



# wwPDB X-ray Structure Validation Summary Report

Mar 5, 2026 – 11:51 AM UTC

PDB ID : 4FAO / pdb\_00004fao  
Title : Specificity and Structure of a high affinity Activin-like 1 (ALK1) signaling complex  
Authors : Townson, S.A.; Martinez-Hackert, E.; Greppi, C.; Lowden, P.; Sako, D.; Liu, J.; Ucran, J.A.; Liharska, K.; Underwood, K.W.; Seehra, J.; Kumar, R.; Grinberg, A.V.  
Deposited on : 2012-05-22  
Resolution : 3.36 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](mailto: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>.

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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)  
Xtrriage (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

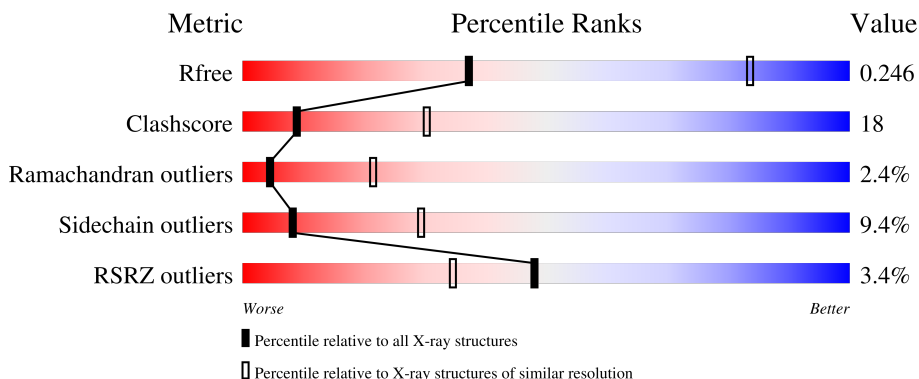
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.36 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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  $\geq 3$ , 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	110	
1	B	110	
1	G	110	
1	H	110	

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Mol	Chain	Length	Quality of chain
1	M	110	
1	N	110	
1	S	110	
1	T	110	
1	a	110	
1	b	110	
1	g	110	
1	h	110	
2	C	106	
2	D	106	
2	I	106	
2	J	106	
2	O	106	
2	P	106	
2	U	106	
2	V	106	
2	c	106	
2	d	106	
2	i	106	
2	j	106	
3	E	124	
3	F	124	
3	K	124	
3	L	124	
3	Q	124	

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Mol	Chain	Length	Quality of chain
3	R	124	<p>2% 48% 22% 27%</p>
3	W	124	<p>3% 45% 24% 27%</p>
3	X	124	<p>2% 49% 22% 27%</p>
3	e	124	<p>50% 20% 27%</p>
3	f	124	<p>2% 48% 22% 27%</p>
3	k	124	<p>2% 46% 23% 27%</p>
3	l	124	<p>4% 48% 22% 27%</p>

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	NAG	F	202	X	-	-	-
4	NAG	K	202	X	-	-	-
4	NAG	L	202	X	-	-	-
4	NAG	X	202	X	-	-	-
4	NAG	k	202	X	-	-	-
4	NAG	l	202	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25411 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 Growth/differentiation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	105	821	528	134	150	9	0	0	0
1	B	105	814	523	133	150	8	0	0	0
1	G	105	810	520	132	150	8	0	0	0
1	H	105	821	528	134	150	9	0	0	0
1	M	105	817	525	133	150	9	0	0	0
1	N	104	801	515	128	149	9	0	0	0
1	S	105	821	528	134	150	9	0	0	0
1	T	105	813	522	132	150	9	0	0	0
1	a	105	806	518	129	150	9	0	0	0
1	b	105	821	528	134	150	9	0	0	0
1	g	105	820	528	133	150	9	0	0	0
1	h	105	821	528	134	150	9	0	0	0

- Molecule 2 is a protein called Serine/threonine-protein kinase receptor R3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	75	567	344	111	102	10	0	0	0
2	D	72	553	333	110	100	10	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	75	Total 556	C 338	N 110	O 98	S 10	0	0	0
2	J	72	Total 539	C 327	N 104	O 98	S 10	0	0	0
2	O	75	Total 531	C 325	N 99	O 97	S 10	0	0	0
2	P	72	Total 549	C 333	N 110	O 96	S 10	0	0	0
2	U	75	Total 572	C 346	N 112	O 104	S 10	0	0	0
2	V	72	Total 553	C 333	N 111	O 99	S 10	0	0	0
2	c	75	Total 561	C 340	N 113	O 98	S 10	0	0	0
2	d	72	Total 539	C 328	N 104	O 97	S 10	0	0	0
2	i	75	Total 559	C 339	N 109	O 101	S 10	0	0	0
2	j	72	Total 559	C 336	N 113	O 100	S 10	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	20	GLY	-	expression tag	UNP P37023
C	21	ALA	-	expression tag	UNP P37023
C	119	SER	-	expression tag	UNP P37023
C	120	GLY	-	expression tag	UNP P37023
C	121	ASP	-	expression tag	UNP P37023
C	122	ASP	-	expression tag	UNP P37023
C	123	ASP	-	expression tag	UNP P37023
C	124	ASP	-	expression tag	UNP P37023
C	125	LYS	-	expression tag	UNP P37023
D	20	GLY	-	expression tag	UNP P37023
D	21	ALA	-	expression tag	UNP P37023
D	119	SER	-	expression tag	UNP P37023
D	120	GLY	-	expression tag	UNP P37023
D	121	ASP	-	expression tag	UNP P37023
D	122	ASP	-	expression tag	UNP P37023
D	123	ASP	-	expression tag	UNP P37023
D	124	ASP	-	expression tag	UNP P37023
D	125	LYS	-	expression tag	UNP P37023
I	20	GLY	-	expression tag	UNP P37023

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Chain	Residue	Modelled	Actual	Comment	Reference
I	21	ALA	-	expression tag	UNP P37023
I	119	SER	-	expression tag	UNP P37023
I	120	GLY	-	expression tag	UNP P37023
I	121	ASP	-	expression tag	UNP P37023
I	122	ASP	-	expression tag	UNP P37023
I	123	ASP	-	expression tag	UNP P37023
I	124	ASP	-	expression tag	UNP P37023
I	125	LYS	-	expression tag	UNP P37023
J	20	GLY	-	expression tag	UNP P37023
J	21	ALA	-	expression tag	UNP P37023
J	119	SER	-	expression tag	UNP P37023
J	120	GLY	-	expression tag	UNP P37023
J	121	ASP	-	expression tag	UNP P37023
J	122	ASP	-	expression tag	UNP P37023
J	123	ASP	-	expression tag	UNP P37023
J	124	ASP	-	expression tag	UNP P37023
J	125	LYS	-	expression tag	UNP P37023
O	20	GLY	-	expression tag	UNP P37023
O	21	ALA	-	expression tag	UNP P37023
O	119	SER	-	expression tag	UNP P37023
O	120	GLY	-	expression tag	UNP P37023
O	121	ASP	-	expression tag	UNP P37023
O	122	ASP	-	expression tag	UNP P37023
O	123	ASP	-	expression tag	UNP P37023
O	124	ASP	-	expression tag	UNP P37023
O	125	LYS	-	expression tag	UNP P37023
P	20	GLY	-	expression tag	UNP P37023
P	21	ALA	-	expression tag	UNP P37023
P	119	SER	-	expression tag	UNP P37023
P	120	GLY	-	expression tag	UNP P37023
P	121	ASP	-	expression tag	UNP P37023
P	122	ASP	-	expression tag	UNP P37023
P	123	ASP	-	expression tag	UNP P37023
P	124	ASP	-	expression tag	UNP P37023
P	125	LYS	-	expression tag	UNP P37023
U	20	GLY	-	expression tag	UNP P37023
U	21	ALA	-	expression tag	UNP P37023
U	119	SER	-	expression tag	UNP P37023
U	120	GLY	-	expression tag	UNP P37023
U	121	ASP	-	expression tag	UNP P37023
U	122	ASP	-	expression tag	UNP P37023
U	123	ASP	-	expression tag	UNP P37023

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Chain	Residue	Modelled	Actual	Comment	Reference
U	124	ASP	-	expression tag	UNP P37023
U	125	LYS	-	expression tag	UNP P37023
V	20	GLY	-	expression tag	UNP P37023
V	21	ALA	-	expression tag	UNP P37023
V	119	SER	-	expression tag	UNP P37023
V	120	GLY	-	expression tag	UNP P37023
V	121	ASP	-	expression tag	UNP P37023
V	122	ASP	-	expression tag	UNP P37023
V	123	ASP	-	expression tag	UNP P37023
V	124	ASP	-	expression tag	UNP P37023
V	125	LYS	-	expression tag	UNP P37023
c	20	GLY	-	expression tag	UNP P37023
c	21	ALA	-	expression tag	UNP P37023
c	119	SER	-	expression tag	UNP P37023
c	120	GLY	-	expression tag	UNP P37023
c	121	ASP	-	expression tag	UNP P37023
c	122	ASP	-	expression tag	UNP P37023
c	123	ASP	-	expression tag	UNP P37023
c	124	ASP	-	expression tag	UNP P37023
c	125	LYS	-	expression tag	UNP P37023
d	20	GLY	-	expression tag	UNP P37023
d	21	ALA	-	expression tag	UNP P37023
d	119	SER	-	expression tag	UNP P37023
d	120	GLY	-	expression tag	UNP P37023
d	121	ASP	-	expression tag	UNP P37023
d	122	ASP	-	expression tag	UNP P37023
d	123	ASP	-	expression tag	UNP P37023
d	124	ASP	-	expression tag	UNP P37023
d	125	LYS	-	expression tag	UNP P37023
i	20	GLY	-	expression tag	UNP P37023
i	21	ALA	-	expression tag	UNP P37023
i	119	SER	-	expression tag	UNP P37023
i	120	GLY	-	expression tag	UNP P37023
i	121	ASP	-	expression tag	UNP P37023
i	122	ASP	-	expression tag	UNP P37023
i	123	ASP	-	expression tag	UNP P37023
i	124	ASP	-	expression tag	UNP P37023
i	125	LYS	-	expression tag	UNP P37023
j	20	GLY	-	expression tag	UNP P37023
j	21	ALA	-	expression tag	UNP P37023
j	119	SER	-	expression tag	UNP P37023
j	120	GLY	-	expression tag	UNP P37023

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Chain	Residue	Modelled	Actual	Comment	Reference
j	121	ASP	-	expression tag	UNP P37023
j	122	ASP	-	expression tag	UNP P37023
j	123	ASP	-	expression tag	UNP P37023
j	124	ASP	-	expression tag	UNP P37023
j	125	LYS	-	expression tag	UNP P37023

- Molecule 3 is a protein called Activin receptor type-2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	91	Total 739	C 457	N 132	O 140	S 10	0	0	0
3	F	91	Total 716	C 445	N 127	O 134	S 10	0	0	0
3	K	91	Total 709	C 441	N 125	O 133	S 10	0	0	0
3	L	91	Total 725	C 448	N 129	O 138	S 10	0	0	0
3	Q	91	Total 736	C 455	N 129	O 142	S 10	0	0	0
3	R	91	Total 718	C 445	N 126	O 137	S 10	0	0	0
3	W	91	Total 726	C 449	N 129	O 138	S 10	0	0	0
3	X	91	Total 711	C 440	N 126	O 135	S 10	0	0	0
3	e	91	Total 718	C 444	N 123	O 141	S 10	0	0	0
3	f	91	Total 725	C 448	N 127	O 140	S 10	0	0	0
3	k	91	Total 710	C 441	N 122	O 137	S 10	0	0	0
3	l	91	Total 712	C 442	N 125	O 135	S 10	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP Q13705
E	0	ALA	-	expression tag	UNP Q13705
E	117	GLY	-	expression tag	UNP Q13705
E	118	ASP	-	expression tag	UNP Q13705
E	119	ASP	-	expression tag	UNP Q13705

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Chain	Residue	Modelled	Actual	Comment	Reference
E	120	ASP	-	expression tag	UNP Q13705
E	121	ASP	-	expression tag	UNP Q13705
E	122	LYS	-	expression tag	UNP Q13705
F	-1	GLY	-	expression tag	UNP Q13705
F	0	ALA	-	expression tag	UNP Q13705
F	117	GLY	-	expression tag	UNP Q13705
F	118	ASP	-	expression tag	UNP Q13705
F	119	ASP	-	expression tag	UNP Q13705
F	120	ASP	-	expression tag	UNP Q13705
F	121	ASP	-	expression tag	UNP Q13705
F	122	LYS	-	expression tag	UNP Q13705
K	-1	GLY	-	expression tag	UNP Q13705
K	0	ALA	-	expression tag	UNP Q13705
K	117	GLY	-	expression tag	UNP Q13705
K	118	ASP	-	expression tag	UNP Q13705
K	119	ASP	-	expression tag	UNP Q13705
K	120	ASP	-	expression tag	UNP Q13705
K	121	ASP	-	expression tag	UNP Q13705
K	122	LYS	-	expression tag	UNP Q13705
L	-1	GLY	-	expression tag	UNP Q13705
L	0	ALA	-	expression tag	UNP Q13705
L	117	GLY	-	expression tag	UNP Q13705
L	118	ASP	-	expression tag	UNP Q13705
L	119	ASP	-	expression tag	UNP Q13705
L	120	ASP	-	expression tag	UNP Q13705
L	121	ASP	-	expression tag	UNP Q13705
L	122	LYS	-	expression tag	UNP Q13705
Q	-1	GLY	-	expression tag	UNP Q13705
Q	0	ALA	-	expression tag	UNP Q13705
Q	117	GLY	-	expression tag	UNP Q13705
Q	118	ASP	-	expression tag	UNP Q13705
Q	119	ASP	-	expression tag	UNP Q13705
Q	120	ASP	-	expression tag	UNP Q13705
Q	121	ASP	-	expression tag	UNP Q13705
Q	122	LYS	-	expression tag	UNP Q13705
R	-1	GLY	-	expression tag	UNP Q13705
R	0	ALA	-	expression tag	UNP Q13705
R	117	GLY	-	expression tag	UNP Q13705
R	118	ASP	-	expression tag	UNP Q13705
R	119	ASP	-	expression tag	UNP Q13705
R	120	ASP	-	expression tag	UNP Q13705
R	121	ASP	-	expression tag	UNP Q13705

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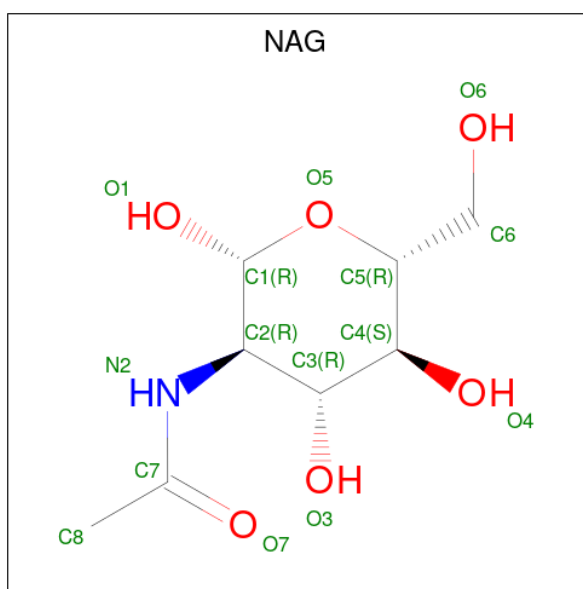
Chain	Residue	Modelled	Actual	Comment	Reference
R	122	LYS	-	expression tag	UNP Q13705
W	-1	GLY	-	expression tag	UNP Q13705
W	0	ALA	-	expression tag	UNP Q13705
W	117	GLY	-	expression tag	UNP Q13705
W	118	ASP	-	expression tag	UNP Q13705
W	119	ASP	-	expression tag	UNP Q13705
W	120	ASP	-	expression tag	UNP Q13705
W	121	ASP	-	expression tag	UNP Q13705
W	122	LYS	-	expression tag	UNP Q13705
X	-1	GLY	-	expression tag	UNP Q13705
X	0	ALA	-	expression tag	UNP Q13705
X	117	GLY	-	expression tag	UNP Q13705
X	118	ASP	-	expression tag	UNP Q13705
X	119	ASP	-	expression tag	UNP Q13705
X	120	ASP	-	expression tag	UNP Q13705
X	121	ASP	-	expression tag	UNP Q13705
X	122	LYS	-	expression tag	UNP Q13705
e	-1	GLY	-	expression tag	UNP Q13705
e	0	ALA	-	expression tag	UNP Q13705
e	117	GLY	-	expression tag	UNP Q13705
e	118	ASP	-	expression tag	UNP Q13705
e	119	ASP	-	expression tag	UNP Q13705
e	120	ASP	-	expression tag	UNP Q13705
e	121	ASP	-	expression tag	UNP Q13705
e	122	LYS	-	expression tag	UNP Q13705
f	-1	GLY	-	expression tag	UNP Q13705
f	0	ALA	-	expression tag	UNP Q13705
f	117	GLY	-	expression tag	UNP Q13705
f	118	ASP	-	expression tag	UNP Q13705
f	119	ASP	-	expression tag	UNP Q13705
f	120	ASP	-	expression tag	UNP Q13705
f	121	ASP	-	expression tag	UNP Q13705
f	122	LYS	-	expression tag	UNP Q13705
k	-1	GLY	-	expression tag	UNP Q13705
k	0	ALA	-	expression tag	UNP Q13705
k	117	GLY	-	expression tag	UNP Q13705
k	118	ASP	-	expression tag	UNP Q13705
k	119	ASP	-	expression tag	UNP Q13705
k	120	ASP	-	expression tag	UNP Q13705
k	121	ASP	-	expression tag	UNP Q13705
k	122	LYS	-	expression tag	UNP Q13705
l	-1	GLY	-	expression tag	UNP Q13705

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Chain	Residue	Modelled	Actual	Comment	Reference
1	0	ALA	-	expression tag	UNP Q13705
1	117	GLY	-	expression tag	UNP Q13705
1	118	ASP	-	expression tag	UNP Q13705
1	119	ASP	-	expression tag	UNP Q13705
1	120	ASP	-	expression tag	UNP Q13705
1	121	ASP	-	expression tag	UNP Q13705
1	122	LYS	-	expression tag	UNP Q13705

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	K	1	Total	C	N	O	0	0
			14	8	1	5		
4	K	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	L	1	Total	C	N	O	0	0
			14	8	1	5		
4	Q	1	Total	C	N	O	0	0
			14	8	1	5		
4	Q	1	Total	C	N	O	0	0
			14	8	1	5		
4	R	1	Total	C	N	O	0	0
			14	8	1	5		
4	R	1	Total	C	N	O	0	0
			14	8	1	5		
4	W	1	Total	C	N	O	0	0
			14	8	1	5		
4	W	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	e	1	Total	C	N	O	0	0
			14	8	1	5		
4	e	1	Total	C	N	O	0	0
			14	8	1	5		
4	f	1	Total	C	N	O	0	0
			14	8	1	5		
4	f	1	Total	C	N	O	0	0
			14	8	1	5		
4	k	1	Total	C	N	O	0	0
			14	8	1	5		
4	k	1	Total	C	N	O	0	0
			14	8	1	5		
4	l	1	Total	C	N	O	0	0
			14	8	1	5		
4	l	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Na	0	0
			1	1		
5	K	1	Total	Na	0	0
			1	1		

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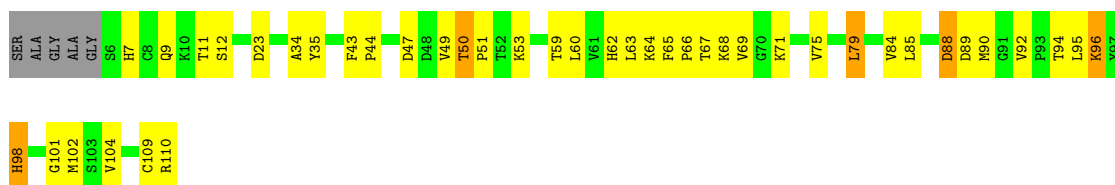
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	R	1	Total 1	Na 1	0	0
5	X	1	Total 1	Na 1	0	0
5	e	1	Total 1	Na 1	0	0
5	k	1	Total 1	Na 1	0	0

### 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.

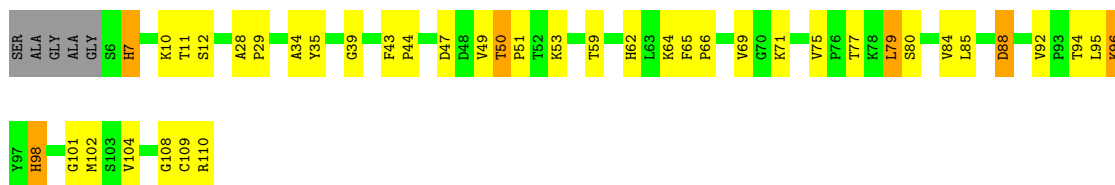
- Molecule 1: Growth/differentiation factor 2

Chain A: 



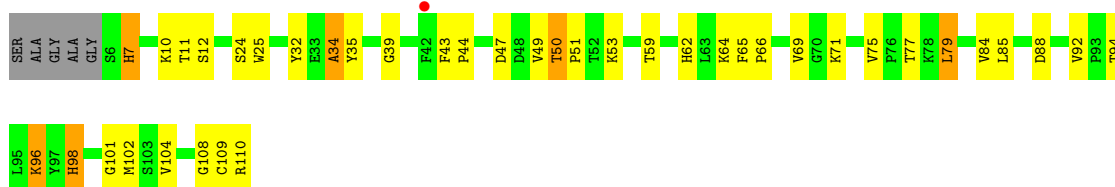
- Molecule 1: Growth/differentiation factor 2

Chain B: 



- Molecule 1: Growth/differentiation factor 2

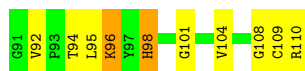
Chain G: 



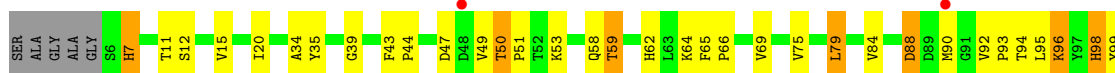
- Molecule 1: Growth/differentiation factor 2

Chain H: 

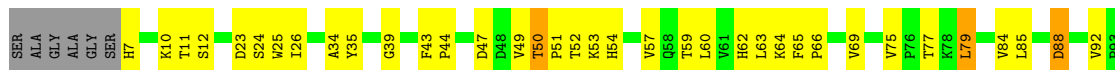




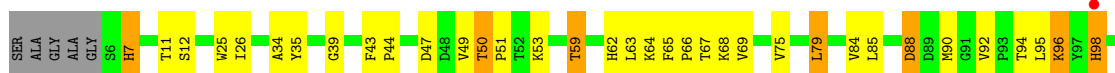
• Molecule 1: Growth/differentiation factor 2



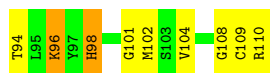
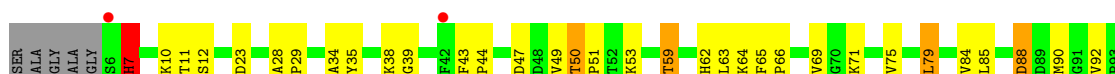
• Molecule 1: Growth/differentiation factor 2



• Molecule 1: Growth/differentiation factor 2

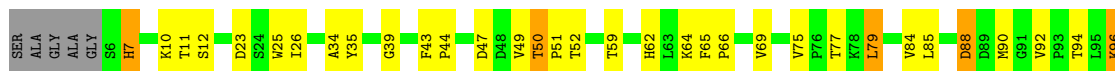


• Molecule 1: Growth/differentiation factor 2

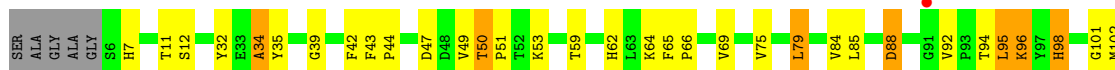


• Molecule 1: Growth/differentiation factor 2

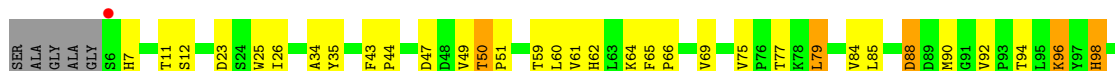




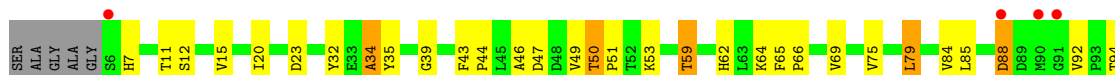
• Molecule 1: Growth/differentiation factor 2



• Molecule 1: Growth/differentiation factor 2



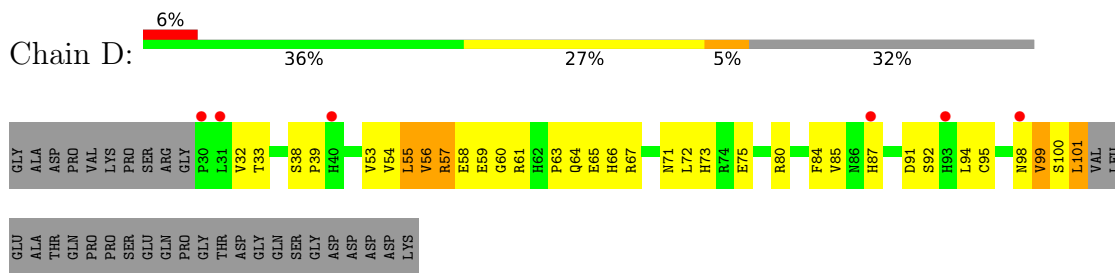
• Molecule 1: Growth/differentiation factor 2



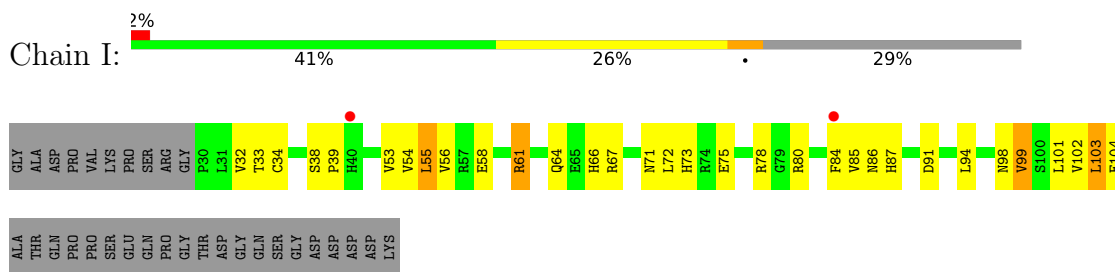
• Molecule 2: Serine/threonine-protein kinase receptor R3



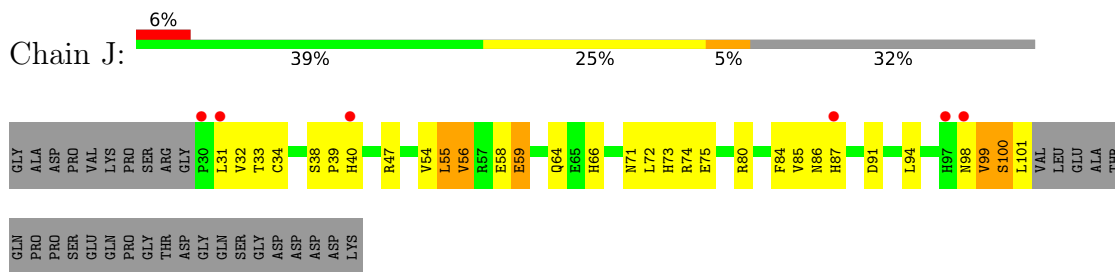
• Molecule 2: Serine/threonine-protein kinase receptor R3



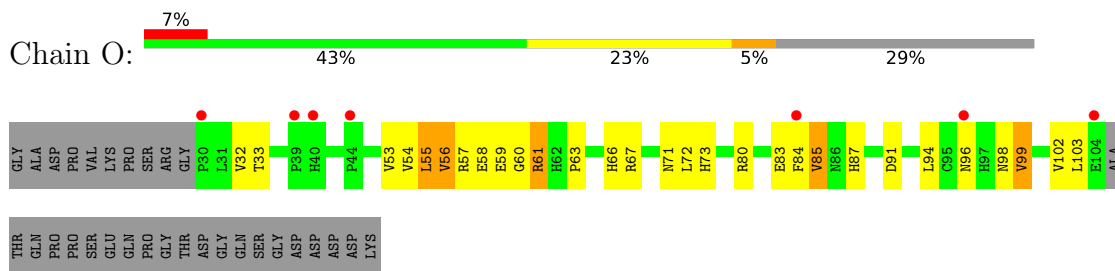
• Molecule 2: Serine/threonine-protein kinase receptor R3



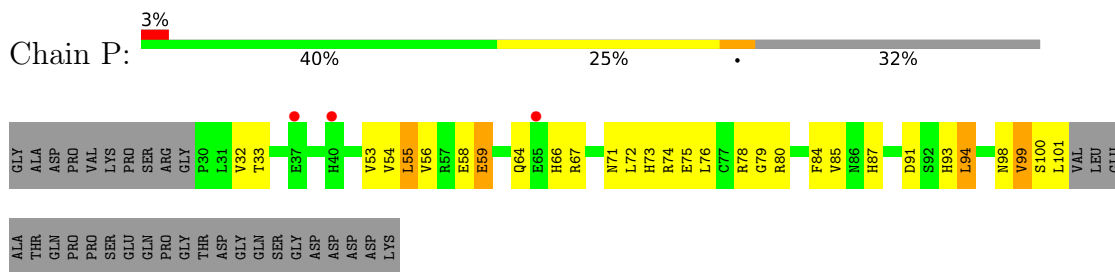
• Molecule 2: Serine/threonine-protein kinase receptor R3



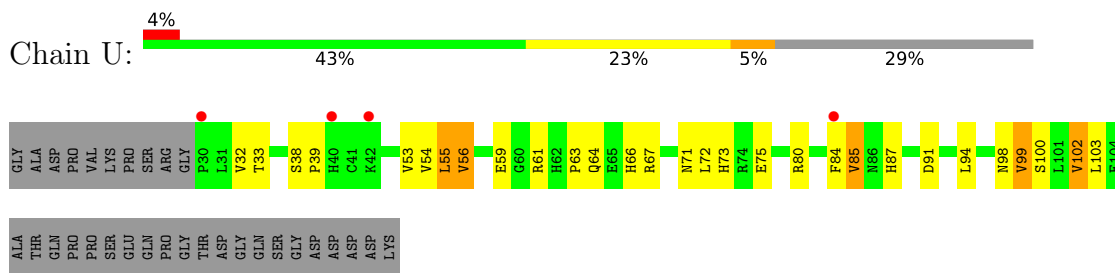
• Molecule 2: Serine/threonine-protein kinase receptor R3



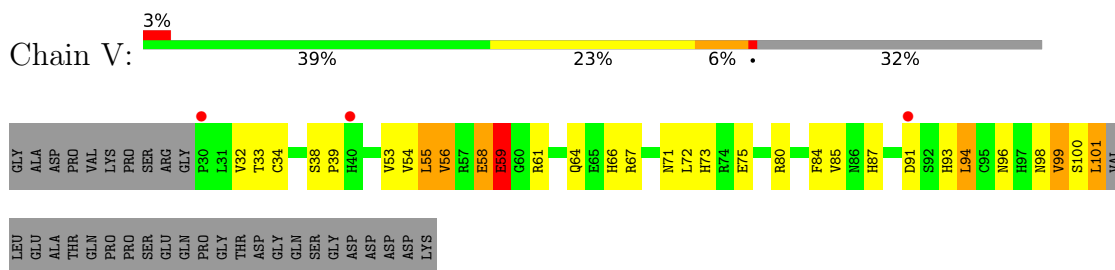
• Molecule 2: Serine/threonine-protein kinase receptor R3



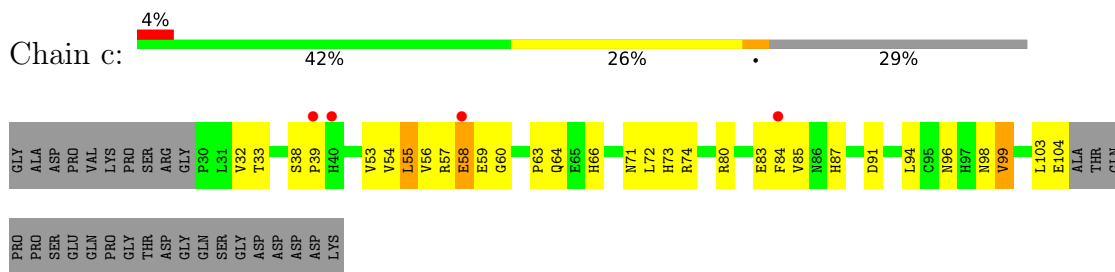
• Molecule 2: Serine/threonine-protein kinase receptor R3



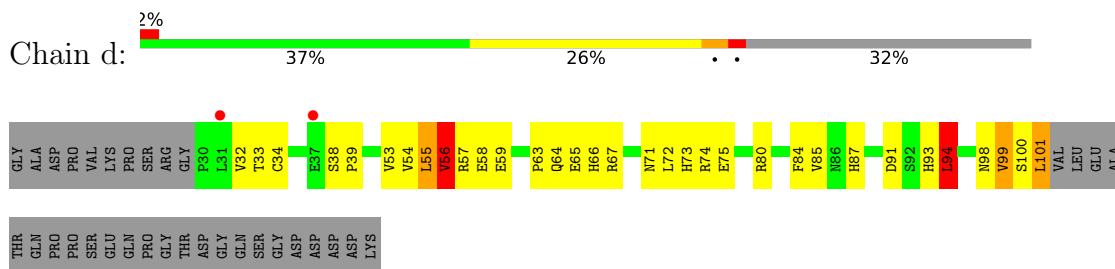
- Molecule 2: Serine/threonine-protein kinase receptor R3



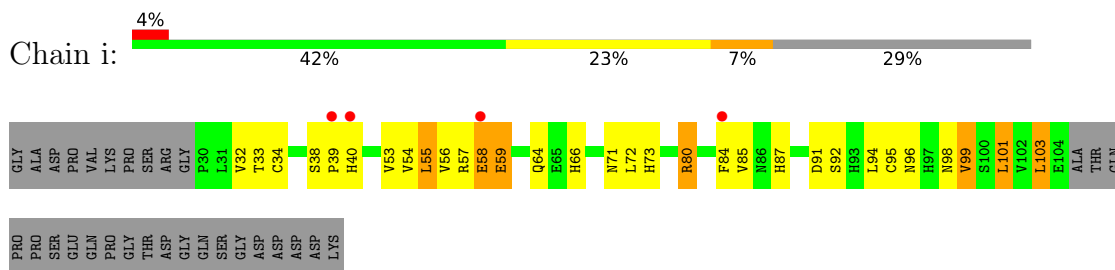
- Molecule 2: Serine/threonine-protein kinase receptor R3



- Molecule 2: Serine/threonine-protein kinase receptor R3



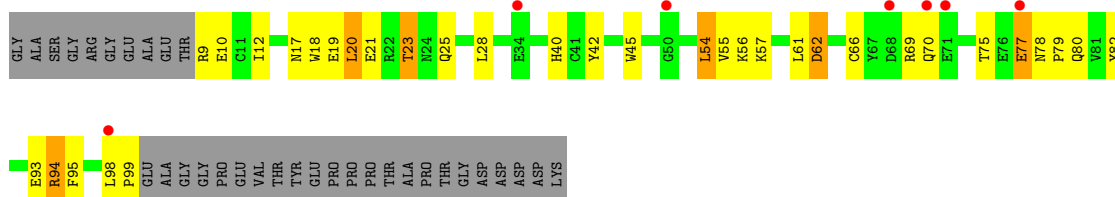
- Molecule 2: Serine/threonine-protein kinase receptor R3



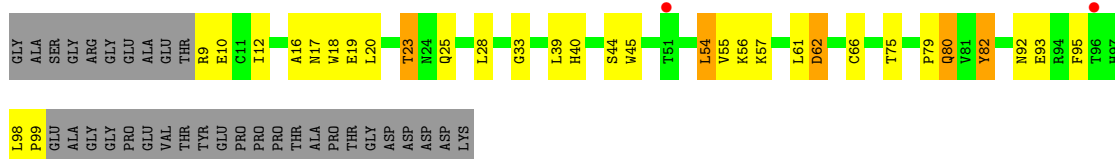
- Molecule 2: Serine/threonine-protein kinase receptor R3



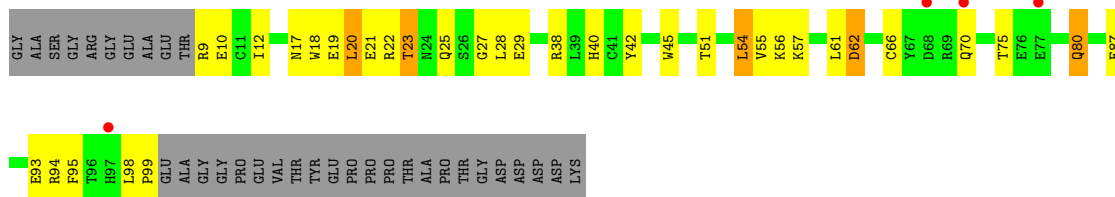
- Molecule 3: Activin receptor type-2B



- Molecule 3: Activin receptor type-2B



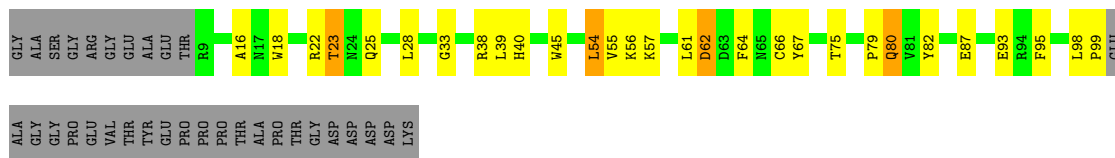
- Molecule 3: Activin receptor type-2B



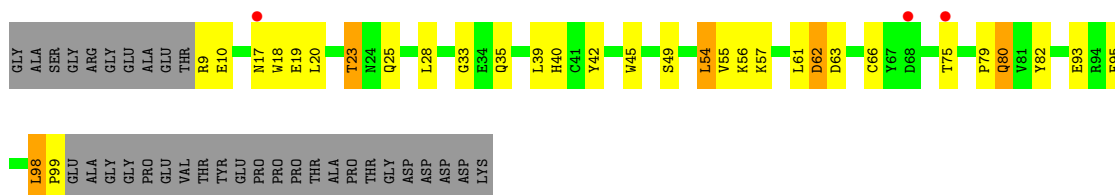
- Molecule 3: Activin receptor type-2B



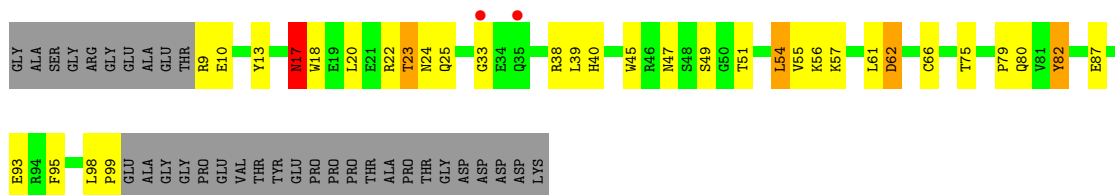
- Molecule 3: Activin receptor type-2B



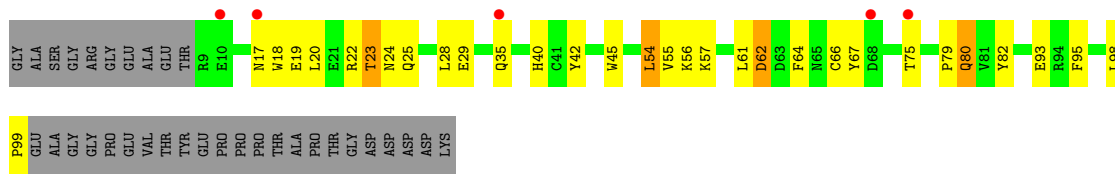
• Molecule 3: Activin receptor type-2B



• Molecule 3: Activin receptor type-2B



• Molecule 3: Activin receptor type-2B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	216.45Å 216.45Å 216.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.85 – 3.36 26.85 – 3.36	Depositor EDS
% Data completeness (in resolution range)	84.0 (26.85-3.36) 82.9 (26.85-3.36)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.47 (at 3.38Å)	Xtrriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, $R_{free}$	0.219 , 0.261 0.207 , 0.246	Depositor DCC
$R_{free}$ test set	2000 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.8	Xtrriage
Anisotropy	0.530	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 73.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	25411	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.68	0/844	1.01	3/1144 (0.3%)
1	B	0.69	0/837	1.03	4/1137 (0.4%)
1	G	0.67	0/833	1.09	6/1133 (0.5%)
1	H	0.67	0/844	1.02	4/1144 (0.3%)
1	M	0.70	0/840	1.00	2/1140 (0.2%)
1	N	0.64	0/823	1.02	5/1119 (0.4%)
1	S	0.70	0/844	1.03	3/1144 (0.3%)
1	T	0.69	0/836	1.06	6/1136 (0.5%)
1	a	0.66	0/828	1.02	4/1126 (0.4%)
1	b	0.67	0/844	1.00	5/1144 (0.4%)
1	g	0.67	0/843	1.03	4/1142 (0.4%)
1	h	0.65	0/844	1.00	2/1144 (0.2%)
2	C	0.57	0/582	0.98	1/792 (0.1%)
2	D	0.52	0/568	0.94	1/772 (0.1%)
2	I	0.51	0/571	0.93	0/778
2	J	0.55	0/553	0.96	1/753 (0.1%)
2	O	0.51	0/545	0.93	1/748 (0.1%)
2	P	0.51	0/564	0.95	0/767
2	U	0.54	0/587	1.00	3/798 (0.4%)
2	V	0.54	0/567	0.95	1/770 (0.1%)
2	c	0.51	0/576	0.91	0/785
2	d	0.50	0/554	0.93	1/755 (0.1%)
2	i	0.50	0/573	0.95	1/780 (0.1%)
2	j	0.50	0/574	0.91	1/779 (0.1%)
3	E	0.62	0/757	0.86	0/1024
3	F	0.54	0/734	0.84	0/996
3	K	0.57	0/727	0.87	0/988
3	L	0.62	0/743	0.84	0/1008
3	Q	0.66	0/754	0.83	0/1021
3	R	0.63	0/736	0.89	0/1000
3	W	0.65	0/744	0.85	0/1009
3	X	0.52	0/729	0.84	0/990

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	e	0.55	0/736	0.82	0/1000
3	f	0.58	0/743	0.83	0/1008
3	k	0.53	0/728	0.84	0/990
3	l	0.60	0/730	0.85	0/992
All	All	0.61	0/25735	0.95	59/34956 (0.2%)

There are no bond length outliers.

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	ALA	N-CA-C	-7.34	99.66	110.52
1	G	7	HIS	CB-CA-C	-7.30	106.56	117.07
1	h	34	ALA	N-CA-C	-7.09	100.03	110.52
1	b	34	ALA	N-CA-C	-6.88	100.34	110.52
1	a	34	ALA	N-CA-C	-6.85	100.38	110.52

There are no chirality outliers.

There are no planarity outliers.

## 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	821	0	801	36	0
1	B	814	0	783	41	0
1	G	810	0	772	38	0
1	H	821	0	801	41	0
1	M	817	0	790	42	0
1	N	801	0	765	48	0
1	S	821	0	801	43	0
1	T	813	0	779	43	0
1	a	806	0	767	37	0
1	b	821	0	801	35	0
1	g	820	0	800	38	0
1	h	821	0	801	40	0
2	C	567	0	509	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	553	0	499	23	0
2	I	556	0	483	19	0
2	J	539	0	478	20	0
2	O	531	0	449	23	0
2	P	549	0	493	20	0
2	U	572	0	514	14	0
2	V	553	0	502	20	0
2	c	561	0	501	23	0
2	d	539	0	476	28	0
2	i	559	0	503	23	0
2	j	559	0	510	29	0
3	E	739	0	637	30	0
3	F	716	0	614	22	0
3	K	709	0	599	18	0
3	L	725	0	620	19	0
3	Q	736	0	634	34	0
3	R	718	0	606	23	0
3	W	726	0	622	33	0
3	X	711	0	599	21	0
3	e	718	0	596	20	0
3	f	725	0	619	23	0
3	k	710	0	594	21	0
3	l	712	0	601	23	0
4	E	28	0	26	0	0
4	F	28	0	26	0	0
4	K	28	0	26	0	0
4	L	28	0	26	2	0
4	Q	28	0	26	1	0
4	R	28	0	26	0	0
4	W	28	0	26	1	0
4	X	28	0	26	7	0
4	e	28	0	26	0	0
4	f	28	0	26	0	0
4	k	28	0	26	6	0
4	l	28	0	26	1	0
5	F	1	0	0	0	0
5	K	1	0	0	0	0
5	R	1	0	0	0	0
5	X	1	0	0	0	0
5	e	1	0	0	0	0
5	k	1	0	0	0	0
All	All	25411	0	23031	895	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 895 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:100:SER:O	2:J:101:LEU:HD23	1.62	0.99
1:M:64:LYS:HB2	2:P:84:PHE:CE1	2.00	0.97
1:S:90:MET:HE1	2:d:57:ARG:HB2	1.45	0.97
1:N:35:TYR:HB2	1:N:104:VAL:HB	1.50	0.93
2:U:55:LEU:HD13	2:U:103:LEU:HD13	1.52	0.92

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	12	38
1	B	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	12	38
1	G	103/110 (94%)	94 (91%)	9 (9%)	0	100	100
1	H	103/110 (94%)	95 (92%)	6 (6%)	2 (2%)	6	25
1	M	103/110 (94%)	95 (92%)	6 (6%)	2 (2%)	6	25
1	N	102/110 (93%)	93 (91%)	8 (8%)	1 (1%)	12	38
1	S	103/110 (94%)	94 (91%)	8 (8%)	1 (1%)	12	38
1	T	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	12	38
1	a	103/110 (94%)	95 (92%)	6 (6%)	2 (2%)	6	25
1	b	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	12	38
1	g	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	12	38
1	h	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	12	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	73/106 (69%)	57 (78%)	12 (16%)	4 (6%)	1	9
2	D	70/106 (66%)	55 (79%)	11 (16%)	4 (6%)	1	8
2	I	73/106 (69%)	54 (74%)	15 (20%)	4 (6%)	1	9
2	J	70/106 (66%)	54 (77%)	12 (17%)	4 (6%)	1	8
2	O	73/106 (69%)	57 (78%)	12 (16%)	4 (6%)	1	9
2	P	70/106 (66%)	56 (80%)	10 (14%)	4 (6%)	1	8
2	U	73/106 (69%)	57 (78%)	13 (18%)	3 (4%)	2	14
2	V	70/106 (66%)	56 (80%)	10 (14%)	4 (6%)	1	8
2	c	73/106 (69%)	54 (74%)	15 (20%)	4 (6%)	1	9
2	d	70/106 (66%)	56 (80%)	11 (16%)	3 (4%)	2	13
2	i	73/106 (69%)	56 (77%)	13 (18%)	4 (6%)	1	9
2	j	70/106 (66%)	55 (79%)	11 (16%)	4 (6%)	1	8
3	E	89/124 (72%)	78 (88%)	10 (11%)	1 (1%)	11	36
3	F	89/124 (72%)	77 (86%)	10 (11%)	2 (2%)	5	23
3	K	89/124 (72%)	76 (85%)	11 (12%)	2 (2%)	5	23
3	L	89/124 (72%)	79 (89%)	9 (10%)	1 (1%)	11	36
3	Q	89/124 (72%)	79 (89%)	9 (10%)	1 (1%)	11	36
3	R	89/124 (72%)	77 (86%)	11 (12%)	1 (1%)	11	36
3	W	89/124 (72%)	78 (88%)	10 (11%)	1 (1%)	11	36
3	X	89/124 (72%)	77 (86%)	11 (12%)	1 (1%)	11	36
3	e	89/124 (72%)	78 (88%)	10 (11%)	1 (1%)	11	36
3	f	89/124 (72%)	79 (89%)	8 (9%)	2 (2%)	5	23
3	k	89/124 (72%)	76 (85%)	11 (12%)	2 (2%)	5	23
3	l	89/124 (72%)	79 (89%)	8 (9%)	2 (2%)	5	23
All	All	3161/4080 (78%)	2736 (87%)	348 (11%)	77 (2%)	4	21

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	62	ASP
3	F	62	ASP
1	H	88	ASP
3	K	62	ASP
3	L	62	ASP

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	91/93 (98%)	86 (94%)	5 (6%)	19	47
1	B	89/93 (96%)	83 (93%)	6 (7%)	15	41
1	G	88/93 (95%)	83 (94%)	5 (6%)	18	46
1	H	91/93 (98%)	86 (94%)	5 (6%)	19	47
1	M	90/93 (97%)	85 (94%)	5 (6%)	19	46
1	N	87/93 (94%)	82 (94%)	5 (6%)	18	46
1	S	91/93 (98%)	86 (94%)	5 (6%)	19	47
1	T	89/93 (96%)	83 (93%)	6 (7%)	15	41
1	a	87/93 (94%)	82 (94%)	5 (6%)	18	46
1	b	91/93 (98%)	86 (94%)	5 (6%)	19	47
1	g	91/93 (98%)	86 (94%)	5 (6%)	19	47
1	h	91/93 (98%)	86 (94%)	5 (6%)	19	47
2	C	63/92 (68%)	54 (86%)	9 (14%)	3	13
2	D	63/92 (68%)	53 (84%)	10 (16%)	2	10
2	I	58/92 (63%)	47 (81%)	11 (19%)	1	6
2	J	59/92 (64%)	49 (83%)	10 (17%)	2	9
2	O	55/92 (60%)	47 (86%)	8 (14%)	3	13
2	P	60/92 (65%)	51 (85%)	9 (15%)	3	11
2	U	64/92 (70%)	54 (84%)	10 (16%)	2	10
2	V	62/92 (67%)	50 (81%)	12 (19%)	1	5
2	c	61/92 (66%)	53 (87%)	8 (13%)	4	15
2	d	59/92 (64%)	47 (80%)	12 (20%)	1	4
2	i	62/92 (67%)	51 (82%)	11 (18%)	2	8
2	j	64/92 (70%)	53 (83%)	11 (17%)	2	8
3	E	76/106 (72%)	70 (92%)	6 (8%)	11	37
3	F	73/106 (69%)	68 (93%)	5 (7%)	14	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	71/106 (67%)	65 (92%)	6 (8%)	10	33
3	L	75/106 (71%)	70 (93%)	5 (7%)	15	41
3	Q	77/106 (73%)	69 (90%)	8 (10%)	7	24
3	R	73/106 (69%)	68 (93%)	5 (7%)	14	41
3	W	75/106 (71%)	67 (89%)	8 (11%)	6	23
3	X	72/106 (68%)	65 (90%)	7 (10%)	8	28
3	e	73/106 (69%)	69 (94%)	4 (6%)	19	47
3	f	76/106 (72%)	71 (93%)	5 (7%)	15	42
3	k	72/106 (68%)	65 (90%)	7 (10%)	8	28
3	l	72/106 (68%)	68 (94%)	4 (6%)	19	46
All	All	2691/3492 (77%)	2438 (91%)	253 (9%)	8	29

5 of 253 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	80	GLN
2	i	54	VAL
2	U	102	VAL
1	h	98	HIS
2	j	80	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	62	HIS
2	j	87	HIS
3	W	65	ASN
2	j	66	HIS
3	k	80	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 6 are monoatomic - leaving 24 for Mogul analysis.

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
4	NAG	R	201	3	14,14,15	0.77	0	17,19,21	1.30	1 (5%)
4	NAG	e	202	3	14,14,15	0.62	0	17,19,21	1.29	1 (5%)
4	NAG	E	201	3	14,14,15	0.67	0	17,19,21	1.35	3 (17%)
4	NAG	e	201	3	14,14,15	0.59	0	17,19,21	1.52	3 (17%)
4	NAG	L	201	3	14,14,15	0.76	0	17,19,21	1.81	2 (11%)
4	NAG	K	202	3	14,14,15	0.81	1 (7%)	17,19,21	2.35	5 (29%)
4	NAG	Q	201	3	14,14,15	0.66	0	17,19,21	1.16	3 (17%)
4	NAG	W	202	3	14,14,15	0.56	0	17,19,21	1.95	4 (23%)
4	NAG	l	201	3	14,14,15	0.71	0	17,19,21	1.33	2 (11%)
4	NAG	k	201	3	14,14,15	0.53	0	17,19,21	2.17	5 (29%)
4	NAG	F	202	3	14,14,15	0.61	0	17,19,21	1.25	3 (17%)
4	NAG	X	201	3	14,14,15	0.56	0	17,19,21	1.29	2 (11%)
4	NAG	f	201	3	14,14,15	0.67	0	17,19,21	1.33	2 (11%)
4	NAG	K	201	3	14,14,15	0.49	0	17,19,21	2.04	3 (17%)
4	NAG	L	202	3	14,14,15	0.78	1 (7%)	17,19,21	1.34	3 (17%)
4	NAG	k	202	3	14,14,15	0.52	0	17,19,21	0.71	0
4	NAG	X	202	3	14,14,15	0.80	0	17,19,21	1.66	5 (29%)
4	NAG	E	202	3	14,14,15	0.68	0	17,19,21	2.26	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	F	201	3	14,14,15	0.48	0	17,19,21	1.51	3 (17%)
4	NAG	R	202	3	14,14,15	0.60	0	17,19,21	1.32	2 (11%)
4	NAG	W	201	3	14,14,15	0.64	0	17,19,21	2.04	2 (11%)
4	NAG	l	202	3	14,14,15	0.60	0	17,19,21	1.31	2 (11%)
4	NAG	f	202	3	14,14,15	0.52	0	17,19,21	1.87	4 (23%)
4	NAG	Q	202	3	14,14,15	0.82	1 (7%)	17,19,21	2.10	5 (29%)

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	NAG	R	201	3	-	2/6/23/26	0/1/1/1
4	NAG	e	202	3	-	4/6/23/26	0/1/1/1
4	NAG	E	201	3	-	2/6/23/26	0/1/1/1
4	NAG	e	201	3	-	2/6/23/26	0/1/1/1
4	NAG	L	201	3	-	2/6/23/26	0/1/1/1
4	NAG	K	202	3	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	Q	201	3	-	2/6/23/26	0/1/1/1
4	NAG	W	202	3	-	5/6/23/26	0/1/1/1
4	NAG	l	201	3	-	2/6/23/26	0/1/1/1
4	NAG	k	201	3	-	0/6/23/26	0/1/1/1
4	NAG	F	202	3	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	X	201	3	-	2/6/23/26	0/1/1/1
4	NAG	f	201	3	-	4/6/23/26	0/1/1/1
4	NAG	K	201	3	-	2/6/23/26	0/1/1/1
4	NAG	L	202	3	1/1/5/7	5/6/23/26	0/1/1/1
4	NAG	k	202	3	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	E	202	3	-	3/6/23/26	0/1/1/1
4	NAG	X	202	3	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	F	201	3	-	4/6/23/26	0/1/1/1
4	NAG	R	202	3	-	5/6/23/26	0/1/1/1
4	NAG	W	201	3	-	2/6/23/26	0/1/1/1
4	NAG	l	202	3	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	f	202	3	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Q	202	3	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	202	NAG	C1-C2	2.47	1.55	1.52
4	K	202	NAG	C1-C2	2.40	1.55	1.52
4	L	202	NAG	C1-C2	2.11	1.55	1.52

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	201	NAG	C2-N2-C7	-6.64	114.00	122.90
4	E	202	NAG	C1-O5-C5	6.16	120.44	112.19
4	k	201	NAG	C1-O5-C5	5.77	119.92	112.19
4	K	201	NAG	C1-O5-C5	5.57	119.66	112.19
4	K	202	NAG	C1-O5-C5	5.57	119.65	112.19

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	202	NAG	C1
4	K	202	NAG	C1
4	L	202	NAG	C1
4	X	202	NAG	C1
4	k	202	NAG	C1

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	202	NAG	C1-C2-N2-C7
4	E	202	NAG	C8-C7-N2-C2
4	E	202	NAG	O7-C7-N2-C2
4	F	202	NAG	C8-C7-N2-C2
4	F	202	NAG	O7-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	l	201	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	k	201	NAG	4	0
4	X	201	NAG	4	0
4	L	202	NAG	2	0
4	k	202	NAG	2	0
4	X	202	NAG	3	0
4	W	201	NAG	1	0
4	Q	202	NAG	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	105/110 (95%)	-0.13	0 <b>100</b> <b>100</b>	35, 57, 90, 111	0
1	B	105/110 (95%)	-0.19	0 <b>100</b> <b>100</b>	31, 60, 89, 111	0
1	G	105/110 (95%)	-0.09	1 (0%) 79 66	34, 61, 90, 113	0
1	H	105/110 (95%)	-0.13	1 (0%) 79 66	31, 59, 90, 110	0
1	M	105/110 (95%)	-0.09	2 (1%) 66 49	39, 59, 90, 110	0
1	N	104/110 (94%)	-0.03	1 (0%) 79 66	41, 65, 92, 124	0
1	S	105/110 (95%)	-0.12	1 (0%) 79 66	32, 58, 89, 110	0
1	T	105/110 (95%)	-0.06	2 (1%) 66 49	32, 59, 91, 112	0
1	a	105/110 (95%)	-0.02	0 <b>100</b> <b>100</b>	39, 62, 97, 116	0
1	b	105/110 (95%)	-0.12	1 (0%) 79 66	38, 62, 91, 111	0
1	g	105/110 (95%)	-0.15	1 (0%) 79 66	36, 62, 92, 111	0
1	h	105/110 (95%)	-0.04	5 (4%) 35 25	35, 60, 90, 110	0
2	C	75/106 (70%)	0.36	4 (5%) 32 23	56, 94, 131, 160	0
2	D	72/106 (67%)	0.66	6 (8%) 17 14	56, 96, 131, 161	0
2	I	75/106 (70%)	0.43	2 (2%) 56 41	59, 95, 131, 159	0
2	J	72/106 (67%)	0.67	6 (8%) 17 14	55, 95, 131, 161	0
2	O	75/106 (70%)	0.88	7 (9%) 14 13	64, 101, 141, 167	0
2	P	72/106 (67%)	0.43	3 (4%) 40 28	58, 96, 130, 164	0
2	U	75/106 (70%)	0.52	4 (5%) 32 23	57, 95, 130, 160	0
2	V	72/106 (67%)	0.56	3 (4%) 40 28	60, 94, 131, 162	0
2	c	75/106 (70%)	0.67	4 (5%) 32 23	63, 99, 131, 159	0
2	d	72/106 (67%)	0.49	2 (2%) 55 40	58, 97, 131, 159	0
2	i	75/106 (70%)	0.72	4 (5%) 32 23	62, 100, 131, 194	0
2	j	72/106 (67%)	0.54	4 (5%) 30 22	60, 97, 131, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	E	91/124 (73%)	0.71	7 (7%) 19 15	48, 79, 120, 158	0
3	F	91/124 (73%)	0.33	3 (3%) 49 35	56, 83, 121, 156	0
3	K	91/124 (73%)	0.47	5 (5%) 30 22	63, 85, 124, 158	0
3	L	91/124 (73%)	0.43	6 (6%) 24 18	45, 79, 119, 157	0
3	Q	91/124 (73%)	0.71	7 (7%) 19 15	46, 78, 118, 158	0
3	R	91/124 (73%)	0.63	2 (2%) 62 46	66, 92, 129, 185	0
3	W	91/124 (73%)	0.77	4 (4%) 39 28	45, 78, 119, 158	0
3	X	91/124 (73%)	0.27	3 (3%) 49 35	57, 82, 122, 158	0
3	e	91/124 (73%)	0.35	0 100 100	63, 85, 122, 157	0
3	f	91/124 (73%)	0.38	3 (3%) 49 35	43, 80, 121, 160	0
3	k	91/124 (73%)	0.35	2 (2%) 62 46	58, 82, 122, 157	0
3	l	91/124 (73%)	0.37	5 (5%) 30 22	44, 80, 120, 158	0
All	All	3233/4080 (79%)	0.28	111 (3%) 48 34	31, 77, 124, 194	0

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	c	58	GLU	5.2
3	E	68	ASP	4.5
2	i	58	GLU	4.4
3	Q	68	ASP	4.1
3	Q	34	GLU	4.0

## 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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NA	e	203	1/1	0.76	0.27	52,52,52,52	0
4	NAG	f	202	14/15	0.79	0.15	60,102,144,150	0
4	NAG	F	202	14/15	0.79	0.13	84,107,120,127	0
5	NA	k	203	1/1	0.80	0.29	62,62,62,62	0
4	NAG	K	202	14/15	0.82	0.14	56,100,139,142	0
5	NA	X	203	1/1	0.82	0.26	37,37,37,37	0
4	NAG	R	202	14/15	0.82	0.12	69,118,135,152	0
4	NAG	e	202	14/15	0.82	0.13	71,123,143,152	0
4	NAG	l	202	14/15	0.85	0.10	62,97,108,117	0
4	NAG	E	202	14/15	0.85	0.10	42,101,122,123	0
4	NAG	R	201	14/15	0.86	0.16	51,78,96,96	0
4	NAG	X	202	14/15	0.87	0.11	59,83,130,148	0
4	NAG	K	201	14/15	0.88	0.13	43,82,92,93	0
4	NAG	k	202	14/15	0.90	0.11	47,105,157,168	0
4	NAG	L	202	14/15	0.90	0.08	45,108,116,117	0
5	NA	K	203	1/1	0.90	0.24	36,36,36,36	0
4	NAG	W	202	14/15	0.91	0.09	28,84,111,118	0
4	NAG	Q	202	14/15	0.91	0.09	29,77,96,102	0
4	NAG	e	201	14/15	0.92	0.11	38,69,83,85	0
5	NA	F	203	1/1	0.92	0.33	44,44,44,44	0
4	NAG	X	201	14/15	0.94	0.10	30,61,82,92	0
4	NAG	k	201	14/15	0.94	0.10	55,77,95,97	0
5	NA	R	203	1/1	0.94	0.30	58,58,58,58	0
4	NAG	F	201	14/15	0.95	0.10	57,72,98,98	0
4	NAG	E	201	14/15	0.96	0.08	28,41,56,67	0
4	NAG	l	201	14/15	0.97	0.08	18,36,51,65	0
4	NAG	W	201	14/15	0.97	0.07	35,47,55,62	0
4	NAG	Q	201	14/15	0.97	0.08	18,34,58,64	0
4	NAG	L	201	14/15	0.97	0.07	30,37,61,63	0
4	NAG	f	201	14/15	0.98	0.06	21,41,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.