	SO4	D	401	5/5	0.93	0.22	57,57,57,57	0
4	SPD	C	404	10/10	0.93	0.27	39,40,40,40	0
3	SO4	C	401	5/5	0.93	0.18	60,60,60,61	0
3	SO4	R	401	5/5	0.94	0.21	89,89,89,89	0
3	SO4	M	401	5/5	0.94	0.18	47,47,47,47	0
3	SO4	H	401	5/5	0.94	0.20	49,49,50,50	0
4	SPD	G	403	10/10	0.94	0.39	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	J	402	5/5	0.94	0.20	66,66,66,66	0
3	SO4	I	403	5/5	0.94	0.22	51,51,51,51	0
4	SPD	K	404	10/10	0.94	0.48	45,45,45,45	0
3	SO4	J	403	5/5	0.95	0.23	54,55,55,55	0
4	SPD	B	405	10/10	0.95	0.42	39,40,40,40	0
3	SO4	B	402	5/5	0.95	0.15	64,64,64,64	0
3	SO4	D	402	5/5	0.95	0.19	55,55,55,55	0
3	SO4	E	403	5/5	0.95	0.17	51,51,51,51	0
3	SO4	A	402	5/5	0.95	0.19	54,54,54,54	0
3	SO4	C	402	5/5	0.95	0.18	53,53,53,53	0
3	SO4	M	403	5/5	0.95	0.24	53,53,54,54	0
4	SPD	I	404	10/10	0.95	0.45	45,45,46,46	0
3	SO4	E	402	5/5	0.96	0.22	60,60,60,60	0
3	SO4	C	403	5/5	0.96	0.16	52,52,52,52	0
3	SO4	M	402	5/5	0.96	0.20	51,51,51,51	0
3	SO4	E	404	5/5	0.96	0.17	56,56,56,56	0
3	SO4	A	401	5/5	0.96	0.17	56,57,57,57	0
3	SO4	B	403	5/5	0.96	0.19	52,52,52,52	0
3	SO4	G	402	5/5	0.96	0.15	49,49,50,50	0
3	SO4	E	401	5/5	0.96	0.16	52,52,52,52	0
3	SO4	H	402	5/5	0.96	0.17	52,52,52,52	0
3	SO4	B	404	5/5	0.97	0.16	54,54,54,54	0
3	SO4	I	402	5/5	0.97	0.11	66,66,66,66	0
3	SO4	F	403	5/5	0.97	0.16	56,56,56,56	0
3	SO4	A	403	5/5	0.97	0.14	54,55,55,55	0
3	SO4	B	401	5/5	0.97	0.18	54,54,54,54	0
3	SO4	D	403	5/5	0.97	0.15	50,51,51,51	0
3	SO4	O	404	5/5	0.97	0.28	92,92,92,92	0
3	SO4	F	401	5/5	0.97	0.17	53,53,53,54	0
3	SO4	K	402	5/5	0.97	0.13	63,63,63,64	0
3	SO4	K	403	5/5	0.97	0.21	56,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.