



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2024 – 06:57 AM EDT

PDB ID : 3QAZ
Title : IL-2 mutant D10 ternary complex
Authors : Levin, A.M.; Bates, D.L.; Ring, A.M.; Lin, J.T.; Su, L.; Krieg, C.; Bowman, G.R.; Novick, P.; Pande, V.S.; Khort, H.E.; Boyman, O.; Gathman, C.G.; Garcia, K.C.
Deposited on : 2011-01-12
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

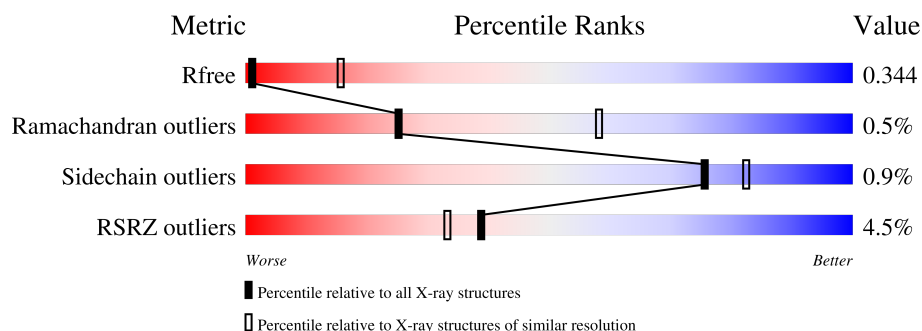
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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.



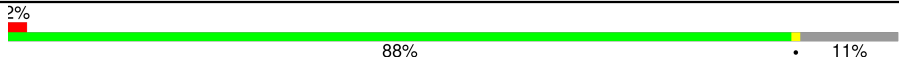
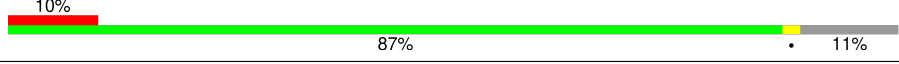
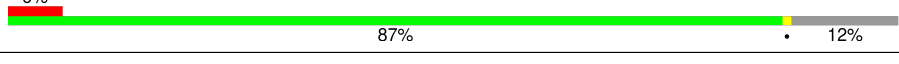


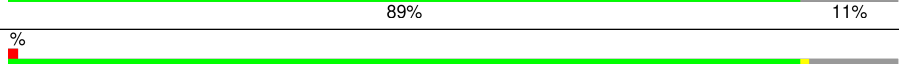
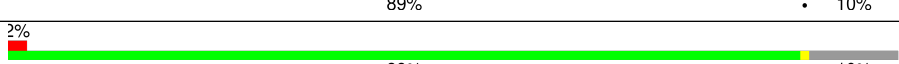
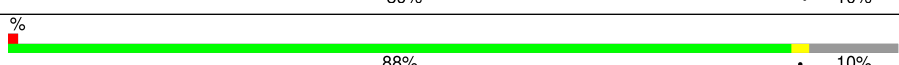
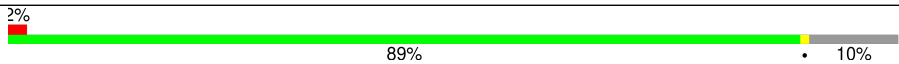


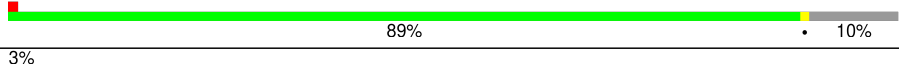
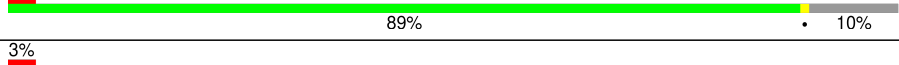
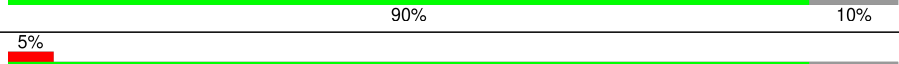

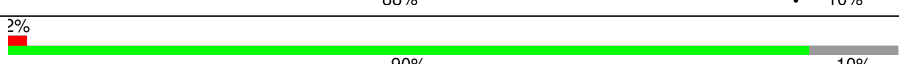
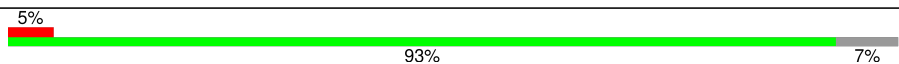
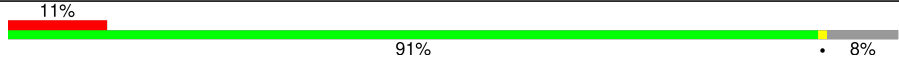
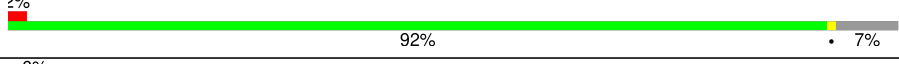
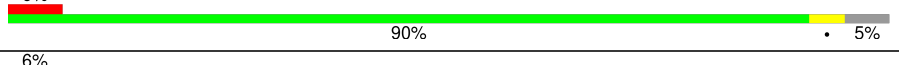
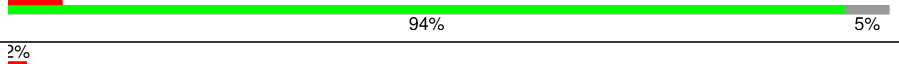
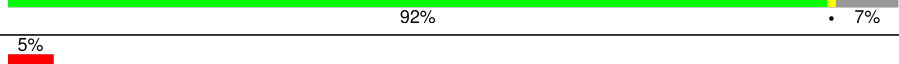
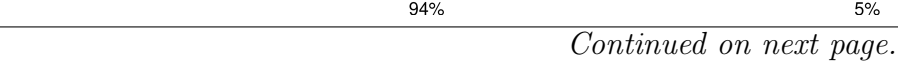


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1025 (3.98-3.62)
Ramachandran outliers	177936	1044 (3.98-3.62)
Sidechain outliers	177891	1039 (3.98-3.62)
RSRZ outliers	164620	1025 (3.98-3.62)

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

Mol	Chain	Length	Quality of chain
1	A	136	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> </div>
1	D	136	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
1	G	136	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>11%</div> </div> </div>
1	J	136	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>11%</div> </div> </div>
1	M	136	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> </div>
1	P	136	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	S	136	
1	V	136	
1	Y	136	
1	b	136	
1	e	136	
1	h	136	
2	B	217	
2	E	217	
2	H	217	
2	K	217	
2	N	217	
2	Q	217	
2	T	217	
2	W	217	
2	Z	217	
2	c	217	
2	f	217	
2	i	217	
3	C	202	
3	F	202	
3	I	202	
3	L	202	
3	O	202	
3	R	202	
3	U	202	

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Mol	Chain	Length	Quality of chain
3	X	202	<div><div></div><div>5%</div><div>94%</div><div>5%</div></div>
3	a	202	<div><div></div><div>11%</div><div>95%</div><div>5%</div></div>
3	d	202	<div><div></div><div>9%</div><div>94%</div><div>5%</div></div>
3	g	202	<div><div></div><div>5%</div><div>94%</div><div>5%</div></div>
3	j	202	<div><div></div><div>8%</div><div>94%</div><div>5%</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 51562 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 Interleukin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	D	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	G	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	J	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	M	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	P	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	S	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	V	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	Y	120	Total	C	N	O	S	0	0	0
			991	643	161	180	7			
1	b	119	Total	C	N	O	S	0	0	0
			983	637	160	179	7			
1	e	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	h	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP P60568
A	-1	ASP	-	expression tag	UNP P60568
A	0	PRO	-	expression tag	UNP P60568
A	74	HIS	GLN	engineered mutation	UNP P60568
A	80	PHE	LEU	engineered mutation	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
A	81	ASP	ARG	engineered mutation	UNP P60568
A	85	VAL	LEU	engineered mutation	UNP P60568
A	86	VAL	ILE	engineered mutation	UNP P60568
A	92	PHE	ILE	engineered mutation	UNP P60568
D	-2	ALA	-	expression tag	UNP P60568
D	-1	ASP	-	expression tag	UNP P60568
D	0	PRO	-	expression tag	UNP P60568
D	74	HIS	GLN	engineered mutation	UNP P60568
D	80	PHE	LEU	engineered mutation	UNP P60568
D	81	ASP	ARG	engineered mutation	UNP P60568
D	85	VAL	LEU	engineered mutation	UNP P60568
D	86	VAL	ILE	engineered mutation	UNP P60568
D	92	PHE	ILE	engineered mutation	UNP P60568
G	-2	ALA	-	expression tag	UNP P60568
G	-1	ASP	-	expression tag	UNP P60568
G	0	PRO	-	expression tag	UNP P60568
G	74	HIS	GLN	engineered mutation	UNP P60568
G	80	PHE	LEU	engineered mutation	UNP P60568
G	81	ASP	ARG	engineered mutation	UNP P60568
G	85	VAL	LEU	engineered mutation	UNP P60568
G	86	VAL	ILE	engineered mutation	UNP P60568
G	92	PHE	ILE	engineered mutation	UNP P60568
J	-2	ALA	-	expression tag	UNP P60568
J	-1	ASP	-	expression tag	UNP P60568
J	0	PRO	-	expression tag	UNP P60568
J	74	HIS	GLN	engineered mutation	UNP P60568
J	80	PHE	LEU	engineered mutation	UNP P60568
J	81	ASP	ARG	engineered mutation	UNP P60568
J	85	VAL	LEU	engineered mutation	UNP P60568
J	86	VAL	ILE	engineered mutation	UNP P60568
J	92	PHE	ILE	engineered mutation	UNP P60568
M	-2	ALA	-	expression tag	UNP P60568
M	-1	ASP	-	expression tag	UNP P60568
M	0	PRO	-	expression tag	UNP P60568
M	74	HIS	GLN	engineered mutation	UNP P60568
M	80	PHE	LEU	engineered mutation	UNP P60568
M	81	ASP	ARG	engineered mutation	UNP P60568
M	85	VAL	LEU	engineered mutation	UNP P60568
M	86	VAL	ILE	engineered mutation	UNP P60568
M	92	PHE	ILE	engineered mutation	UNP P60568
P	-2	ALA	-	expression tag	UNP P60568
P	-1	ASP	-	expression tag	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
P	0	PRO	-	expression tag	UNP P60568
P	74	HIS	GLN	engineered mutation	UNP P60568
P	80	PHE	LEU	engineered mutation	UNP P60568
P	81	ASP	ARG	engineered mutation	UNP P60568
P	85	VAL	LEU	engineered mutation	UNP P60568
P	86	VAL	ILE	engineered mutation	UNP P60568
P	92	PHE	ILE	engineered mutation	UNP P60568
S	-2	ALA	-	expression tag	UNP P60568
S	-1	ASP	-	expression tag	UNP P60568
S	0	PRO	-	expression tag	UNP P60568
S	74	HIS	GLN	engineered mutation	UNP P60568
S	80	PHE	LEU	engineered mutation	UNP P60568
S	81	ASP	ARG	engineered mutation	UNP P60568
S	85	VAL	LEU	engineered mutation	UNP P60568
S	86	VAL	ILE	engineered mutation	UNP P60568
S	92	PHE	ILE	engineered mutation	UNP P60568
V	-2	ALA	-	expression tag	UNP P60568
V	-1	ASP	-	expression tag	UNP P60568
V	0	PRO	-	expression tag	UNP P60568
V	74	HIS	GLN	engineered mutation	UNP P60568
V	80	PHE	LEU	engineered mutation	UNP P60568
V	81	ASP	ARG	engineered mutation	UNP P60568
V	85	VAL	LEU	engineered mutation	UNP P60568
V	86	VAL	ILE	engineered mutation	UNP P60568
V	92	PHE	ILE	engineered mutation	UNP P60568
Y	-2	ALA	-	expression tag	UNP P60568
Y	-1	ASP	-	expression tag	UNP P60568
Y	0	PRO	-	expression tag	UNP P60568
Y	74	HIS	GLN	engineered mutation	UNP P60568
Y	80	PHE	LEU	engineered mutation	UNP P60568
Y	81	ASP	ARG	engineered mutation	UNP P60568
Y	85	VAL	LEU	engineered mutation	UNP P60568
Y	86	VAL	ILE	engineered mutation	UNP P60568
Y	92	PHE	ILE	engineered mutation	UNP P60568
b	-2	ALA	-	expression tag	UNP P60568
b	-1	ASP	-	expression tag	UNP P60568
b	0	PRO	-	expression tag	UNP P60568
b	74	HIS	GLN	engineered mutation	UNP P60568
b	80	PHE	LEU	engineered mutation	UNP P60568
b	81	ASP	ARG	engineered mutation	UNP P60568
b	85	VAL	LEU	engineered mutation	UNP P60568
b	86	VAL	ILE	engineered mutation	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
b	92	PHE	ILE	engineered mutation	UNP P60568
e	-2	ALA	-	expression tag	UNP P60568
e	-1	ASP	-	expression tag	UNP P60568
e	0	PRO	-	expression tag	UNP P60568
e	74	HIS	GLN	engineered mutation	UNP P60568
e	80	PHE	LEU	engineered mutation	UNP P60568
e	81	ASP	ARG	engineered mutation	UNP P60568
e	85	VAL	LEU	engineered mutation	UNP P60568
e	86	VAL	ILE	engineered mutation	UNP P60568
e	92	PHE	ILE	engineered mutation	UNP P60568
h	-2	ALA	-	expression tag	UNP P60568
h	-1	ASP	-	expression tag	UNP P60568
h	0	PRO	-	expression tag	UNP P60568
h	74	HIS	GLN	engineered mutation	UNP P60568
h	80	PHE	LEU	engineered mutation	UNP P60568
h	81	ASP	ARG	engineered mutation	UNP P60568
h	85	VAL	LEU	engineered mutation	UNP P60568
h	86	VAL	ILE	engineered mutation	UNP P60568
h	92	PHE	ILE	engineered mutation	UNP P60568

- Molecule 2 is a protein called Interleukin-2 receptor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	0	0	0
			1612	1031	285	286	10			
2	E	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			
2	H	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			
2	K	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			
2	N	195	Total	C	N	O	S	0	0	0
			1612	1031	285	286	10			
2	Q	195	Total	C	N	O	S	0	0	0
			1612	1031	285	286	10			
2	T	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			
2	W	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			
2	Z	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			
2	c	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	f	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			
2	i	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ASP	SER	engineered mutation	UNP P14784
B	0	PRO	ALA	engineered mutation	UNP P14784
B	3	GLN	ASN	engineered mutation	UNP P14784
B	17	GLN	ASN	engineered mutation	UNP P14784
B	45	GLN	ASN	engineered mutation	UNP P14784
E	-1	ASP	SER	engineered mutation	UNP P14784
E	0	PRO	ALA	engineered mutation	UNP P14784
E	3	GLN	ASN	engineered mutation	UNP P14784
E	17	GLN	ASN	engineered mutation	UNP P14784
E	45	GLN	ASN	engineered mutation	UNP P14784
H	-1	ASP	SER	engineered mutation	UNP P14784
H	0	PRO	ALA	engineered mutation	UNP P14784
H	3	GLN	ASN	engineered mutation	UNP P14784
H	17	GLN	ASN	engineered mutation	UNP P14784
H	45	GLN	ASN	engineered mutation	UNP P14784
K	-1	ASP	SER	engineered mutation	UNP P14784
K	0	PRO	ALA	engineered mutation	UNP P14784
K	3	GLN	ASN	engineered mutation	UNP P14784
K	17	GLN	ASN	engineered mutation	UNP P14784
K	45	GLN	ASN	engineered mutation	UNP P14784
N	-1	ASP	SER	engineered mutation	UNP P14784
N	0	PRO	ALA	engineered mutation	UNP P14784
N	3	GLN	ASN	engineered mutation	UNP P14784
N	17	GLN	ASN	engineered mutation	UNP P14784
N	45	GLN	ASN	engineered mutation	UNP P14784
Q	-1	ASP	SER	engineered mutation	UNP P14784
Q	0	PRO	ALA	engineered mutation	UNP P14784
Q	3	GLN	ASN	engineered mutation	UNP P14784
Q	17	GLN	ASN	engineered mutation	UNP P14784
Q	45	GLN	ASN	engineered mutation	UNP P14784
T	-1	ASP	SER	engineered mutation	UNP P14784
T	0	PRO	ALA	engineered mutation	UNP P14784
T	3	GLN	ASN	engineered mutation	UNP P14784
T	17	GLN	ASN	engineered mutation	UNP P14784

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Chain	Residue	Modelled	Actual	Comment	Reference
T	45	GLN	ASN	engineered mutation	UNP P14784
W	-1	ASP	SER	engineered mutation	UNP P14784
W	0	PRO	ALA	engineered mutation	UNP P14784
W	3	GLN	ASN	engineered mutation	UNP P14784
W	17	GLN	ASN	engineered mutation	UNP P14784
W	45	GLN	ASN	engineered mutation	UNP P14784
Z	-1	ASP	SER	engineered mutation	UNP P14784
Z	0	PRO	ALA	engineered mutation	UNP P14784
Z	3	GLN	ASN	engineered mutation	UNP P14784
Z	17	GLN	ASN	engineered mutation	UNP P14784
Z	45	GLN	ASN	engineered mutation	UNP P14784
c	-1	ASP	SER	engineered mutation	UNP P14784
c	0	PRO	ALA	engineered mutation	UNP P14784
c	3	GLN	ASN	engineered mutation	UNP P14784
c	17	GLN	ASN	engineered mutation	UNP P14784
c	45	GLN	ASN	engineered mutation	UNP P14784
f	-1	ASP	SER	engineered mutation	UNP P14784
f	0	PRO	ALA	engineered mutation	UNP P14784
f	3	GLN	ASN	engineered mutation	UNP P14784
f	17	GLN	ASN	engineered mutation	UNP P14784
f	45	GLN	ASN	engineered mutation	UNP P14784
i	-1	ASP	SER	engineered mutation	UNP P14784
i	0	PRO	ALA	engineered mutation	UNP P14784
i	3	GLN	ASN	engineered mutation	UNP P14784
i	17	GLN	ASN	engineered mutation	UNP P14784
i	45	GLN	ASN	engineered mutation	UNP P14784

- Molecule 3 is a protein called Cytokine receptor common subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	188	Total	C	N	O	S	0	0	0
			1605	1022	286	289	8			
3	F	186	Total	C	N	O	S	0	0	0
			1592	1014	284	286	8			
3	I	188	Total	C	N	O	S	0	0	0
			1605	1022	286	289	8			
3	L	191	Total	C	N	O	S	0	0	0
			1630	1037	290	295	8			
3	O	191	Total	C	N	O	S	0	0	0
			1630	1037	290	295	8			
3	R	188	Total	C	N	O	S	0	0	0
			1612	1028	287	289	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	U	191	Total	C	N	O	S	0	0	0
			1630	1037	290	295	8			
3	X	191	Total	C	N	O	S	0	0	0
			1630	1037	290	295	8			
3	a	191	Total	C	N	O	S	0	0	0
			1630	1037	290	295	8			
3	d	191	Total	C	N	O	S	0	0	0
			1630	1037	290	295	8			
3	g	191	Total	C	N	O	S	0	0	0
			1630	1037	290	295	8			
3	j	191	Total	C	N	O	S	0	0	0
			1630	1037	290	295	8			

There are 48 discrepancies between the modelled and reference sequences:

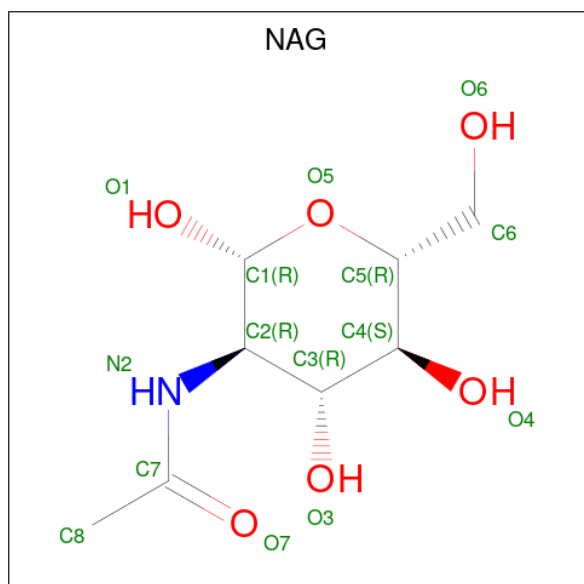
Chain	Residue	Modelled	Actual	Comment	Reference
C	31	ALA	-	expression tag	UNP P31785
C	32	ASP	-	expression tag	UNP P31785
C	33	PRO	-	expression tag	UNP P31785
C	53	GLN	ASN	engineered mutation	UNP P31785
F	31	ALA	-	expression tag	UNP P31785
F	32	ASP	-	expression tag	UNP P31785
F	33	PRO	-	expression tag	UNP P31785
F	53	GLN	ASN	engineered mutation	UNP P31785
I	31	ALA	-	expression tag	UNP P31785
I	32	ASP	-	expression tag	UNP P31785
I	33	PRO	-	expression tag	UNP P31785
I	53	GLN	ASN	engineered mutation	UNP P31785
L	31	ALA	-	expression tag	UNP P31785
L	32	ASP	-	expression tag	UNP P31785
L	33	PRO	-	expression tag	UNP P31785
L	53	GLN	ASN	engineered mutation	UNP P31785
O	31	ALA	-	expression tag	UNP P31785
O	32	ASP	-	expression tag	UNP P31785
O	33	PRO	-	expression tag	UNP P31785
O	53	GLN	ASN	engineered mutation	UNP P31785
R	31	ALA	-	expression tag	UNP P31785
R	32	ASP	-	expression tag	UNP P31785
R	33	PRO	-	expression tag	UNP P31785
R	53	GLN	ASN	engineered mutation	UNP P31785
U	31	ALA	-	expression tag	UNP P31785
U	32	ASP	-	expression tag	UNP P31785
U	33	PRO	-	expression tag	UNP P31785

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Chain	Residue	Modelled	Actual	Comment	Reference
U	53	GLN	ASN	engineered mutation	UNP P31785
X	31	ALA	-	expression tag	UNP P31785
X	32	ASP	-	expression tag	UNP P31785
X	33	PRO	-	expression tag	UNP P31785
X	53	GLN	ASN	engineered mutation	UNP P31785
a	31	ALA	-	expression tag	UNP P31785
a	32	ASP	-	expression tag	UNP P31785
a	33	PRO	-	expression tag	UNP P31785
a	53	GLN	ASN	engineered mutation	UNP P31785
d	31	ALA	-	expression tag	UNP P31785
d	32	ASP	-	expression tag	UNP P31785
d	33	PRO	-	expression tag	UNP P31785
d	53	GLN	ASN	engineered mutation	UNP P31785
g	31	ALA	-	expression tag	UNP P31785
g	32	ASP	-	expression tag	UNP P31785
g	33	PRO	-	expression tag	UNP P31785
g	53	GLN	ASN	engineered mutation	UNP P31785
j	31	ALA	-	expression tag	UNP P31785
j	32	ASP	-	expression tag	UNP P31785
j	33	PRO	-	expression tag	UNP P31785
j	53	GLN	ASN	engineered mutation	UNP P31785

- 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	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	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	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	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		
4	N	1	Total	C	N	O	0	0
			14	8	1	5		
4	O	1	Total	C	N	O	0	0
			14	8	1	5		
4	O	1	Total	C	N	O	0	0
			14	8	1	5		
4	O	1	Total	C	N	O	0	0
			14	8	1	5		
4	O	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	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	R	1	Total	C	N	O	0	0
			14	8	1	5		
4	T	1	Total	C	N	O	0	0
			14	8	1	5		
4	U	1	Total	C	N	O	0	0
			14	8	1	5		
4	U	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	Z	1	Total	C	N	O	0	0
			14	8	1	5		

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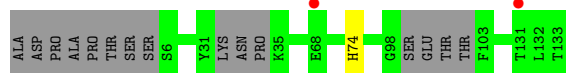
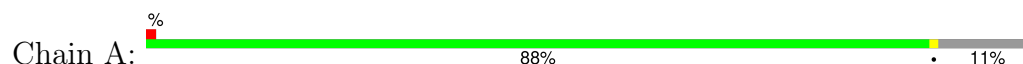
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	a	1	Total	C	N	O	0	0
			14	8	1	5		
4	a	1	Total	C	N	O	0	0
			14	8	1	5		
4	c	1	Total	C	N	O	0	0
			14	8	1	5		
4	c	1	Total	C	N	O	0	0
			14	8	1	5		
4	d	1	Total	C	N	O	0	0
			14	8	1	5		
4	f	1	Total	C	N	O	0	0
			14	8	1	5		
4	g	1	Total	C	N	O	0	0
			14	8	1	5		
4	g	1	Total	C	N	O	0	0
			14	8	1	5		
4	i	1	Total	C	N	O	0	0
			14	8	1	5		
4	i	1	Total	C	N	O	0	0
			14	8	1	5		
4	j	1	Total	C	N	O	0	0
			14	8	1	5		

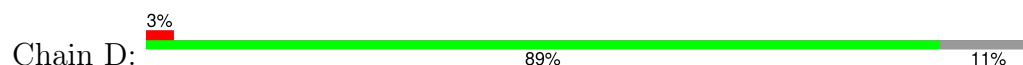
3 Residue-property plots [i](#)

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.

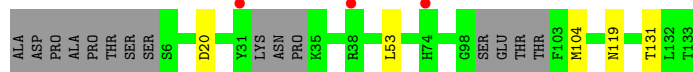
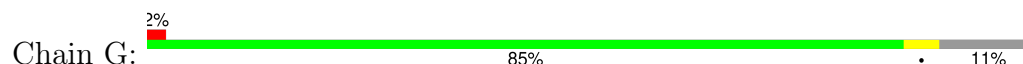
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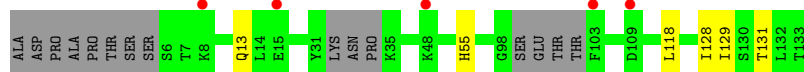
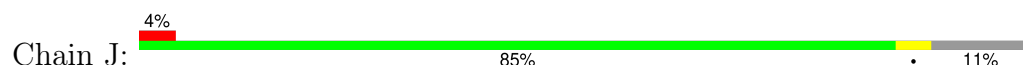
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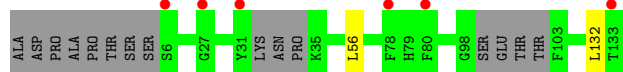
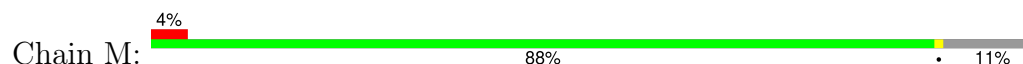
- Molecule 1: Interleukin-2



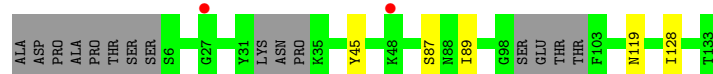
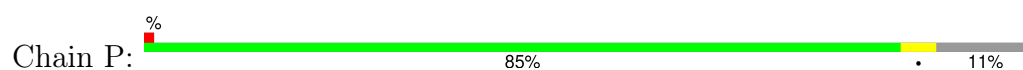
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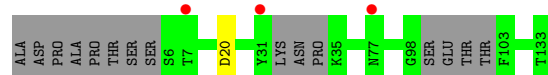
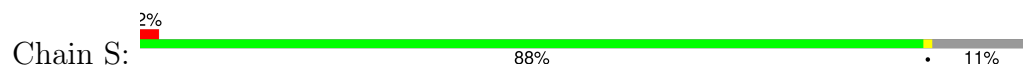
- Molecule 1: Interleukin-2



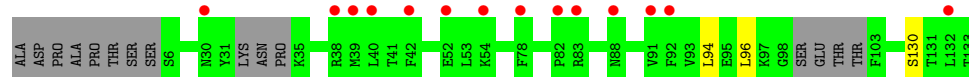
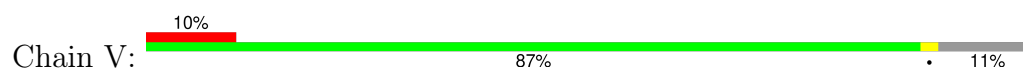
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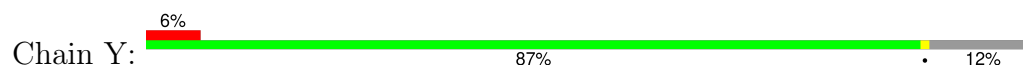
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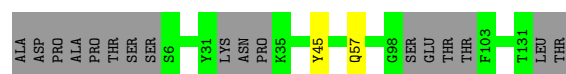
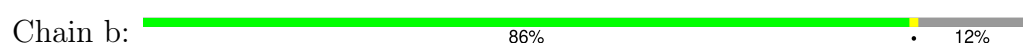
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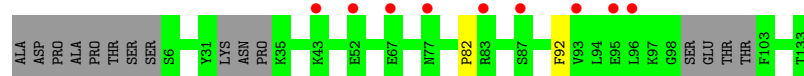
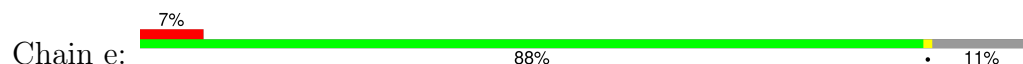
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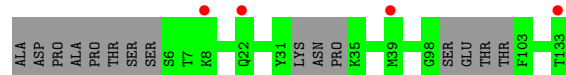
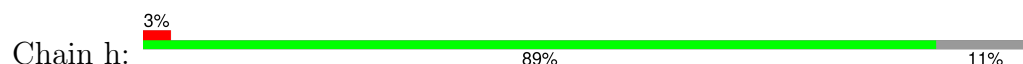
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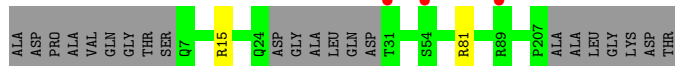
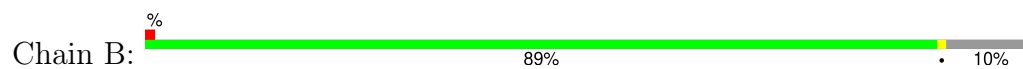
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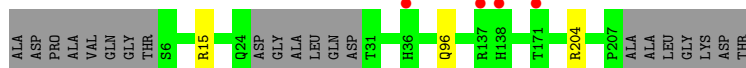
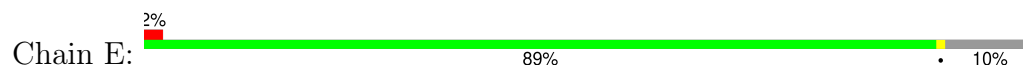
- Molecule 1: Interleukin-2



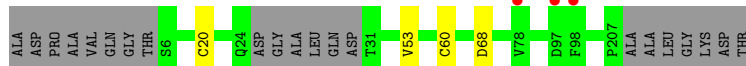
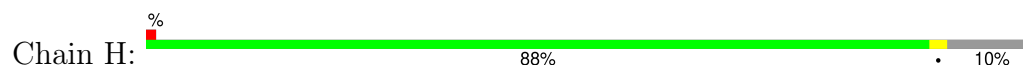
- Molecule 2: Interleukin-2 receptor subunit beta



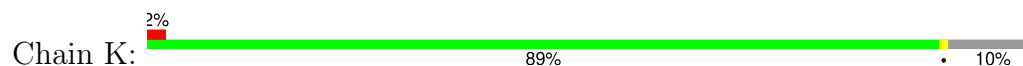
- Molecule 2: Interleukin-2 receptor subunit beta



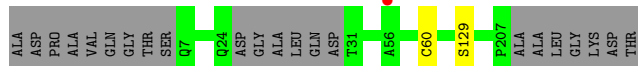
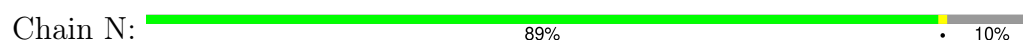
- Molecule 2: Interleukin-2 receptor subunit beta



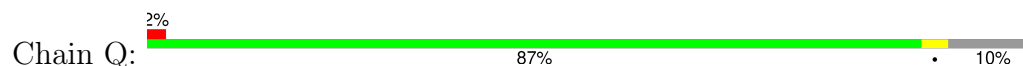
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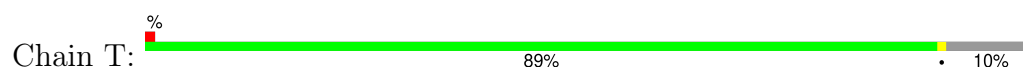
- Molecule 2: Interleukin-2 receptor subunit beta



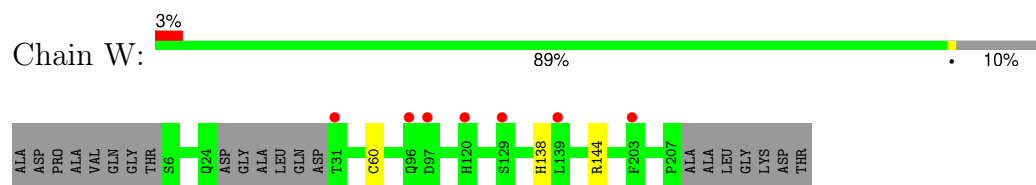
- Molecule 2: Interleukin-2 receptor subunit beta



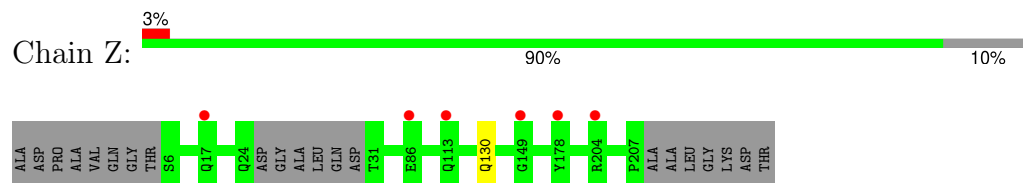
- Molecule 2: Interleukin-2 receptor subunit beta



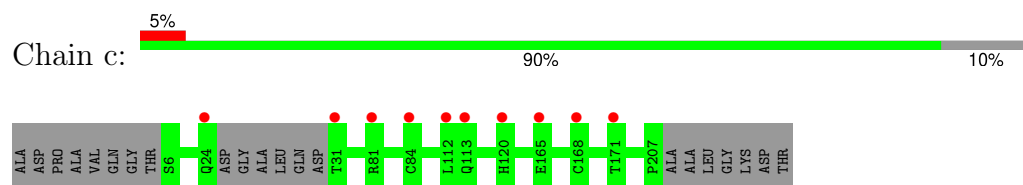
- Molecule 2: Interleukin-2 receptor subunit beta



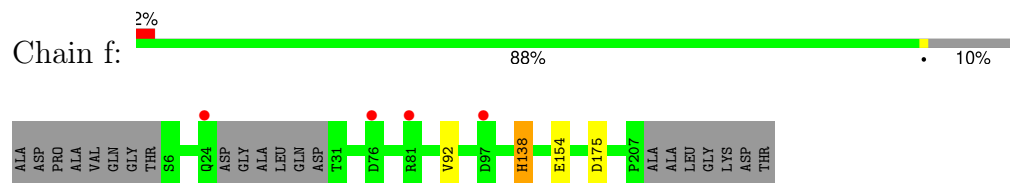
- Molecule 2: Interleukin-2 receptor subunit beta



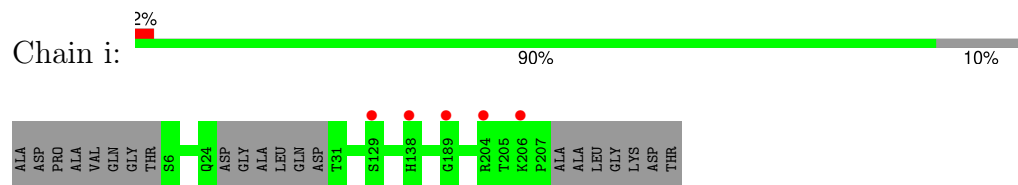
- Molecule 2: Interleukin-2 receptor subunit beta



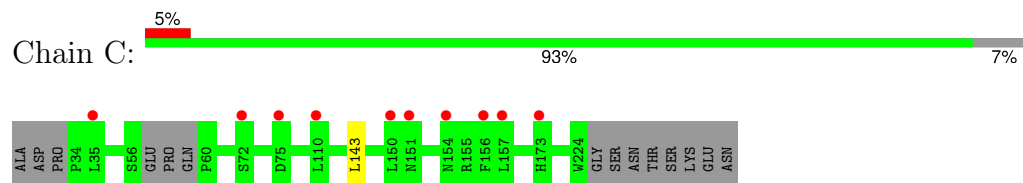
- Molecule 2: Interleukin-2 receptor subunit beta



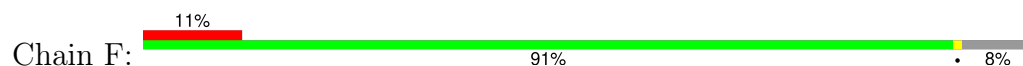
- Molecule 2: Interleukin-2 receptor subunit beta

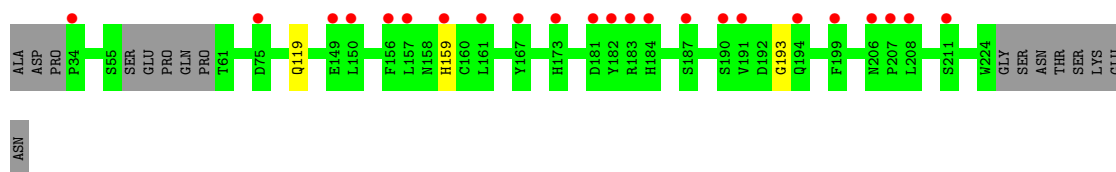


- Molecule 3: Cytokine receptor common subunit gamma

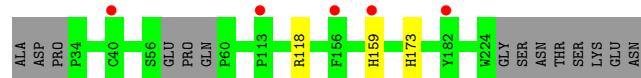
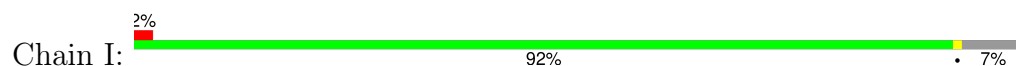


- Molecule 3: Cytokine receptor common subunit gamma

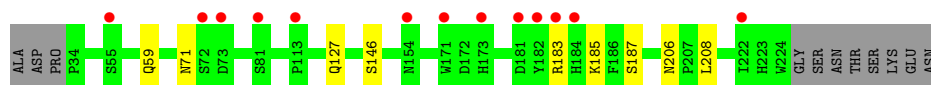
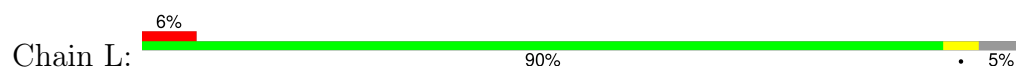




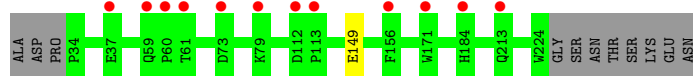
- Molecule 3: Cytokine receptor common subunit gamma



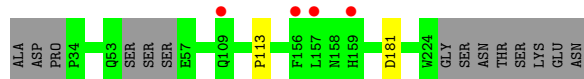
- Molecule 3: Cytokine receptor common subunit gamma



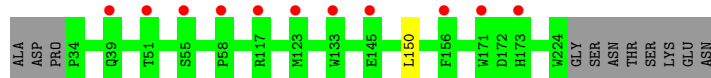
- Molecule 3: Cytokine receptor common subunit gamma



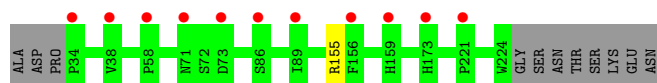
- Molecule 3: Cytokine receptor common subunit gamma



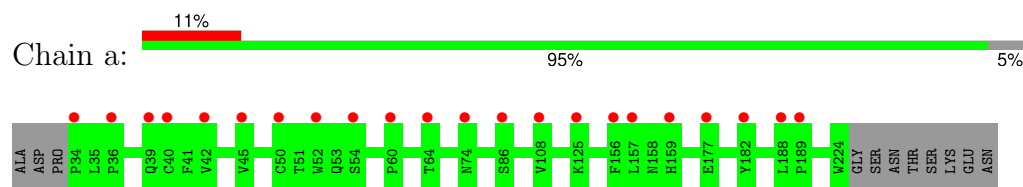
- Molecule 3: Cytokine receptor common subunit gamma



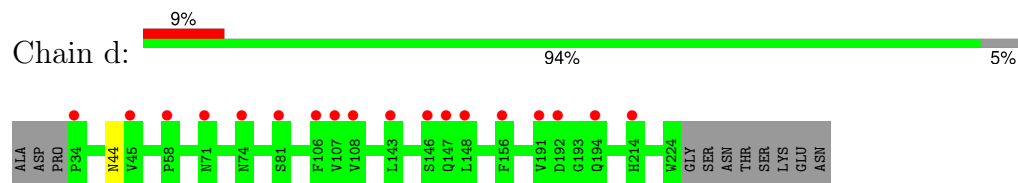
- Molecule 3: Cytokine receptor common subunit gamma



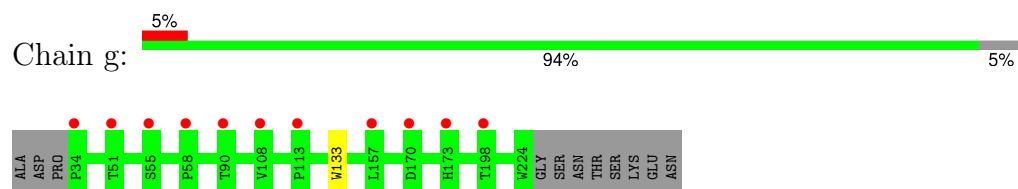
● Molecule 3: Cytokine receptor common subunit gamma



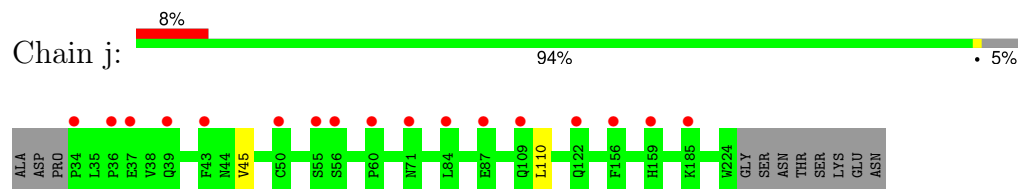
● Molecule 3: Cytokine receptor common subunit gamma



● Molecule 3: Cytokine receptor common subunit gamma



● Molecule 3: Cytokine receptor common subunit gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	118.23Å 118.10Å 236.12Å 99.86° 99.86° 99.74°	Depositor
Resolution (Å)	52.19 – 3.80 52.19 – 3.80	Depositor EDS
% Data completeness (in resolution range)	93.2 (52.19-3.80) 94.5 (52.19-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_621)	Depositor
R, R_{free}	0.291 , 0.344 0.285 , 0.344	Depositor DCC
R_{free} test set	1881 reflections (1.67%)	wwPDB-VP
Wilson B-factor (Å ²)	82.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 92.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.036 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	51562	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7576e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.33	0/1015	0.52	0/1367
1	D	0.36	0/1015	0.57	0/1367
1	G	0.36	0/1015	0.53	0/1367
1	J	0.36	0/1015	0.56	0/1367
1	M	0.31	0/1015	0.51	0/1367
1	P	0.36	0/1015	0.53	0/1367
1	S	0.32	0/1015	0.51	0/1367
1	V	0.38	0/1015	0.60	1/1367 (0.1%)
1	Y	0.34	0/1008	0.53	0/1357
1	b	0.38	0/1000	0.57	0/1346
1	e	0.45	0/1015	0.65	0/1367
1	h	0.34	0/1015	0.53	0/1367
2	B	0.35	0/1660	0.55	0/2264
2	E	0.34	0/1666	0.57	0/2272
2	H	0.34	0/1666	0.54	0/2272
2	K	0.38	0/1666	0.60	0/2272
2	N	0.32	0/1660	0.54	0/2264
2	Q	0.37	0/1660	0.57	0/2264
2	T	0.33	0/1666	0.54	0/2272
2	W	0.36	0/1666	0.57	0/2272
2	Z	0.34	0/1666	0.56	0/2272
2	c	0.35	0/1666	0.53	0/2272
2	f	0.37	0/1666	0.56	0/2272
2	i	0.33	0/1666	0.54	0/2272
3	C	0.34	0/1658	0.53	0/2254
3	F	0.34	0/1644	0.59	0/2235
3	I	0.31	0/1658	0.53	0/2254
3	L	0.39	0/1685	0.62	1/2294 (0.0%)
3	O	0.32	0/1685	0.55	0/2294
3	R	0.31	0/1666	0.53	0/2267
3	U	0.26	0/1685	0.47	0/2294
3	X	0.26	0/1685	0.47	0/2294

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	a	0.27	0/1685	0.47	0/2294
3	d	0.26	0/1685	0.47	0/2294
3	g	0.26	0/1685	0.48	0/2294
3	j	0.29	0/1685	0.49	0/2294
All	All	0.34	0/52238	0.54	2/70975 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	208	LEU	CB-CG-CD2	-6.00	100.79	111.00
1	V	96	LEU	CA-CB-CG	-5.37	102.95	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	115/136 (85%)	96 (84%)	18 (16%)	1 (1%)	14	45
1	D	115/136 (85%)	98 (85%)	17 (15%)	0	100	100
1	G	115/136 (85%)	102 (89%)	12 (10%)	1 (1%)	14	45
1	J	115/136 (85%)	108 (94%)	7 (6%)	0	100	100
1	M	115/136 (85%)	103 (90%)	10 (9%)	2 (2%)	7	34
1	P	115/136 (85%)	103 (90%)	10 (9%)	2 (2%)	7	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	115/136 (85%)	99 (86%)	16 (14%)	0	100	100
1	V	115/136 (85%)	100 (87%)	13 (11%)	2 (2%)	7	34
1	Y	114/136 (84%)	101 (89%)	12 (10%)	1 (1%)	14	45
1	b	113/136 (83%)	93 (82%)	19 (17%)	1 (1%)	14	45
1	e	115/136 (85%)	100 (87%)	13 (11%)	2 (2%)	7	34
1	h	115/136 (85%)	101 (88%)	14 (12%)	0	100	100
2	B	191/217 (88%)	180 (94%)	11 (6%)	0	100	100
2	E	192/217 (88%)	179 (93%)	13 (7%)	0	100	100
2	H	192/217 (88%)	175 (91%)	16 (8%)	1 (0%)	25	58
2	K	192/217 (88%)	176 (92%)	15 (8%)	1 (0%)	25	58
2	N	191/217 (88%)	179 (94%)	12 (6%)	0	100	100
2	Q	191/217 (88%)	179 (94%)	11 (6%)	1 (0%)	25	58
2	T	192/217 (88%)	176 (92%)	15 (8%)	1 (0%)	25	58
2	W	192/217 (88%)	172 (90%)	20 (10%)	0	100	100
2	Z	192/217 (88%)	175 (91%)	17 (9%)	0	100	100
2	c	192/217 (88%)	178 (93%)	14 (7%)	0	100	100
2	f	192/217 (88%)	181 (94%)	8 (4%)	3 (2%)	8	36
2	i	192/217 (88%)	180 (94%)	12 (6%)	0	100	100
3	C	184/202 (91%)	174 (95%)	10 (5%)	0	100	100
3	F	182/202 (90%)	169 (93%)	12 (7%)	1 (0%)	25	58
3	I	184/202 (91%)	165 (90%)	19 (10%)	0	100	100
3	L	189/202 (94%)	172 (91%)	13 (7%)	4 (2%)	5	32
3	O	189/202 (94%)	172 (91%)	17 (9%)	0	100	100
3	R	184/202 (91%)	169 (92%)	13 (7%)	2 (1%)	12	42
3	U	189/202 (94%)	179 (95%)	10 (5%)	0	100	100
3	X	189/202 (94%)	180 (95%)	8 (4%)	1 (0%)	25	58
3	a	189/202 (94%)	179 (95%)	10 (5%)	0	100	100
3	d	189/202 (94%)	173 (92%)	16 (8%)	0	100	100
3	g	189/202 (94%)	176 (93%)	13 (7%)	0	100	100
3	j	189/202 (94%)	174 (92%)	14 (7%)	1 (0%)	25	58
All	All	5924/6660 (89%)	5416 (91%)	480 (8%)	28 (0%)	25	58

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	71	ASN
3	L	127	GLN
2	Q	88	VAL
1	Y	66	LEU
3	L	187	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	115/128 (90%)	115 (100%)	0	100	100
1	D	115/128 (90%)	115 (100%)	0	100	100
1	G	115/128 (90%)	111 (96%)	4 (4%)	31	54
1	J	115/128 (90%)	109 (95%)	6 (5%)	19	44
1	M	115/128 (90%)	115 (100%)	0	100	100
1	P	115/128 (90%)	113 (98%)	2 (2%)	56	72
1	S	115/128 (90%)	114 (99%)	1 (1%)	75	82
1	V	115/128 (90%)	115 (100%)	0	100	100
1	Y	114/128 (89%)	113 (99%)	1 (1%)	75	82
1	b	113/128 (88%)	113 (100%)	0	100	100
1	e	115/128 (90%)	115 (100%)	0	100	100
1	h	115/128 (90%)	115 (100%)	0	100	100
2	B	179/194 (92%)	177 (99%)	2 (1%)	70	79
2	E	180/194 (93%)	178 (99%)	2 (1%)	70	79
2	H	180/194 (93%)	177 (98%)	3 (2%)	56	72
2	K	180/194 (93%)	178 (99%)	2 (1%)	70	79
2	N	179/194 (92%)	177 (99%)	2 (1%)	70	79
2	Q	179/194 (92%)	175 (98%)	4 (2%)	47	64
2	T	180/194 (93%)	178 (99%)	2 (1%)	70	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	W	180/194 (93%)	177 (98%)	3 (2%)	56	72
2	Z	180/194 (93%)	179 (99%)	1 (1%)	84	88
2	c	180/194 (93%)	180 (100%)	0	100	100
2	f	180/194 (93%)	179 (99%)	1 (1%)	84	88
2	i	180/194 (93%)	180 (100%)	0	100	100
3	C	182/194 (94%)	181 (100%)	1 (0%)	86	90
3	F	180/194 (93%)	178 (99%)	2 (1%)	70	79
3	I	182/194 (94%)	180 (99%)	2 (1%)	70	79
3	L	185/194 (95%)	181 (98%)	4 (2%)	47	64
3	O	185/194 (95%)	184 (100%)	1 (0%)	86	90
3	R	182/194 (94%)	182 (100%)	0	100	100
3	U	185/194 (95%)	184 (100%)	1 (0%)	86	90
3	X	185/194 (95%)	185 (100%)	0	100	100
3	a	185/194 (95%)	185 (100%)	0	100	100
3	d	185/194 (95%)	184 (100%)	1 (0%)	86	90
3	g	185/194 (95%)	184 (100%)	1 (0%)	86	90
3	j	185/194 (95%)	184 (100%)	1 (0%)	86	90
All	All	5740/6192 (93%)	5690 (99%)	50 (1%)	75	82

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	60	CYS
2	Q	68	ASP
3	j	110	LEU
2	N	129	SER
1	P	128	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 156 such sidechains are listed below:

Mol	Chain	Res	Type
3	d	109	GLN
2	i	177	GLN
3	d	178	GLN
3	g	62	ASN

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Mol	Chain	Res	Type
3	j	147	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

54 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	215	-	14,14,15	0.52	0	17,19,21	1.13	1 (5%)
4	NAG	c	215	-	14,14,15	0.70	0	17,19,21	1.65	4 (23%)
4	NAG	a	233	-	14,14,15	0.50	0	17,19,21	1.93	4 (23%)
4	NAG	F	233	-	14,14,15	0.52	0	17,19,21	1.87	3 (17%)
4	NAG	L	233	-	14,14,15	0.56	0	17,19,21	1.23	1 (5%)
4	NAG	T	215	-	14,14,15	0.72	0	17,19,21	1.46	2 (11%)
4	NAG	i	216	-	14,14,15	0.46	0	17,19,21	2.07	6 (35%)
4	NAG	g	300	-	14,14,15	0.47	0	17,19,21	0.97	0
4	NAG	d	300	-	14,14,15	0.48	0	17,19,21	0.67	0
4	NAG	C	400	-	14,14,15	0.53	0	17,19,21	0.77	1 (5%)
4	NAG	Z	215	-	14,14,15	0.60	0	17,19,21	1.57	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	233	-	14,14,15	0.59	0	17,19,21	1.36	1 (5%)
4	NAG	C	235	-	14,14,15	0.50	0	17,19,21	0.97	1 (5%)
4	NAG	K	215	-	14,14,15	0.66	0	17,19,21	1.85	4 (23%)
4	NAG	X	300	-	14,14,15	0.50	0	17,19,21	0.58	0
4	NAG	R	400	-	14,14,15	0.54	0	17,19,21	0.67	0
4	NAG	F	300	-	14,14,15	0.54	0	17,19,21	1.17	2 (11%)
4	NAG	X	233	-	14,14,15	0.55	0	17,19,21	2.06	6 (35%)
4	NAG	C	234	-	14,14,15	0.52	0	17,19,21	1.50	3 (17%)
4	NAG	E	215	-	14,14,15	0.73	0	17,19,21	1.51	2 (11%)
4	NAG	O	234	-	14,14,15	0.45	0	17,19,21	1.06	1 (5%)
4	NAG	I	234	-	14,14,15	0.41	0	17,19,21	1.55	1 (5%)
4	NAG	R	235	-	14,14,15	0.54	0	17,19,21	0.72	0
4	NAG	O	235	-	14,14,15	0.50	0	17,19,21	1.00	1 (5%)
4	NAG	R	233	-	14,14,15	0.60	0	17,19,21	1.33	2 (11%)
4	NAG	L	300	-	14,14,15	0.55	0	17,19,21	1.55	3 (17%)
4	NAG	F	235	-	14,14,15	0.49	0	17,19,21	0.69	0
4	NAG	F	400	-	14,14,15	0.56	0	17,19,21	0.78	0
4	NAG	U	233	-	14,14,15	0.56	0	17,19,21	2.13	5 (29%)
4	NAG	i	215	-	14,14,15	0.66	0	17,19,21	1.56	3 (17%)
4	NAG	L	234	-	14,14,15	0.52	0	17,19,21	0.92	1 (5%)
4	NAG	O	300	-	14,14,15	0.53	0	17,19,21	1.73	4 (23%)
4	NAG	c	216	-	14,14,15	0.52	0	17,19,21	1.96	4 (23%)
4	NAG	F	234	-	14,14,15	0.44	0	17,19,21	1.93	2 (11%)
4	NAG	f	215	-	14,14,15	0.70	0	17,19,21	1.39	3 (17%)
4	NAG	I	300	-	14,14,15	0.53	0	17,19,21	1.43	2 (11%)
4	NAG	I	235	-	14,14,15	0.53	0	17,19,21	0.63	0
4	NAG	R	300	-	14,14,15	0.61	0	17,19,21	1.38	2 (11%)
4	NAG	I	233	-	14,14,15	0.67	0	17,19,21	1.46	2 (11%)
4	NAG	H	215	-	14,14,15	0.62	0	17,19,21	1.38	2 (11%)
4	NAG	N	215	-	14,14,15	0.70	0	17,19,21	1.65	3 (17%)
4	NAG	U	300	-	14,14,15	0.58	0	17,19,21	0.75	0
4	NAG	R	234	-	14,14,15	0.36	0	17,19,21	2.38	4 (23%)
4	NAG	a	300	-	14,14,15	0.47	0	17,19,21	0.87	1 (5%)
4	NAG	K	216	-	14,14,15	0.49	0	17,19,21	1.84	5 (29%)
4	NAG	O	400	-	14,14,15	0.48	0	17,19,21	0.86	0
4	NAG	L	400	-	14,14,15	0.59	0	17,19,21	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	O	233	-	14,14,15	0.64	0	17,19,21	1.41	2 (11%)
4	NAG	C	300	-	14,14,15	0.56	0	17,19,21	1.40	4 (23%)
4	NAG	j	300	-	14,14,15	0.53	0	17,19,21	0.74	0
4	NAG	W	215	-	14,14,15	0.61	0	17,19,21	0.98	1 (5%)
4	NAG	Q	215	-	14,14,15	0.60	0	17,19,21	1.91	5 (29%)
4	NAG	I	400	-	14,14,15	0.56	0	17,19,21	0.60	0
4	NAG	g	233	-	14,14,15	0.54	0	17,19,21	1.94	7 (41%)

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	B	215	-	-	2/6/23/26	0/1/1/1
4	NAG	c	215	-	-	3/6/23/26	0/1/1/1
4	NAG	a	233	-	-	0/6/23/26	0/1/1/1
4	NAG	F	233	-	-	2/6/23/26	0/1/1/1
4	NAG	L	233	-	-	3/6/23/26	0/1/1/1
4	NAG	T	215	-	-	3/6/23/26	0/1/1/1
4	NAG	i	216	-	-	2/6/23/26	0/1/1/1
4	NAG	g	300	-	-	2/6/23/26	0/1/1/1
4	NAG	d	300	-	-	4/6/23/26	0/1/1/1
4	NAG	C	400	-	-	2/6/23/26	0/1/1/1
4	NAG	Z	215	-	-	5/6/23/26	0/1/1/1
4	NAG	C	233	-	-	2/6/23/26	0/1/1/1
4	NAG	C	235	-	-	4/6/23/26	0/1/1/1
4	NAG	K	215	-	-	4/6/23/26	0/1/1/1
4	NAG	X	300	-	-	4/6/23/26	0/1/1/1
4	NAG	R	400	-	-	2/6/23/26	0/1/1/1
4	NAG	F	300	-	-	3/6/23/26	0/1/1/1
4	NAG	X	233	-	-	2/6/23/26	0/1/1/1
4	NAG	C	234	-	-	4/6/23/26	0/1/1/1
4	NAG	E	215	-	-	2/6/23/26	0/1/1/1
4	NAG	O	234	-	-	3/6/23/26	0/1/1/1
4	NAG	I	234	-	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	R	235	-	-	2/6/23/26	0/1/1/1
4	NAG	O	235	-	-	2/6/23/26	0/1/1/1
4	NAG	R	233	-	-	0/6/23/26	0/1/1/1
4	NAG	L	300	-	-	4/6/23/26	0/1/1/1
4	NAG	F	235	-	-	2/6/23/26	0/1/1/1
4	NAG	F	400	-	-	2/6/23/26	0/1/1/1
4	NAG	U	233	-	-	2/6/23/26	0/1/1/1
4	NAG	i	215	-	-	3/6/23/26	0/1/1/1
4	NAG	L	234	-	-	4/6/23/26	0/1/1/1
4	NAG	O	300	-	-	3/6/23/26	0/1/1/1
4	NAG	c	216	-	-	1/6/23/26	0/1/1/1
4	NAG	F	234	-	-	3/6/23/26	0/1/1/1
4	NAG	f	215	-	-	2/6/23/26	0/1/1/1
4	NAG	I	300	-	-	4/6/23/26	0/1/1/1
4	NAG	I	235	-	-	2/6/23/26	0/1/1/1
4	NAG	R	300	-	-	4/6/23/26	0/1/1/1
4	NAG	I	233	-	-	2/6/23/26	0/1/1/1
4	NAG	H	215	-	-	4/6/23/26	0/1/1/1
4	NAG	N	215	-	-	0/6/23/26	0/1/1/1
4	NAG	U	300	-	-	4/6/23/26	0/1/1/1
4	NAG	R	234	-	-	3/6/23/26	0/1/1/1
4	NAG	a	300	-	-	2/6/23/26	0/1/1/1
4	NAG	K	216	-	-	1/6/23/26	0/1/1/1
4	NAG	O	400	-	-	2/6/23/26	0/1/1/1
4	NAG	L	400	-	-	2/6/23/26	0/1/1/1
4	NAG	O	233	-	-	0/6/23/26	0/1/1/1
4	NAG	C	300	-	-	4/6/23/26	0/1/1/1
4	NAG	j	300	-	-	2/6/23/26	0/1/1/1
4	NAG	W	215	-	-	0/6/23/26	0/1/1/1
4	NAG	Q	215	-	-	1/6/23/26	0/1/1/1
4	NAG	I	400	-	-	2/6/23/26	0/1/1/1
4	NAG	g	233	-	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	234	NAG	C1-O5-C5	8.05	122.97	112.19
4	F	234	NAG	C1-O5-C5	6.31	120.64	112.19
4	a	233	NAG	C1-O5-C5	5.41	119.44	112.19
4	U	233	NAG	C1-O5-C5	5.10	119.02	112.19
4	Z	215	NAG	O5-C1-C2	5.02	119.06	111.29

There are no chirality outliers.

5 of 135 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	234	NAG	C3-C2-N2-C7
4	C	300	NAG	C8-C7-N2-C2
4	C	300	NAG	O7-C7-N2-C2
4	C	400	NAG	C8-C7-N2-C2
4	C	400	NAG	O7-C7-N2-C2

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	121/136 (88%)	-0.07	2 (1%) 69 53	39, 76, 123, 170	0
1	D	121/136 (88%)	0.14	4 (3%) 49 40	34, 71, 130, 159	0
1	G	121/136 (88%)	0.02	3 (2%) 58 46	35, 75, 134, 184	0
1	J	121/136 (88%)	0.05	5 (4%) 42 35	30, 73, 117, 142	0
1	M	121/136 (88%)	0.05	6 (4%) 35 31	37, 75, 126, 167	0
1	P	121/136 (88%)	-0.11	2 (1%) 69 53	30, 73, 128, 153	0
1	S	121/136 (88%)	0.03	3 (2%) 58 46	46, 91, 137, 201	0
1	V	121/136 (88%)	0.64	14 (11%) 11 14	24, 88, 151, 419	0
1	Y	120/136 (88%)	0.25	8 (6%) 25 24	45, 100, 152, 199	0
1	b	119/136 (87%)	0.11	0 100 100	45, 96, 153, 177	0
1	e	121/136 (88%)	0.54	9 (7%) 22 22	22, 80, 131, 165	0
1	h	121/136 (88%)	0.31	4 (3%) 49 40	50, 93, 132, 185	0
2	B	195/217 (89%)	0.01	3 (1%) 71 56	45, 76, 126, 155	0
2	E	196/217 (90%)	0.14	4 (2%) 64 50	30, 74, 118, 190	0
2	H	196/217 (90%)	-0.03	3 (1%) 71 56	41, 73, 122, 150	0
2	K	196/217 (90%)	0.18	4 (2%) 64 50	25, 72, 117, 135	0
2	N	195/217 (89%)	-0.06	1 (0%) 87 75	43, 74, 111, 141	0
2	Q	195/217 (89%)	-0.02	5 (2%) 57 44	29, 69, 111, 146	0
2	T	196/217 (90%)	0.25	3 (1%) 71 56	36, 89, 140, 175	0
2	W	196/217 (90%)	0.14	7 (3%) 46 38	25, 88, 138, 210	0
2	Z	196/217 (90%)	0.10	6 (3%) 51 41	45, 80, 125, 176	0
2	c	196/217 (90%)	0.23	10 (5%) 34 30	46, 82, 138, 208	0
2	f	196/217 (90%)	0.11	4 (2%) 64 50	23, 85, 133, 168	0
2	i	196/217 (90%)	0.24	5 (2%) 57 44	39, 94, 143, 168	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	C	188/202 (93%)	0.38	10 (5%) 33 29	42, 93, 157, 226	0
3	F	186/202 (92%)	0.52	23 (12%) 9 13	33, 86, 149, 214	0
3	I	188/202 (93%)	0.17	5 (2%) 56 44	56, 90, 158, 217	0
3	L	191/202 (94%)	0.41	13 (6%) 25 24	21, 82, 153, 218	0
3	O	191/202 (94%)	0.26	12 (6%) 27 25	38, 88, 156, 196	0
3	R	188/202 (93%)	0.10	4 (2%) 63 49	41, 86, 154, 231	0
3	U	191/202 (94%)	0.61	11 (5%) 30 27	83, 151, 224, 267	0
3	X	191/202 (94%)	0.65	11 (5%) 30 27	81, 156, 229, 291	0
3	a	191/202 (94%)	0.85	22 (11%) 11 14	80, 149, 221, 369	0
3	d	191/202 (94%)	0.61	18 (9%) 15 17	77, 149, 229, 281	0
3	g	191/202 (94%)	0.58	11 (5%) 30 27	82, 143, 195, 287	0
3	j	191/202 (94%)	0.61	17 (8%) 17 17	69, 140, 196, 284	0
All	All	6076/6660 (91%)	0.26	272 (4%) 39 33	21, 90, 178, 419	0

The worst 5 of 272 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	159	HIS	7.0
3	F	156	PHE	6.2
3	d	71	ASN	5.0
1	V	83	ARG	5.0
3	a	156	PHE	4.9

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	O	400	14/15	0.31	0.21	139,147,151,153	0
4	NAG	a	300	14/15	0.36	0.14	123,141,146,148	0
4	NAG	d	300	14/15	0.36	0.20	176,185,189,191	0
4	NAG	X	300	14/15	0.40	0.14	195,203,206,208	0
4	NAG	g	300	14/15	0.40	0.19	157,173,179,182	0
4	NAG	a	233	14/15	0.41	0.19	119,129,137,142	0
4	NAG	L	400	14/15	0.41	0.20	198,202,205,206	0
4	NAG	I	235	14/15	0.43	0.18	131,142,148,150	0
4	NAG	F	400	14/15	0.47	0.22	158,167,171,172	0
4	NAG	j	300	14/15	0.50	0.17	162,174,182,183	0
4	NAG	F	235	14/15	0.53	0.14	137,148,151,153	0
4	NAG	I	400	14/15	0.53	0.19	161,169,176,177	0
4	NAG	R	235	14/15	0.54	0.12	138,149,151,152	0
4	NAG	R	400	14/15	0.54	0.20	200,203,210,211	0
4	NAG	C	300	14/15	0.62	0.19	61,73,86,95	0
4	NAG	i	216	14/15	0.67	0.17	128,143,156,164	0
4	NAG	O	235	14/15	0.68	0.13	91,111,120,122	0
4	NAG	C	235	14/15	0.69	0.14	108,136,143,147	0
4	NAG	F	300	14/15	0.70	0.14	69,80,84,88	0
4	NAG	L	234	14/15	0.70	0.13	120,132,140,140	0
4	NAG	X	233	14/15	0.71	0.14	120,128,156,157	0
4	NAG	U	233	14/15	0.73	0.19	98,118,139,142	0
4	NAG	U	300	14/15	0.74	0.14	172,177,180,182	0
4	NAG	L	300	14/15	0.75	0.14	88,97,104,106	0
4	NAG	C	400	14/15	0.76	0.14	153,161,167,167	0
4	NAG	O	300	14/15	0.77	0.17	86,91,109,113	0
4	NAG	I	300	14/15	0.80	0.12	51,83,96,99	0
4	NAG	O	233	14/15	0.81	0.14	70,78,86,93	0
4	NAG	c	216	14/15	0.81	0.13	91,113,121,123	0
4	NAG	K	216	14/15	0.82	0.16	78,88,92,93	0
4	NAG	R	300	14/15	0.82	0.12	79,87,94,96	0
4	NAG	F	234	14/15	0.85	0.13	81,109,119,125	0
4	NAG	g	233	14/15	0.86	0.11	114,126,139,140	0
4	NAG	C	233	14/15	0.86	0.12	79,85,94,97	0
4	NAG	C	234	14/15	0.87	0.11	89,105,113,116	0
4	NAG	I	233	14/15	0.87	0.12	64,81,91,92	0
4	NAG	R	234	14/15	0.88	0.10	94,111,117,122	0
4	NAG	F	233	14/15	0.88	0.12	81,91,97,97	0
4	NAG	W	215	14/15	0.89	0.11	62,71,83,86	0
4	NAG	O	234	14/15	0.89	0.09	59,77,90,93	0
4	NAG	L	233	14/15	0.89	0.09	66,89,100,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	Z	215	14/15	0.89	0.12	68,76,81,85	0
4	NAG	I	234	14/15	0.90	0.10	78,101,110,111	0
4	NAG	R	233	14/15	0.91	0.12	74,84,92,93	0
4	NAG	c	215	14/15	0.91	0.10	58,66,80,84	0
4	NAG	T	215	14/15	0.91	0.12	38,53,67,68	0
4	NAG	K	215	14/15	0.91	0.12	57,65,73,77	0
4	NAG	i	215	14/15	0.93	0.09	52,67,74,82	0
4	NAG	E	215	14/15	0.93	0.10	35,58,79,86	0
4	NAG	f	215	14/15	0.93	0.09	63,70,87,90	0
4	NAG	B	215	14/15	0.94	0.10	33,46,76,79	0
4	NAG	N	215	14/15	0.94	0.08	47,54,79,80	0
4	NAG	Q	215	14/15	0.95	0.10	38,48,65,67	0
4	NAG	H	215	14/15	0.95	0.09	41,53,80,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.