wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:56 AM GMT

PDB ID	:	2ERJ
Title	:	Crystal structure of the heterotrimeric interleukin-2 receptor in complex with interleukin-2
Authors	:	Debler, E.W.; Stauber, D.J.; Wilson, I.A.
Deposited on	:	2005-10-25
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

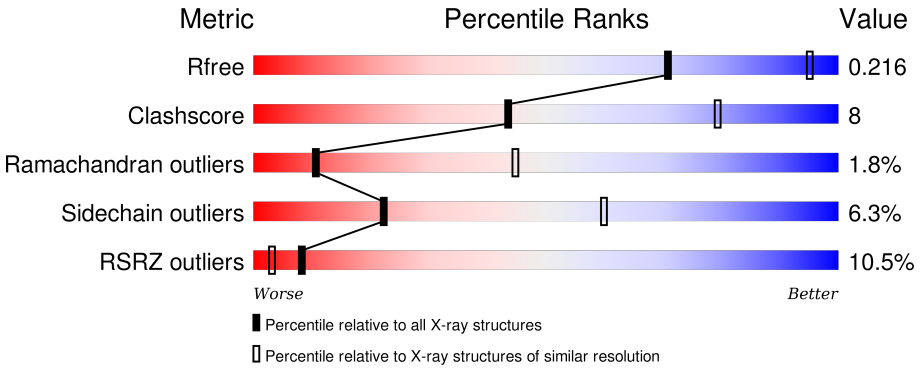
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	225	9% 40% 15% • 42%
1	E	225	8% 43% 14% • 42%
2	B	219	7% 71% 20% • 7%
2	F	219	5% 73% 17% • 8%
3	C	247	4% 60% 17% • 21%

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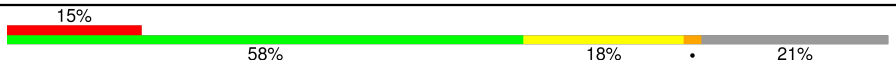
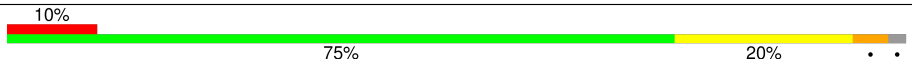
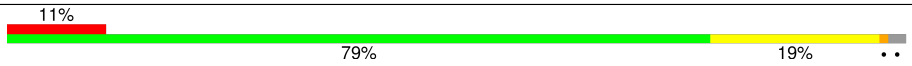
Mol	Chain	Length	Quality of chain
3	G	247	
4	D	133	
4	H	133	

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
8	NAG	G	300	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 11187 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 receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			1028	637	185	191	15			
1	E	131	Total	C	N	O	S	0	0	0
			1033	640	186	192	15			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	CLONING ARTIFACT	UNP P01589
A	-3	MET	-	CLONING ARTIFACT	UNP P01589
A	-2	LEU	-	CLONING ARTIFACT	UNP P01589
A	-1	SER	-	CLONING ARTIFACT	UNP P01589
A	0	LEU	-	CLONING ARTIFACT	UNP P01589
A	49	SER	ASN	ENGINEERED	UNP P01589
A	68	SER	ASN	ENGINEERED	UNP P01589
A	213	THR	-	EXPRESSION TAG	UNP P01589
A	214	GLY	-	EXPRESSION TAG	UNP P01589
A	215	HIS	-	EXPRESSION TAG	UNP P01589
A	216	HIS	-	EXPRESSION TAG	UNP P01589
A	217	HIS	-	EXPRESSION TAG	UNP P01589
A	218	HIS	-	EXPRESSION TAG	UNP P01589
A	219	HIS	-	EXPRESSION TAG	UNP P01589
A	220	HIS	-	EXPRESSION TAG	UNP P01589
E	-4	GLY	-	CLONING ARTIFACT	UNP P01589
E	-3	MET	-	CLONING ARTIFACT	UNP P01589
E	-2	LEU	-	CLONING ARTIFACT	UNP P01589
E	-1	SER	-	CLONING ARTIFACT	UNP P01589
E	0	LEU	-	CLONING ARTIFACT	UNP P01589
E	49	SER	ASN	ENGINEERED	UNP P01589
E	68	SER	ASN	ENGINEERED	UNP P01589
E	213	THR	-	EXPRESSION TAG	UNP P01589
E	214	GLY	-	EXPRESSION TAG	UNP P01589
E	215	HIS	-	EXPRESSION TAG	UNP P01589

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Chain	Residue	Modelled	Actual	Comment	Reference
E	216	HIS	-	EXPRESSION TAG	UNP P01589
E	217	HIS	-	EXPRESSION TAG	UNP P01589
E	218	HIS	-	EXPRESSION TAG	UNP P01589
E	219	HIS	-	EXPRESSION TAG	UNP P01589
E	220	HIS	-	EXPRESSION TAG	UNP P01589

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	204	Total	C	N	O	S	0	0	0
			1676	1065	298	303	10			
2	F	201	Total	C	N	O	S	0	0	0
			1654	1051	294	299	10			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	CLONING ARTIFACT	UNP P14784
B	-3	MET	-	CLONING ARTIFACT	UNP P14784
B	-2	LEU	-	CLONING ARTIFACT	UNP P14784
B	-1	SER	-	CLONING ARTIFACT	UNP P14784
B	0	LEU	-	CLONING ARTIFACT	UNP P14784
B	207	THR	-	EXPRESSION TAG	UNP P14784
B	208	GLY	-	EXPRESSION TAG	UNP P14784
B	209	HIS	-	EXPRESSION TAG	UNP P14784
B	210	HIS	-	EXPRESSION TAG	UNP P14784
B	211	HIS	-	EXPRESSION TAG	UNP P14784
B	212	HIS	-	EXPRESSION TAG	UNP P14784
B	213	HIS	-	EXPRESSION TAG	UNP P14784
B	214	HIS	-	EXPRESSION TAG	UNP P14784
F	-4	GLY	-	CLONING ARTIFACT	UNP P14784
F	-3	MET	-	CLONING ARTIFACT	UNP P14784
F	-2	LEU	-	CLONING ARTIFACT	UNP P14784
F	-1	SER	-	CLONING ARTIFACT	UNP P14784
F	0	LEU	-	CLONING ARTIFACT	UNP P14784
F	207	THR	-	EXPRESSION TAG	UNP P14784
F	208	GLY	-	EXPRESSION TAG	UNP P14784
F	209	HIS	-	EXPRESSION TAG	UNP P14784
F	210	HIS	-	EXPRESSION TAG	UNP P14784
F	211	HIS	-	EXPRESSION TAG	UNP P14784
F	212	HIS	-	EXPRESSION TAG	UNP P14784
F	213	HIS	-	EXPRESSION TAG	UNP P14784

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Chain	Residue	Modelled	Actual	Comment	Reference
F	214	HIS	-	EXPRESSION TAG	UNP P14784

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	195	Total	C	N	O	S	0	0	0
			1655	1052	294	301	8			
3	G	195	Total	C	N	O	S	0	0	0
			1655	1052	294	301	8			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	CLONING ARTIFACT	UNP P31785
C	-3	MET	-	CLONING ARTIFACT	UNP P31785
C	-2	LEU	-	CLONING ARTIFACT	UNP P31785
C	-1	SER	-	CLONING ARTIFACT	UNP P31785
C	0	LEU	-	CLONING ARTIFACT	UNP P31785
C	53	GLN	ASN	ENGINEERED	UNP P31785
C	234	ARG	-	EXPRESSION TAG	UNP P31785
C	235	THR	-	EXPRESSION TAG	UNP P31785
C	236	GLY	-	EXPRESSION TAG	UNP P31785
C	237	HIS	-	EXPRESSION TAG	UNP P31785
C	238	HIS	-	EXPRESSION TAG	UNP P31785
C	239	HIS	-	EXPRESSION TAG	UNP P31785
C	240	HIS	-	EXPRESSION TAG	UNP P31785
C	241	HIS	-	EXPRESSION TAG	UNP P31785
C	242	HIS	-	EXPRESSION TAG	UNP P31785
G	-4	GLY	-	CLONING ARTIFACT	UNP P31785
G	-3	MET	-	CLONING ARTIFACT	UNP P31785
G	-2	LEU	-	CLONING ARTIFACT	UNP P31785
G	-1	SER	-	CLONING ARTIFACT	UNP P31785
G	0	LEU	-	CLONING ARTIFACT	UNP P31785
G	53	GLN	ASN	ENGINEERED	UNP P31785
G	234	ARG	-	EXPRESSION TAG	UNP P31785
G	235	THR	-	EXPRESSION TAG	UNP P31785
G	236	GLY	-	EXPRESSION TAG	UNP P31785
G	237	HIS	-	EXPRESSION TAG	UNP P31785
G	238	HIS	-	EXPRESSION TAG	UNP P31785
G	239	HIS	-	EXPRESSION TAG	UNP P31785
G	240	HIS	-	EXPRESSION TAG	UNP P31785
G	241	HIS	-	EXPRESSION TAG	UNP P31785

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Chain	Residue	Modelled	Actual	Comment	Reference
G	242	HIS	-	EXPRESSION TAG	UNP P31785

- Molecule 4 is a protein called Interleukin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	131	Total	C	N	O	S	0	0	0
			1068	685	176	201	6			
4	H	131	Total	C	N	O	S	0	0	0
			1068	685	176	201	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	125	ALA	CYS	ENGINEERED	UNP P60568
H	125	ALA	CYS	ENGINEERED	UNP P60568

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	4	Total	C	N	O	0	0
			49	28	2	19		
5	F	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	2	Total	C	N	O	0	0
			24	14	1	9		

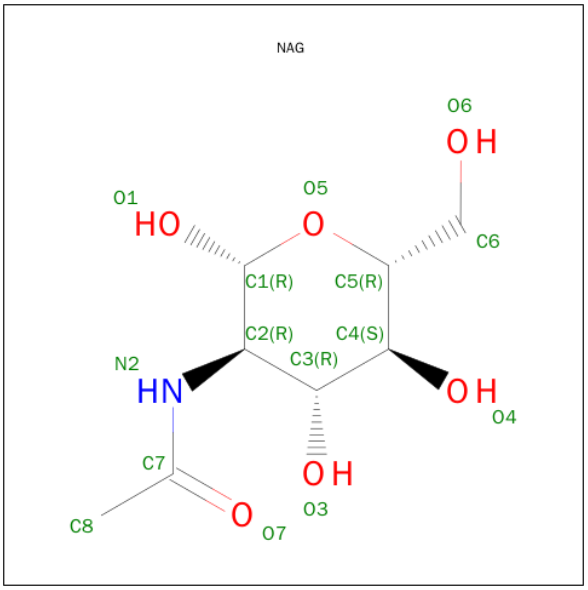
- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	3	Total	C	N	O	0	0
			39	22	2	15		
7	F	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	2	Total C N O 28 16 2 10	0	0
8	G	2	Total C N O 28 16 2 10	0	0

- Molecule 9 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

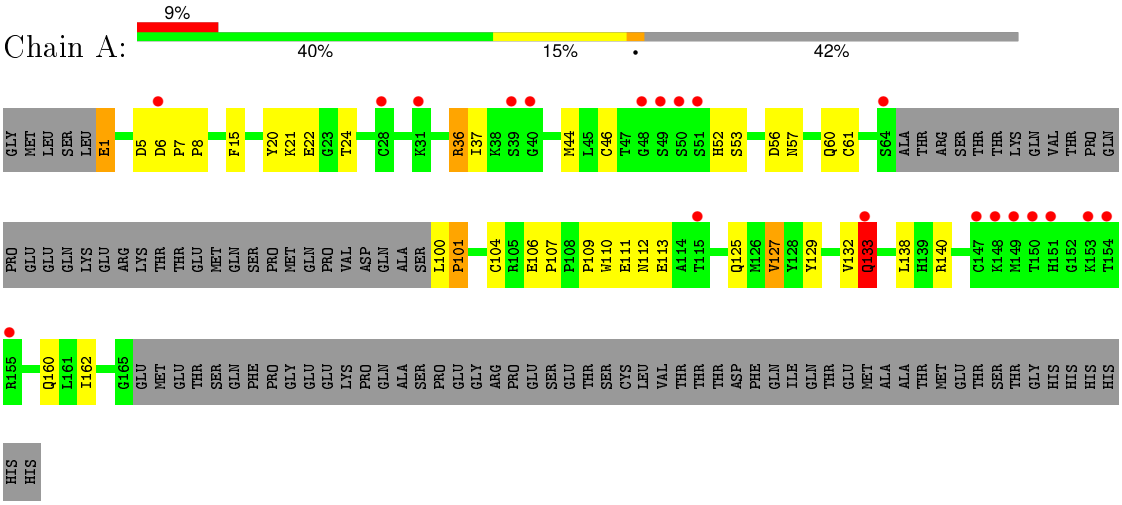
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	F	3	Total C N O 38 22 2 14	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

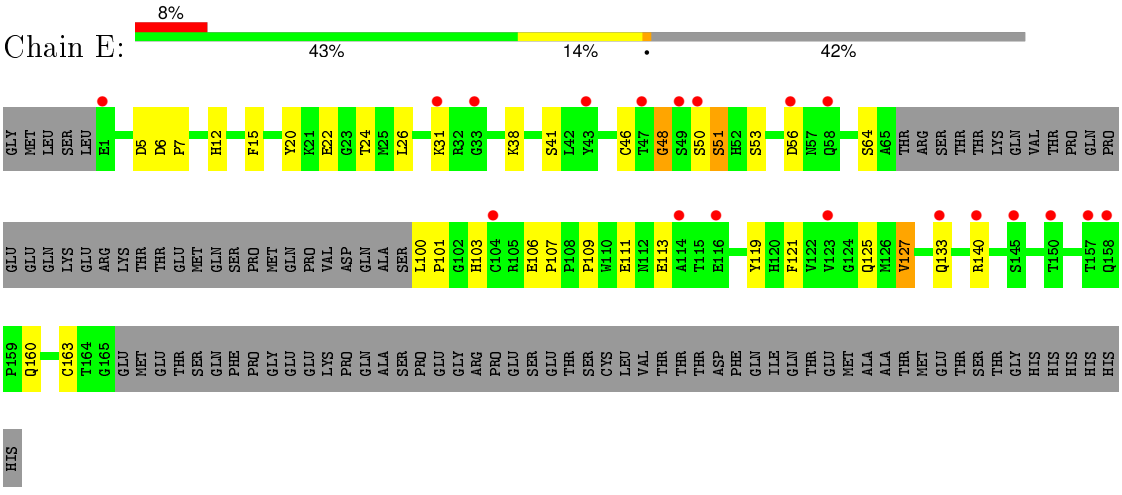
- Molecule 1: Interleukin-2 receptor alpha chain

Chain A:



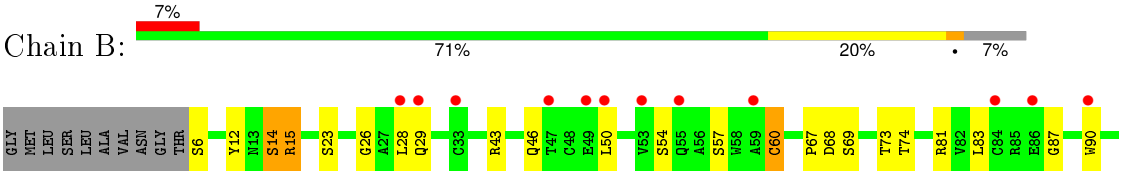
- Molecule 1: Interleukin-2 receptor alpha chain

Chain E:



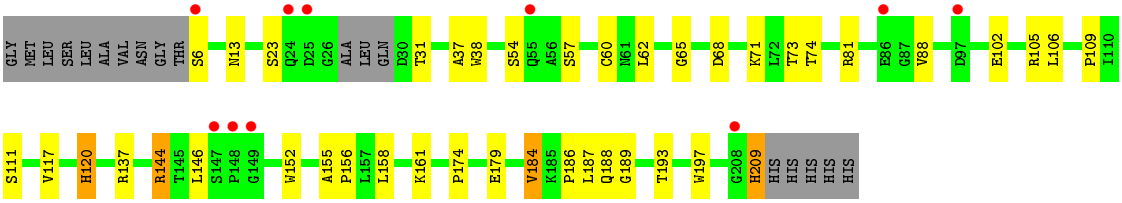
- Molecule 2: Interleukin-2 receptor beta chain

Chain B:



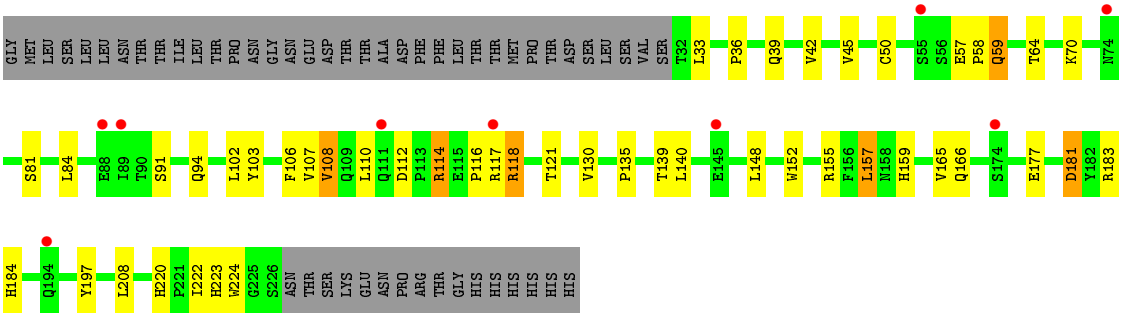
• Molecule 2: Interleukin-2 receptor beta chain

Chain F:



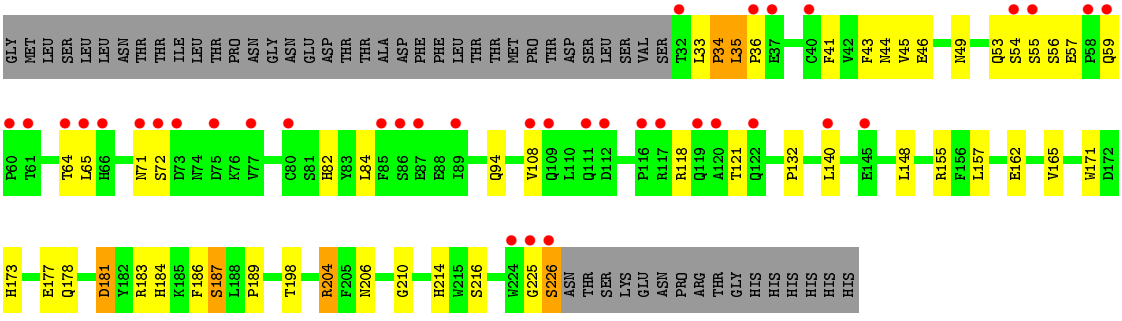
• Molecule 3: Cytokine receptor common gamma chain

Chain C:



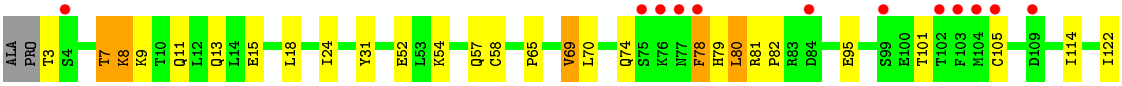
• Molecule 3: Cytokine receptor common gamma chain

Chain G:



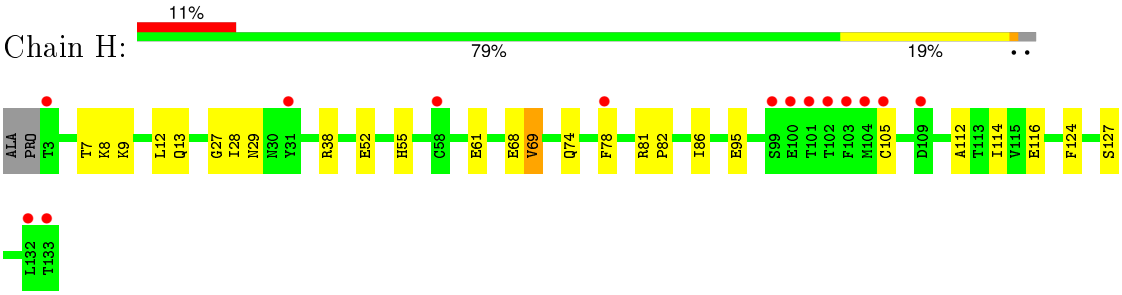
• Molecule 4: Interleukin-2

Chain D:



- Molecule 4: Interleukin-2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.27Å 70.55Å 129.24Å 83.85° 82.45° 89.72°	Depositor
Resolution (Å)	129.10 – 3.00 45.45 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.4 (129.10-3.00) 90.8 (45.45-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.263 0.220 , 0.216	Depositor DCC
R_{free} test set	1861 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	78.4	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 102.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 37243 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11187	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BMA, NAG, FUC

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	0.43	0/1056	0.55	0/1427
1	E	0.39	0/1061	0.53	0/1434
2	B	0.52	0/1725	0.62	0/2353
2	F	0.54	0/1702	0.62	0/2320
3	C	0.48	0/1710	0.65	0/2329
3	G	0.43	0/1710	0.61	0/2329
4	D	0.48	0/1085	0.61	1/1464 (0.1%)
4	H	0.45	0/1085	0.58	0/1464
All	All	0.47	0/11134	0.60	1/15120 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	80	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1028	0	967	20	0
1	E	1033	0	972	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1676	0	1615	32	0
2	F	1654	0	1590	31	0
3	C	1655	0	1555	26	0
3	G	1655	0	1555	26	0
4	D	1068	0	1103	16	0
4	H	1068	0	1103	15	0
5	B	49	0	43	0	0
5	F	49	0	43	2	0
6	B	24	0	22	1	0
7	B	39	0	34	0	0
7	F	39	0	34	0	0
8	C	28	0	25	0	0
8	G	28	0	25	0	0
9	C	28	0	26	0	0
9	G	28	0	26	0	0
10	F	38	0	34	3	0
All	All	11187	0	10772	177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 177 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:TYR:HB3	1:A:24:THR:HG21	1.50	0.93
3:G:33:LEU:N	3:G:34:PRO:HD2	1.89	0.86
1:E:20:TYR:HB3	1:E:24:THR:HG21	1.58	0.85
2:F:81:ARG:NH2	10:F:220:FUC:H61	1.95	0.81
4:H:69:VAL:HG11	4:H:114:ILE:HD12	1.63	0.81

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	126/225 (56%)	108 (86%)	15 (12%)	3 (2%)	7 35
1	E	127/225 (56%)	110 (87%)	14 (11%)	3 (2%)	7 35
2	B	202/219 (92%)	185 (92%)	14 (7%)	3 (2%)	13 50
2	F	197/219 (90%)	181 (92%)	16 (8%)	0	100 100
3	C	193/247 (78%)	171 (89%)	16 (8%)	6 (3%)	5 28
3	G	193/247 (78%)	168 (87%)	19 (10%)	6 (3%)	5 28
4	D	129/133 (97%)	120 (93%)	8 (6%)	1 (1%)	24 66
4	H	129/133 (97%)	121 (94%)	7 (5%)	1 (1%)	24 66
All	All	1296/1648 (79%)	1164 (90%)	109 (8%)	23 (2%)	11 45

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	GLU
1	A	133	GLN
3	C	117	ARG
2	B	148	PRO
3	C	181	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	114/200 (57%)	106 (93%)	8 (7%)	19 55
1	E	114/200 (57%)	109 (96%)	5 (4%)	35 74
2	B	186/198 (94%)	174 (94%)	12 (6%)	21 58
2	F	184/198 (93%)	173 (94%)	11 (6%)	24 62
3	C	188/236 (80%)	177 (94%)	11 (6%)	24 63
3	G	188/236 (80%)	173 (92%)	15 (8%)	15 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	124/125 (99%)	114 (92%)	10 (8%)	15 47
4	H	124/125 (99%)	119 (96%)	5 (4%)	38 77
All	All	1222/1518 (80%)	1145 (94%)	77 (6%)	22 60

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	58	CYS
1	E	64	SER
3	G	226	SER
4	D	69	VAL
4	D	105	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	139	HIS
4	H	119	ASN
2	F	36	HIS
4	D	119	ASN
3	G	82	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

23 carbohydrates 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	$\#\|Z\| > 2$
5	NAG	B	215	2,5	14,14,15	0.55	0	15,19,21	0.94	0
5	FUC	B	216	5	10,10,11	0.74	0	14,14,16	0.95	0
5	NAG	B	217	5	14,14,15	0.58	0	15,19,21	0.95	1 (6%)
5	BMA	B	218	5	11,11,12	0.69	0	14,15,17	1.56	2 (14%)
6	NAG	B	219	2,6	14,14,15	0.49	0	15,19,21	1.53	3 (20%)
6	FUC	B	220	6	10,10,11	0.62	0	14,14,16	0.81	1 (7%)
7	NAG	B	221	2,7	14,14,15	0.59	0	15,19,21	0.81	0
7	NAG	B	222	7	14,14,15	0.50	0	15,19,21	0.96	1 (6%)
7	BMA	B	223	7	11,11,12	0.48	0	14,15,17	1.35	2 (14%)
8	NAG	C	300	8,3	14,14,15	0.64	0	15,19,21	1.20	1 (6%)
8	NAG	C	301	8	14,14,15	0.66	0	15,19,21	1.53	3 (20%)
5	NAG	F	215	2,5	14,14,15	0.62	0	15,19,21	0.80	0
5	FUC	F	216	5	10,10,11	0.71	0	14,14,16	1.01	2 (14%)
5	NAG	F	217	5	14,14,15	0.53	0	15,19,21	0.89	1 (6%)
5	BMA	F	218	5	11,11,12	0.63	0	14,15,17	2.05	3 (21%)
10	NAG	F	219	10,2	14,14,15	0.44	0	15,19,21	1.48	2 (13%)
10	FUC	F	220	10	10,10,11	0.58	0	14,14,16	1.28	2 (14%)
10	NAG	F	221	10	14,14,15	0.42	0	15,19,21	1.42	1 (6%)
7	NAG	F	222	2,7	14,14,15	0.59	0	15,19,21	0.91	0
7	NAG	F	223	7	14,14,15	0.52	0	15,19,21	1.29	1 (6%)
7	BMA	F	224	7	11,11,12	0.63	0	14,15,17	1.09	2 (14%)
8	NAG	G	300	8,3	14,14,15	0.64	0	15,19,21	0.80	0
8	NAG	G	301	8	14,14,15	0.64	0	15,19,21	1.31	2 (13%)

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
5	NAG	B	215	2,5	-	0/6/23/26	0/1/1/1
5	FUC	B	216	5	-	0/0/17/20	0/1/1/1
5	NAG	B	217	5	-	0/6/23/26	0/1/1/1
5	BMA	B	218	5	-	0/2/19/22	0/1/1/1
6	NAG	B	219	2,6	-	0/6/23/26	0/1/1/1
6	FUC	B	220	6	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	221	2,7	-	0/6/23/26	0/1/1/1
7	NAG	B	222	7	-	0/6/23/26	0/1/1/1
7	BMA	B	223	7	-	0/2/19/22	0/1/1/1
8	NAG	C	300	8,3	-	0/6/23/26	0/1/1/1
8	NAG	C	301	8	-	0/6/23/26	0/1/1/1
5	NAG	F	215	2,5	-	0/6/23/26	0/1/1/1
5	FUC	F	216	5	-	0/0/17/20	0/1/1/1
5	NAG	F	217	5	-	0/6/23/26	0/1/1/1
5	BMA	F	218	5	-	0/2/19/22	0/1/1/1
10	NAG	F	219	10,2	-	0/6/23/26	0/1/1/1
10	FUC	F	220	10	-	0/0/17/20	0/1/1/1
10	NAG	F	221	10	-	0/6/23/26	0/1/1/1
7	NAG	F	222	2,7	-	0/6/23/26	0/1/1/1
7	NAG	F	223	7	-	0/6/23/26	0/1/1/1
7	BMA	F	224	7	-	0/2/19/22	0/1/1/1
8	NAG	G	300	8,3	-	0/6/23/26	0/1/1/1
8	NAG	G	301	8	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	219	NAG	C2-N2-C7	-3.27	118.84	123.04
6	B	219	NAG	C4-C3-C2	-2.61	107.16	111.23
5	F	216	FUC	O5-C1-C2	-2.50	106.81	110.86
6	B	219	NAG	C2-N2-C7	-2.43	119.92	123.04
7	B	222	NAG	C2-N2-C7	-2.39	119.97	123.04

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	G	301	NAG	O7-C7-N2-C2
8	G	301	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	220	FUC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	216	FUC	2	0
10	F	219	NAG	1	0
10	F	220	FUC	2	0

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
9	NAG	C	400	3	14,14,15	0.37	0	15,19,21	1.74	2 (13%)
9	NAG	C	500	3	14,14,15	0.52	0	15,19,21	1.31	3 (20%)
9	NAG	G	400	3	14,14,15	0.53	0	15,19,21	1.57	3 (20%)
9	NAG	G	500	3	14,14,15	0.51	0	15,19,21	0.97	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	C	400	3	-	0/6/23/26	0/1/1/1
9	NAG	C	500	3	-	0/6/23/26	0/1/1/1
9	NAG	G	400	3	-	0/6/23/26	0/1/1/1
9	NAG	G	500	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	500	NAG	C3-C4-C5	-2.21	106.35	110.20
9	G	400	NAG	C2-N2-C7	2.12	125.76	123.04
9	C	500	NAG	O5-C5-C6	2.24	112.19	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	400	NAG	O5-C5-C6	2.25	112.22	107.35
9	G	400	NAG	O5-C5-C6	2.68	113.15	107.35

There are no chirality outliers.

There are no torsion outliers.

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	130/225 (57%)	0.99	20 (15%) 3 1	85, 91, 96, 97	0
1	E	131/225 (58%)	0.85	19 (14%) 3 1	86, 92, 96, 98	0
2	B	204/219 (93%)	0.62	16 (7%) 16 6	82, 91, 96, 100	0
2	F	201/219 (91%)	0.45	10 (4%) 32 13	82, 92, 96, 100	0
3	C	195/247 (78%)	0.56	9 (4%) 36 14	88, 92, 97, 102	0
3	G	195/247 (78%)	1.11	37 (18%) 2 1	87, 93, 97, 102	0
4	D	131/133 (98%)	0.77	13 (9%) 9 4	83, 92, 100, 103	0
4	H	131/133 (98%)	0.76	14 (10%) 8 3	84, 92, 100, 105	0
All	All	1318/1648 (79%)	0.75	138 (10%) 8 3	82, 92, 97, 105	0

The worst 5 of 138 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	54	SER	12.6
4	H	102	THR	9.2
2	F	25	ASP	8.1
1	A	49	SER	7.9
3	G	59	GLN	7.9

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	B	215	14/15	0.84	0.27	0.48	77,85,88,94	0
8	NAG	G	300	14/15	0.77	0.48	0.34	105,107,110,112	0
7	NAG	B	221	14/15	0.90	0.20	-0.59	85,86,87,90	0
7	NAG	F	222	14/15	0.93	0.19	-0.64	74,75,78,79	0
8	NAG	C	300	14/15	0.91	0.22	-1.14	88,89,91,95	0
6	NAG	B	219	14/15	0.88	0.16	-1.28	94,95,96,97	0
5	NAG	F	215	14/15	0.93	0.16	-2.10	73,79,81,86	0
5	FUC	F	216	10/11	0.94	0.14	-2.73	70,70,72,72	0
5	FUC	B	216	10/11	0.92	0.13	-3.83	72,74,75,76	0
10	NAG	F	221	14/15	0.72	0.33	-	108,111,112,113	0
5	NAG	B	217	14/15	0.79	0.47	-	101,105,108,111	0
7	BMA	B	223	11/12	0.62	0.33	-	106,108,109,109	0
7	NAG	B	222	14/15	0.78	0.28	-	94,96,99,103	0
6	FUC	B	220	10/11	0.90	0.35	-	96,97,97,97	0
5	BMA	B	218	11/12	0.79	0.28	-	114,116,117,117	0
8	NAG	C	301	14/15	0.80	0.52	-	97,99,101,102	0
7	NAG	F	223	14/15	0.85	0.22	-	80,86,88,93	0
8	NAG	G	301	14/15	0.71	0.39	-	114,116,117,117	0
7	BMA	F	224	11/12	0.77	0.28	-	97,99,100,101	0
5	BMA	F	218	11/12	0.67	0.31	-	108,110,112,113	0
10	FUC	F	220	10/11	0.81	0.30	-	102,102,102,102	0
10	NAG	F	219	14/15	0.72	0.32	-	97,98,101,105	0
5	NAG	F	217	14/15	0.87	0.23	-	91,94,99,104	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
9	NAG	G	500	14/15	0.66	0.23	-0.48	99,101,104,104	0
9	NAG	C	500	14/15	0.66	0.24	-0.69	94,95,96,96	0
9	NAG	C	400	14/15	0.87	0.13	-1.43	85,88,88,89	0
9	NAG	G	400	14/15	0.75	0.18	-	101,103,104,105	0

6.5 Other polymers (i)

There are no such residues in this entry.