Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2024 – 01:39 PM EDT

PDB ID	:	4FAO
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

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

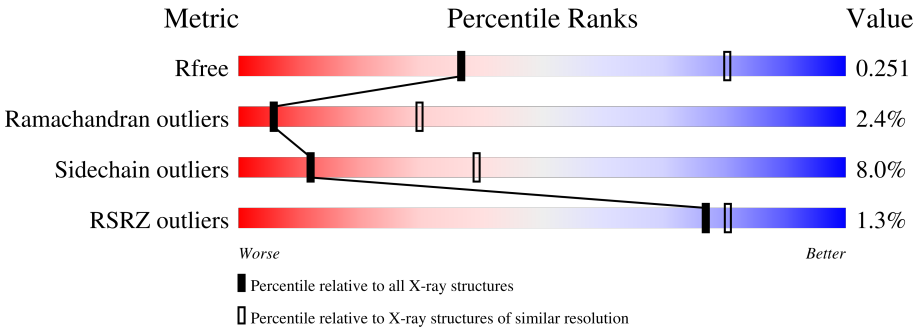
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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}	130704	1558 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	110	92% · 5%
1	B	110	91% 5% 5%
1	G	110	93% · 5%
1	H	110	91% 5% 5%
1	M	110	91% 5% 5%
1	N	110	91% · 5%

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Mol	Chain	Length	Quality of chain
1	S	110	92% • 5%
1	T	110	91% 5% 5%
1	a	110	91% 5% 5%
1	b	110	92% • 5%
1	g	110	92% • 5%
1	h	110	92% • 5%
2	C	106	61% 8% • 29%
2	D	106	57% 10% • 32%
2	I	106	2% 59% 10% • 29%
2	J	106	% 58% 9% • 32%
2	O	106	5% 61% 8% • 29%
2	P	106	2% 58% 8% • 32%
2	U	106	3% 60% 9% • 29%
2	V	106	2% 58% 8% • 32%
2	c	106	% 61% 8% • 29%
2	d	106	3% 58% 8% • 32%
2	i	106	60% 9% • 29%
2	j	106	2% 57% 10% • 32%
3	E	124	68% 6% 27%
3	F	124	% 68% 6% 27%
3	K	124	2% 68% 6% 27%
3	L	124	2% 68% 6% 27%
3	Q	124	% 65% 9% 27%
3	R	124	4% 67% 6% 27%
3	W	124	% 65% 8% 27%

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Mol	Chain	Length	Quality of chain
3	X	124	2% 66% 7% 27%
3	e	124	69% 5% 27%
3	f	124	% 67% 6% 27%
3	k	124	2% 67% 6% 27%
3	l	124	2% 66% 7% 27%

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

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

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

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

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

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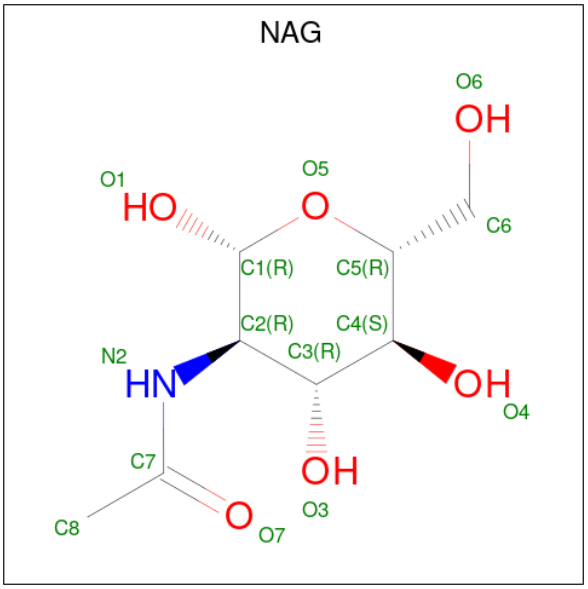
Chain	Residue	Modelled	Actual	Comment	Reference
l	0	ALA	-	expression tag	UNP Q13705
l	117	GLY	-	expression tag	UNP Q13705
l	118	ASP	-	expression tag	UNP Q13705
l	119	ASP	-	expression tag	UNP Q13705
l	120	ASP	-	expression tag	UNP Q13705
l	121	ASP	-	expression tag	UNP Q13705
l	122	LYS	-	expression tag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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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 (three-letter code: 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		

Continued on next page...

Continued from previous page...

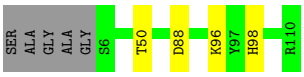
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	R	1	Total Na 1 1	0	0
5	X	1	Total Na 1 1	0	0
5	e	1	Total Na 1 1	0	0
5	k	1	Total Na 1 1	0	0

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.

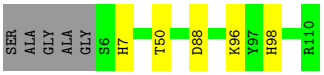
• Molecule 1: Growth/differentiation factor 2

Chain A:



• Molecule 1: Growth/differentiation factor 2

Chain B:

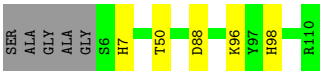


• Molecule 1: Growth/differentiation factor 2

Chain G:

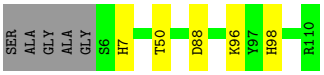
• Molecule 1: Growth/differentiation factor 2

Chain H:



• Molecule 1: Growth/differentiation factor 2

Chain M:

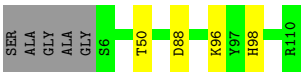


• Molecule 1: Growth/differentiation factor 2

Chain N:

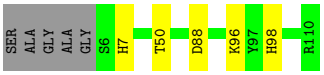
• Molecule 1: Growth/differentiation factor 2

Chain S:



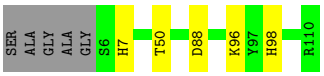
• Molecule 1: Growth/differentiation factor 2

Chain T:



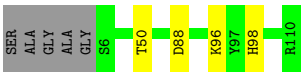
• Molecule 1: Growth/differentiation factor 2

Chain a:



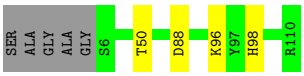
• Molecule 1: Growth/differentiation factor 2

Chain b:



• Molecule 1: Growth/differentiation factor 2

Chain g:

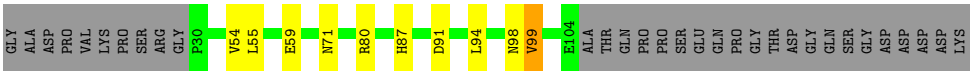


• Molecule 1: Growth/differentiation factor 2

Chain h:

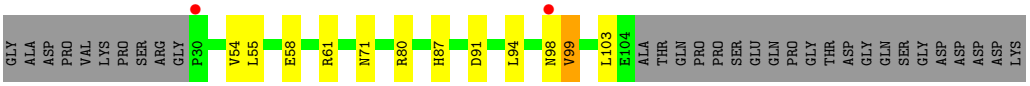
• Molecule 2: Serine/threonine-protein kinase receptor R3

Chain C:

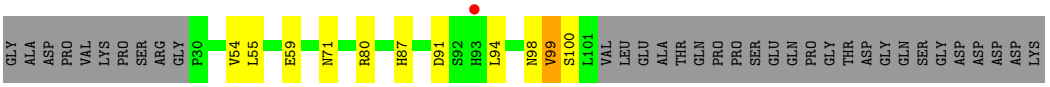


• Molecule 2: Serine/threonine-protein kinase receptor R3

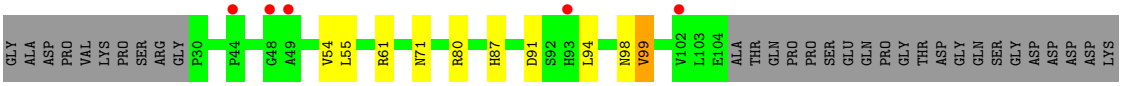
• Molecule 2: Serine/threonine-protein kinase receptor R3



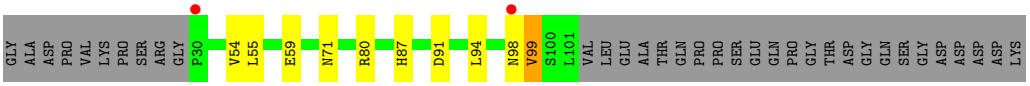
• Molecule 2: Serine/threonine-protein kinase receptor R3



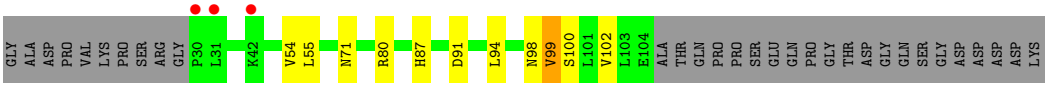
• Molecule 2: Serine/threonine-protein kinase receptor R3



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

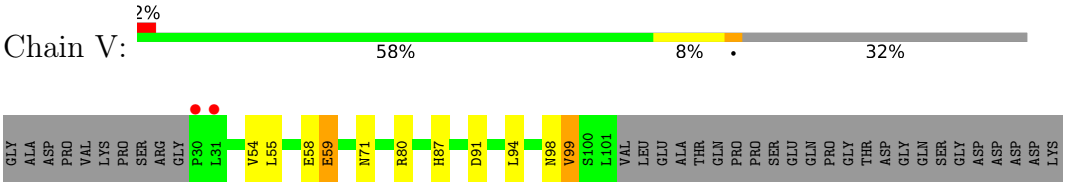


• Molecule 2: Serine/threonine-protein kinase receptor R3



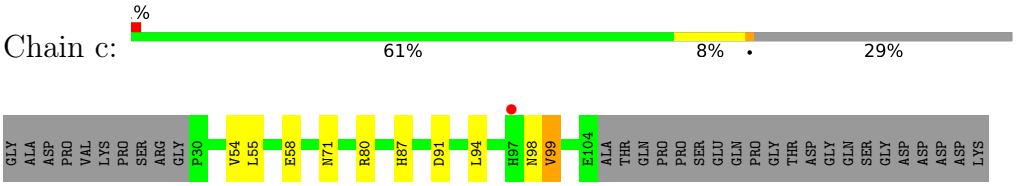
• Molecule 2: Serine/threonine-protein kinase receptor R3

Chain V:



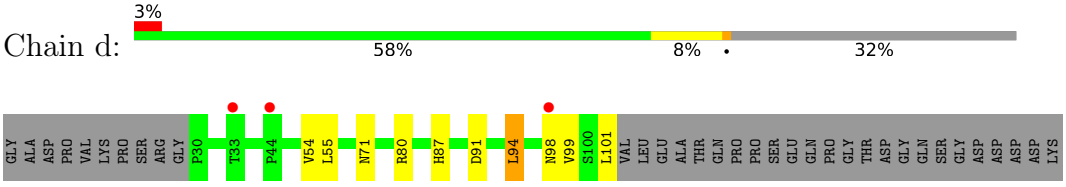
• Molecule 2: Serine/threonine-protein kinase receptor R3

Chain c:



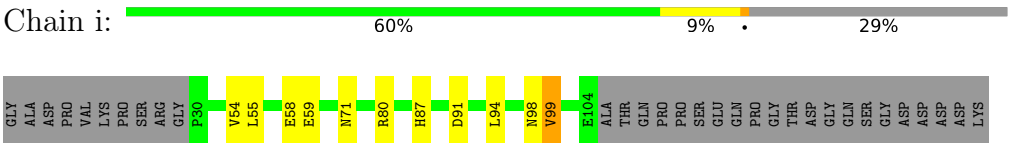
• Molecule 2: Serine/threonine-protein kinase receptor R3

Chain d:



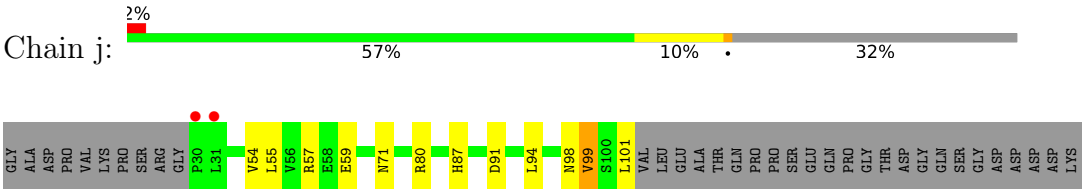
• Molecule 2: Serine/threonine-protein kinase receptor R3

Chain i:



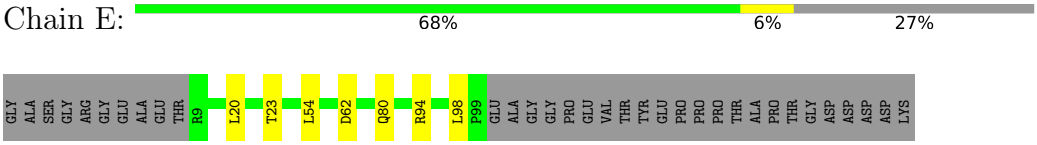
• Molecule 2: Serine/threonine-protein kinase receptor R3

Chain j:



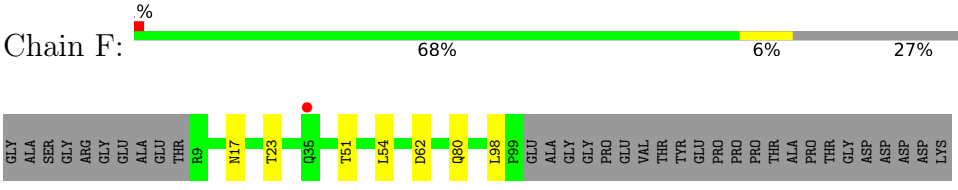
• Molecule 3: Activin receptor type-2B

Chain E:



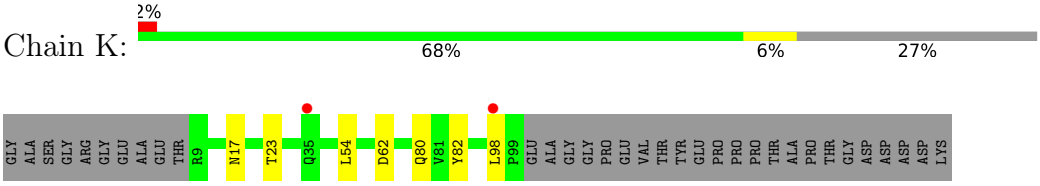
• Molecule 3: Activin receptor type-2B

Chain F:



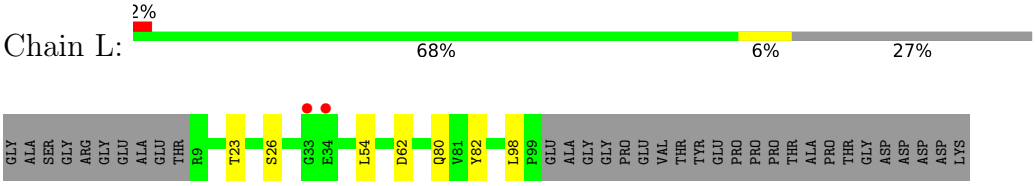
• Molecule 3: Activin receptor type-2B

Chain K:



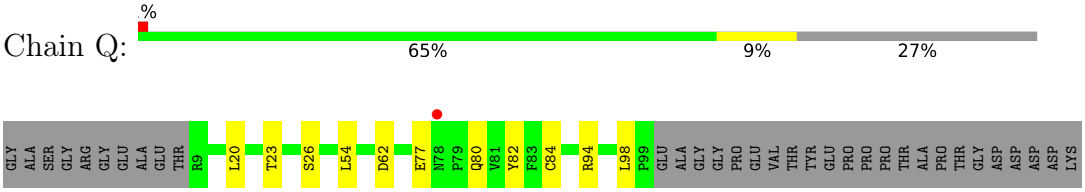
• Molecule 3: Activin receptor type-2B

Chain L:



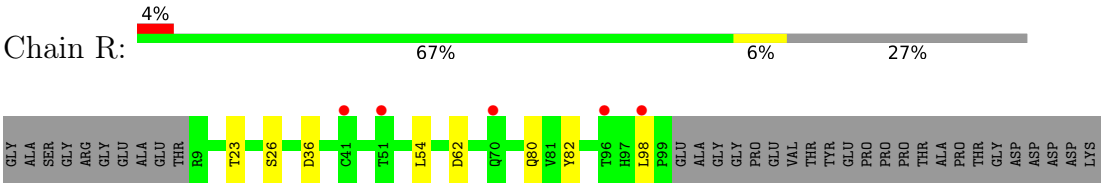
• Molecule 3: Activin receptor type-2B

Chain Q:



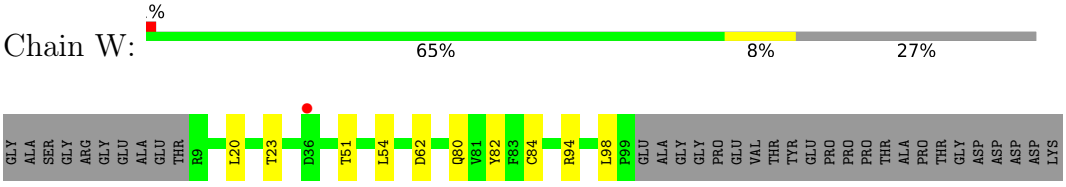
• Molecule 3: Activin receptor type-2B

Chain R:



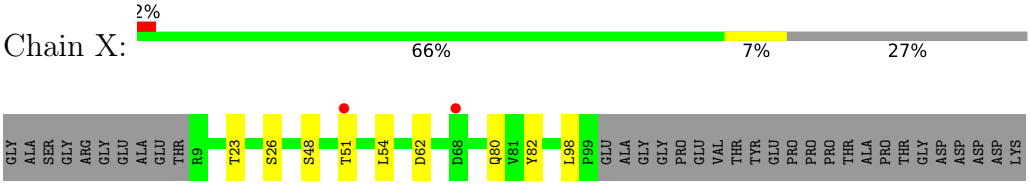
• Molecule 3: Activin receptor type-2B

Chain W:



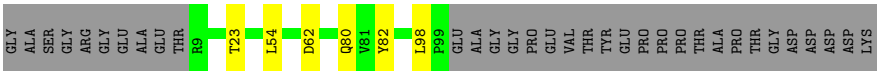
• Molecule 3: Activin receptor type-2B

Chain X:



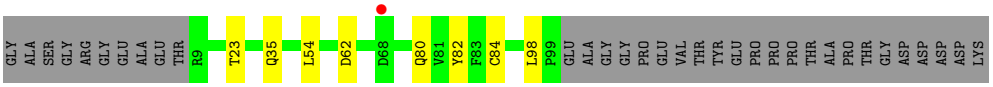
• Molecule 3: Activin receptor type-2B

Chain e:



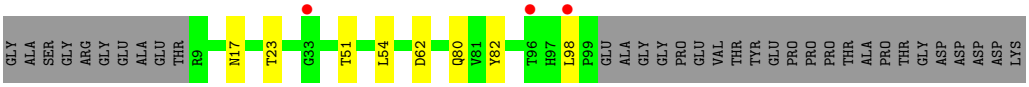
• Molecule 3: Activin receptor type-2B

Chain f:



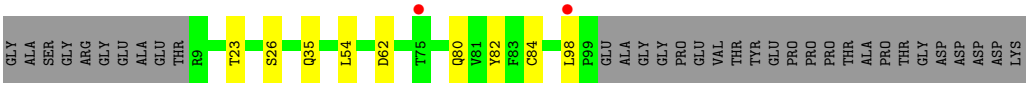
• Molecule 3: Activin receptor type-2B

Chain k:



• Molecule 3: Activin receptor type-2B

Chain l:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α, β, γ	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) 83.0 (26.85-3.36)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.47 (at 3.38Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.219 , 0.261 0.209 , 0.251	Depositor DCC
R_{free} test set	2000 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å^2)	60.8	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 66.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	25411	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.56	0/844	0.63	0/1144
1	B	0.54	0/837	0.64	0/1137
1	G	0.54	0/833	0.65	0/1133
1	H	0.53	0/844	0.63	0/1144
1	M	0.56	0/840	0.62	0/1140
1	N	0.54	0/823	0.64	0/1119
1	S	0.56	0/844	0.62	0/1144
1	T	0.54	0/836	0.64	0/1136
1	a	0.53	0/828	0.65	0/1126
1	b	0.55	0/844	0.62	0/1144
1	g	0.54	0/843	0.63	0/1142
1	h	0.53	0/844	0.62	0/1144
2	C	0.48	0/582	0.60	0/792
2	D	0.45	0/568	0.64	0/772
2	I	0.46	0/571	0.60	0/778
2	J	0.41	0/553	0.63	0/753
2	O	0.38	0/545	0.57	0/748
2	P	0.41	0/564	0.61	0/767
2	U	0.46	0/587	0.60	0/798
2	V	0.44	0/567	0.65	0/770
2	c	0.40	0/576	0.58	0/785
2	d	0.40	0/554	0.61	0/755
2	i	0.40	0/573	0.60	0/780
2	j	0.40	0/574	0.60	0/779
3	E	0.54	0/757	0.60	0/1024
3	F	0.46	0/734	0.57	0/996
3	K	0.50	0/727	0.61	0/988
3	L	0.52	0/743	0.58	0/1008
3	Q	0.54	0/754	0.59	0/1021
3	R	0.56	0/736	0.60	0/1000
3	W	0.53	0/744	0.60	0/1009
3	X	0.44	0/729	0.57	0/990

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
3	e	0.47	0/736	0.58	0/1000
3	f	0.48	0/743	0.58	0/1008
3	k	0.47	0/728	0.57	0/990
3	l	0.51	0/730	0.58	0/992
All	All	0.50	0/25735	0.61	0/34956

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	15 49
1	B	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	15 49
1	G	103/110 (94%)	94 (91%)	9 (9%)	0	100 100
1	H	103/110 (94%)	95 (92%)	6 (6%)	2 (2%)	8 34
1	M	103/110 (94%)	95 (92%)	6 (6%)	2 (2%)	8 34
1	N	102/110 (93%)	93 (91%)	8 (8%)	1 (1%)	15 49
1	S	103/110 (94%)	94 (91%)	8 (8%)	1 (1%)	15 49
1	T	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	15 49
1	a	103/110 (94%)	95 (92%)	6 (6%)	2 (2%)	8 34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	15	49
1	g	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	15	49
1	h	103/110 (94%)	95 (92%)	7 (7%)	1 (1%)	15	49
2	C	73/106 (69%)	57 (78%)	12 (16%)	4 (6%)	2	13
2	D	70/106 (66%)	55 (79%)	11 (16%)	4 (6%)	1	12
2	I	73/106 (69%)	54 (74%)	15 (20%)	4 (6%)	2	13
2	J	70/106 (66%)	54 (77%)	12 (17%)	4 (6%)	1	12
2	O	73/106 (69%)	57 (78%)	12 (16%)	4 (6%)	2	13
2	P	70/106 (66%)	56 (80%)	10 (14%)	4 (6%)	1	12
2	U	73/106 (69%)	57 (78%)	13 (18%)	3 (4%)	3	19
2	V	70/106 (66%)	56 (80%)	10 (14%)	4 (6%)	1	12
2	c	73/106 (69%)	54 (74%)	15 (20%)	4 (6%)	2	13
2	d	70/106 (66%)	56 (80%)	11 (16%)	3 (4%)	2	18
2	i	73/106 (69%)	56 (77%)	13 (18%)	4 (6%)	2	13
2	j	70/106 (66%)	55 (79%)	11 (16%)	4 (6%)	1	12
3	E	89/124 (72%)	78 (88%)	10 (11%)	1 (1%)	14	46
3	F	89/124 (72%)	77 (86%)	10 (11%)	2 (2%)	6	32
3	K	89/124 (72%)	76 (85%)	11 (12%)	2 (2%)	6	32
3	L	89/124 (72%)	79 (89%)	9 (10%)	1 (1%)	14	46
3	Q	89/124 (72%)	79 (89%)	9 (10%)	1 (1%)	14	46
3	R	89/124 (72%)	77 (86%)	11 (12%)	1 (1%)	14	46
3	W	89/124 (72%)	78 (88%)	10 (11%)	1 (1%)	14	46
3	X	89/124 (72%)	77 (86%)	11 (12%)	1 (1%)	14	46
3	e	89/124 (72%)	78 (88%)	10 (11%)	1 (1%)	14	46
3	f	89/124 (72%)	79 (89%)	8 (9%)	2 (2%)	6	32
3	k	89/124 (72%)	76 (85%)	11 (12%)	2 (2%)	6	32
3	l	89/124 (72%)	79 (89%)	8 (9%)	2 (2%)	6	32
All	All	3161/4080 (78%)	2736 (87%)	348 (11%)	77 (2%)	6	30

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	62	ASP

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Mol	Chain	Res	Type
3	F	62	ASP
1	H	88	ASP
3	K	62	ASP
3	L	62	ASP
1	M	88	ASP
2	O	61	ARG
2	P	59	GLU
3	Q	62	ASP
3	R	62	ASP
3	W	62	ASP
3	X	62	ASP
3	e	62	ASP
3	f	62	ASP
2	i	58	GLU
2	j	59	GLU
3	k	62	ASP
3	l	62	ASP
1	A	88	ASP
1	B	88	ASP
2	C	59	GLU
2	D	61	ARG
2	J	59	GLU
1	S	88	ASP
1	T	88	ASP
2	V	59	GLU
1	a	7	HIS
1	a	88	ASP
1	b	88	ASP
2	c	58	GLU
1	h	88	ASP
2	C	94	LEU
2	C	98	ASN
2	D	94	LEU
2	I	94	LEU
2	I	98	ASN
2	J	94	LEU
2	J	98	ASN
1	N	88	ASP
2	P	94	LEU
2	U	98	ASN
2	c	94	LEU
2	c	98	ASN

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Mol	Chain	Res	Type
2	i	94	LEU
2	i	98	ASN
2	j	94	LEU
2	D	98	ASN
1	H	7	HIS
2	I	61	ARG
3	K	17	ASN
2	O	98	ASN
2	P	98	ASN
2	V	98	ASN
2	d	94	LEU
2	d	98	ASN
3	f	35	GLN
1	g	88	ASP
2	j	98	ASN
2	C	99	VAL
2	D	99	VAL
3	F	17	ASN
2	I	99	VAL
2	J	99	VAL
2	O	94	LEU
2	O	99	VAL
2	U	94	LEU
2	V	94	LEU
2	V	99	VAL
2	c	99	VAL
2	d	99	VAL
2	i	99	VAL
1	M	7	HIS
2	P	99	VAL
2	U	99	VAL
2	j	99	VAL
3	k	17	ASN
3	l	35	GLN

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%)	88 (97%)	3 (3%)	38	67
1	B	89/93 (96%)	85 (96%)	4 (4%)	27	59
1	G	88/93 (95%)	85 (97%)	3 (3%)	37	66
1	H	91/93 (98%)	88 (97%)	3 (3%)	38	67
1	M	90/93 (97%)	87 (97%)	3 (3%)	38	67
1	N	87/93 (94%)	84 (97%)	3 (3%)	37	66
1	S	91/93 (98%)	88 (97%)	3 (3%)	38	67
1	T	89/93 (96%)	85 (96%)	4 (4%)	27	59
1	a	87/93 (94%)	84 (97%)	3 (3%)	37	66
1	b	91/93 (98%)	88 (97%)	3 (3%)	38	67
1	g	91/93 (98%)	88 (97%)	3 (3%)	38	67
1	h	91/93 (98%)	88 (97%)	3 (3%)	38	67
2	C	63/92 (68%)	56 (89%)	7 (11%)	6	24
2	D	63/92 (68%)	54 (86%)	9 (14%)	3	14
2	I	58/92 (63%)	49 (84%)	9 (16%)	2	12
2	J	59/92 (64%)	51 (86%)	8 (14%)	3	16
2	O	55/92 (60%)	48 (87%)	7 (13%)	4	18
2	P	60/92 (65%)	53 (88%)	7 (12%)	5	21
2	U	64/92 (70%)	55 (86%)	9 (14%)	3	15
2	V	62/92 (67%)	53 (86%)	9 (14%)	3	14
2	c	61/92 (66%)	54 (88%)	7 (12%)	5	22
2	d	59/92 (64%)	51 (86%)	8 (14%)	3	16
2	i	62/92 (67%)	54 (87%)	8 (13%)	4	17
2	j	64/92 (70%)	55 (86%)	9 (14%)	3	15
3	E	76/106 (72%)	70 (92%)	6 (8%)	12	40
3	F	73/106 (69%)	68 (93%)	5 (7%)	16	46
3	K	71/106 (67%)	66 (93%)	5 (7%)	15	45
3	L	75/106 (71%)	69 (92%)	6 (8%)	12	39
3	Q	77/106 (73%)	67 (87%)	10 (13%)	4	17
3	R	73/106 (69%)	66 (90%)	7 (10%)	8	30
3	W	75/106 (71%)	66 (88%)	9 (12%)	5	20
3	X	72/106 (68%)	64 (89%)	8 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	e	73/106 (69%)	68 (93%)	5 (7%)	16 46
3	f	76/106 (72%)	70 (92%)	6 (8%)	12 40
3	k	72/106 (68%)	66 (92%)	6 (8%)	11 37
3	l	72/106 (68%)	65 (90%)	7 (10%)	8 30
All	All	2691/3492 (77%)	2476 (92%)	215 (8%)	12 39

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	THR
1	A	96	LYS
1	A	98	HIS
1	B	7	HIS
1	B	50	THR
1	B	96	LYS
1	B	98	HIS
2	C	54	VAL
2	C	55	LEU
2	C	71	ASN
2	C	80	ARG
2	C	87	HIS
2	C	91	ASP
2	C	99	VAL
2	D	54	VAL
2	D	55	LEU
2	D	57	ARG
2	D	71	ASN
2	D	80	ARG
2	D	87	HIS
2	D	91	ASP
2	D	99	VAL
2	D	101	LEU
3	E	20	LEU
3	E	23	THR
3	E	54	LEU
3	E	80	GLN
3	E	94	ARG
3	E	98	LEU
3	F	23	THR
3	F	51	THR
3	F	54	LEU

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Mol	Chain	Res	Type
3	F	80	GLN
3	F	98	LEU
1	G	50	THR
1	G	96	LYS
1	G	98	HIS
1	H	50	THR
1	H	96	LYS
1	H	98	HIS
2	I	54	VAL
2	I	55	LEU
2	I	58	GLU
2	I	71	ASN
2	I	80	ARG
2	I	87	HIS
2	I	91	ASP
2	I	99	VAL
2	I	103	LEU
2	J	54	VAL
2	J	55	LEU
2	J	71	ASN
2	J	80	ARG
2	J	87	HIS
2	J	91	ASP
2	J	99	VAL
2	J	100	SER
3	K	23	THR
3	K	54	LEU
3	K	80	GLN
3	K	82	TYR
3	K	98	LEU
3	L	23	THR
3	L	26	SER
3	L	54	LEU
3	L	80	GLN
3	L	82	TYR
3	L	98	LEU
1	M	50	THR
1	M	96	LYS
1	M	98	HIS
1	N	50	THR
1	N	96	LYS
1	N	98	HIS

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Mol	Chain	Res	Type
2	O	54	VAL
2	O	55	LEU
2	O	71	ASN
2	O	80	ARG
2	O	87	HIS
2	O	91	ASP
2	O	99	VAL
2	P	54	VAL
2	P	55	LEU
2	P	71	ASN
2	P	80	ARG
2	P	87	HIS
2	P	91	ASP
2	P	99	VAL
3	Q	20	LEU
3	Q	23	THR
3	Q	26	SER
3	Q	54	LEU
3	Q	77	GLU
3	Q	80	GLN
3	Q	82	TYR
3	Q	84	CYS
3	Q	94	ARG
3	Q	98	LEU
3	R	23	THR
3	R	26	SER
3	R	36	ASP
3	R	54	LEU
3	R	80	GLN
3	R	82	TYR
3	R	98	LEU
1	S	50	THR
1	S	96	LYS
1	S	98	HIS
1	T	7	HIS
1	T	50	THR
1	T	96	LYS
1	T	98	HIS
2	U	54	VAL
2	U	55	LEU
2	U	71	ASN
2	U	80	ARG

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Mol	Chain	Res	Type
2	U	87	HIS
2	U	91	ASP
2	U	99	VAL
2	U	100	SER
2	U	102	VAL
2	V	54	VAL
2	V	55	LEU
2	V	58	GLU
2	V	59	GLU
2	V	71	ASN
2	V	80	ARG
2	V	87	HIS
2	V	91	ASP
2	V	99	VAL
3	W	20	LEU
3	W	23	THR
3	W	51	THR
3	W	54	LEU
3	W	80	GLN
3	W	82	TYR
3	W	84	CYS
3	W	94	ARG
3	W	98	LEU
3	X	23	THR
3	X	26	SER
3	X	48	SER
3	X	51	THR
3	X	54	LEU
3	X	80	GLN
3	X	82	TYR
3	X	98	LEU
1	a	50	THR
1	a	96	LYS
1	a	98	HIS
1	b	50	THR
1	b	96	LYS
1	b	98	HIS
2	c	54	VAL
2	c	55	LEU
2	c	71	ASN
2	c	80	ARG
2	c	87	HIS

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Mol	Chain	Res	Type
2	c	91	ASP
2	c	99	VAL
2	d	54	VAL
2	d	55	LEU
2	d	71	ASN
2	d	80	ARG
2	d	87	HIS
2	d	91	ASP
2	d	94	LEU
2	d	101	LEU
3	e	23	THR
3	e	54	LEU
3	e	80	GLN
3	e	82	TYR
3	e	98	LEU
3	f	23	THR
3	f	54	LEU
3	f	80	GLN
3	f	82	TYR
3	f	84	CYS
3	f	98	LEU
1	g	50	THR
1	g	96	LYS
1	g	98	HIS
1	h	50	THR
1	h	96	LYS
1	h	98	HIS
2	i	54	VAL
2	i	55	LEU
2	i	59	GLU
2	i	71	ASN
2	i	80	ARG
2	i	87	HIS
2	i	91	ASP
2	i	99	VAL
2	j	54	VAL
2	j	55	LEU
2	j	57	ARG
2	j	71	ASN
2	j	80	ARG
2	j	87	HIS
2	j	91	ASP

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Mol	Chain	Res	Type
2	j	99	VAL
2	j	101	LEU
3	k	23	THR
3	k	51	THR
3	k	54	LEU
3	k	80	GLN
3	k	82	TYR
3	k	98	LEU
3	l	23	THR
3	l	26	SER
3	l	54	LEU
3	l	80	GLN
3	l	82	TYR
3	l	84	CYS
3	l	98	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	B	62	HIS
2	C	66	HIS
3	E	17	ASN
3	F	17	ASN
1	G	62	HIS
1	H	62	HIS
3	K	17	ASN
3	L	17	ASN
1	M	62	HIS
1	N	62	HIS
2	P	93	HIS
3	R	17	ASN
1	S	62	HIS
1	T	62	HIS
2	U	66	HIS
2	V	66	HIS
2	V	93	HIS
3	X	17	ASN
1	a	62	HIS
1	b	7	HIS
1	b	62	HIS
2	d	93	HIS

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Mol	Chain	Res	Type
3	e	17	ASN
3	f	17	ASN
1	g	62	HIS
1	h	54	HIS
1	h	62	HIS
3	k	17	ASN
3	l	17	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	E	201	3	14,14,15	0.69	0	17,19,21	1.35	3 (17%)
4	NAG	f	201	3	14,14,15	0.68	0	17,19,21	1.36	2 (11%)
4	NAG	L	202	3	14,14,15	0.75	0	17,19,21	1.34	3 (17%)
4	NAG	W	201	3	14,14,15	0.64	0	17,19,21	2.01	4 (23%)
4	NAG	f	202	3	14,14,15	0.51	0	17,19,21	1.90	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	X	201	3	14,14,15	0.57	0	17,19,21	1.29	2 (11%)
4	NAG	K	202	3	14,14,15	0.77	1 (7%)	17,19,21	2.32	5 (29%)
4	NAG	R	201	3	14,14,15	0.78	0	17,19,21	1.30	2 (11%)
4	NAG	Q	201	3	14,14,15	0.68	0	17,19,21	1.25	3 (17%)
4	NAG	W	202	3	14,14,15	0.55	0	17,19,21	1.98	6 (35%)
4	NAG	F	201	3	14,14,15	0.47	0	17,19,21	1.60	3 (17%)
4	NAG	L	201	3	14,14,15	0.77	0	17,19,21	1.76	2 (11%)
4	NAG	F	202	3	14,14,15	0.58	0	17,19,21	1.32	3 (17%)
4	NAG	e	202	3	14,14,15	0.61	0	17,19,21	1.35	2 (11%)
4	NAG	K	201	3	14,14,15	0.50	0	17,19,21	2.00	3 (17%)
4	NAG	E	202	3	14,14,15	0.65	0	17,19,21	2.25	6 (35%)
4	NAG	l	201	3	14,14,15	0.72	0	17,19,21	1.32	2 (11%)
4	NAG	X	202	3	14,14,15	0.78	0	17,19,21	1.63	5 (29%)
4	NAG	k	201	3	14,14,15	0.51	0	17,19,21	2.16	4 (23%)
4	NAG	l	202	3	14,14,15	0.58	0	17,19,21	1.29	2 (11%)
4	NAG	R	202	3	14,14,15	0.57	0	17,19,21	1.36	3 (17%)
4	NAG	k	202	3	14,14,15	0.51	0	17,19,21	0.75	0
4	NAG	Q	202	3	14,14,15	0.78	1 (7%)	17,19,21	2.20	5 (29%)
4	NAG	e	201	3	14,14,15	0.61	0	17,19,21	1.50	3 (17%)

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	E	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	L	202	3	1/1/5/7	5/6/23/26	0/1/1/1
4	NAG	W	201	3	-	2/6/23/26	0/1/1/1
4	NAG	f	202	3	-	5/6/23/26	0/1/1/1
4	NAG	X	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	R	201	3	-	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	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	201	3	-	4/6/23/26	0/1/1/1
4	NAG	L	201	3	-	2/6/23/26	0/1/1/1
4	NAG	F	202	3	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	e	202	3	-	4/6/23/26	0/1/1/1
4	NAG	K	201	3	-	2/6/23/26	0/1/1/1
4	NAG	E	202	3	-	3/6/23/26	0/1/1/1
4	NAG	l	201	3	-	2/6/23/26	0/1/1/1
4	NAG	X	202	3	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	k	201	3	-	0/6/23/26	0/1/1/1
4	NAG	l	202	3	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	R	202	3	-	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	Q	202	3	-	3/6/23/26	0/1/1/1
4	NAG	e	201	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	202	NAG	C1-C2	2.26	1.55	1.52
4	K	202	NAG	C1-C2	2.20	1.55	1.52

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	W	201	NAG	C2-N2-C7	-6.25	114.00	122.90
4	E	202	NAG	C1-O5-C5	6.09	120.44	112.19
4	k	201	NAG	C1-O5-C5	5.71	119.92	112.19
4	K	201	NAG	C1-O5-C5	5.51	119.66	112.19
4	K	202	NAG	C1-O5-C5	5.50	119.65	112.19
4	K	202	NAG	O5-C1-C2	5.38	119.78	111.29
4	Q	202	NAG	C1-O5-C5	5.38	119.48	112.19
4	W	202	NAG	C1-O5-C5	5.13	119.14	112.19
4	Q	202	NAG	O5-C5-C6	4.45	114.18	107.20
4	L	201	NAG	O5-C1-C2	-4.43	104.29	111.29
4	e	201	NAG	C1-O5-C5	4.38	118.12	112.19
4	f	202	NAG	C4-C3-C2	-4.38	104.60	111.02
4	k	201	NAG	C4-C3-C2	-4.32	104.69	111.02
4	L	201	NAG	C2-N2-C7	-3.86	117.40	122.90
4	K	201	NAG	C4-C3-C2	-3.79	105.46	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	X	201	NAG	C1-O5-C5	3.62	117.09	112.19
4	K	201	NAG	C1-C2-N2	3.52	116.50	110.49
4	W	202	NAG	O5-C1-C2	3.51	116.83	111.29
4	E	202	NAG	C4-C3-C2	-3.39	106.05	111.02
4	R	201	NAG	C4-C3-C2	3.33	115.90	111.02
4	l	202	NAG	C1-O5-C5	3.27	116.62	112.19
4	f	202	NAG	C1-O5-C5	3.26	116.61	112.19
4	F	201	NAG	C6-C5-C4	-3.25	105.40	113.00
4	Q	202	NAG	C3-C4-C5	-3.23	104.48	110.24
4	e	201	NAG	C4-C3-C2	-3.15	106.39	111.02
4	W	201	NAG	C4-C3-C2	-3.15	106.41	111.02
4	E	202	NAG	C2-N2-C7	3.13	127.36	122.90
4	Q	201	NAG	O5-C5-C6	3.00	111.91	107.20
4	F	201	NAG	O5-C5-C6	2.99	111.89	107.20
4	F	201	NAG	C1-O5-C5	2.91	116.13	112.19
4	X	202	NAG	C3-C4-C5	-2.90	105.06	110.24
4	k	201	NAG	C1-C2-N2	2.84	115.34	110.49
4	F	202	NAG	O5-C5-C6	2.78	111.57	107.20
4	E	201	NAG	C1-O5-C5	2.78	115.95	112.19
4	f	202	NAG	O5-C5-C6	2.72	111.46	107.20
4	e	202	NAG	O5-C5-C6	2.70	111.44	107.20
4	K	202	NAG	O3-C3-C2	2.68	115.01	109.47
4	e	202	NAG	C4-C3-C2	2.67	114.93	111.02
4	W	202	NAG	O5-C5-C6	2.61	111.29	107.20
4	f	202	NAG	C3-C4-C5	-2.59	105.62	110.24
4	l	201	NAG	C2-N2-C7	-2.53	119.30	122.90
4	Q	202	NAG	C6-C5-C4	-2.52	107.09	113.00
4	K	202	NAG	C2-N2-C7	2.52	126.49	122.90
4	R	202	NAG	O5-C5-C6	2.48	111.09	107.20
4	E	202	NAG	C1-C2-N2	2.45	114.67	110.49
4	L	202	NAG	C1-O5-C5	2.42	115.48	112.19
4	W	201	NAG	O5-C5-C6	2.41	110.99	107.20
4	K	202	NAG	C3-C4-C5	-2.38	105.99	110.24
4	X	202	NAG	C2-N2-C7	2.36	126.26	122.90
4	R	202	NAG	C3-C4-C5	-2.35	106.04	110.24
4	E	202	NAG	C3-C4-C5	-2.35	106.05	110.24
4	E	201	NAG	C3-C4-C5	2.32	114.38	110.24
4	F	202	NAG	O5-C1-C2	2.31	114.94	111.29
4	X	202	NAG	C4-C3-C2	2.29	114.37	111.02
4	L	202	NAG	C3-C4-C5	-2.27	106.18	110.24
4	Q	202	NAG	C4-C3-C2	-2.23	107.75	111.02
4	e	201	NAG	O3-C3-C4	2.22	115.47	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	X	201	NAG	C1-C2-N2	-2.21	106.71	110.49
4	R	202	NAG	C2-N2-C7	2.21	126.05	122.90
4	E	202	NAG	O5-C5-C6	2.20	110.65	107.20
4	Q	201	NAG	C1-O5-C5	2.19	115.16	112.19
4	W	202	NAG	C2-N2-C7	-2.19	119.78	122.90
4	l	202	NAG	C2-N2-C7	-2.18	119.80	122.90
4	f	202	NAG	C1-C2-N2	2.18	114.20	110.49
4	L	202	NAG	C4-C3-C2	2.16	114.19	111.02
4	f	201	NAG	C6-C5-C4	-2.16	107.96	113.00
4	F	202	NAG	C3-C4-C5	-2.15	106.41	110.24
4	E	201	NAG	C2-N2-C7	-2.15	119.84	122.90
4	k	201	NAG	C6-C5-C4	-2.13	108.01	113.00
4	l	201	NAG	C6-C5-C4	-2.13	108.01	113.00
4	W	202	NAG	C6-C5-C4	-2.11	108.06	113.00
4	f	201	NAG	O7-C7-N2	2.05	125.72	121.95
4	X	202	NAG	C1-O5-C5	2.05	114.97	112.19
4	Q	201	NAG	C2-N2-C7	-2.03	120.02	122.90
4	W	201	NAG	C6-C5-C4	-2.01	108.29	113.00
4	X	202	NAG	O7-C7-C8	-2.00	118.33	122.06
4	W	202	NAG	C3-C4-C5	-2.00	106.67	110.24
4	R	201	NAG	C3-C4-C5	2.00	113.81	110.24

All (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
4	l	202	NAG	C1

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
4	K	201	NAG	C8-C7-N2-C2
4	K	201	NAG	O7-C7-N2-C2
4	L	201	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	L	201	NAG	O7-C7-N2-C2
4	L	202	NAG	C3-C2-N2-C7
4	L	202	NAG	C8-C7-N2-C2
4	L	202	NAG	O7-C7-N2-C2
4	Q	202	NAG	C8-C7-N2-C2
4	Q	202	NAG	O7-C7-N2-C2
4	R	201	NAG	C8-C7-N2-C2
4	R	201	NAG	O7-C7-N2-C2
4	R	202	NAG	C1-C2-N2-C7
4	R	202	NAG	C8-C7-N2-C2
4	R	202	NAG	O7-C7-N2-C2
4	W	202	NAG	C3-C2-N2-C7
4	W	202	NAG	C8-C7-N2-C2
4	W	202	NAG	O7-C7-N2-C2
4	X	201	NAG	C8-C7-N2-C2
4	X	201	NAG	O7-C7-N2-C2
4	X	202	NAG	C3-C2-N2-C7
4	X	202	NAG	C8-C7-N2-C2
4	X	202	NAG	O7-C7-N2-C2
4	e	202	NAG	C3-C2-N2-C7
4	f	202	NAG	C8-C7-N2-C2
4	f	202	NAG	O7-C7-N2-C2
4	k	202	NAG	C8-C7-N2-C2
4	k	202	NAG	O7-C7-N2-C2
4	l	202	NAG	C8-C7-N2-C2
4	l	202	NAG	O7-C7-N2-C2
4	l	201	NAG	O5-C5-C6-O6
4	Q	201	NAG	O5-C5-C6-O6
4	F	201	NAG	C8-C7-N2-C2
4	F	201	NAG	O7-C7-N2-C2
4	R	202	NAG	O5-C5-C6-O6
4	k	202	NAG	O5-C5-C6-O6
4	l	201	NAG	C4-C5-C6-O6
4	f	201	NAG	O5-C5-C6-O6
4	K	202	NAG	C8-C7-N2-C2
4	f	202	NAG	C1-C2-N2-C7
4	f	202	NAG	C4-C5-C6-O6
4	L	202	NAG	C4-C5-C6-O6
4	Q	201	NAG	C4-C5-C6-O6
4	E	201	NAG	C8-C7-N2-C2
4	E	201	NAG	O7-C7-N2-C2
4	K	202	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	e	201	NAG	C8-C7-N2-C2
4	e	202	NAG	C8-C7-N2-C2
4	f	201	NAG	C4-C5-C6-O6
4	e	202	NAG	O7-C7-N2-C2
4	k	202	NAG	C4-C5-C6-O6
4	F	201	NAG	O5-C5-C6-O6
4	f	202	NAG	O5-C5-C6-O6
4	R	202	NAG	C4-C5-C6-O6
4	W	201	NAG	C8-C7-N2-C2
4	e	201	NAG	O7-C7-N2-C2
4	L	202	NAG	O5-C5-C6-O6
4	F	202	NAG	C4-C5-C6-O6
4	F	202	NAG	O5-C5-C6-O6
4	E	202	NAG	C1-C2-N2-C7
4	W	201	NAG	O7-C7-N2-C2
4	e	202	NAG	C1-C2-N2-C7
4	f	201	NAG	C8-C7-N2-C2
4	F	201	NAG	C4-C5-C6-O6
4	f	201	NAG	O7-C7-N2-C2
4	W	202	NAG	O5-C5-C6-O6
4	Q	202	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	105/110 (95%)	-0.47	0	100	100	35, 57, 90, 111	0
1	B	105/110 (95%)	-0.56	0	100	100	31, 60, 89, 111	0
1	G	105/110 (95%)	-0.54	0	100	100	34, 61, 90, 113	0
1	H	105/110 (95%)	-0.46	0	100	100	31, 59, 90, 110	0
1	M	105/110 (95%)	-0.47	0	100	100	39, 59, 90, 110	0
1	N	104/110 (94%)	-0.39	0	100	100	41, 65, 92, 124	0
1	S	105/110 (95%)	-0.44	0	100	100	32, 58, 89, 110	0
1	T	105/110 (95%)	-0.47	0	100	100	32, 59, 91, 112	0
1	a	105/110 (95%)	-0.48	0	100	100	39, 62, 97, 116	0
1	b	105/110 (95%)	-0.51	0	100	100	38, 62, 91, 111	0
1	g	105/110 (95%)	-0.44	0	100	100	36, 62, 92, 111	0
1	h	105/110 (95%)	-0.49	0	100	100	35, 60, 90, 110	0
2	C	75/106 (70%)	0.02	0	100	100	56, 94, 131, 160	0
2	D	72/106 (67%)	0.02	0	100	100	56, 96, 131, 161	0
2	I	75/106 (70%)	-0.02	2 (2%)	54	57	59, 95, 131, 159	0
2	J	72/106 (67%)	0.00	1 (1%)	75	78	55, 95, 131, 161	0
2	O	75/106 (70%)	0.53	5 (6%)	17	20	64, 101, 141, 167	0
2	P	72/106 (67%)	-0.03	2 (2%)	53	55	58, 96, 130, 164	0
2	U	75/106 (70%)	0.05	3 (4%)	38	40	57, 95, 130, 160	0
2	V	72/106 (67%)	-0.01	2 (2%)	53	55	60, 94, 131, 162	0
2	c	75/106 (70%)	0.19	1 (1%)	77	80	63, 99, 131, 159	0
2	d	72/106 (67%)	0.08	3 (4%)	36	38	58, 97, 131, 159	0
2	i	75/106 (70%)	0.21	0	100	100	62, 100, 131, 194	0
2	j	72/106 (67%)	0.00	2 (2%)	53	55	60, 97, 131, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	E	91/124 (73%)	-0.09	0 100 100	48, 79, 120, 158	0
3	F	91/124 (73%)	-0.04	1 (1%) 80 84	56, 83, 121, 156	0
3	K	91/124 (73%)	-0.11	2 (2%) 62 65	63, 85, 124, 158	0
3	L	91/124 (73%)	-0.10	2 (2%) 62 65	45, 79, 119, 157	0
3	Q	91/124 (73%)	0.02	1 (1%) 80 84	46, 78, 118, 158	0
3	R	91/124 (73%)	0.31	5 (5%) 25 27	66, 92, 129, 185	0
3	W	91/124 (73%)	-0.08	1 (1%) 80 84	45, 78, 119, 158	0
3	X	91/124 (73%)	-0.05	2 (2%) 62 65	57, 82, 122, 158	0
3	e	91/124 (73%)	-0.04	0 100 100	63, 85, 122, 157	0
3	f	91/124 (73%)	-0.05	1 (1%) 80 84	43, 80, 121, 160	0
3	k	91/124 (73%)	-0.06	3 (3%) 46 48	58, 82, 122, 157	0
3	l	91/124 (73%)	-0.13	2 (2%) 62 65	44, 80, 120, 158	0
All	All	3233/4080 (79%)	-0.17	41 (1%) 77 80	31, 77, 124, 194	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	j	30	PRO	4.9
3	R	96	THR	4.8
2	P	30	PRO	3.6
2	O	48	GLY	3.4
3	L	34	GLU	3.3
2	V	30	PRO	3.2
2	P	98	ASN	3.1
2	j	31	LEU	3.1
2	V	31	LEU	3.0
3	R	51	THR	3.0
2	U	31	LEU	3.0
2	I	30	PRO	2.8
2	O	44	PRO	2.6
2	I	98	ASN	2.5
2	d	98	ASN	2.4
3	f	68	ASP	2.4
3	R	70	GLN	2.4
2	O	93	HIS	2.3
2	O	49	ALA	2.2
3	L	33	GLY	2.2
3	k	33	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	c	97	HIS	2.2
2	U	42	LYS	2.2
3	Q	78	ASN	2.2
2	d	44	PRO	2.2
2	U	30	PRO	2.2
3	X	51	THR	2.2
2	J	93	HIS	2.1
3	k	96	THR	2.1
3	l	98	LEU	2.1
3	l	75	THR	2.1
3	R	41	CYS	2.1
3	F	35	GLN	2.1
2	O	102	VAL	2.1
3	X	68	ASP	2.1
3	k	98	LEU	2.1
3	K	35	GLN	2.0
3	W	36	ASP	2.0
3	K	98	LEU	2.0
2	d	33	THR	2.0
3	R	98	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	F	202	14/15	0.88	0.20	84,107,120,127	0
4	NAG	R	202	14/15	0.88	0.28	69,118,135,152	0
5	NA	e	203	1/1	0.88	0.33	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	f	202	14/15	0.89	0.26	60,102,144,150	0
4	NAG	e	202	14/15	0.89	0.29	71,123,143,152	0
4	NAG	E	202	14/15	0.90	0.23	42,101,122,123	0
5	NA	k	203	1/1	0.90	0.22	62,62,62,62	0
4	NAG	l	202	14/15	0.91	0.19	62,97,108,117	0
4	NAG	K	202	14/15	0.91	0.19	56,100,139,142	0
4	NAG	k	202	14/15	0.91	0.23	47,105,157,168	0
5	NA	R	203	1/1	0.92	0.17	58,58,58,58	0
4	NAG	L	202	14/15	0.92	0.24	45,108,116,117	0
4	NAG	W	202	14/15	0.92	0.25	28,84,111,118	0
4	NAG	X	202	14/15	0.93	0.24	59,83,130,148	0
4	NAG	Q	202	14/15	0.94	0.25	29,77,96,102	0
5	NA	X	203	1/1	0.94	0.21	37,37,37,37	0
5	NA	F	203	1/1	0.94	0.32	44,44,44,44	0
5	NA	K	203	1/1	0.94	0.27	36,36,36,36	0
4	NAG	F	201	14/15	0.95	0.17	57,72,98,98	0
4	NAG	R	201	14/15	0.95	0.16	51,78,96,96	0
4	NAG	K	201	14/15	0.95	0.13	43,82,92,93	0
4	NAG	k	201	14/15	0.96	0.14	55,77,95,97	0
4	NAG	E	201	14/15	0.97	0.13	28,41,56,67	0
4	NAG	e	201	14/15	0.97	0.14	38,69,83,85	0
4	NAG	Q	201	14/15	0.97	0.14	18,34,58,64	0
4	NAG	W	201	14/15	0.97	0.13	35,47,55,62	0
4	NAG	L	201	14/15	0.97	0.14	30,37,61,63	0
4	NAG	X	201	14/15	0.97	0.15	30,61,82,92	0
4	NAG	l	201	14/15	0.97	0.13	18,36,51,65	0
4	NAG	f	201	14/15	0.98	0.14	21,41,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.