



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 25, 2026 – 01:17 AM UTC

PDB ID : 6IKM / pdb_00006ikm
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

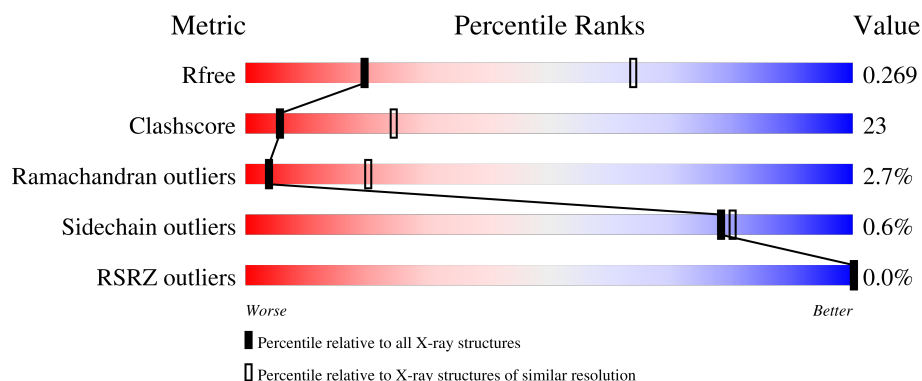
1 Overall quality at a glance

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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 $\leq 5\%$. 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	69% 29% ..
1	B	340	68% 30% ..
1	C	340	71% 28% .
1	D	340	69% 29% .
1	E	340	63% 35% .

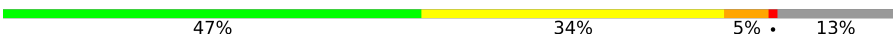
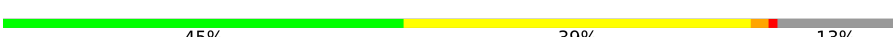
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Mol	Chain	Length	Quality of chain
1	F	340	
1	G	340	
1	H	340	
1	I	340	
1	J	340	
1	K	340	
1	L	340	
1	M	340	
1	N	340	
1	O	340	
1	P	340	
1	Q	340	
1	R	340	
2	a	258	
2	b	258	
2	c	258	
2	d	258	
2	e	258	
2	f	258	
2	g	258	
2	h	258	
2	i	258	
2	j	258	
2	k	258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

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Mol	Chain	Length	Quality of chain
2	m	258	
2	n	258	
2	o	258	
2	p	258	
2	q	258	
2	r	258	

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
3	SO4	A	403	-	-	X	-
3	SO4	G	401	-	-	X	-
3	SO4	I	402	-	-	X	-
3	SO4	M	401	-	-	X	-
3	SO4	M	402	-	-	X	-
3	SO4	N	404	-	-	X	-
3	SO4	N	406	-	-	X	-
3	SO4	O	406	-	-	X	-
3	SO4	R	401	-	-	X	-
4	SPD	N	407	-	-	X	-
4	SPD	O	407	-	-	X	-
4	SPD	Q	401	-	-	X	-

2 Entry composition

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.

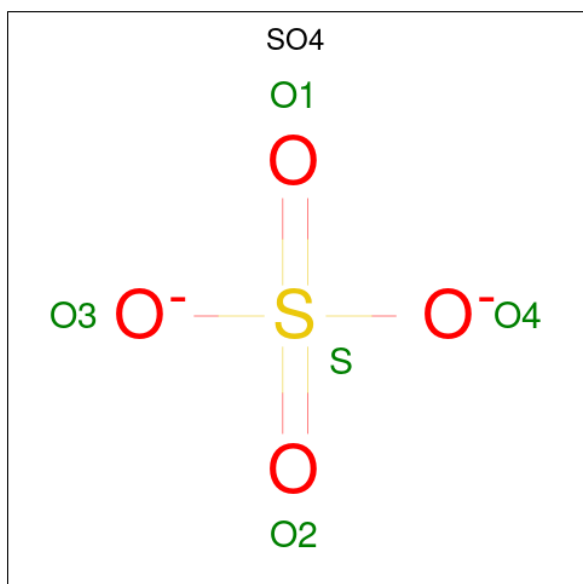
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0
2	b	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0
2	c	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0
2	d	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0
2	e	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0
2	f	225	Total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

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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 (CCD ID: SO4) (formula: O₄S).



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	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		

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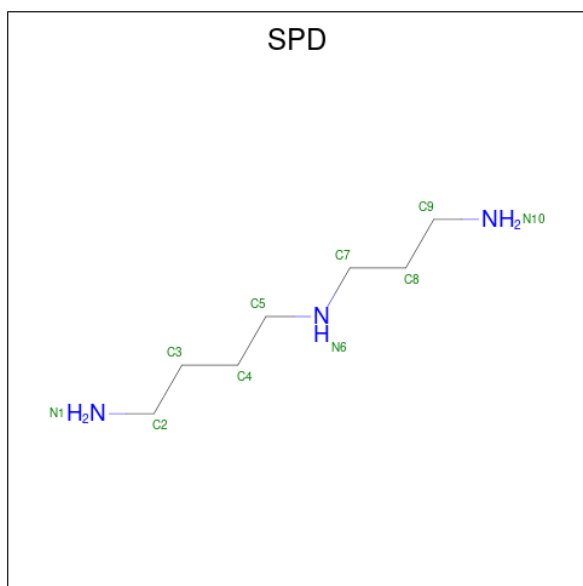
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total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

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

- Molecule 4 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



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

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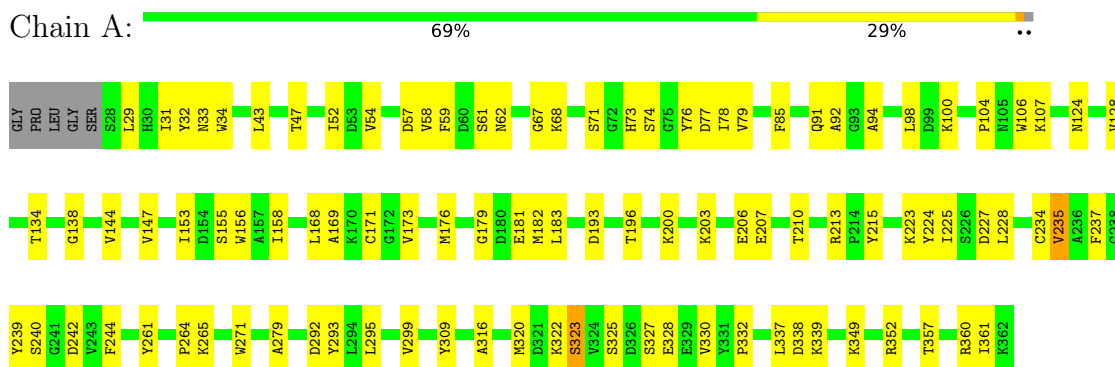
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	N	0	0
			10	7	3		
4	F	1	Total	C	N	0	0
			10	7	3		
4	G	1	Total	C	N	0	0
			10	7	3		
4	H	1	Total	C	N	0	0
			10	7	3		
4	I	1	Total	C	N	0	0
			10	7	3		
4	J	1	Total	C	N	0	0
			10	7	3		
4	K	1	Total	C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

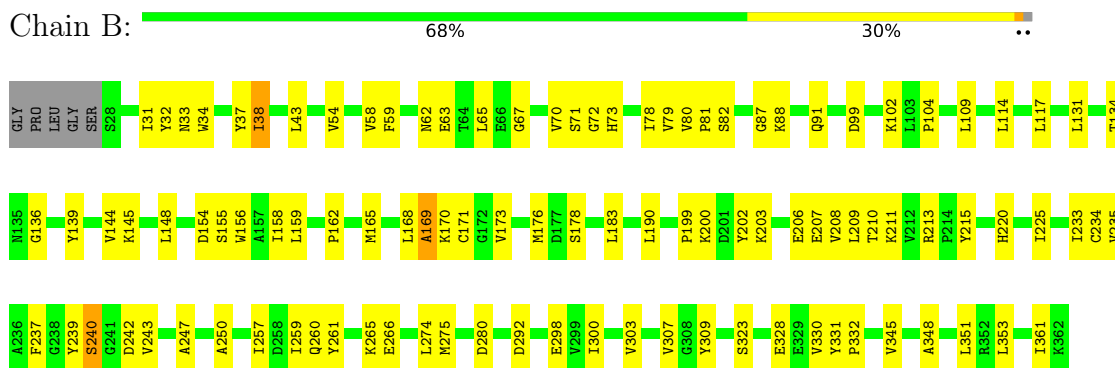
3 Residue-property plots

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.

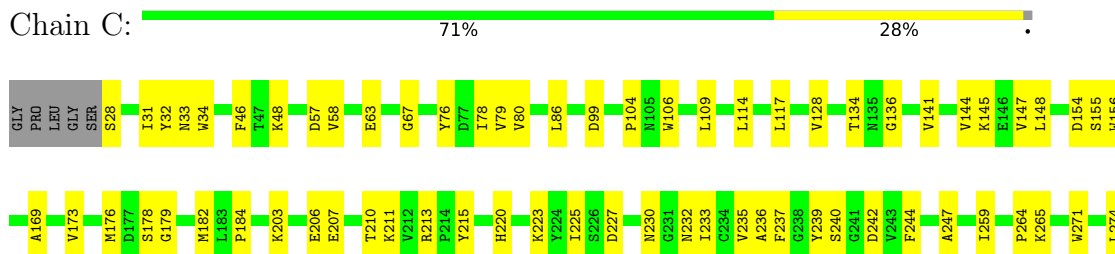
• Molecule 1: Polyamine transport protein



• Molecule 1: Polyamine transport protein



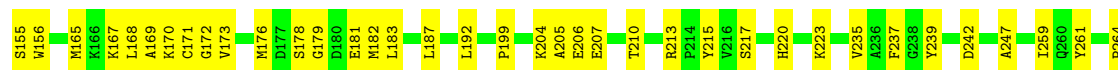
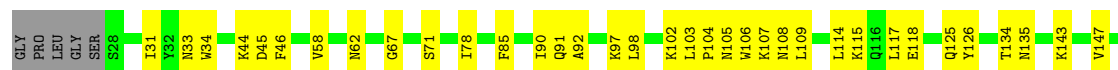
• Molecule 1: Polyamine transport protein





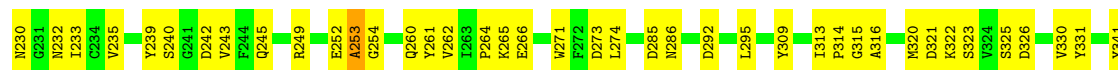
• Molecule 1: Polyamine transport protein

Chain D: 69% 29% .



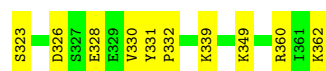
• Molecule 1: Polyamine transport protein

Chain E: 63% 35% .

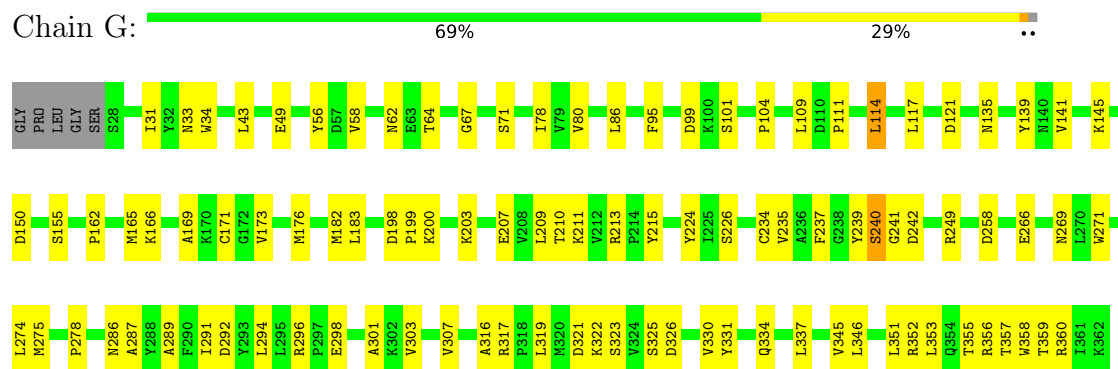


• Molecule 1: Polyamine transport protein

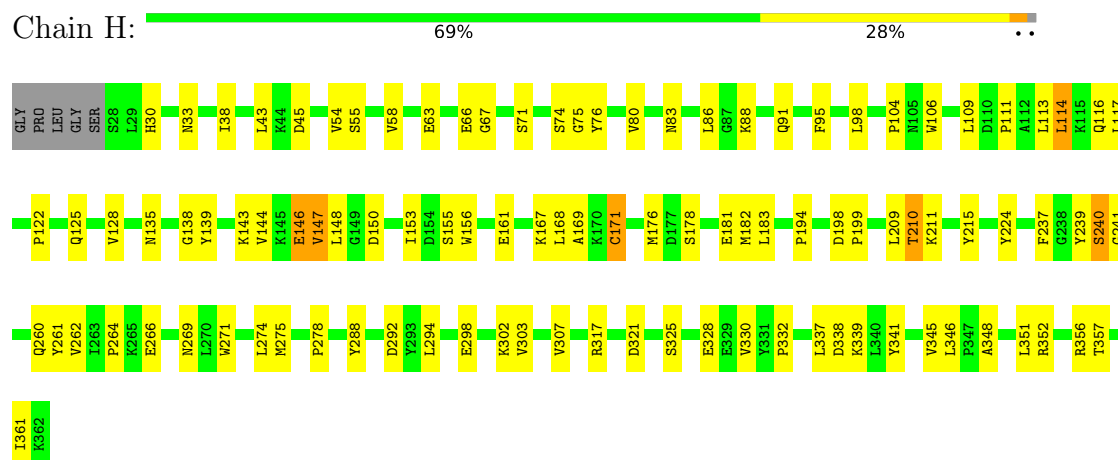
Chain F: 64% 34% ..



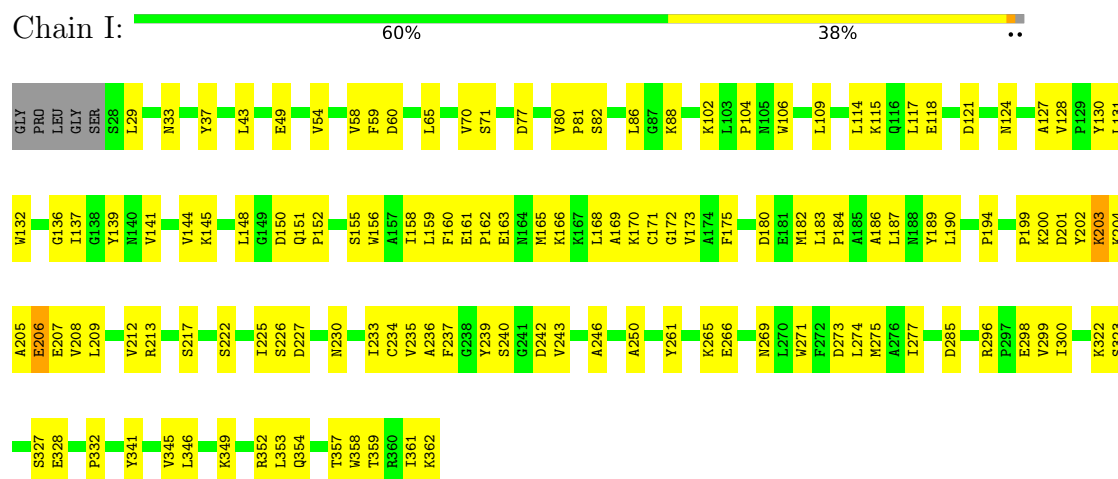
• Molecule 1: Polyamine transport protein



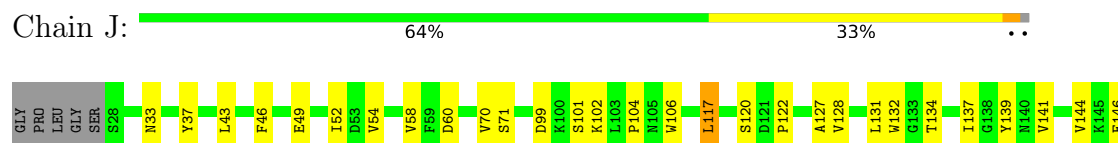
• Molecule 1: Polyamine transport protein

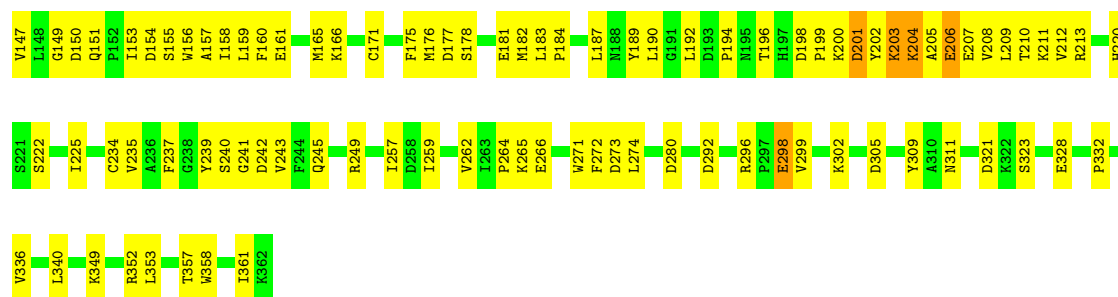


• Molecule 1: Polyamine transport protein



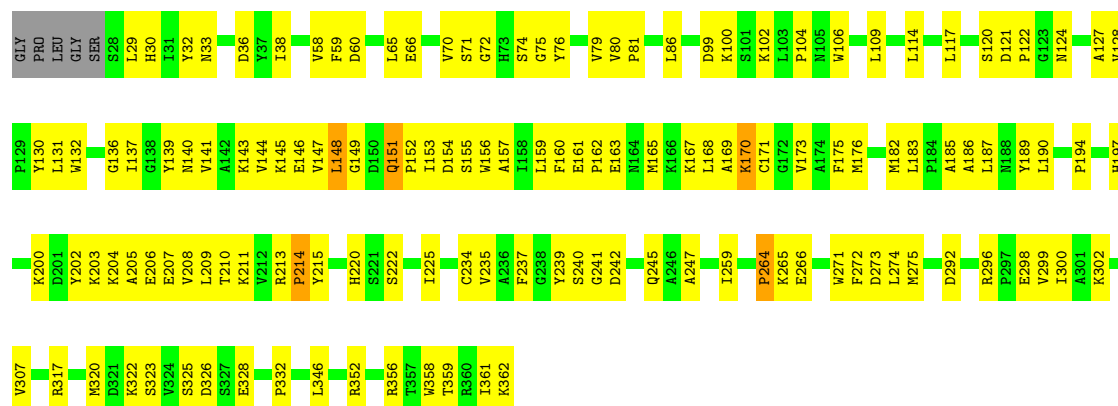
• Molecule 1: Polyamine transport protein





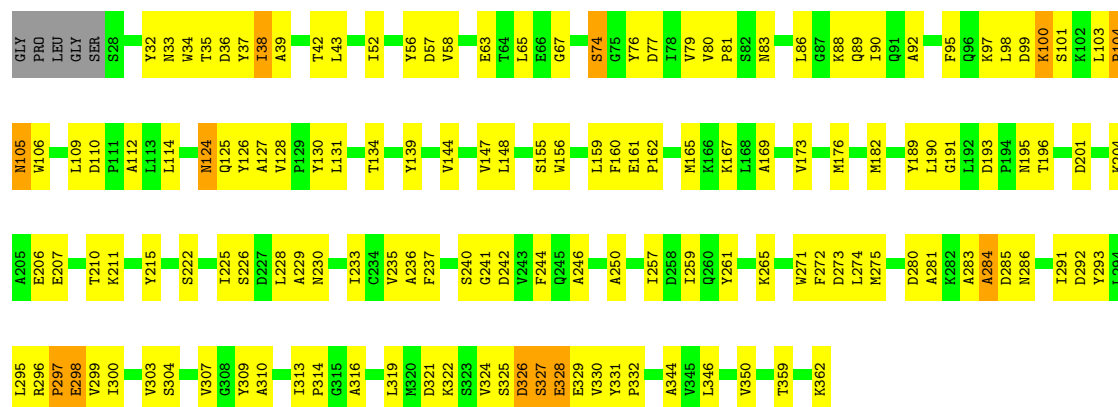
• Molecule 1: Polyamine transport protein

Chain K: 58% 39% ..



• Molecule 1: Polyamine transport protein

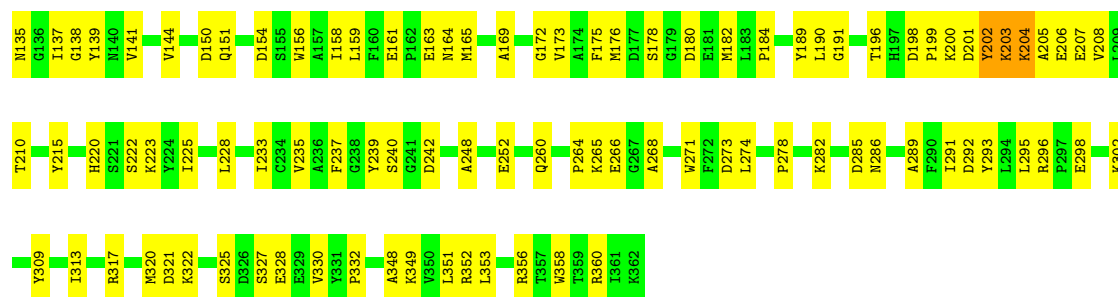
Chain L: 56% 39% ..



• Molecule 1: Polyamine transport protein

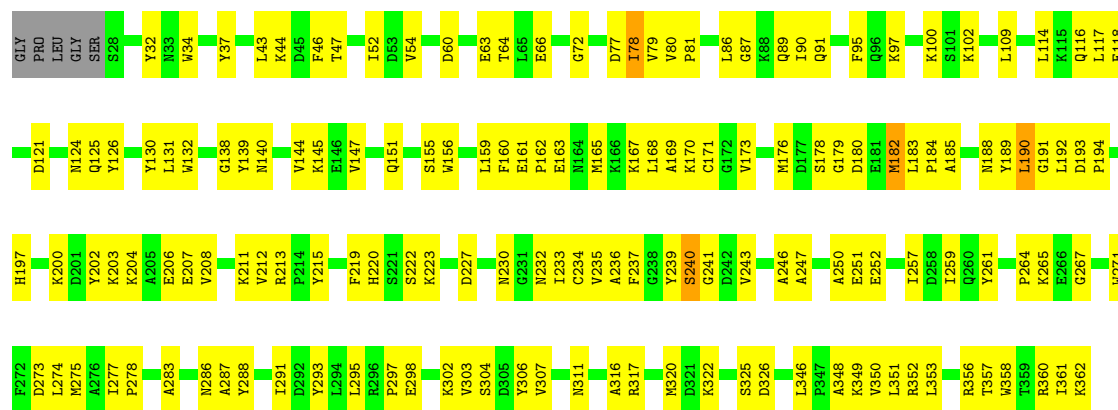
Chain M: 62% 36% ..





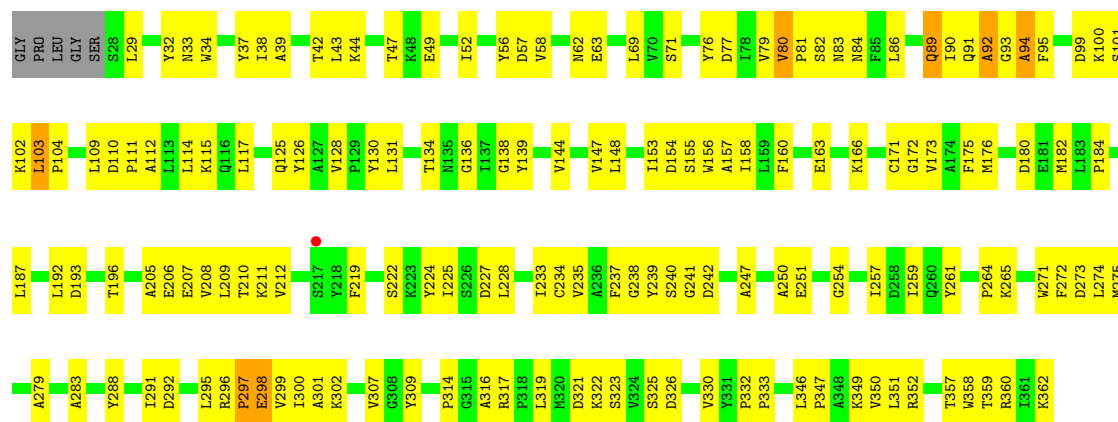
• Molecule 1: Polyamine transport protein

Chain N: 53% 44% ..



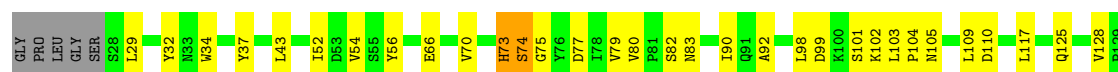
• Molecule 1: Polyamine transport protein

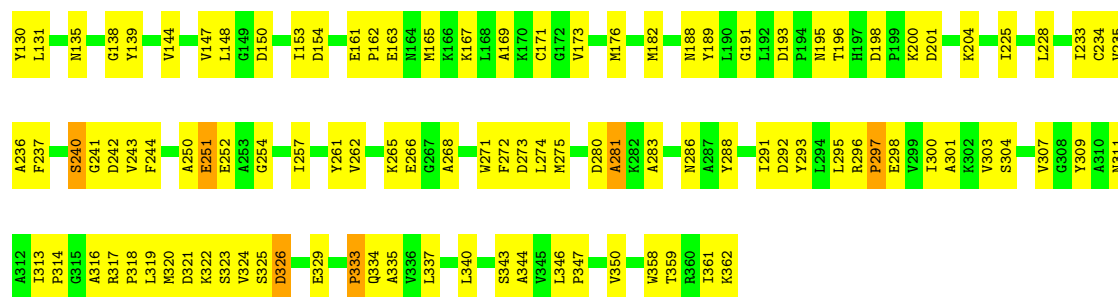
Chain O: 52% 44% ..



• Molecule 1: Polyamine transport protein

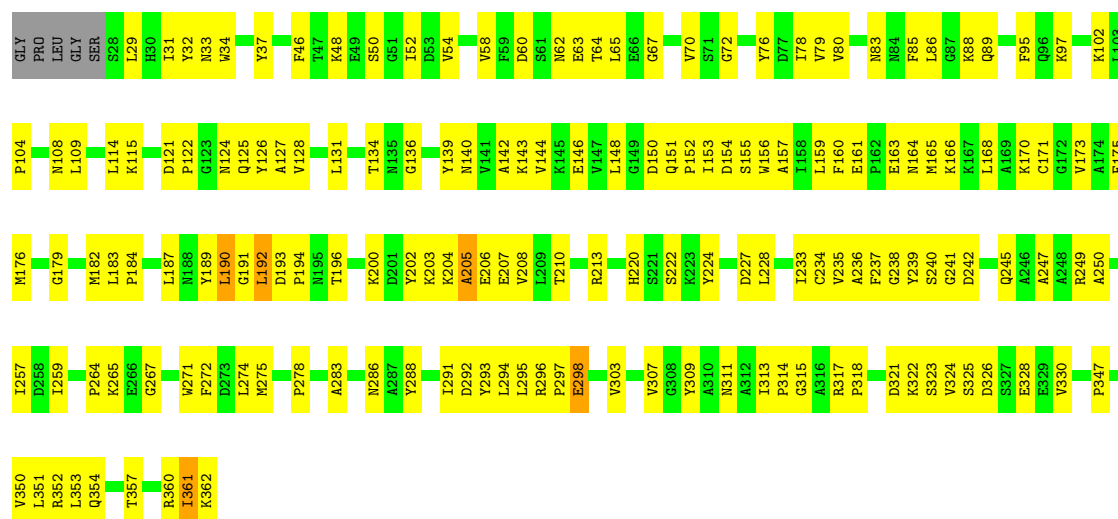
Chain P: 58% 38% ..





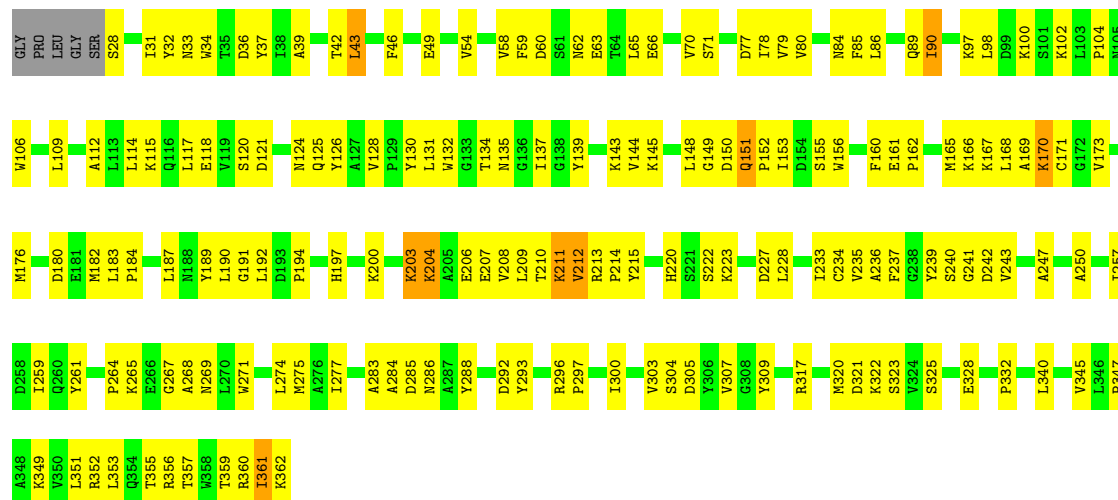
• Molecule 1: Polyamine transport protein

Chain Q: 50% 47% ..



• Molecule 1: Polyamine transport protein

Chain R: 49% 47% ..



• Molecule 2: ScFv5

Device Type	Percentage
Smartphones	50%
Tablets	35%
Other mobile devices	13%



Response	Percentage
Yes	49%
No	37%
Don't know	13%



Device Type	Percentage
Smartphone	52%
Tablet	34%
Feature Phone	13%



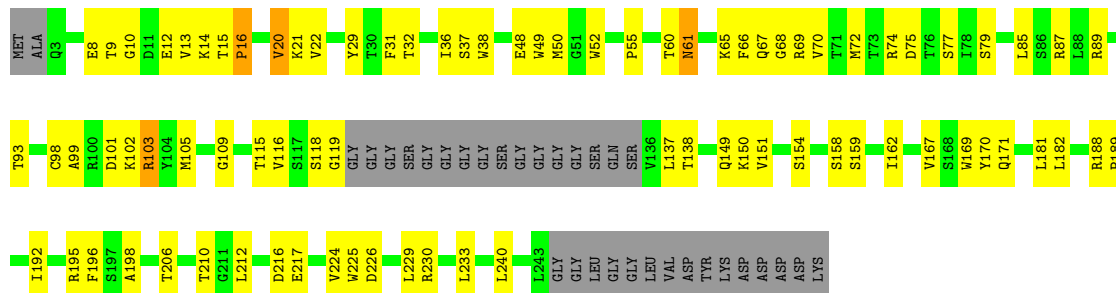
App Type	Percentage
Shopping app	60%
Social media app	26%
Health app	1%
Productivity app	13%





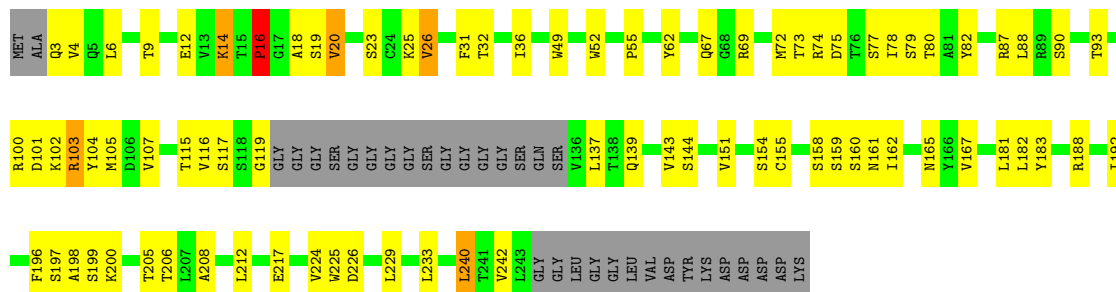
• Molecule 2: ScFv5

Chain e: 55% 31% 13%



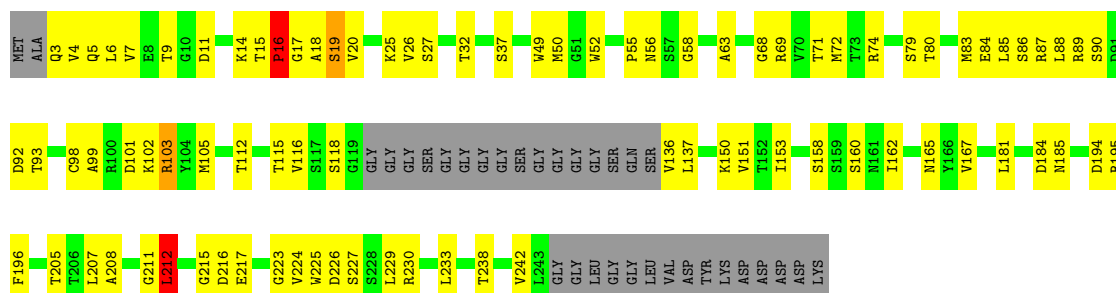
• Molecule 2: ScFv5

Chain f: 55% 29% 13%



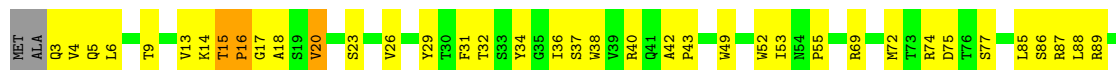
• Molecule 2: ScFv5

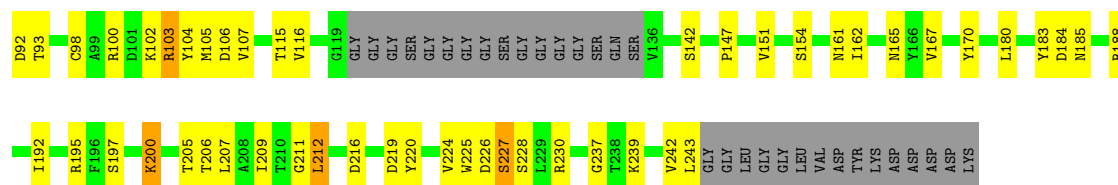
Chain g: 53% 32% 13%



• Molecule 2: ScFv5

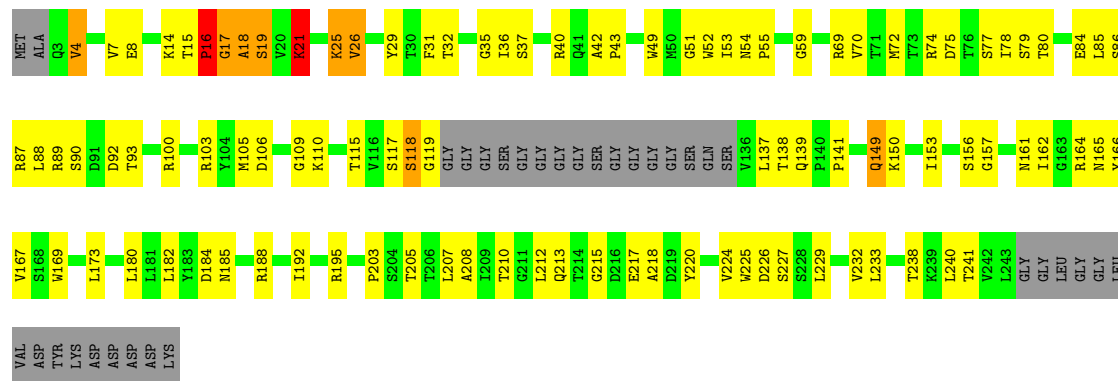
Chain h: 53% 31% 13%





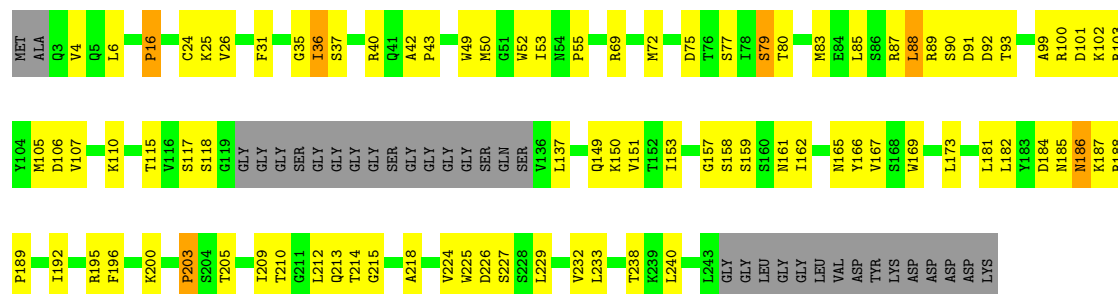
• Molecule 2: ScFv5

Chain i: 48% 35% 13%



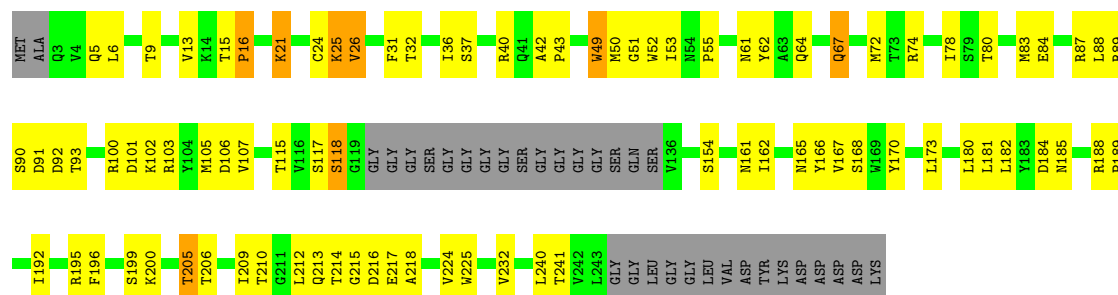
• Molecule 2: ScFv5

Chain j: 52% 33% 13%

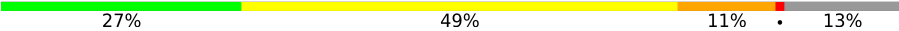


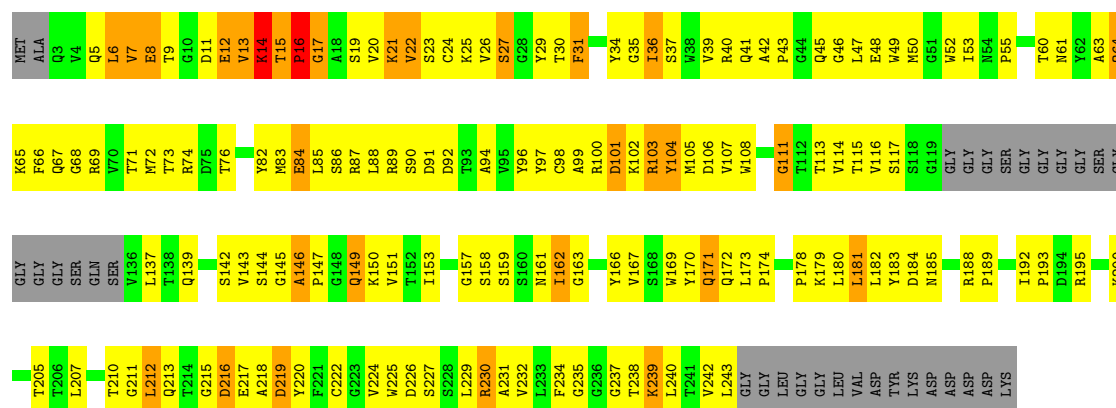
• Molecule 2: ScFv5

Chain k: 53% 31% 13%



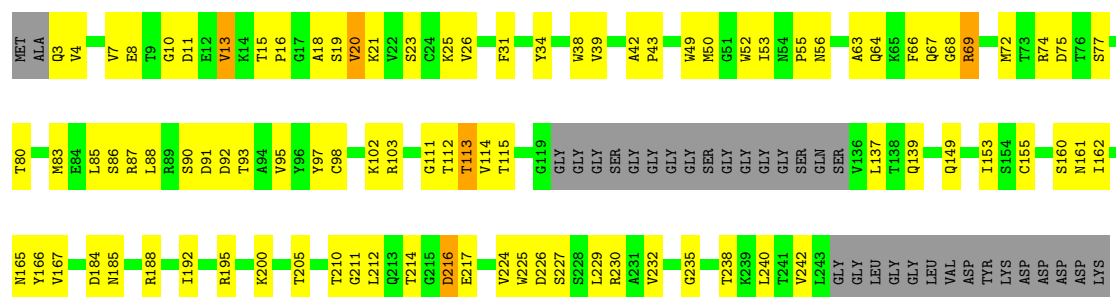
• Molecule 2: ScFv5

Chain l:  27% 49% 11% 13%

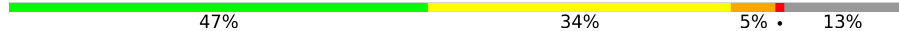


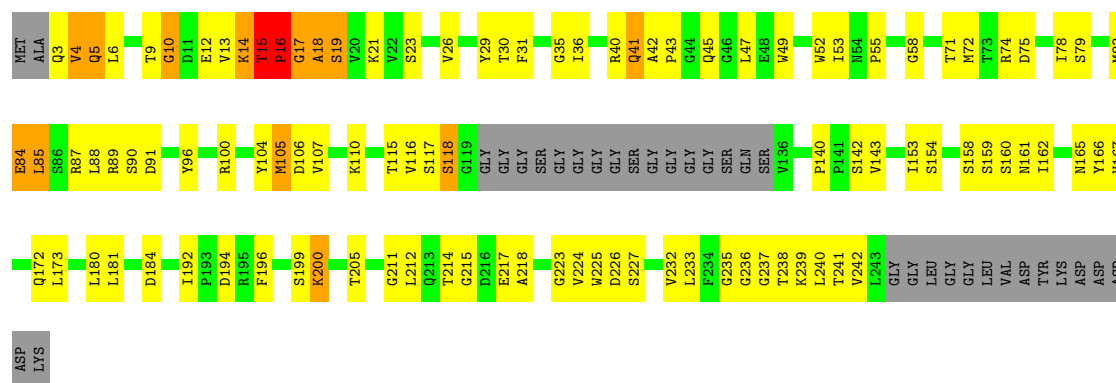
• Molecule 2: ScFv5

Chain m:  51% 34% 13%



• Molecule 2: ScFv5

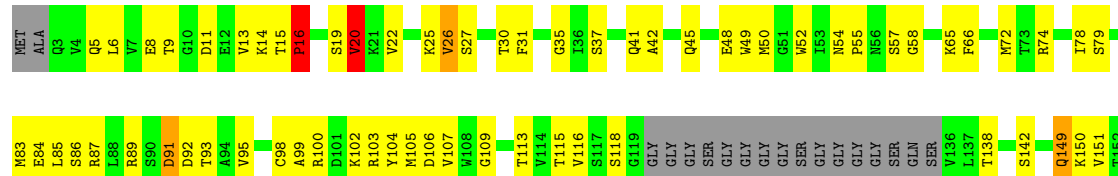
Chain n:  47% 34% 5% 13%



• Molecule 2: ScFv5

Chain o:  47% 38% 13%







4 Data and refinement statistics

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 46.47 – 3.40	Depositor EDS
% Data completeness (in resolution range)	89.5 (46.47-3.40) 89.4 (46.47-3.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.228 , 0.268 0.231 , 0.269	Depositor DCC
R_{free} test set	10759 reflections (4.50%)	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 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.21	0/2684	0.49	0/3653
1	B	0.23	0/2684	0.54	0/3653
1	C	0.24	0/2684	0.50	0/3653
1	D	0.23	0/2684	0.52	0/3653
1	E	0.28	0/2684	0.60	2/3653 (0.1%)
1	F	0.24	0/2684	0.55	0/3653
1	G	0.24	0/2684	0.52	0/3653
1	H	0.24	0/2684	0.65	4/3653 (0.1%)
1	I	0.35	2/2684 (0.1%)	0.67	2/3653 (0.1%)
1	J	0.29	0/2684	0.62	2/3653 (0.1%)
1	K	0.29	0/2684	0.64	2/3653 (0.1%)
1	L	0.28	0/2684	0.58	0/3653
1	M	0.25	0/2684	0.57	1/3653 (0.0%)
1	N	0.26	0/2684	0.54	0/3653
1	O	0.33	1/2684 (0.0%)	0.66	2/3653 (0.1%)
1	P	0.28	0/2684	0.62	2/3653 (0.1%)
1	Q	0.32	0/2684	0.64	2/3653 (0.1%)
1	R	0.30	0/2684	0.67	1/3653 (0.0%)
2	a	0.42	1/1736 (0.1%)	0.80	8/2358 (0.3%)
2	b	0.36	1/1736 (0.1%)	0.68	1/2358 (0.0%)
2	c	0.44	1/1736 (0.1%)	0.72	1/2358 (0.0%)
2	d	0.34	0/1736	0.66	0/2358
2	e	0.35	1/1736 (0.1%)	0.66	0/2358
2	f	0.40	2/1736 (0.1%)	0.66	1/2358 (0.0%)
2	g	0.39	1/1736 (0.1%)	0.76	2/2358 (0.1%)
2	h	0.38	0/1736	0.69	1/2358 (0.0%)
2	i	0.39	1/1736 (0.1%)	0.71	4/2358 (0.2%)
2	j	0.34	0/1736	0.70	1/2358 (0.0%)
2	k	0.46	2/1736 (0.1%)	0.79	8/2358 (0.3%)
2	l	0.47	0/1736	1.00	7/2358 (0.3%)
2	m	0.37	0/1736	0.63	0/2358
2	n	0.40	0/1736	0.88	4/2358 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	o	0.42	1/1736 (0.1%)	0.80	8/2358 (0.3%)
2	p	0.42	1/1736 (0.1%)	0.80	8/2358 (0.3%)
2	q	0.42	0/1736	0.84	3/2358 (0.1%)
2	r	0.48	1/1736 (0.1%)	0.86	4/2358 (0.2%)
All	All	0.33	16/79560 (0.0%)	0.66	81/108198 (0.1%)

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 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	r	238	THR	CB-CG2	10.74	1.88	1.52
2	k	26	VAL	CB-CG2	7.92	1.78	1.52
2	i	26	VAL	CB-CG2	7.36	1.76	1.52
2	c	16	PRO	C-O	-7.36	1.18	1.24
1	I	137	ILE	C-N	6.06	1.36	1.33

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	147	VAL	N-CA-C	-13.36	99.60	112.96
2	g	212	LEU	CB-CG-CD2	10.82	143.15	110.70
2	n	85	LEU	CA-CB-CG	10.03	151.39	116.30
1	H	146	GLU	CA-C-N	-8.78	111.92	121.84
1	H	146	GLU	C-N-CA	-8.78	111.92	121.84

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](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2618	0	2580	80	0
1	B	2618	0	2580	79	0
1	C	2618	0	2580	67	0
1	D	2618	0	2580	76	0
1	E	2618	0	2578	102	0
1	F	2618	0	2580	87	1
1	G	2618	0	2580	77	0
1	H	2618	0	2576	75	1
1	I	2618	0	2580	109	0
1	J	2618	0	2580	129	0
1	K	2618	0	2576	127	0
1	L	2618	0	2579	124	0
1	M	2618	0	2580	110	0
1	N	2618	0	2580	148	0
1	O	2618	0	2580	151	0
1	P	2618	0	2580	127	0
1	Q	2618	0	2580	159	0
1	R	2618	0	2580	167	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	a	1699	0	1659	78	0
2	b	1699	0	1659	101	0
2	c	1699	0	1659	94	0
2	d	1699	0	1659	64	0
2	e	1699	0	1659	65	1
2	f	1699	0	1659	69	4
2	g	1699	0	1659	96	0
2	h	1699	0	1659	123	1
2	i	1699	0	1658	128	0
2	j	1699	0	1659	68	0
2	k	1699	0	1659	96	0
2	l	1699	0	1659	234	0
2	m	1699	0	1659	76	0
2	n	1699	0	1659	111	0
2	o	1699	0	1659	121	3
2	p	1699	0	1658	120	1
2	q	1699	0	1659	90	0
2	r	1699	0	1659	101	0
3	A	15	0	0	3	0
3	B	20	0	0	0	0
3	C	15	0	0	1	0
3	D	15	0	0	1	0
3	E	20	0	0	2	0
3	F	15	0	0	2	0
3	G	10	0	0	3	0
3	H	10	0	0	1	0
3	I	15	0	0	3	0
3	J	15	0	0	1	0
3	K	15	0	0	1	0
3	L	15	0	0	1	0
3	M	15	0	0	4	0
3	N	30	0	0	6	0
3	O	30	0	0	3	0
3	R	15	0	0	3	0
4	A	10	0	19	5	0
4	B	10	0	17	2	0
4	C	10	0	17	3	0
4	D	10	0	19	5	0
4	E	10	0	17	5	0
4	F	10	0	19	3	0
4	G	10	0	19	2	0
4	H	10	0	19	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	10	0	17	1	0
4	J	10	0	19	3	0
4	K	10	0	19	3	0
4	L	10	0	19	2	0
4	M	10	0	17	3	0
4	N	10	0	17	6	0
4	O	10	0	17	6	0
4	P	10	0	17	5	0
4	Q	10	0	19	7	0
4	R	10	0	17	3	0
All	All	78156	0	76613	3615	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 3615 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:26:VAL:CB	2:k:26:VAL:CG2	1.78	1.56
2:i:26:VAL:CB	2:i:26:VAL:CG2	1.76	1.56
2:g:18:ALA:CB	2:g:88:LEU:H	1.18	1.53
2:r:238:THR:CB	2:r:238:THR:CG2	1.88	1.49
2:h:225:TRP:CZ3	2:h:227:SER:HA	1.47	1.48

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:119:GLY:O	2:o:64:GLN:OE1[2_657]	1.51	0.69
2:f:119:GLY:O	2:o:64:GLN:CG[2_657]	1.59	0.61
2:f:119:GLY:O	2:o:64:GLN:CD[2_657]	1.66	0.54
1:F:163:GLU:OE1	2:h:142:SER:OG[2_757]	2.09	0.11
2:e:119:GLY:O	2:p:64:GLN:CG[1_554]	2.16	0.04

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%)	10	35
1	B	333/340 (98%)	300 (90%)	28 (8%)	5 (2%)	8	30
1	C	333/340 (98%)	301 (90%)	28 (8%)	4 (1%)	10	35
1	D	333/340 (98%)	305 (92%)	24 (7%)	4 (1%)	10	35
1	E	333/340 (98%)	298 (90%)	30 (9%)	5 (2%)	8	30
1	F	333/340 (98%)	297 (89%)	28 (8%)	8 (2%)	4	22
1	G	333/340 (98%)	304 (91%)	26 (8%)	3 (1%)	14	42
1	H	333/340 (98%)	305 (92%)	21 (6%)	7 (2%)	5	24
1	I	333/340 (98%)	291 (87%)	39 (12%)	3 (1%)	14	42
1	J	333/340 (98%)	281 (84%)	44 (13%)	8 (2%)	4	22
1	K	333/340 (98%)	293 (88%)	31 (9%)	9 (3%)	4	20
1	L	333/340 (98%)	284 (85%)	34 (10%)	15 (4%)	2	12
1	M	333/340 (98%)	293 (88%)	35 (10%)	5 (2%)	8	30
1	N	333/340 (98%)	282 (85%)	40 (12%)	11 (3%)	3	17
1	O	333/340 (98%)	285 (86%)	39 (12%)	9 (3%)	4	20
1	P	333/340 (98%)	281 (84%)	46 (14%)	6 (2%)	6	26
1	Q	333/340 (98%)	275 (83%)	49 (15%)	9 (3%)	4	20
1	R	333/340 (98%)	274 (82%)	49 (15%)	10 (3%)	3	18
2	a	221/258 (86%)	187 (85%)	28 (13%)	6 (3%)	4	20
2	b	221/258 (86%)	197 (89%)	18 (8%)	6 (3%)	4	20
2	c	221/258 (86%)	193 (87%)	21 (10%)	7 (3%)	3	17
2	d	221/258 (86%)	187 (85%)	26 (12%)	8 (4%)	2	16
2	e	221/258 (86%)	202 (91%)	16 (7%)	3 (1%)	9	31
2	f	221/258 (86%)	196 (89%)	24 (11%)	1 (0%)	24	54
2	g	221/258 (86%)	187 (85%)	29 (13%)	5 (2%)	5	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	h	221/258 (86%)	190 (86%)	25 (11%)	6 (3%)	4	20
2	i	221/258 (86%)	189 (86%)	24 (11%)	8 (4%)	2	16
2	j	221/258 (86%)	185 (84%)	29 (13%)	7 (3%)	3	17
2	k	221/258 (86%)	189 (86%)	25 (11%)	7 (3%)	3	17
2	l	221/258 (86%)	146 (66%)	46 (21%)	29 (13%)	0	1
2	m	221/258 (86%)	181 (82%)	37 (17%)	3 (1%)	9	31
2	n	221/258 (86%)	173 (78%)	32 (14%)	16 (7%)	1	5
2	o	221/258 (86%)	186 (84%)	29 (13%)	6 (3%)	4	20
2	p	221/258 (86%)	186 (84%)	29 (13%)	6 (3%)	4	20
2	q	221/258 (86%)	171 (77%)	36 (16%)	14 (6%)	1	7
2	r	221/258 (86%)	179 (81%)	32 (14%)	10 (4%)	2	12
All	All	9972/10764 (93%)	8574 (86%)	1125 (11%)	273 (3%)	4	20

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 ⓘ

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%)	279 (100%)	0	100	100
1	B	279/282 (99%)	279 (100%)	0	100	100
1	C	279/282 (99%)	279 (100%)	0	100	100
1	D	279/282 (99%)	279 (100%)	0	100	100
1	E	279/282 (99%)	279 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	279/282 (99%)	279 (100%)	0	100	100
1	G	279/282 (99%)	279 (100%)	0	100	100
1	H	279/282 (99%)	279 (100%)	0	100	100
1	I	279/282 (99%)	277 (99%)	2 (1%)	76	78
1	J	279/282 (99%)	279 (100%)	0	100	100
1	K	279/282 (99%)	279 (100%)	0	100	100
1	L	279/282 (99%)	279 (100%)	0	100	100
1	M	279/282 (99%)	278 (100%)	1 (0%)	84	83
1	N	279/282 (99%)	279 (100%)	0	100	100
1	O	279/282 (99%)	279 (100%)	0	100	100
1	P	279/282 (99%)	277 (99%)	2 (1%)	76	78
1	Q	279/282 (99%)	279 (100%)	0	100	100
1	R	279/282 (99%)	277 (99%)	2 (1%)	76	78
2	a	186/203 (92%)	185 (100%)	1 (0%)	81	81
2	b	186/203 (92%)	184 (99%)	2 (1%)	65	74
2	c	186/203 (92%)	186 (100%)	0	100	100
2	d	186/203 (92%)	186 (100%)	0	100	100
2	e	186/203 (92%)	181 (97%)	5 (3%)	39	60
2	f	186/203 (92%)	182 (98%)	4 (2%)	45	63
2	g	186/203 (92%)	182 (98%)	4 (2%)	45	63
2	h	186/203 (92%)	184 (99%)	2 (1%)	65	74
2	i	186/203 (92%)	183 (98%)	3 (2%)	55	68
2	j	186/203 (92%)	185 (100%)	1 (0%)	81	81
2	k	186/203 (92%)	185 (100%)	1 (0%)	81	81
2	l	186/203 (92%)	182 (98%)	4 (2%)	45	63
2	m	186/203 (92%)	181 (97%)	5 (3%)	39	60
2	n	186/203 (92%)	182 (98%)	4 (2%)	45	63
2	o	186/203 (92%)	185 (100%)	1 (0%)	81	81
2	p	186/203 (92%)	185 (100%)	1 (0%)	81	81
2	q	186/203 (92%)	182 (98%)	4 (2%)	45	63
2	r	186/203 (92%)	184 (99%)	2 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	8370/8730 (96%)	8319 (99%)	51 (1%)	78 80

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	l	21	LYS
2	n	14	LYS
2	r	16	PRO
1	M	88	LYS
2	m	19	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
2	n	5	GLN
2	q	61	ASN
2	n	54	ASN
1	P	91	GLN
1	R	197	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	403	-	4,4,4	0.85	0	6,6,6	0.58	0
4	SPD	L	404	-	9,9,9	0.41	0	8,8,8	1.33	2 (25%)
4	SPD	F	404	-	9,9,9	0.42	0	8,8,8	1.00	0
4	SPD	O	407	-	9,9,9	0.41	0	8,8,8	0.96	0
3	SO4	G	401	-	4,4,4	0.86	0	6,6,6	0.52	0
3	SO4	L	401	-	4,4,4	0.83	0	6,6,6	0.53	0
3	SO4	N	402	-	4,4,4	0.85	0	6,6,6	0.54	0
3	SO4	I	402	-	4,4,4	0.85	0	6,6,6	0.53	0
4	SPD	H	403	-	9,9,9	0.42	0	8,8,8	1.00	0
3	SO4	K	401	-	4,4,4	0.83	0	6,6,6	0.56	0
3	SO4	E	402	-	4,4,4	0.86	0	6,6,6	0.52	0
3	SO4	L	402	-	4,4,4	0.87	0	6,6,6	0.63	0
3	SO4	R	402	-	4,4,4	0.85	0	6,6,6	0.54	0
3	SO4	A	402	-	4,4,4	0.85	0	6,6,6	0.59	0
3	SO4	J	401	-	4,4,4	0.86	0	6,6,6	0.53	0
3	SO4	K	402	-	4,4,4	0.81	0	6,6,6	0.55	0
3	SO4	A	403	-	4,4,4	0.86	0	6,6,6	0.57	0
3	SO4	B	403	-	4,4,4	0.86	0	6,6,6	0.51	0
3	SO4	E	404	-	4,4,4	0.85	0	6,6,6	0.58	0
3	SO4	N	403	-	4,4,4	0.85	0	6,6,6	0.53	0
3	SO4	O	401	-	4,4,4	0.82	0	6,6,6	0.62	0
3	SO4	E	403	-	4,4,4	0.84	0	6,6,6	0.50	0
3	SO4	M	402	-	4,4,4	0.86	0	6,6,6	0.56	0
3	SO4	H	402	-	4,4,4	0.87	0	6,6,6	0.53	0
3	SO4	E	401	-	4,4,4	0.85	0	6,6,6	0.59	0
4	SPD	J	404	-	9,9,9	0.43	0	8,8,8	1.03	0
4	SPD	Q	401	-	9,9,9	0.43	0	8,8,8	0.91	0
3	SO4	G	402	-	4,4,4	0.86	0	6,6,6	0.57	0
3	SO4	F	403	-	4,4,4	0.85	0	6,6,6	0.55	0
3	SO4	A	401	-	4,4,4	0.85	0	6,6,6	0.56	0
3	SO4	O	405	-	4,4,4	0.82	0	6,6,6	0.49	0
3	SO4	D	402	-	4,4,4	0.87	0	6,6,6	0.57	0
4	SPD	N	407	-	9,9,9	0.41	0	8,8,8	1.06	0
4	SPD	K	404	-	9,9,9	0.40	0	8,8,8	0.82	0
4	SPD	C	404	-	9,9,9	0.42	0	8,8,8	1.09	0
3	SO4	O	404	-	4,4,4	0.85	0	6,6,6	0.54	0
3	SO4	D	403	-	4,4,4	0.86	0	6,6,6	0.54	0
3	SO4	I	401	-	4,4,4	0.85	0	6,6,6	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	402	-	4,4,4	0.86	0	6,6,6	0.50	0
3	SO4	N	401	-	4,4,4	0.85	0	6,6,6	0.52	0
3	SO4	H	401	-	4,4,4	0.85	0	6,6,6	0.55	0
3	SO4	N	406	-	4,4,4	0.86	0	6,6,6	0.60	0
3	SO4	O	406	-	4,4,4	0.84	0	6,6,6	0.55	0
4	SPD	G	403	-	9,9,9	0.42	0	8,8,8	0.93	0
4	SPD	P	401	-	9,9,9	0.43	0	8,8,8	1.22	2 (25%)
3	SO4	M	403	-	4,4,4	0.86	0	6,6,6	0.53	0
3	SO4	O	402	-	4,4,4	0.86	0	6,6,6	0.55	0
4	SPD	I	404	-	9,9,9	0.44	0	8,8,8	0.76	0
3	SO4	N	405	-	4,4,4	0.85	0	6,6,6	0.55	0
3	SO4	B	404	-	4,4,4	0.84	0	6,6,6	0.57	0
3	SO4	D	401	-	4,4,4	0.84	0	6,6,6	0.56	0
3	SO4	N	404	-	4,4,4	0.85	0	6,6,6	0.53	0
4	SPD	D	404	-	9,9,9	0.42	0	8,8,8	1.10	1 (12%)
4	SPD	E	405	-	9,9,9	0.41	0	8,8,8	0.89	0
3	SO4	C	403	-	4,4,4	0.86	0	6,6,6	0.53	0
3	SO4	B	401	-	4,4,4	0.84	0	6,6,6	0.56	0
4	SPD	M	404	-	9,9,9	0.42	0	8,8,8	0.88	0
3	SO4	M	401	-	4,4,4	0.83	0	6,6,6	0.56	0
3	SO4	R	403	-	4,4,4	0.85	0	6,6,6	0.50	0
4	SPD	A	404	-	9,9,9	0.43	0	8,8,8	0.71	0
4	SPD	B	405	-	9,9,9	0.41	0	8,8,8	0.85	0
4	SPD	R	404	-	9,9,9	0.40	0	8,8,8	1.13	1 (12%)
3	SO4	L	403	-	4,4,4	0.85	0	6,6,6	0.57	0
3	SO4	C	402	-	4,4,4	0.87	0	6,6,6	0.55	0
3	SO4	R	401	-	4,4,4	0.83	0	6,6,6	0.57	0
3	SO4	F	401	-	4,4,4	0.83	0	6,6,6	0.58	0
3	SO4	J	402	-	4,4,4	0.85	0	6,6,6	0.51	0
3	SO4	K	403	-	4,4,4	0.85	0	6,6,6	0.50	0
3	SO4	J	403	-	4,4,4	0.84	0	6,6,6	0.51	0
3	SO4	I	403	-	4,4,4	0.82	0	6,6,6	0.56	0
3	SO4	C	401	-	4,4,4	0.86	0	6,6,6	0.55	0
3	SO4	F	402	-	4,4,4	0.85	0	6,6,6	0.59	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	L	404	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SPD	F	404	-	-	3/7/7/7	-
4	SPD	J	404	-	-	6/7/7/7	-
4	SPD	M	404	-	-	4/7/7/7	-
4	SPD	G	403	-	-	5/7/7/7	-
4	SPD	A	404	-	-	4/7/7/7	-
4	SPD	B	405	-	-	5/7/7/7	-
4	SPD	H	403	-	-	3/7/7/7	-
4	SPD	O	407	-	-	3/7/7/7	-
4	SPD	I	404	-	-	3/7/7/7	-
4	SPD	P	401	-	-	3/7/7/7	-
4	SPD	Q	401	-	-	3/7/7/7	-
4	SPD	R	404	-	-	4/7/7/7	-
4	SPD	N	407	-	-	5/7/7/7	-
4	SPD	D	404	-	-	3/7/7/7	-
4	SPD	K	404	-	-	5/7/7/7	-
4	SPD	C	404	-	-	3/7/7/7	-
4	SPD	E	405	-	-	6/7/7/7	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	404	SPD	C7-C8-C9	-2.41	105.54	114.17
4	R	404	SPD	C4-C5-N6	-2.32	105.84	112.07
4	P	401	SPD	C4-C5-N6	-2.21	106.14	112.07
4	L	404	SPD	C4-C5-N6	-2.21	106.15	112.07
4	P	401	SPD	C8-C7-N6	-2.16	106.26	112.07

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.

42 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	403	SO4	1	0
4	L	404	SPD	2	0
4	F	404	SPD	3	0
4	O	407	SPD	6	0
3	G	401	SO4	2	0
3	L	401	SO4	1	0
3	I	402	SO4	2	0
4	H	403	SPD	4	0
3	K	401	SO4	1	0
3	E	402	SO4	1	0
3	R	402	SO4	1	0
3	A	403	SO4	2	0
3	E	404	SO4	1	0
3	M	402	SO4	2	0
4	J	404	SPD	3	0
4	Q	401	SPD	7	0
3	G	402	SO4	1	0
3	F	403	SO4	1	0
3	A	401	SO4	1	0
4	N	407	SPD	6	0
4	K	404	SPD	3	0
4	C	404	SPD	3	0
3	H	401	SO4	1	0
3	N	406	SO4	3	0
3	O	406	SO4	2	0
4	G	403	SPD	2	0
4	P	401	SPD	5	0
4	I	404	SPD	1	0
3	D	401	SO4	1	0
3	N	404	SO4	3	0
4	D	404	SPD	5	0
4	E	405	SPD	5	0
4	M	404	SPD	3	0
3	M	401	SO4	2	0
4	A	404	SPD	5	0
4	B	405	SPD	2	0
4	R	404	SPD	3	0
3	R	401	SO4	2	0
3	J	402	SO4	1	0
3	I	403	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	SO4	1	0
3	F	402	SO4	1	0

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, 95th 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%)	-1.13	0	100	100	35, 45, 60, 64	0
1	B	335/340 (98%)	-1.08	0	100	100	33, 47, 62, 71	0
1	C	335/340 (98%)	-1.09	0	100	100	34, 45, 58, 62	0
1	D	335/340 (98%)	-1.13	0	100	100	33, 45, 58, 65	0
1	E	335/340 (98%)	-1.11	0	100	100	35, 47, 60, 65	0
1	F	335/340 (98%)	-1.12	0	100	100	35, 47, 61, 71	0
1	G	335/340 (98%)	-1.13	0	100	100	34, 43, 51, 59	0
1	H	335/340 (98%)	-1.15	0	100	100	34, 44, 52, 59	0
1	I	335/340 (98%)	-1.08	0	100	100	37, 50, 72, 78	0
1	J	335/340 (98%)	-1.03	0	100	100	38, 52, 73, 77	0
1	K	335/340 (98%)	-1.03	0	100	100	36, 52, 72, 78	0
1	L	335/340 (98%)	-0.95	0	100	100	63, 73, 84, 87	0
1	M	335/340 (98%)	-1.09	0	100	100	34, 44, 52, 63	0
1	N	335/340 (98%)	-1.00	0	100	100	62, 74, 82, 86	0
1	O	335/340 (98%)	-0.91	1 (0%)	90	84	62, 72, 82, 86	0
1	P	335/340 (98%)	-0.98	0	100	100	62, 72, 82, 88	0
1	Q	335/340 (98%)	-0.94	0	100	100	62, 74, 84, 89	0
1	R	335/340 (98%)	-0.91	0	100	100	61, 73, 84, 90	0
2	a	225/258 (87%)	-1.10	0	100	100	44, 56, 64, 75	0
2	b	225/258 (87%)	-1.11	0	100	100	38, 45, 59, 89	0
2	c	225/258 (87%)	-1.09	0	100	100	42, 52, 61, 82	0
2	d	225/258 (87%)	-1.10	0	100	100	42, 52, 61, 74	0
2	e	225/258 (87%)	-1.12	0	100	100	38, 45, 59, 102	0
2	f	225/258 (87%)	-1.16	0	100	100	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%)	-1.05	0 100 100	46, 53, 66, 79	0
2	h	225/258 (87%)	-1.03	0 100 100	46, 55, 67, 85	0
2	i	225/258 (87%)	-1.10	0 100 100	40, 49, 68, 102	0
2	j	225/258 (87%)	-1.03	0 100 100	43, 50, 70, 106	0
2	k	225/258 (87%)	-1.02	0 100 100	42, 49, 69, 103	0
2	l	225/258 (87%)	-0.71	0 100 100	80, 102, 121, 126	0
2	m	225/258 (87%)	-1.07	0 100 100	46, 53, 65, 79	0
2	n	225/258 (87%)	-0.88	0 100 100	59, 72, 84, 102	0
2	o	225/258 (87%)	-0.89	0 100 100	44, 56, 64, 75	0
2	p	225/258 (87%)	-0.92	0 100 100	44, 56, 64, 75	0
2	q	225/258 (87%)	-0.84	1 (0%) 88 81	58, 73, 85, 102	0
2	r	225/258 (87%)	-0.80	0 100 100	56, 72, 83, 103	0
All	All	10080/10764 (93%)	-1.03	2 (0%) 100 100	33, 53, 81, 126	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	217	SER	2.7
2	q	191	GLY	2.4

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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
3	SO4	O	404	5/5	0.96	0.09	92,92,92,92	0
4	SPD	O	407	10/10	0.96	0.10	67,67,67,67	0
3	SO4	L	402	5/5	0.97	0.12	93,93,93,93	0
4	SPD	G	403	10/10	0.97	0.09	37,37,37,37	0
4	SPD	L	404	10/10	0.97	0.11	67,67,67,68	0
3	SO4	N	401	5/5	0.97	0.06	88,88,88,88	0
3	SO4	N	402	5/5	0.98	0.05	87,87,87,87	0
3	SO4	N	404	5/5	0.98	0.08	93,93,94,94	0
3	SO4	O	402	5/5	0.98	0.06	92,92,93,93	0
3	SO4	K	401	5/5	0.98	0.06	79,79,80,80	0
3	SO4	R	402	5/5	0.98	0.07	90,90,90,91	0
3	SO4	R	403	5/5	0.98	0.07	85,86,86,86	0
4	SPD	A	404	10/10	0.98	0.08	38,38,38,38	0
4	SPD	B	405	10/10	0.98	0.07	39,40,40,40	0
4	SPD	D	404	10/10	0.98	0.08	38,38,39,39	0
3	SO4	L	401	5/5	0.98	0.05	83,83,83,84	0
4	SPD	H	403	10/10	0.98	0.08	37,37,37,37	0
4	SPD	I	404	10/10	0.98	0.07	45,45,46,46	0
3	SO4	E	402	5/5	0.98	0.11	60,60,60,60	0
4	SPD	M	404	10/10	0.98	0.07	36,36,36,37	0
3	SO4	I	401	5/5	0.98	0.08	76,76,76,76	0
4	SPD	P	401	10/10	0.98	0.08	65,65,65,65	0
4	SPD	Q	401	10/10	0.98	0.08	64,65,66,66	0
4	SPD	R	404	10/10	0.98	0.08	67,68,68,68	0
3	SO4	J	403	5/5	0.99	0.06	54,55,55,55	0
3	SO4	B	401	5/5	0.99	0.03	54,54,54,54	0
3	SO4	K	402	5/5	0.99	0.04	63,63,63,64	0
3	SO4	B	402	5/5	0.99	0.03	64,64,64,64	0
3	SO4	C	401	5/5	0.99	0.04	60,60,60,61	0
3	SO4	L	403	5/5	0.99	0.03	84,84,84,84	0
3	SO4	M	401	5/5	0.99	0.07	47,47,47,47	0
3	SO4	M	402	5/5	0.99	0.04	51,51,51,51	0
3	SO4	M	403	5/5	0.99	0.05	53,53,54,54	0
3	SO4	C	402	5/5	0.99	0.06	53,53,53,53	0
3	SO4	C	403	5/5	0.99	0.03	52,52,52,52	0
3	SO4	N	403	5/5	0.99	0.03	83,83,83,83	0
3	SO4	D	401	5/5	0.99	0.06	57,57,57,57	0
3	SO4	N	405	5/5	0.99	0.05	86,86,86,86	0
3	SO4	N	406	5/5	0.99	0.04	90,90,90,90	0
3	SO4	O	401	5/5	0.99	0.04	95,95,95,95	0
3	SO4	D	402	5/5	0.99	0.06	55,55,55,55	0
3	SO4	O	403	5/5	0.99	0.07	88,88,88,88	0
3	SO4	D	403	5/5	0.99	0.03	50,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	O	405	5/5	0.99	0.09	85,85,85,85	0
3	SO4	O	406	5/5	0.99	0.04	85,85,86,86	0
3	SO4	R	401	5/5	0.99	0.05	89,89,89,89	0
3	SO4	E	401	5/5	0.99	0.03	52,52,52,52	0
3	SO4	A	402	5/5	0.99	0.05	54,54,54,54	0
3	SO4	E	403	5/5	0.99	0.03	51,51,51,51	0
3	SO4	E	404	5/5	0.99	0.05	56,56,56,56	0
4	SPD	C	404	10/10	0.99	0.05	39,40,40,40	0
3	SO4	F	401	5/5	0.99	0.03	53,53,53,54	0
4	SPD	E	405	10/10	0.99	0.06	39,39,39,39	0
4	SPD	F	404	10/10	0.99	0.06	39,39,39,39	0
3	SO4	F	402	5/5	0.99	0.10	65,65,66,66	0
3	SO4	G	401	5/5	0.99	0.07	50,50,50,50	0
3	SO4	G	402	5/5	0.99	0.03	49,49,50,50	0
4	SPD	J	404	10/10	0.99	0.06	45,45,46,46	0
4	SPD	K	404	10/10	0.99	0.06	45,45,45,45	0
3	SO4	H	401	5/5	0.99	0.05	49,49,50,50	0
3	SO4	H	402	5/5	0.99	0.03	52,52,52,52	0
4	SPD	N	407	10/10	0.99	0.06	67,67,67,67	0
3	SO4	A	403	5/5	0.99	0.04	54,55,55,55	0
3	SO4	I	402	5/5	0.99	0.04	66,66,66,66	0
3	SO4	J	401	5/5	0.99	0.03	76,76,76,76	0
3	SO4	J	402	5/5	0.99	0.06	66,66,66,66	0
3	SO4	B	403	5/5	1.00	0.03	52,52,52,52	0
3	SO4	I	403	5/5	1.00	0.04	51,51,51,51	0
3	SO4	K	403	5/5	1.00	0.03	56,56,56,56	0
3	SO4	B	404	5/5	1.00	0.02	54,54,54,54	0
3	SO4	F	403	5/5	1.00	0.03	56,56,56,56	0
3	SO4	A	401	5/5	1.00	0.04	56,57,57,57	0

6.5 Other polymers

There are no such residues in this entry.