Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

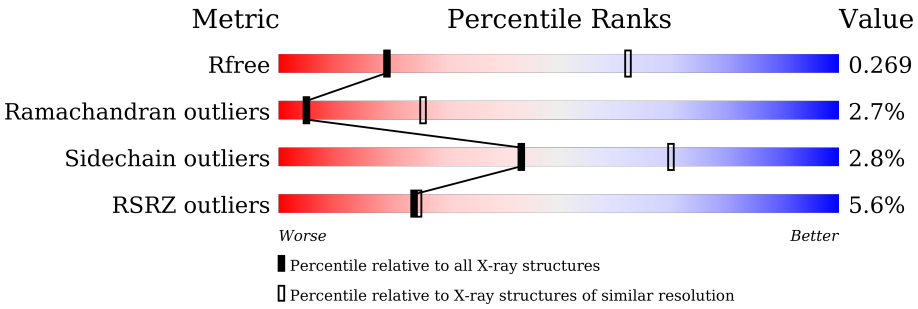
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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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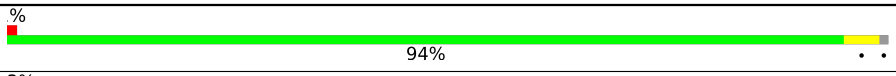
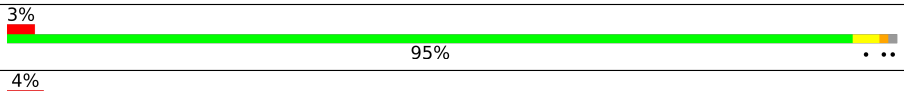
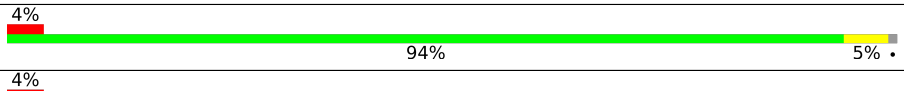
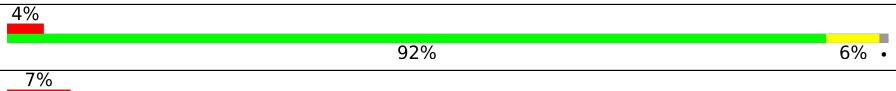
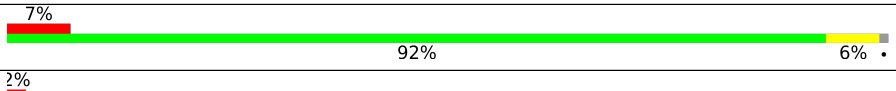
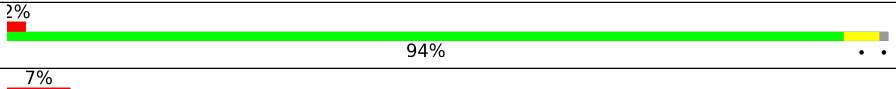
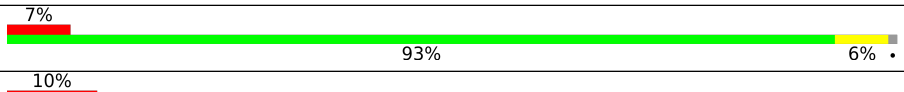
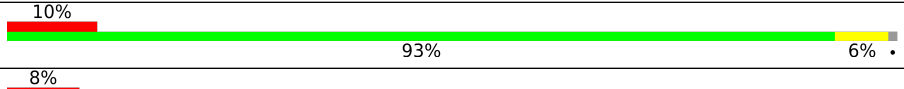
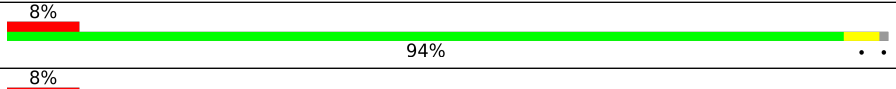
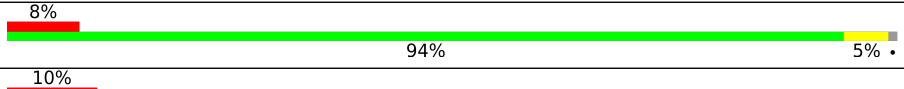
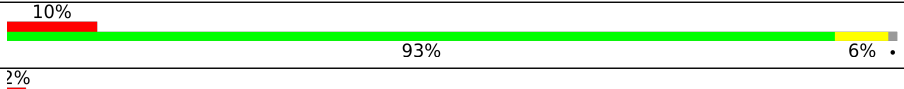
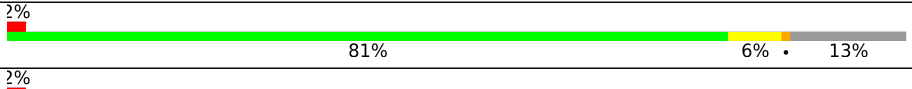
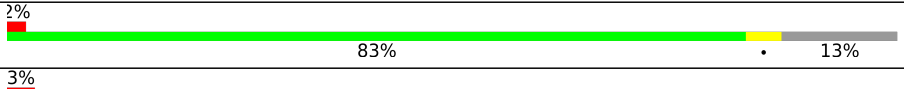
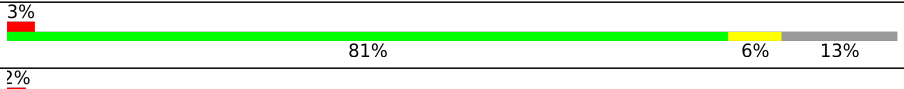
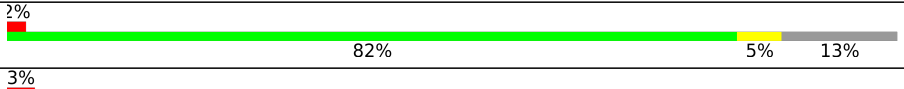
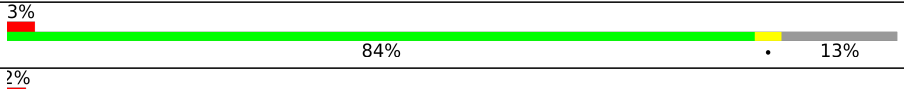
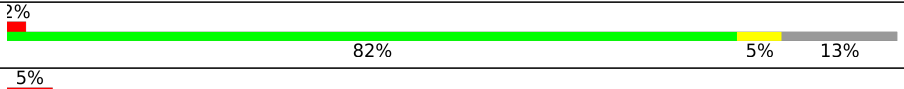
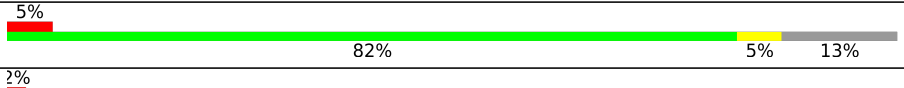
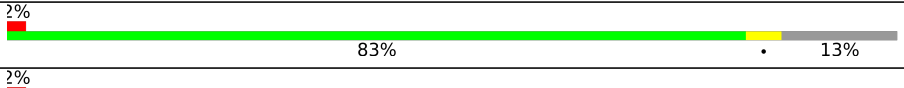
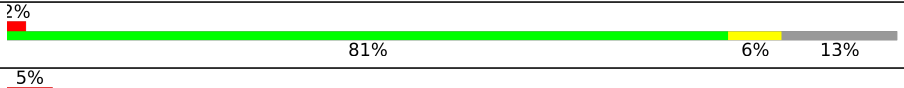
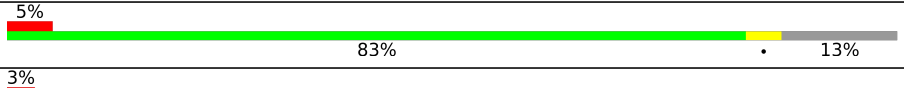
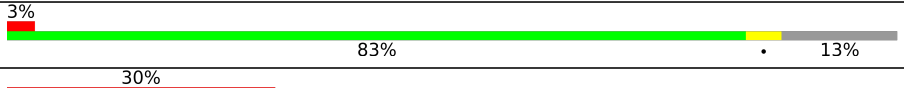
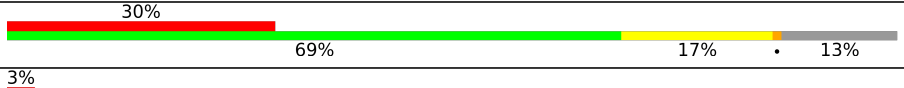
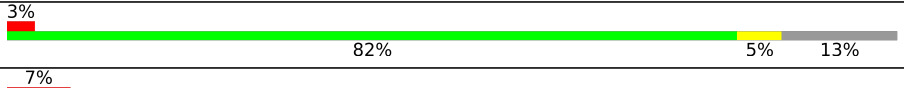
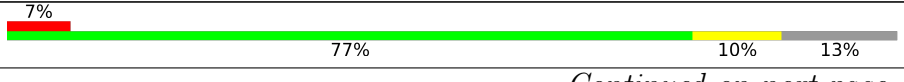
Mol	Chain	Length	Quality of chain
1	H	340	
1	I	340	
1	J	340	
1	K	340	
1	L	340	
1	M	340	
1	N	340	
1	O	340	
1	P	340	
1	Q	340	
1	R	340	
2	a	258	
2	b	258	
2	c	258	
2	d	258	
2	e	258	
2	f	258	
2	g	258	
2	h	258	
2	i	258	
2	j	258	
2	k	258	
2	l	258	
2	m	258	
2	n	258	

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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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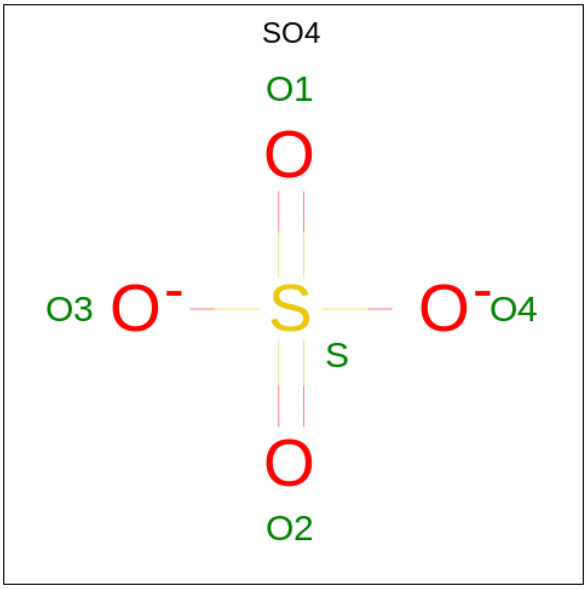
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	m	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	n	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	o	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	p	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	q	225	Total	C	N	O	S	0	0	0
			1699	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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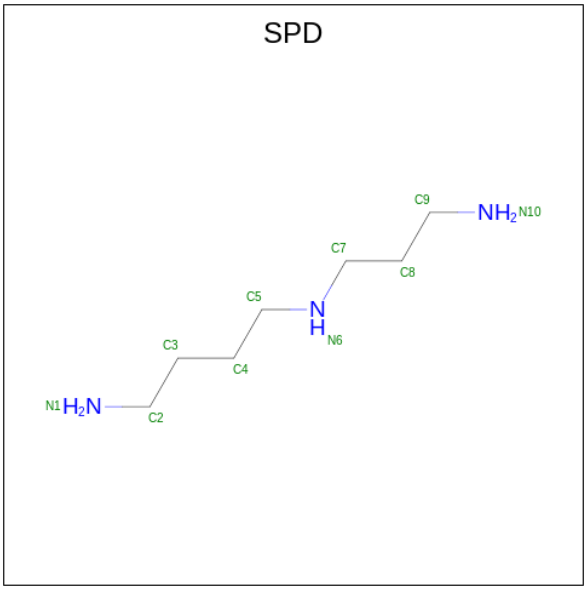
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0
3	R	1	Total O S 5 4 1	0	0
3	R	1	Total O S 5 4 1	0	0
3	R	1	Total O S 5 4 1	0	0

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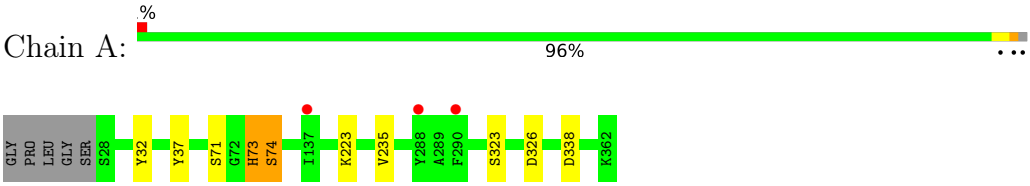
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C N 10 7 3	0	0
4	F	1	Total C N 10 7 3	0	0
4	G	1	Total C N 10 7 3	0	0
4	H	1	Total C N 10 7 3	0	0
4	I	1	Total C N 10 7 3	0	0
4	J	1	Total C N 10 7 3	0	0
4	K	1	Total C N 10 7 3	0	0
4	L	1	Total C N 10 7 3	0	0
4	M	1	Total C N 10 7 3	0	0
4	N	1	Total C N 10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

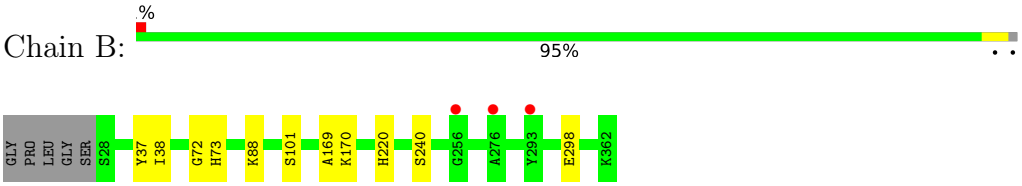
• Molecule 1: Polyamine transport protein

Chain A:



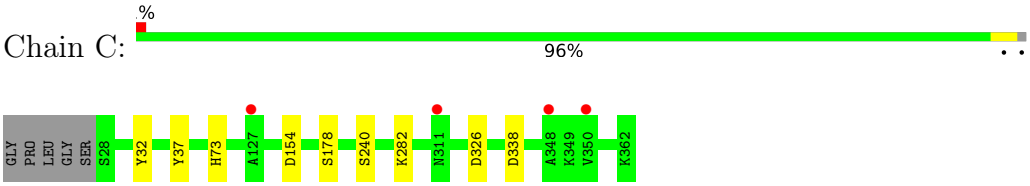
• Molecule 1: Polyamine transport protein

Chain B:



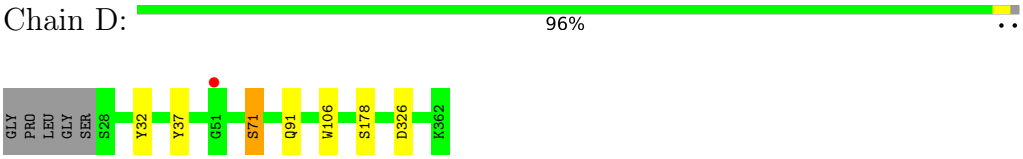
• Molecule 1: Polyamine transport protein

Chain C:



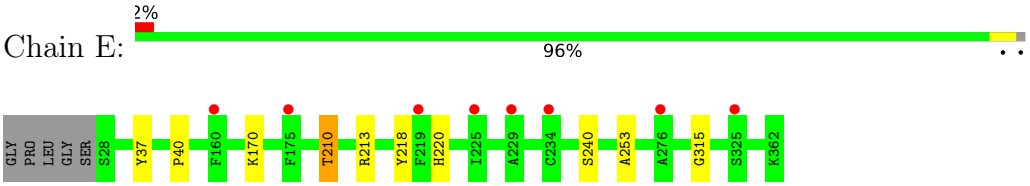
• Molecule 1: Polyamine transport protein

Chain D:



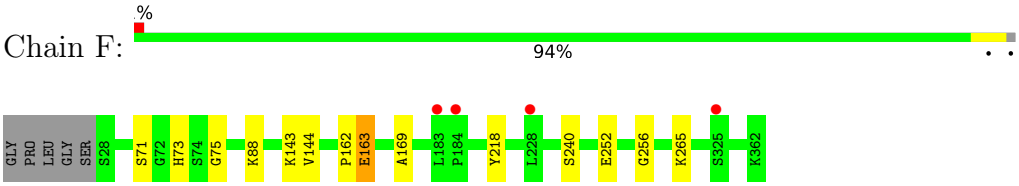
• Molecule 1: Polyamine transport protein

Chain E:



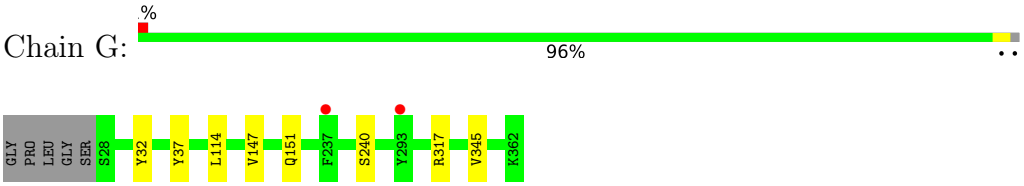
• Molecule 1: Polyamine transport protein

Chain F:



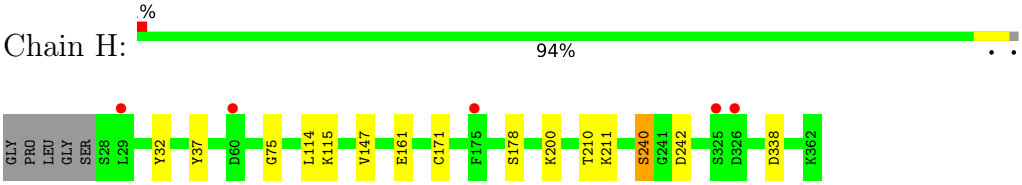
• Molecule 1: Polyamine transport protein

Chain G:



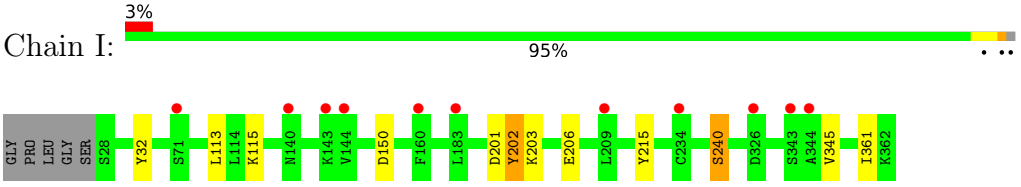
• Molecule 1: Polyamine transport protein

Chain H:



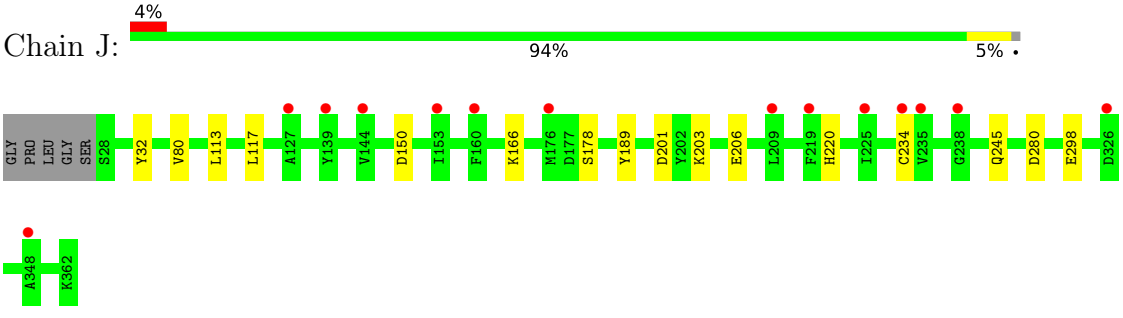
• Molecule 1: Polyamine transport protein

Chain I:



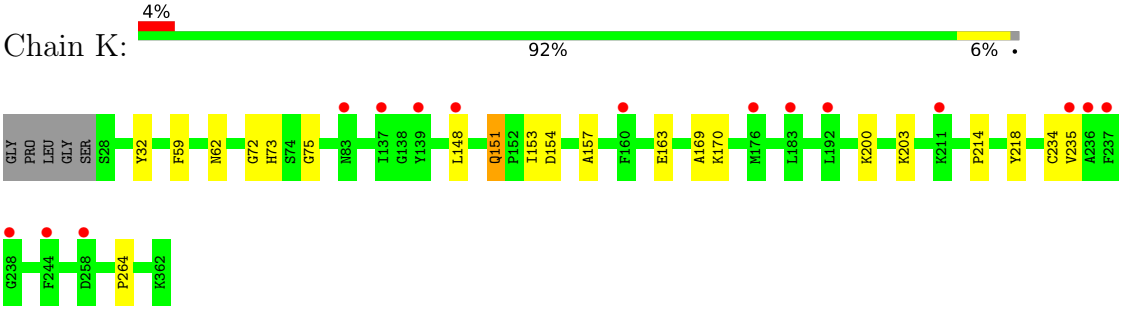
• Molecule 1: Polyamine transport protein

Chain J:



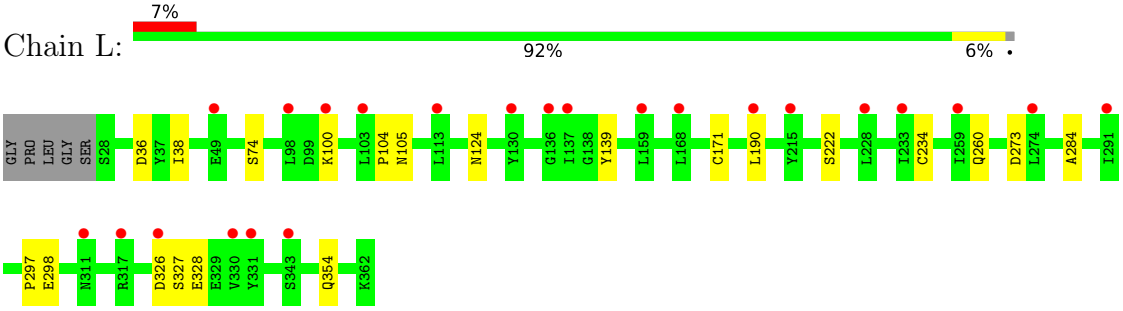
• Molecule 1: Polyamine transport protein

Chain K:



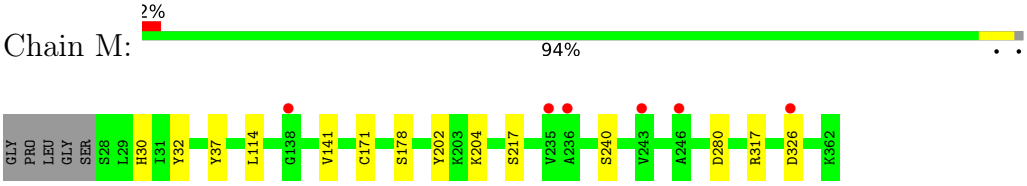
• Molecule 1: Polyamine transport protein

Chain L:



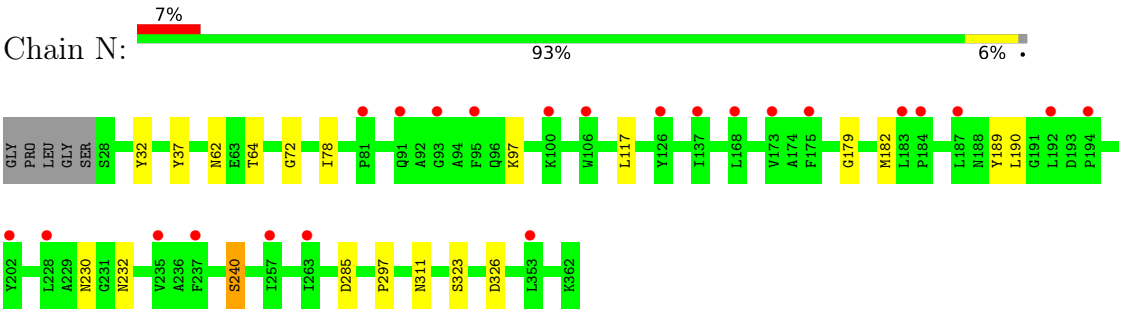
• Molecule 1: Polyamine transport protein

Chain M:



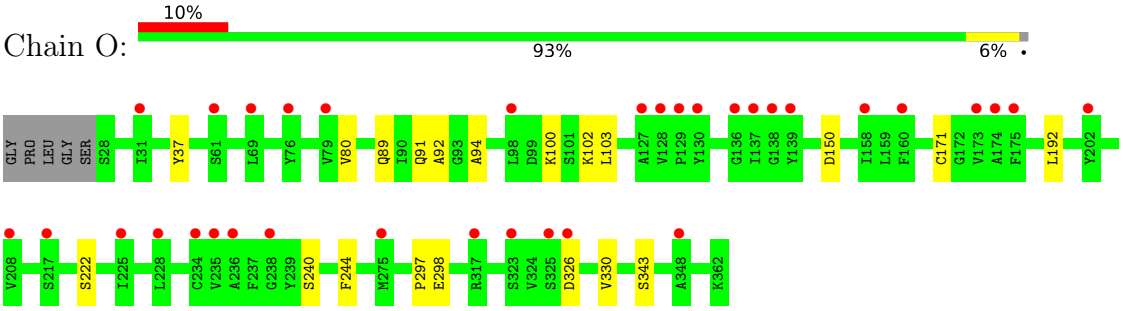
• Molecule 1: Polyamine transport protein

Chain N:



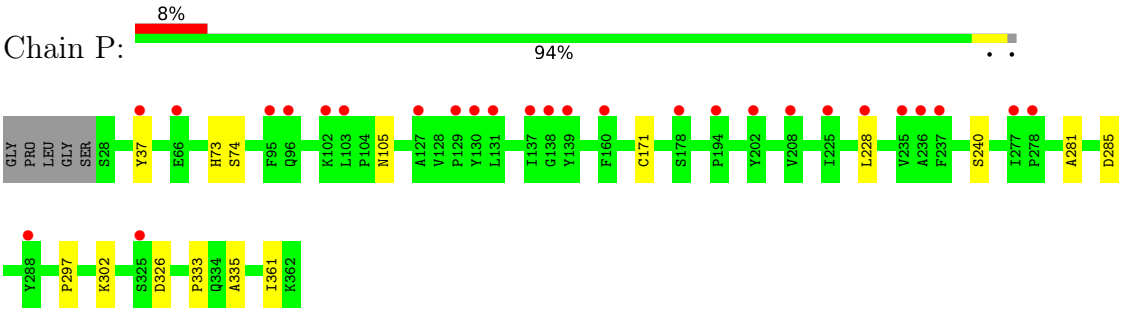
• Molecule 1: Polyamine transport protein

Chain O:



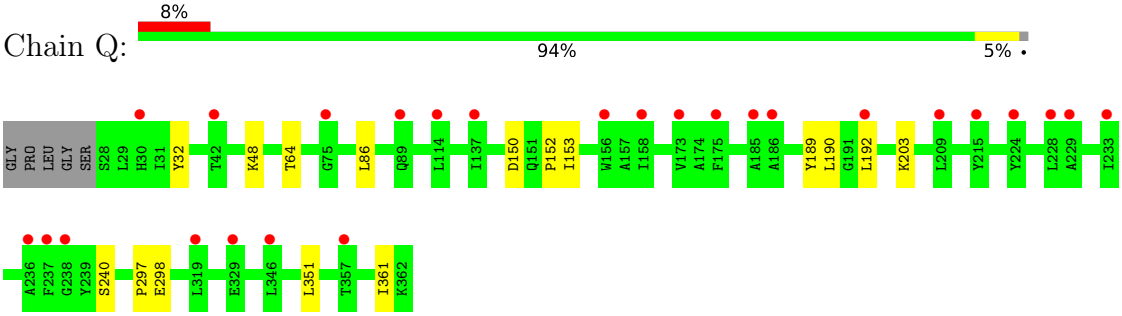
• Molecule 1: Polyamine transport protein

Chain P:



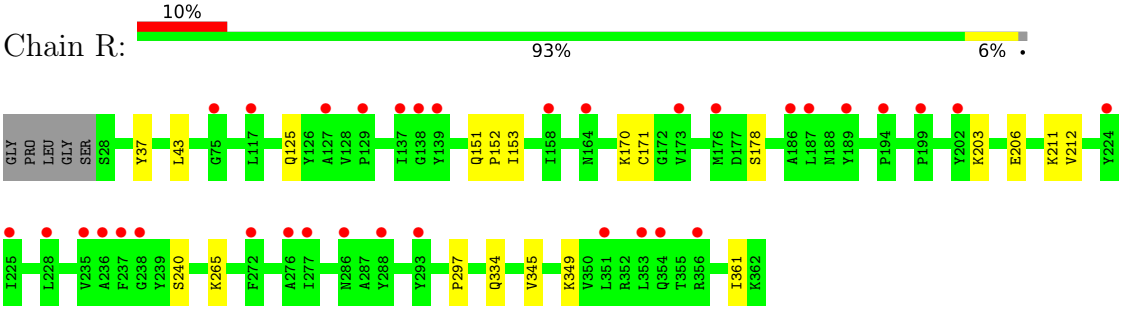
• Molecule 1: Polyamine transport protein

Chain Q:



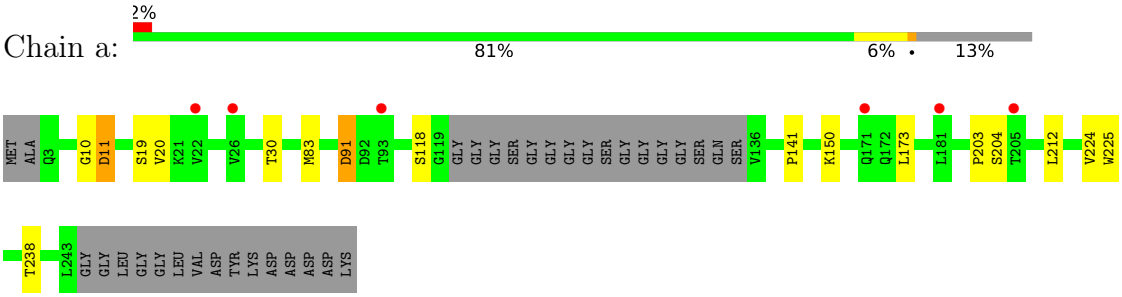
• Molecule 1: Polyamine transport protein

Chain R:



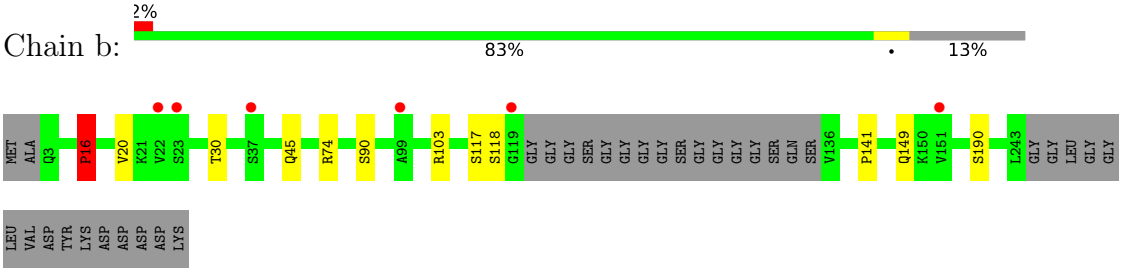
• Molecule 2: ScFv5

Chain a:



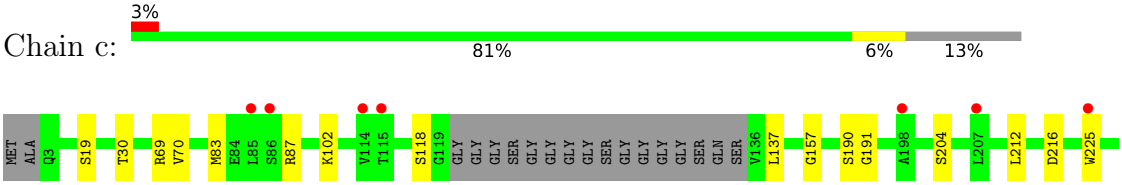
• Molecule 2: ScFv5

Chain b:



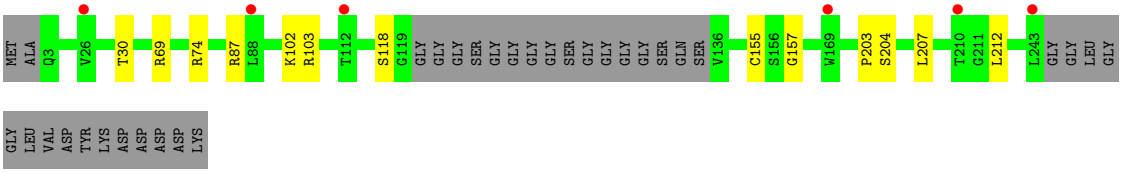
• Molecule 2: ScFv5

Chain c:



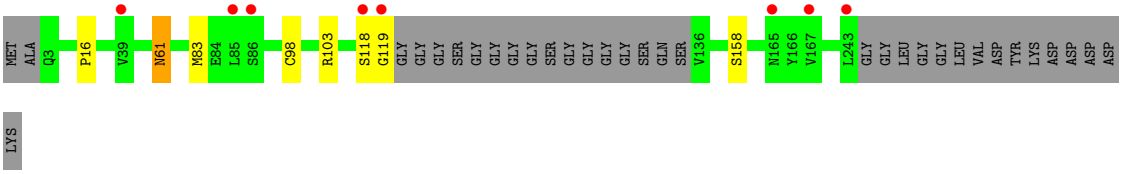
• Molecule 2: ScFv5

Chain d:



• Molecule 2: ScFv5

Chain e:

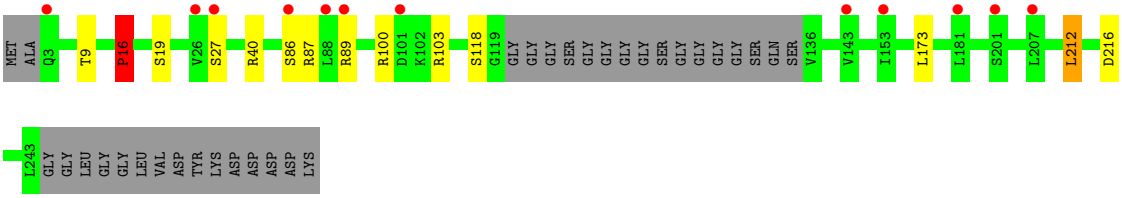


• Molecule 2: ScFv5

Chain f:

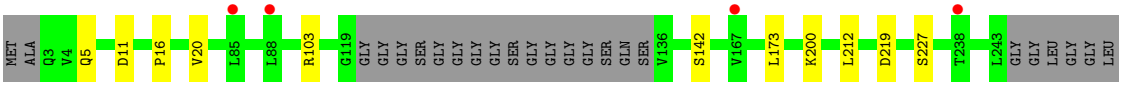
• Molecule 2: ScFv5

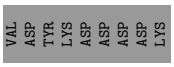
Chain g:



• Molecule 2: ScFv5

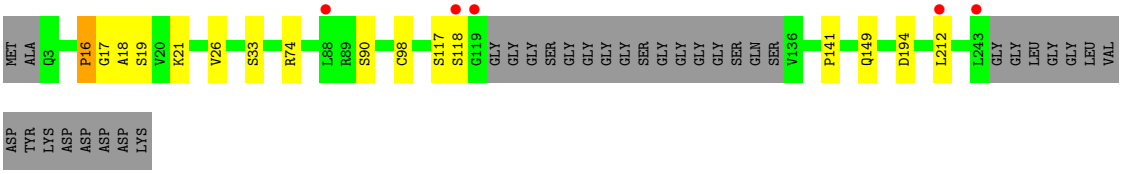
Chain h:





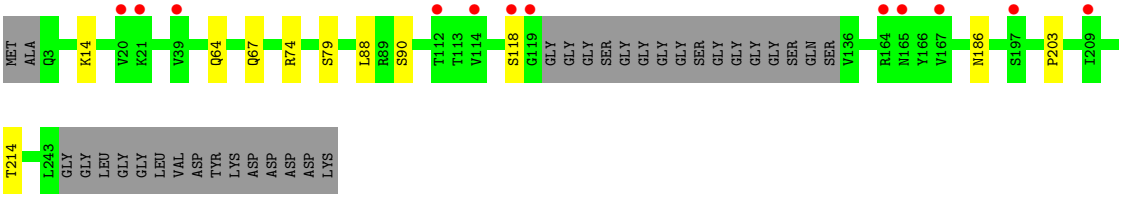
• Molecule 2: ScFv5

Chain i:



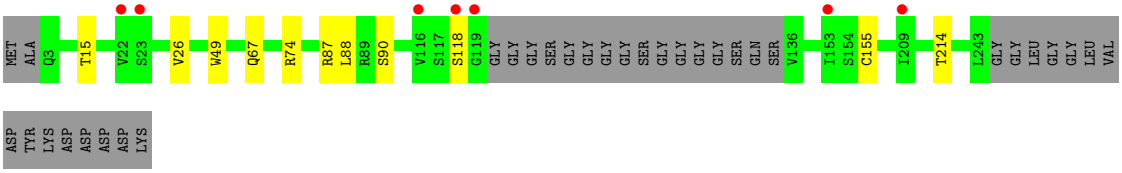
• Molecule 2: ScFv5

Chain j:



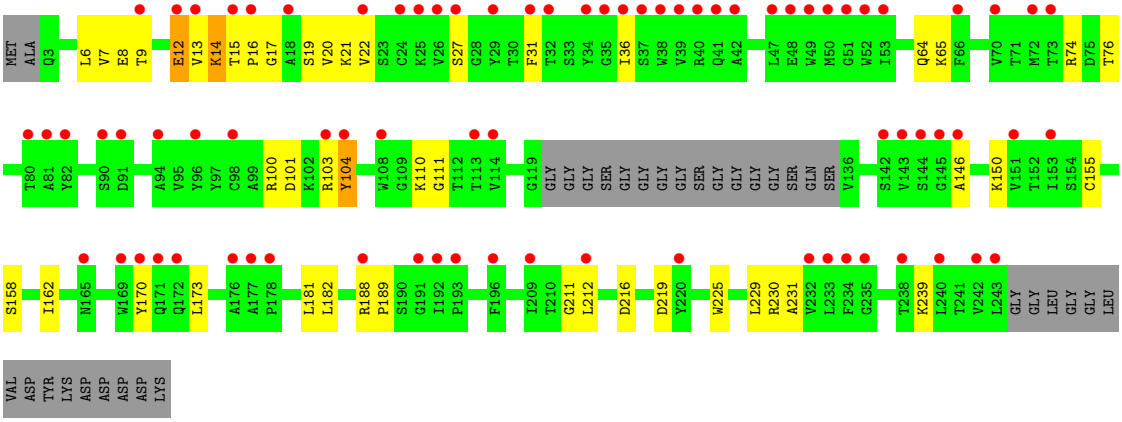
• Molecule 2: ScFv5

Chain k:



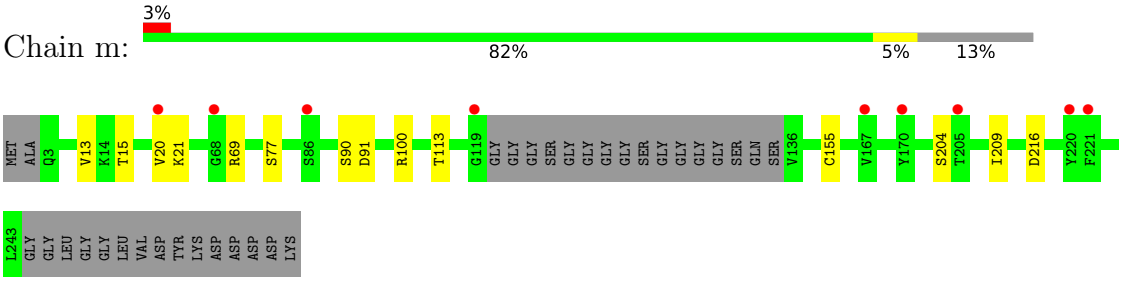
• Molecule 2: ScFv5

Chain l:



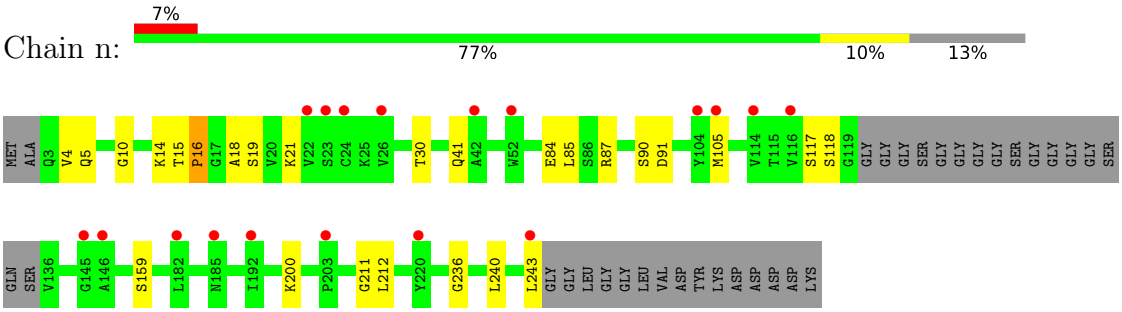
• Molecule 2: ScFv5

Chain m:



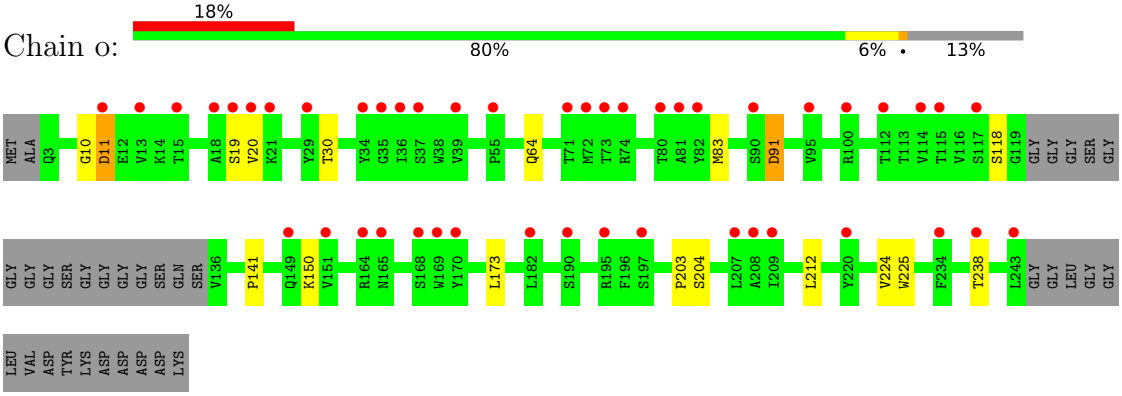
• Molecule 2: ScFv5

Chain n:



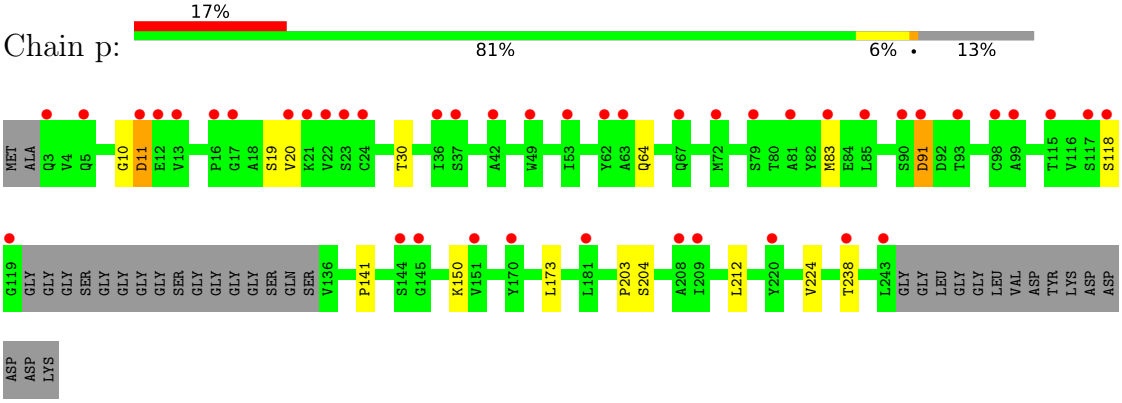
• Molecule 2: ScFv5

Chain o:



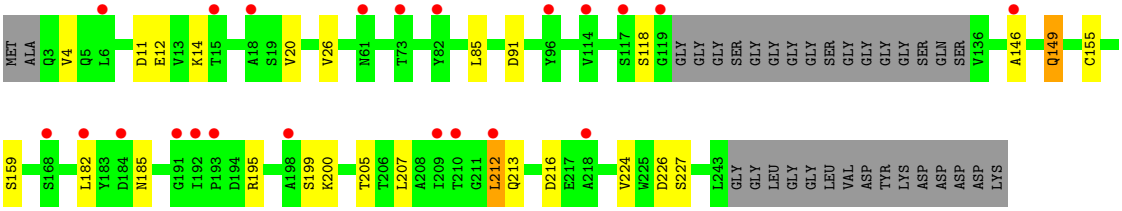
• Molecule 2: ScFv5

Chain p:

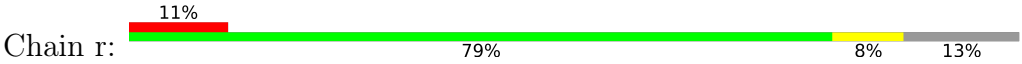


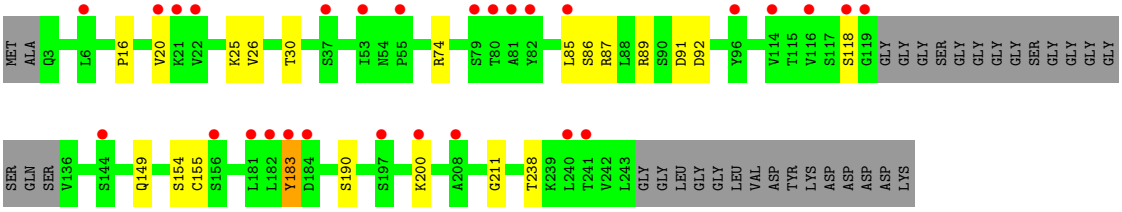
• Molecule 2: ScFv5

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

5.1 Standard geometry

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

All (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
1	I	345	VAL	CB-CG2	8.10	1.69	1.52
2	f	26	VAL	CB-CG2	7.87	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	345	VAL	CB-CG1	7.46	1.68	1.52
2	i	26	VAL	CB-CG1	7.19	1.68	1.52
1	I	202	TYR	CD2-CE2	-7.04	1.28	1.39
1	O	330	VAL	CB-CG2	6.57	1.66	1.52
1	K	235	VAL	CB-CG2	6.48	1.66	1.52
2	l	12	GLU	CB-CG	6.38	1.64	1.52
1	G	147	VAL	CB-CG2	5.42	1.64	1.52
2	c	19	SER	CA-CB	-5.38	1.44	1.52
1	Q	203	LYS	CE-NZ	5.25	1.62	1.49
2	o	238	THR	CB-CG2	5.25	1.69	1.52
2	p	238	THR	CB-CG2	5.24	1.69	1.52
2	a	238	THR	CB-CG2	5.24	1.69	1.52
1	F	144	VAL	CB-CG2	5.23	1.63	1.52
2	p	224	VAL	CB-CG1	5.19	1.63	1.52
2	a	224	VAL	CB-CG1	5.18	1.63	1.52
2	o	224	VAL	CB-CG1	5.17	1.63	1.52
1	J	80	VAL	CB-CG2	5.16	1.63	1.52
2	q	224	VAL	CB-CG2	5.11	1.63	1.52
2	c	70	VAL	CB-CG2	5.02	1.63	1.52

All (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
1	O	80	VAL	CG1-CB-CG2	11.13	128.70	110.90
2	l	181	LEU	CB-CG-CD2	-10.72	92.78	111.00
1	O	103	LEU	CB-CG-CD2	-10.31	93.47	111.00
1	I	345	VAL	CG1-CB-CG2	10.02	126.93	110.90
1	H	147	VAL	CG1-CB-CG2	8.64	124.72	110.90
2	q	212	LEU	CA-CB-CG	7.22	131.91	115.30
2	k	26	VAL	CG1-CB-CG2	7.16	122.36	110.90
1	I	202	TYR	CB-CG-CD2	-7.00	116.80	121.00
2	q	227	SER	CA-C-N	6.80	132.15	117.20
2	r	183	TYR	CB-CG-CD2	-6.79	116.92	121.00
2	i	26	VAL	CG1-CB-CG2	6.75	121.70	110.90
2	r	183	TYR	CB-CG-CD1	6.75	125.05	121.00
2	n	240	LEU	CB-CG-CD1	6.71	122.40	111.00
2	n	240	LEU	CB-CG-CD2	-6.70	99.60	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	c	83	MET	CB-CG-SD	6.52	131.97	112.40
2	l	181	LEU	CA-CB-CG	-6.46	100.45	115.30
2	d	207	LEU	CA-CB-CG	6.40	130.02	115.30
2	f	212	LEU	CA-CB-CG	6.25	129.67	115.30
2	j	14	LYS	C-N-CA	5.86	136.35	121.70
2	g	16	PRO	N-CA-C	5.85	127.31	112.10
2	o	224	VAL	CG1-CB-CG2	5.80	120.18	110.90
2	a	224	VAL	CG1-CB-CG2	5.78	120.14	110.90
2	p	224	VAL	CG1-CB-CG2	5.77	120.13	110.90
2	q	227	SER	CA-C-O	-5.75	108.03	120.10
2	r	92	ASP	CB-CG-OD1	-5.63	113.23	118.30
2	a	238	THR	OG1-CB-CG2	5.57	122.81	110.00
2	p	238	THR	OG1-CB-CG2	5.57	122.80	110.00
2	o	238	THR	OG1-CB-CG2	5.55	122.77	110.00
2	c	70	VAL	CG1-CB-CG2	-5.54	102.03	110.90
1	G	147	VAL	CG1-CB-CG2	5.53	119.75	110.90
1	K	235	VAL	CG1-CB-CG2	5.51	119.71	110.90
2	b	16	PRO	N-CA-CB	-5.43	96.62	102.60
2	l	173	LEU	CA-CB-CG	5.43	127.79	115.30
2	q	85	LEU	CA-CB-CG	5.42	127.77	115.30
1	E	210	THR	OG1-CB-CG2	5.42	122.46	110.00
1	I	206	GLU	CA-CB-CG	5.36	125.19	113.40
1	E	213	ARG	NE-CZ-NH1	-5.35	117.62	120.30
2	n	243	LEU	CA-CB-CG	5.33	127.56	115.30
1	P	228	LEU	CA-CB-CG	5.19	127.24	115.30
2	r	85	LEU	CB-CG-CD1	-5.12	102.30	111.00
2	q	182	LEU	CB-CG-CD2	-5.10	102.34	111.00
2	n	212	LEU	CA-CB-CG	5.09	127.00	115.30
2	m	209	ILE	CG1-CB-CG2	-5.07	100.24	111.40
1	O	150	ASP	C-N-CA	-5.03	109.13	121.70
1	M	280	ASP	CB-CG-OD1	-5.03	113.78	118.30
1	E	210	THR	CA-CB-CG2	5.02	119.43	112.40
2	l	229	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	73	HIS	Peptide
1	I	203	LYS	Peptide
1	I	361	ILE	Peptide
1	K	169	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	L	273	ASP	Peptide
1	M	202	TYR	Peptide
1	P	333	PRO	Peptide
1	P	361	ILE	Peptide
1	R	361	ILE	Peptide
2	a	10	GLY	Peptide
2	a	11	ASP	Peptide
2	b	117	SER	Peptide
2	c	157	GLY	Peptide
2	d	157	GLY	Peptide
2	g	86	SER	Peptide
2	l	101	ASP	Peptide
2	l	219	ASP	Peptide
2	l	36	ILE	Peptide
2	m	216	ASP	Peptide
2	m	90	SER	Peptide
2	n	84	GLU	Peptide
2	n	90	SER	Peptide
2	o	10	GLY	Peptide
2	o	11	ASP	Peptide
2	p	10	GLY	Peptide
2	p	11	ASP	Peptide
2	q	212	LEU	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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

All (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
2	c	118	SER
2	d	118	SER
2	d	155	CYS
2	e	61	ASN
2	e	118	SER
1	F	73	HIS
1	F	163	GLU
2	g	9	THR
2	g	118	SER
1	H	114	LEU
2	h	103	ARG
2	h	212	LEU
2	i	16	PRO
1	J	201	ASP
1	J	206	GLU
2	j	88	LEU
2	j	90	SER
2	j	118	SER
1	L	36	ASP
1	L	38	ILE
1	L	105	ASN
1	L	297	PRO
1	L	298	GLU
1	L	328	GLU
2	l	6	LEU
2	l	9	THR
2	l	12	GLU

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Mol	Chain	Res	Type
2	l	14	LYS
2	l	15	THR
2	l	22	VAL
2	l	27	SER
2	l	104	TYR
2	l	146	ALA
2	l	150	LYS
2	l	162	ILE
2	l	216	ASP
2	l	239	LYS
2	m	91	ASP
1	N	232	ASN
1	N	240	SER
2	n	30	THR
2	n	41	GLN
2	n	87	ARG
2	n	91	ASP
2	n	105	MET
2	n	118	SER
1	O	91	GLN
1	O	94	ALA
1	O	297	PRO
1	O	298	GLU
2	o	118	SER
1	P	74	SER
1	P	335	ALA
2	p	118	SER
2	q	4	VAL
2	q	11	ASP
2	q	12	GLU
2	q	118	SER
2	q	149	GLN
2	q	155	CYS
2	q	200	LYS
1	R	170	LYS
2	r	16	PRO
2	r	87	ARG
2	r	149	GLN
2	r	155	CYS
2	a	212	LEU
1	B	72	GLY
1	B	169	ALA

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Mol	Chain	Res	Type
1	B	240	SER
2	b	30	THR
2	b	103	ARG
2	c	30	THR
2	c	190	SER
2	d	103	ARG
1	E	253	ALA
2	e	103	ARG
1	F	75	GLY
1	F	252	GLU
2	f	103	ARG
1	G	114	LEU
2	g	16	PRO
2	g	27	SER
1	H	171	CYS
1	H	240	SER
2	h	227	SER
1	I	201	ASP
2	i	90	SER
2	i	149	GLN
2	j	214	THR
1	K	72	GLY
1	K	75	GLY
1	K	153	ILE
2	k	87	ARG
2	k	88	LEU
2	k	90	SER
2	k	214	THR
1	L	74	SER
1	L	104	PRO
1	L	124	ASN
1	L	190	LEU
1	L	284	ALA
1	L	327	SER
2	l	8	GLU
2	l	17	GLY
2	l	65	LYS
2	l	76	THR
2	l	103	ARG
2	l	111	GLY
2	l	231	ALA
1	M	114	LEU

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Mol	Chain	Res	Type
1	M	204	LYS
1	N	117	LEU
2	n	10	GLY
2	n	19	SER
2	n	236	GLY
2	o	212	LEU
1	P	281	ALA
2	p	212	LEU
1	Q	64	THR
1	Q	190	LEU
1	Q	351	LEU
2	q	91	ASP
2	q	185	ASN
1	R	153	ILE
1	R	203	LYS
1	A	323	SER
2	a	19	SER
2	a	30	THR
1	C	338	ASP
2	c	87	ARG
1	D	71	SER
1	D	91	GLN
2	d	69	ARG
1	E	315	GLY
1	F	169	ALA
1	G	240	SER
2	g	103	ARG
1	H	338	ASP
2	h	5	GLN
2	h	16	PRO
1	I	240	SER
2	i	17	GLY
1	J	150	ASP
1	J	166	LYS
1	J	298	GLU
1	K	151	GLN
1	K	170	LYS
2	k	49	TRP
2	k	67	GLN
2	k	118	SER
1	L	100	LYS
1	L	326	ASP

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Mol	Chain	Res	Type
2	l	31	PHE
2	l	211	GLY
2	l	212	LEU
2	l	230	ARG
1	M	141	VAL
1	M	240	SER
2	m	69	ARG
1	N	64	THR
1	N	190	LEU
2	n	5	GLN
2	n	16	PRO
2	n	18	ALA
2	n	159	SER
1	O	100	LYS
1	O	192	LEU
2	o	19	SER
2	o	30	THR
1	P	297	PRO
2	p	19	SER
2	p	30	THR
1	R	43	LEU
1	R	212	VAL
2	r	30	THR
2	r	91	ASP
1	A	74	SER
2	a	203	PRO
1	C	178	SER
1	D	106	TRP
2	d	30	THR
1	E	210	THR
1	F	240	SER
2	h	200	LYS
2	i	18	ALA
2	i	19	SER
1	J	117	LEU
2	j	79	SER
2	j	186	ASN
1	L	222	SER
2	l	7	VAL
2	l	64	GLN
1	N	78	ILE
1	O	89	GLN

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Mol	Chain	Res	Type
1	O	92	ALA
1	O	222	SER
2	o	203	PRO
2	p	203	PRO
2	q	226	ASP
1	B	298	GLU
2	c	69	ARG
2	c	212	LEU
2	d	87	ARG
2	d	212	LEU
1	E	240	SER
1	I	150	ASP
1	J	178	SER
1	J	280	ASP
1	K	148	LEU
1	K	157	ALA
2	l	16	PRO
2	l	189	PRO
1	M	178	SER
2	m	113	THR
1	N	182	MET
1	N	311	ASN
2	n	200	LYS
1	P	105	ASN
1	P	240	SER
1	Q	192	LEU
2	q	159	SER
1	R	152	PRO
1	R	206	GLU
1	R	211	LYS
2	r	20	VAL
2	r	118	SER
1	C	154	ASP
1	C	240	SER
1	D	178	SER
1	G	345	VAL
1	H	75	GLY
1	H	178	SER
1	H	210	THR
2	i	118	SER
1	N	179	GLY
1	N	297	PRO

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Mol	Chain	Res	Type
2	n	211	GLY
1	Q	297	PRO
1	Q	298	GLU
2	r	211	GLY
2	c	191	GLY
1	F	256	GLY
1	Q	153	ILE
2	q	146	ALA
1	R	297	PRO
1	B	38	ILE
2	l	13	VAL
1	N	72	GLY
1	Q	361	ILE
2	b	141	PRO
2	d	203	PRO
1	K	214	PRO
2	n	4	VAL
2	q	26	VAL
2	r	26	VAL
1	A	235	VAL
2	a	141	PRO
1	F	162	PRO
2	j	203	PRO
1	K	264	PRO
2	o	141	PRO
2	p	141	PRO
1	Q	152	PRO
1	E	40	PRO
2	i	141	PRO
2	q	20	VAL
1	R	345	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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

All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
1	A	37	TYR
1	A	71	SER
1	A	73	HIS
1	A	74	SER
1	A	223	LYS
1	A	326	ASP
2	a	11	ASP
2	a	20	VAL
2	a	83	MET
2	a	91	ASP
2	a	150	LYS
2	a	173	LEU
2	a	204	SER
2	a	225	TRP
1	B	37	TYR
1	B	73	HIS
1	B	88	LYS
1	B	101	SER
1	B	170	LYS
1	B	220	HIS
2	b	16	PRO
2	b	20	VAL
2	b	45	GLN
2	b	74	ARG
2	b	149	GLN
2	b	190	SER
1	C	32	TYR
1	C	37	TYR

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Mol	Chain	Res	Type
1	C	73	HIS
1	C	282	LYS
1	C	326	ASP
2	c	102	LYS
2	c	137	LEU
2	c	204	SER
2	c	216	ASP
2	c	225	TRP
1	D	32	TYR
1	D	37	TYR
1	D	71	SER
1	D	326	ASP
2	d	74	ARG
2	d	102	LYS
2	d	204	SER
1	E	37	TYR
1	E	170	LYS
1	E	218	TYR
1	E	220	HIS
2	e	16	PRO
2	e	61	ASN
2	e	83	MET
2	e	98	CYS
2	e	158	SER
1	F	71	SER
1	F	88	LYS
1	F	143	LYS
1	F	218	TYR
1	F	265	LYS
2	f	14	LYS
2	f	16	PRO
2	f	20	VAL
2	f	74	ARG
2	f	77	SER
2	f	98	CYS
2	f	155	CYS
2	f	201	SER
2	f	228	SER
1	G	32	TYR
1	G	37	TYR
1	G	151	GLN
1	G	317	ARG

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Mol	Chain	Res	Type
2	g	16	PRO
2	g	19	SER
2	g	40	ARG
2	g	87	ARG
2	g	89	ARG
2	g	100	ARG
2	g	173	LEU
2	g	212	LEU
2	g	216	ASP
1	H	32	TYR
1	H	37	TYR
1	H	115	LYS
1	H	200	LYS
1	H	211	LYS
1	H	240	SER
1	H	242	ASP
2	h	11	ASP
2	h	20	VAL
2	h	173	LEU
2	h	219	ASP
1	I	32	TYR
1	I	113	LEU
1	I	115	LYS
1	I	202	TYR
1	I	215	TYR
1	I	240	SER
2	i	16	PRO
2	i	21	LYS
2	i	33	SER
2	i	74	ARG
2	i	98	CYS
2	i	117	SER
2	i	194	ASP
2	i	212	LEU
1	J	32	TYR
1	J	113	LEU
1	J	189	TYR
1	J	203	LYS
1	J	220	HIS
1	J	234	CYS
1	J	245	GLN
2	j	64	GLN

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Mol	Chain	Res	Type
2	j	67	GLN
2	j	74	ARG
1	K	32	TYR
1	K	59	PHE
1	K	62	ASN
1	K	73	HIS
1	K	151	GLN
1	K	154	ASP
1	K	163	GLU
1	K	200	LYS
1	K	203	LYS
1	K	218	TYR
1	K	234	CYS
2	k	15	THR
2	k	74	ARG
2	k	155	CYS
1	L	139	TYR
1	L	171	CYS
1	L	234	CYS
1	L	260	GLN
1	L	354	GLN
2	l	14	LYS
2	l	19	SER
2	l	20	VAL
2	l	21	LYS
2	l	74	ARG
2	l	100	ARG
2	l	104	TYR
2	l	110	LYS
2	l	155	CYS
2	l	158	SER
2	l	170	TYR
2	l	182	LEU
2	l	188	ARG
2	l	225	TRP
1	M	30	HIS
1	M	32	TYR
1	M	37	TYR
1	M	171	CYS
1	M	217	SER
1	M	317	ARG
1	M	326	ASP

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Mol	Chain	Res	Type
2	m	13	VAL
2	m	15	THR
2	m	20	VAL
2	m	21	LYS
2	m	77	SER
2	m	100	ARG
2	m	155	CYS
2	m	204	SER
1	N	32	TYR
1	N	37	TYR
1	N	62	ASN
1	N	97	LYS
1	N	189	TYR
1	N	230	ASN
1	N	240	SER
1	N	285	ASP
1	N	323	SER
1	N	326	ASP
2	n	14	LYS
2	n	15	THR
2	n	16	PRO
2	n	21	LYS
2	n	117	SER
1	O	37	TYR
1	O	102	LYS
1	O	171	CYS
1	O	240	SER
1	O	244	PHE
1	O	326	ASP
1	O	343	SER
2	o	11	ASP
2	o	20	VAL
2	o	83	MET
2	o	91	ASP
2	o	150	LYS
2	o	173	LEU
2	o	204	SER
2	o	225	TRP
1	P	37	TYR
1	P	73	HIS
1	P	171	CYS
1	P	285	ASP

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Mol	Chain	Res	Type
1	P	302	LYS
1	P	326	ASP
2	p	11	ASP
2	p	20	VAL
2	p	83	MET
2	p	91	ASP
2	p	150	LYS
2	p	173	LEU
2	p	204	SER
1	Q	32	TYR
1	Q	48	LYS
1	Q	86	LEU
1	Q	150	ASP
1	Q	189	TYR
1	Q	240	SER
2	q	14	LYS
2	q	149	GLN
2	q	195	ARG
2	q	199	SER
2	q	205	THR
2	q	207	LEU
2	q	213	GLN
2	q	216	ASP
1	R	37	TYR
1	R	125	GLN
1	R	151	GLN
1	R	171	CYS
1	R	178	SER
1	R	240	SER
1	R	265	LYS
1	R	334	GLN
1	R	349	LYS
2	r	25	LYS
2	r	74	ARG
2	r	86	SER
2	r	89	ARG
2	r	154	SER
2	r	183	TYR
2	r	190	SER
2	r	200	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	a	54	ASN
1	D	220	HIS
1	E	230	ASN
2	e	54	ASN
1	G	232	ASN
2	g	185	ASN
2	i	139	GLN
1	J	62	ASN
2	j	3	GLN
1	K	164	ASN
2	l	149	GLN
1	M	151	GLN
1	M	232	ASN
2	m	56	ASN
2	m	64	GLN
1	N	89	GLN
2	n	5	GLN
2	n	41	GLN
2	n	54	ASN
1	O	62	ASN
1	O	105	ASN
2	o	64	GLN
2	p	64	GLN
2	q	149	GLN
2	r	149	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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.

All (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
4	L	404	SPD	C8-C7-N6	-2.08	106.52	112.14

There are no chirality outliers.

All (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

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Mol	Chain	Res	Type	Atoms
4	D	404	SPD	C3-C4-C5-N6
4	P	401	SPD	C3-C4-C5-N6
4	A	404	SPD	C3-C4-C5-N6
4	F	404	SPD	N6-C7-C8-C9
4	B	405	SPD	C3-C4-C5-N6
4	J	404	SPD	N6-C7-C8-C9
4	R	404	SPD	C8-C7-N6-C5
4	H	403	SPD	N6-C7-C8-C9
4	K	404	SPD	N6-C7-C8-C9
4	O	407	SPD	N6-C7-C8-C9
4	Q	401	SPD	N6-C7-C8-C9
4	G	403	SPD	N6-C7-C8-C9
4	G	403	SPD	C4-C5-N6-C7
4	I	404	SPD	C8-C7-N6-C5
4	J	404	SPD	C8-C7-N6-C5
4	L	404	SPD	C8-C7-N6-C5
4	L	404	SPD	C3-C4-C5-N6
4	N	407	SPD	C8-C7-N6-C5
4	K	404	SPD	C3-C4-C5-N6
4	N	407	SPD	C3-C4-C5-N6
4	G	403	SPD	C7-C8-C9-N10
4	H	403	SPD	C7-C8-C9-N10
4	I	404	SPD	C7-C8-C9-N10
4	N	407	SPD	C7-C8-C9-N10
4	O	407	SPD	C7-C8-C9-N10
4	P	401	SPD	C7-C8-C9-N10
4	R	404	SPD	C7-C8-C9-N10
4	G	403	SPD	C3-C4-C5-N6
4	K	404	SPD	N1-C2-C3-C4
4	R	404	SPD	C3-C4-C5-N6
4	Q	401	SPD	C2-C3-C4-C5
4	Q	401	SPD	C4-C5-N6-C7
4	J	404	SPD	C2-C3-C4-C5
4	K	404	SPD	C2-C3-C4-C5
4	M	404	SPD	C3-C4-C5-N6
4	M	404	SPD	C2-C3-C4-C5
4	A	404	SPD	C8-C7-N6-C5
4	B	405	SPD	C7-C8-C9-N10
4	L	404	SPD	C7-C8-C9-N10
4	B	405	SPD	C8-C7-N6-C5
4	F	404	SPD	C4-C5-N6-C7
4	L	404	SPD	C4-C5-N6-C7

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Mol	Chain	Res	Type	Atoms
4	H	403	SPD	C8-C7-N6-C5
4	A	404	SPD	N1-C2-C3-C4
4	R	404	SPD	N1-C2-C3-C4
4	C	404	SPD	N1-C2-C3-C4
4	D	404	SPD	N1-C2-C3-C4
4	G	403	SPD	N1-C2-C3-C4
4	M	404	SPD	N1-C2-C3-C4
4	B	405	SPD	N6-C7-C8-C9
4	E	405	SPD	C8-C7-N6-C5
4	N	407	SPD	C4-C5-N6-C7
4	C	404	SPD	C7-C8-C9-N10
4	A	404	SPD	C2-C3-C4-C5
4	B	405	SPD	N1-C2-C3-C4
4	N	407	SPD	N1-C2-C3-C4
4	I	404	SPD	C4-C5-N6-C7
4	J	404	SPD	C4-C5-N6-C7
4	K	404	SPD	C8-C7-N6-C5
4	F	404	SPD	C8-C7-N6-C5
4	E	405	SPD	N1-C2-C3-C4
4	E	405	SPD	C7-C8-C9-N10
4	M	404	SPD	C7-C8-C9-N10
4	D	404	SPD	C4-C5-N6-C7
4	J	404	SPD	N1-C2-C3-C4
4	E	405	SPD	C3-C4-C5-N6
4	C	404	SPD	C3-C4-C5-N6
4	E	405	SPD	C4-C5-N6-C7

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

All (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
2	j	118	SER	5.3
2	l	82	TYR	5.3
2	o	117	SER	5.1
2	l	234	PHE	5.0
2	l	47	LEU	4.9
2	p	243	LEU	4.9
2	n	192	ILE	4.9
1	R	138	GLY	4.9
1	R	354	GLN	4.8
2	o	170	TYR	4.8
2	l	9	THR	4.8
2	p	90	SER	4.7
2	a	26	VAL	4.4
2	l	193	PRO	4.4
2	e	119	GLY	4.4
1	P	236	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
2	k	119	GLY	4.4
2	l	196	PHE	4.2
2	l	18	ALA	4.2
2	l	232	VAL	4.2
2	r	80	THR	4.1
2	l	212	LEU	4.1
2	o	208	ALA	4.1
1	I	144	VAL	4.1
2	p	220	TYR	4.1
2	p	13	VAL	4.0
2	l	24	CYS	4.0
2	o	13	VAL	3.9
2	o	114	VAL	3.9
2	l	48	GLU	3.9
2	l	90	SER	3.9
1	L	100	LYS	3.9
2	l	40	ARG	3.9
1	P	288	TYR	3.9
2	l	12	GLU	3.8
2	o	112	THR	3.8
2	l	34	TYR	3.8
2	l	53	ILE	3.8
1	I	343	SER	3.8
1	O	175	PHE	3.8
1	P	235	VAL	3.8
2	l	39	VAL	3.7
2	q	191	GLY	3.7
2	r	81	ALA	3.7
2	k	22	VAL	3.7
2	q	119	GLY	3.7
2	l	37	SER	3.7
2	r	119	GLY	3.7
2	p	117	SER	3.7
2	n	23	SER	3.6
1	P	96	GLN	3.6
2	o	18	ALA	3.6
1	N	183	LEU	3.6
1	J	160	PHE	3.6
1	O	76	TYR	3.6
2	l	72	MET	3.6
1	R	127	ALA	3.6
2	p	63	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	l	66	PHE	3.5
2	l	171	GLN	3.5
1	K	258	ASP	3.5
1	O	174	ALA	3.5
2	o	115	THR	3.5
2	h	88	LEU	3.5
2	o	81	ALA	3.4
2	q	6	LEU	3.4
1	O	138	GLY	3.4
1	N	202	TYR	3.4
2	l	25	LYS	3.4
2	o	39	VAL	3.4
2	l	15	THR	3.4
2	l	96	TYR	3.4
2	o	90	SER	3.4
2	p	23	SER	3.4
1	L	259	ILE	3.4
2	f	119	GLY	3.4
1	N	168	LEU	3.4
2	l	108	TRP	3.4
1	P	237	PHE	3.4
2	l	50	MET	3.4
2	l	191	GLY	3.4
1	J	235	VAL	3.3
2	l	178	PRO	3.3
2	l	51	GLY	3.3
2	r	118	SER	3.3
2	l	31	PHE	3.3
2	o	149	GLN	3.3
1	O	348	ALA	3.3
2	l	73	THR	3.3
1	N	93	GLY	3.3
2	p	151	VAL	3.3
2	c	86	SER	3.3
2	o	197	SER	3.3
2	l	192	ILE	3.3
2	l	13	VAL	3.3
2	p	20	VAL	3.3
2	r	55	PRO	3.3
2	p	16	PRO	3.3
1	L	136	GLY	3.3
2	p	36	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	O	127	ALA	3.2
2	q	18	ALA	3.2
1	R	236	ALA	3.2
1	L	228	LEU	3.2
2	l	153	ILE	3.2
2	p	12	GLU	3.2
2	n	185	ASN	3.2
2	o	207	LEU	3.2
2	o	243	LEU	3.2
1	O	325	SER	3.2
2	l	52	TRP	3.2
1	J	209	LEU	3.1
2	l	26	VAL	3.1
1	I	209	LEU	3.1
1	R	187	LEU	3.1
2	l	27	SER	3.1
1	Q	175	PHE	3.1
2	g	153	ILE	3.1
2	i	119	GLY	3.1
2	r	20	VAL	3.1
1	L	343	SER	3.1
1	I	234	CYS	3.1
2	l	49	TRP	3.0
1	P	103	LEU	3.0
2	k	118	SER	3.0
2	c	114	VAL	3.0
2	p	99	ALA	3.0
2	n	26	VAL	3.0
2	o	11	ASP	3.0
1	O	234	CYS	3.0
2	m	119	GLY	3.0
1	Q	237	PHE	3.0
2	l	32	THR	3.0
2	q	114	VAL	3.0
1	P	228	LEU	3.0
2	l	238	THR	3.0
1	J	219	PHE	3.0
2	k	23	SER	3.0
1	R	194	PRO	3.0
2	q	198	ALA	3.0
2	e	39	VAL	3.0
2	q	146	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	j	164	ARG	2.9
2	l	242	VAL	2.9
1	N	194	PRO	2.9
1	O	130	TYR	2.9
2	r	184	ASP	2.9
1	N	228	LEU	2.9
1	O	160	PHE	2.9
2	p	208	ALA	2.9
1	Q	346	LEU	2.9
2	n	243	LEU	2.9
2	o	82	TYR	2.9
2	o	238	THR	2.9
2	p	72	MET	2.9
2	q	210	THR	2.9
2	l	29	TYR	2.9
2	p	115	THR	2.9
1	L	291	ILE	2.9
2	r	96	TYR	2.9
1	Q	114	LEU	2.9
2	l	114	VAL	2.9
2	g	86	SER	2.9
2	r	6	LEU	2.9
2	l	22	VAL	2.8
2	l	233	LEU	2.8
2	m	68	GLY	2.8
2	o	37	SER	2.8
2	l	91	ASP	2.8
2	l	81	ALA	2.8
2	l	170	TYR	2.8
1	R	237	PHE	2.8
2	r	208	ALA	2.8
2	l	209	ILE	2.8
1	I	326	ASP	2.8
2	o	169	TRP	2.8
2	g	88	LEU	2.8
2	l	145	GLY	2.8
1	J	225	ILE	2.8
2	o	74	ARG	2.8
2	p	85	LEU	2.8
2	p	145	GLY	2.8
1	O	129	PRO	2.8
2	r	79	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	R	276	ALA	2.7
1	R	199	PRO	2.7
2	l	80	THR	2.7
1	O	275	MET	2.7
1	Q	30	HIS	2.7
1	R	117	LEU	2.7
2	m	167	VAL	2.7
2	k	153	ILE	2.7
1	O	69	LEU	2.7
1	L	331	TYR	2.7
1	N	173	VAL	2.7
2	m	20	VAL	2.7
1	N	81	PRO	2.7
2	n	105	MET	2.7
2	h	238	THR	2.7
1	L	330	VAL	2.7
1	L	233	ILE	2.7
2	l	35	GLY	2.7
2	o	151	VAL	2.7
1	I	183	LEU	2.7
2	p	3	GLN	2.7
1	P	138	GLY	2.7
1	O	236	ALA	2.7
1	N	100	LYS	2.7
1	Q	329	GLU	2.7
2	p	24	CYS	2.7
2	n	182	LEU	2.7
2	r	182	LEU	2.7
1	I	71	SER	2.6
2	o	220	TYR	2.6
1	N	106	TRP	2.6
2	p	83	MET	2.6
2	n	146	ALA	2.6
1	R	129	PRO	2.6
2	g	3	GLN	2.6
2	o	72	MET	2.6
2	l	103	ARG	2.6
1	J	234	CYS	2.6
1	N	126	TYR	2.6
1	N	137	ILE	2.6
2	l	220	TYR	2.6
2	p	93	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	238	GLY	2.6
2	m	86	SER	2.6
2	l	240	LEU	2.6
2	n	203	PRO	2.6
2	d	26	VAL	2.6
1	J	176	MET	2.6
1	O	225	ILE	2.6
1	R	351	LEU	2.6
2	f	88	LEU	2.6
1	E	225	ILE	2.6
1	O	98	LEU	2.6
1	Q	158	ILE	2.6
2	r	53	ILE	2.6
2	l	143	VAL	2.6
2	n	145	GLY	2.6
1	R	228	LEU	2.6
1	N	175	PHE	2.6
1	J	139	TYR	2.6
1	Q	186	ALA	2.6
1	J	144	VAL	2.6
2	o	35	GLY	2.5
2	r	241	THR	2.5
2	q	82	TYR	2.5
2	a	22	VAL	2.5
2	q	212	LEU	2.5
2	o	165	ASN	2.5
1	R	293	TYR	2.5
2	o	34	TYR	2.5
1	P	131	LEU	2.5
2	c	85	LEU	2.5
2	b	23	SER	2.5
2	p	53	ILE	2.5
1	O	202	TYR	2.5
1	R	137	ILE	2.5
1	R	238	GLY	2.5
2	r	144	SER	2.5
1	R	235	VAL	2.5
2	p	21	LYS	2.5
1	K	139	TYR	2.5
2	p	11	ASP	2.5
2	r	116	VAL	2.5
1	K	148	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	49	GLU	2.5
1	B	276	ALA	2.5
2	n	42	ALA	2.5
2	p	119	GLY	2.5
1	Q	89	GLN	2.5
1	D	51	GLY	2.5
1	L	274	LEU	2.5
1	R	186	ALA	2.5
2	c	198	ALA	2.5
2	j	119	GLY	2.5
2	n	22	VAL	2.5
2	o	20	VAL	2.5
2	o	168	SER	2.5
2	p	79	SER	2.5
1	E	234	CYS	2.5
2	o	71	THR	2.5
1	P	202	TYR	2.5
1	H	326	ASP	2.5
1	L	137	ILE	2.5
1	O	31	ILE	2.5
1	K	83	ASN	2.4
1	J	348	ALA	2.4
1	N	95	PHE	2.4
1	O	137	ILE	2.4
1	K	235	VAL	2.4
2	d	243	LEU	2.4
2	e	167	VAL	2.4
2	p	238	THR	2.4
1	C	350	VAL	2.4
2	i	88	LEU	2.4
1	G	293	TYR	2.4
1	O	139	TYR	2.4
2	l	176	ALA	2.4
1	R	225	ILE	2.4
2	i	118	SER	2.4
1	I	140	ASN	2.4
1	Q	137	ILE	2.4
1	E	175	PHE	2.4
1	R	158	ILE	2.4
1	O	136	GLY	2.4
1	R	224	TYR	2.4
2	l	98	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	344	ALA	2.4
2	l	177	ALA	2.4
2	l	151	VAL	2.4
1	E	160	PHE	2.4
2	e	165	ASN	2.4
2	p	67	GLN	2.4
2	p	98	CYS	2.4
1	P	225	ILE	2.4
1	M	326	ASP	2.4
1	Q	209	LEU	2.4
2	n	52	TRP	2.4
2	q	182	LEU	2.4
1	Q	229	ALA	2.4
1	R	202	TYR	2.4
1	L	190	LEU	2.4
1	R	75	GLY	2.3
1	P	66	GLU	2.3
2	g	181	LEU	2.3
2	q	192	ILE	2.3
2	g	101	ASP	2.3
2	l	169	TRP	2.3
2	o	21	LYS	2.3
1	Q	215	TYR	2.3
2	o	19	SER	2.3
2	f	9	THR	2.3
1	N	192	LEU	2.3
1	O	217	SER	2.3
1	P	102	LYS	2.3
1	Q	173	VAL	2.3
2	l	165	ASN	2.3
1	N	91	GLN	2.3
2	q	184	ASP	2.3
1	F	184	PRO	2.3
1	F	325	SER	2.3
1	P	278	PRO	2.3
2	h	167	VAL	2.3
2	o	195	ARG	2.3
1	N	263	ILE	2.3
2	c	207	LEU	2.3
1	R	356	ARG	2.3
1	P	127	ALA	2.3
1	R	139	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	m	170	TYR	2.3
1	A	290	PHE	2.3
2	g	27	SER	2.3
1	O	158	ILE	2.3
2	q	218	ALA	2.3
1	P	194	PRO	2.3
2	p	144	SER	2.3
2	q	117	SER	2.3
2	r	200	LYS	2.3
1	O	228	LEU	2.3
1	Q	319	LEU	2.3
2	d	169	TRP	2.3
1	J	127	ALA	2.3
2	l	146	ALA	2.3
2	o	190	SER	2.3
2	l	41	GLN	2.3
2	m	220	TYR	2.3
2	n	220	TYR	2.3
2	o	29	TYR	2.3
2	p	49	TRP	2.3
2	j	165	ASN	2.3
2	r	21	LYS	2.3
1	H	325	SER	2.3
2	p	37	SER	2.3
2	b	119	GLY	2.3
1	L	159	LEU	2.3
1	K	211	LYS	2.3
1	K	244	PHE	2.3
1	N	257	ILE	2.3
2	b	151	VAL	2.3
2	e	118	SER	2.3
2	r	156	SER	2.3
2	p	91	ASP	2.2
2	j	21	LYS	2.2
2	g	26	VAL	2.2
2	j	167	VAL	2.2
1	K	238	GLY	2.2
2	q	168	SER	2.2
2	r	37	SER	2.2
2	g	89	ARG	2.2
1	K	183	LEU	2.2
1	L	103	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	311	ASN	2.2
2	n	24	CYS	2.2
1	E	219	PHE	2.2
1	P	95	PHE	2.2
2	o	209	ILE	2.2
2	q	73	THR	2.2
1	L	215	TYR	2.2
2	p	170	TYR	2.2
1	L	98	LEU	2.2
1	Q	192	LEU	2.2
1	R	353	LEU	2.2
2	d	88	LEU	2.2
1	P	160	PHE	2.2
1	M	243	VAL	2.2
1	O	173	VAL	2.2
1	Q	357	THR	2.2
2	o	80	THR	2.2
1	C	348	ALA	2.2
1	F	183	LEU	2.2
2	b	37	SER	2.2
1	N	184	PRO	2.2
2	e	85	LEU	2.2
1	K	237	PHE	2.2
1	O	208	VAL	2.2
2	b	22	VAL	2.2
2	j	39	VAL	2.2
2	l	70	VAL	2.2
2	o	36	ILE	2.2
1	J	326	ASP	2.2
2	l	113	THR	2.2
1	N	187	LEU	2.2
2	o	182	LEU	2.2
1	R	277	ILE	2.2
1	M	138	GLY	2.2
1	Q	228	LEU	2.2
1	R	286	ASN	2.2
2	g	207	LEU	2.2
2	l	172	GLN	2.2
2	o	55	PRO	2.2
2	c	115	THR	2.2
2	l	144	SER	2.2
1	E	276	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	Q	185	ALA	2.2
2	r	183	TYR	2.2
1	P	129	PRO	2.2
2	p	62	TYR	2.2
2	q	96	TYR	2.2
1	H	175	PHE	2.2
1	Q	233	ILE	2.2
1	E	229	ALA	2.2
1	K	192	LEU	2.2
1	O	323	SER	2.2
1	Q	236	ALA	2.2
1	I	160	PHE	2.2
1	K	137	ILE	2.2
1	P	208	VAL	2.2
2	a	93	THR	2.2
1	I	143	LYS	2.2
2	h	85	LEU	2.2
2	r	181	LEU	2.1
1	K	236	ALA	2.1
1	M	246	ALA	2.1
1	Q	224	TYR	2.1
2	b	99	ALA	2.1
1	O	128	VAL	2.1
1	L	113	LEU	2.1
1	L	130	TYR	2.1
2	p	42	ALA	2.1
2	k	209	ILE	2.1
2	n	116	VAL	2.1
1	Q	238	GLY	2.1
1	L	326	ASP	2.1
2	r	240	LEU	2.1
1	A	288	TYR	2.1
2	r	82	TYR	2.1
2	n	114	VAL	2.1
1	K	160	PHE	2.1
2	l	188	ARG	2.1
1	N	235	VAL	2.1
1	O	238	GLY	2.1
2	l	235	GLY	2.1
2	j	197	SER	2.1
2	o	234	PHE	2.1
1	C	311	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	137	ILE	2.1
2	r	114	VAL	2.1
2	e	86	SER	2.1
2	l	42	ALA	2.1
2	c	225	TRP	2.1
2	p	209	ILE	2.1
2	q	209	ILE	2.1
2	o	15	THR	2.1
2	o	164	ARG	2.1
2	p	5	GLN	2.1
2	p	17	GLY	2.1
1	G	237	PHE	2.1
2	l	104	TYR	2.1
1	O	326	ASP	2.1
2	o	100	ARG	2.1
1	R	164	ASN	2.1
1	R	173	VAL	2.1
2	f	23	SER	2.1
2	j	114	VAL	2.1
1	L	168	LEU	2.1
2	i	212	LEU	2.1
2	i	243	LEU	2.1
2	a	171	GLN	2.1
1	N	237	PHE	2.1
2	d	210	THR	2.1
1	R	288	TYR	2.1
1	M	235	VAL	2.1
2	p	22	VAL	2.1
2	e	243	LEU	2.1
1	P	130	TYR	2.1
2	m	205	THR	2.1
2	j	20	VAL	2.1
2	k	116	VAL	2.1
2	l	94	ALA	2.1
1	P	37	TYR	2.0
1	R	189	TYR	2.0
2	a	205	THR	2.0
2	o	95	VAL	2.0
2	q	15	THR	2.0
1	B	256	GLY	2.0
1	N	353	LEU	2.0
2	a	181	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	60	ASP	2.0
1	O	61	SER	2.0
1	Q	156	TRP	2.0
1	R	176	MET	2.0
1	P	139	TYR	2.0
1	Q	42	THR	2.0
1	Q	75	GLY	2.0
2	d	112	THR	2.0
2	j	209	ILE	2.0
2	r	85	LEU	2.0
1	K	176	MET	2.0
1	R	272	PHE	2.0
1	E	325	SER	2.0
1	P	178	SER	2.0
1	P	325	SER	2.0
2	g	201	SER	2.0
2	l	142	SER	2.0
2	n	104	TYR	2.0
1	A	137	ILE	2.0
1	H	29	LEU	2.0
2	p	181	LEU	2.0
2	m	221	PHE	2.0
2	q	61	ASN	2.0
1	O	79	VAL	2.0
2	r	22	VAL	2.0
1	M	236	ALA	2.0
2	p	81	ALA	2.0
1	O	317	ARG	2.0
2	j	112	THR	2.0
1	B	293	TYR	2.0
2	p	118	SER	2.0
2	r	197	SER	2.0
1	C	127	ALA	2.0
1	J	153	ILE	2.0
1	P	277	ILE	2.0
2	q	193	PRO	2.0
1	F	228	LEU	2.0
1	L	317	ARG	2.0
1	O	235	VAL	2.0
2	g	143	VAL	2.0

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

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

6.3 Carbohydrates (i)

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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.