



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:15 AM GMT

PDB ID : 3L89  
Title : Human Adenovirus type 21 knob in complex with domains SCR1 and SCR2  
of CD46 (membrane cofactor protein, MCP)  
Authors : Cupelli, K.; Stehle, T.  
Deposited on : 2009-12-30  
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

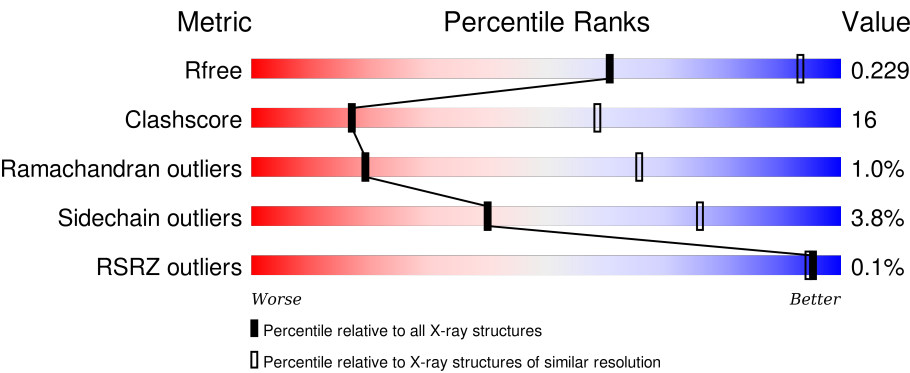
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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.













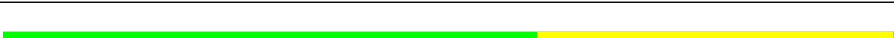


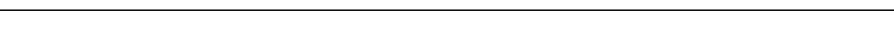
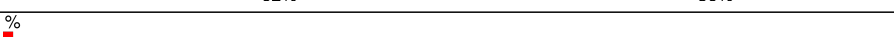
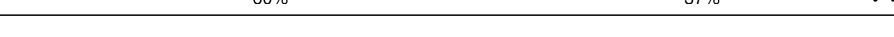



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	201	<div><div></div><div>67%21%•9%</div></div>
1	B	201	<div><div></div><div>65%25%•8%</div></div>
1	C	201	<div><div></div><div>67%22%•8%</div></div>
1	D	201	<div><div></div><div>58%30%•9%</div></div>
1	E	201	<div><div></div><div>56%33%•8%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	201	
1	G	201	
1	H	201	
1	I	201	
1	J	201	
1	K	201	
1	L	201	
2	M	126	
2	N	126	
2	O	126	
2	P	126	
2	Q	126	
2	R	126	
2	S	126	
2	T	126	
2	U	126	
2	V	126	
2	W	126	
2	X	126	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29017 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 Fiber protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1411	895	231	279	6			
1	B	184	Total	C	N	O	S	0	0	0
			1428	904	234	284	6			
1	C	184	Total	C	N	O	S	0	0	0
			1426	903	234	283	6			
1	D	183	Total	C	N	O	S	0	0	0
			1415	896	232	281	6			
1	E	184	Total	C	N	O	S	0	0	0
			1434	907	234	287	6			
1	F	185	Total	C	N	O	S	0	0	0
			1437	908	236	287	6			
1	G	182	Total	C	N	O	S	0	0	0
			1419	901	232	280	6			
1	H	183	Total	C	N	O	S	0	0	0
			1428	903	234	285	6			
1	I	186	Total	C	N	O	S	0	0	0
			1447	915	237	289	6			
1	J	182	Total	C	N	O	S	0	0	0
			1417	900	231	280	6			
1	K	185	Total	C	N	O	S	0	0	0
			1428	905	235	282	6			
1	L	186	Total	C	N	O	S	0	0	0
			1441	913	236	286	6			

- Molecule 2 is a protein called Membrane cofactor protein.

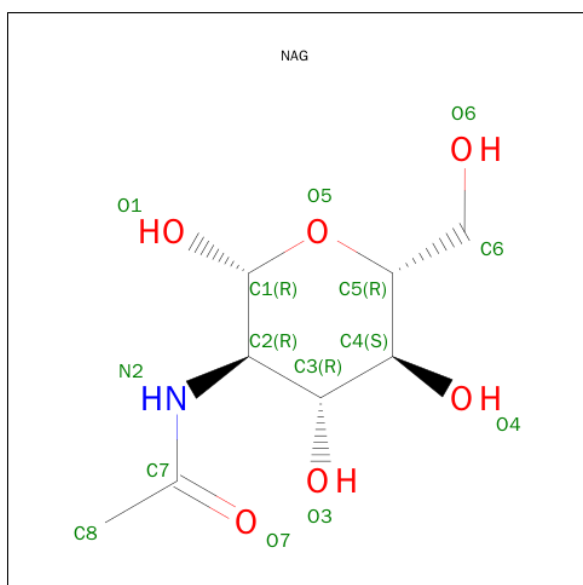
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	126	Total	C	N	O	S	0	0	0
			987	641	153	183	10			
2	N	126	Total	C	N	O	S	0	0	0
			991	641	153	187	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	126	Total	C	N	O	S	0	0	0
			1011	653	158	190	10			
2	P	126	Total	C	N	O	S	0	0	0
			977	631	151	185	10			
2	Q	125	Total	C	N	O	S	0	0	0
			962	622	149	181	10			
2	R	126	Total	C	N	O	S	0	0	0
			997	645	154	188	10			
2	S	126	Total	C	N	O	S	0	0	0
			976	628	154	184	10			
2	T	124	Total	C	N	O	S	0	0	0
			958	619	148	181	10			
2	U	126	Total	C	N	O	S	0	0	0
			996	645	154	187	10			
2	V	126	Total	C	N	O	S	0	0	0
			991	640	155	186	10			
2	W	125	Total	C	N	O	S	0	0	0
			983	637	154	182	10			
2	X	126	Total	C	N	O	S	0	0	0
			1001	649	156	186	10			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	S	1	Total	C	N	O	0	0
			14	8	1	5		

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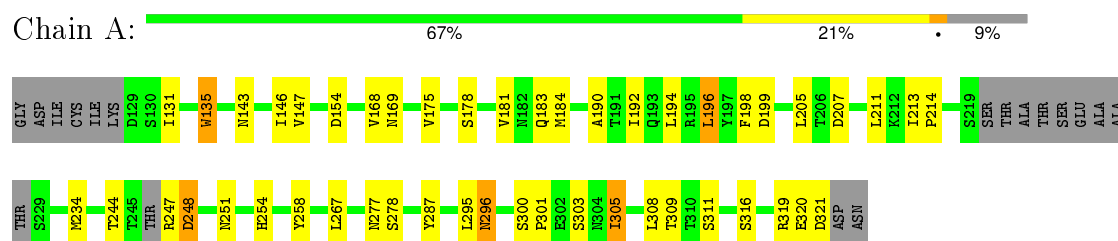
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	M	1	Total	C	N	O	0	0
			14	8	1	5		
3	P	1	Total	C	N	O	0	0
			14	8	1	5		
3	V	1	Total	C	N	O	0	0
			14	8	1	5		

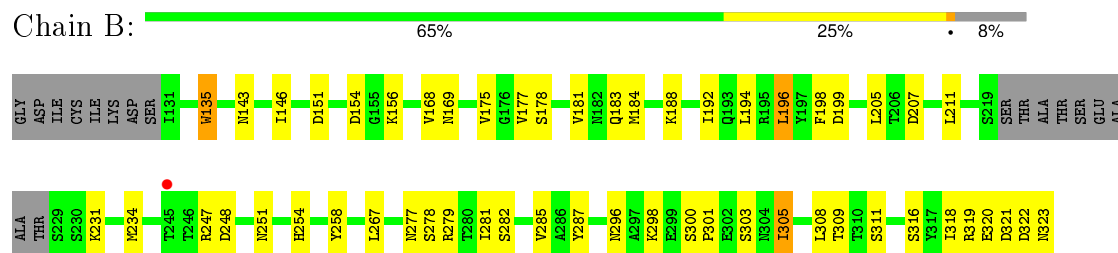
### 3 Residue-property plots

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.

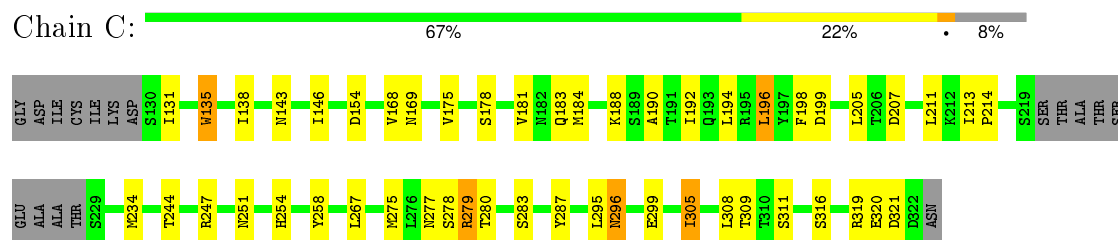
#### • Molecule 1: Fiber protein



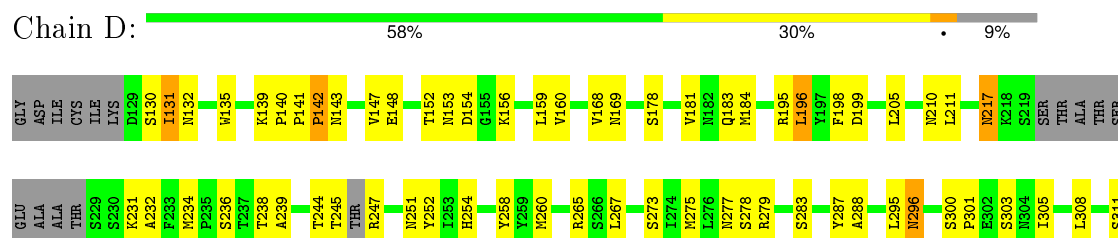
#### • Molecule 1: Fiber protein



#### • Molecule 1: Fiber protein



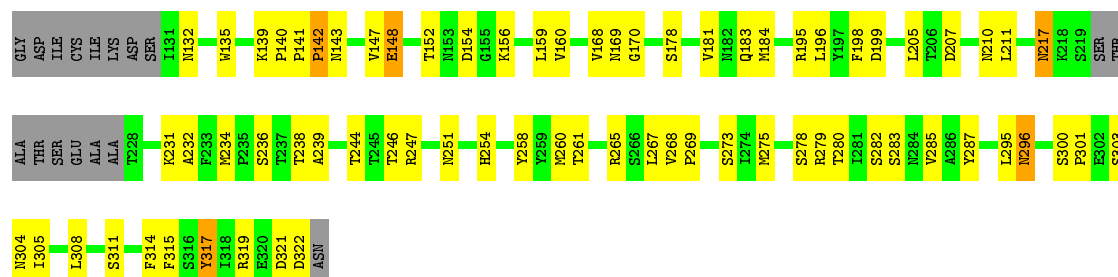
#### • Molecule 1: Fiber protein





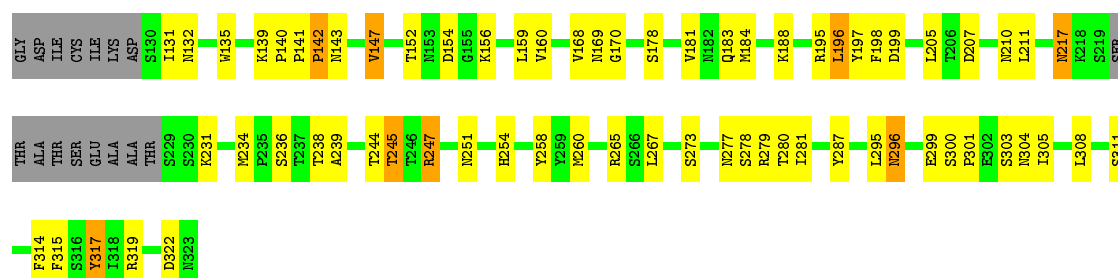
• Molecule 1: Fiber protein

Chain E: 56% 33% 8%



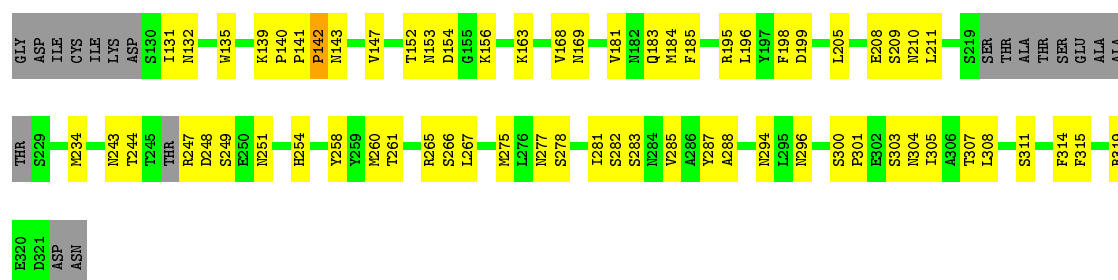
• Molecule 1: Fiber protein

Chain F: 58% 30% 8%



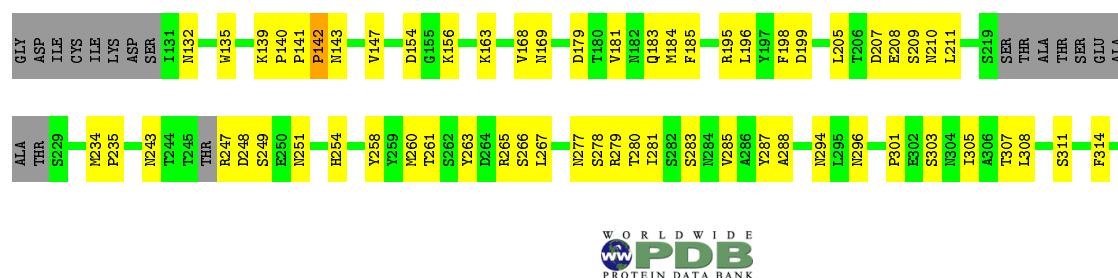
• Molecule 1: Fiber protein

Chain G: 58% 32% 9%



• Molecule 1: Fiber protein

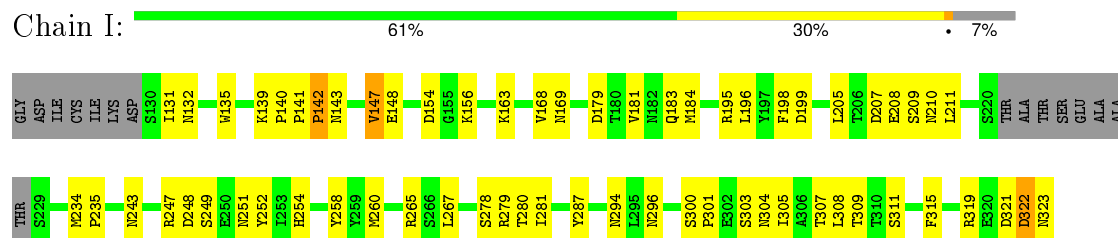
Chain H: 60% 30% 9%



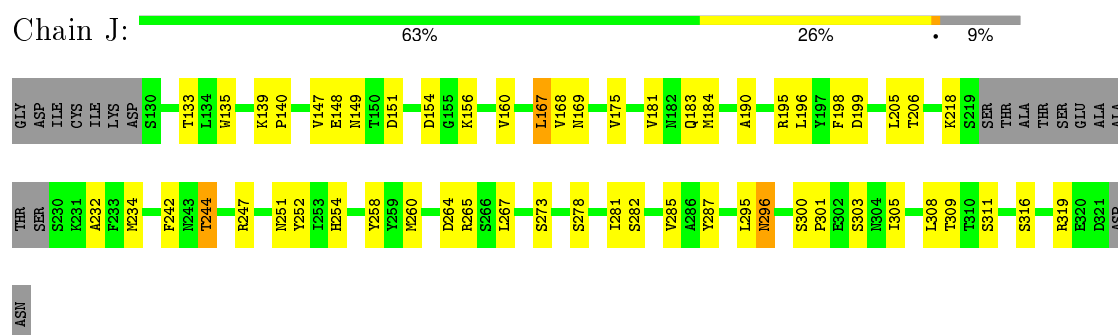




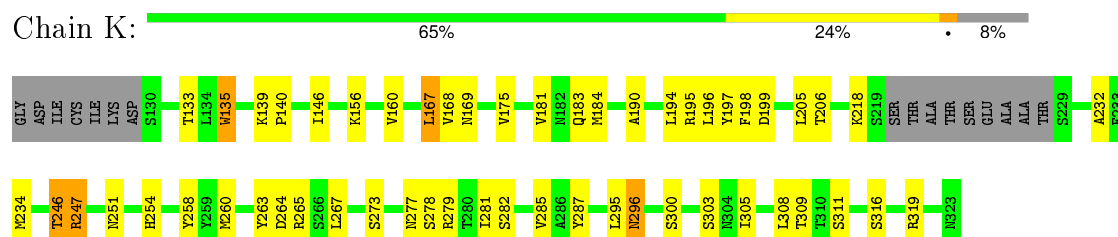
- Molecule 1: Fiber protein



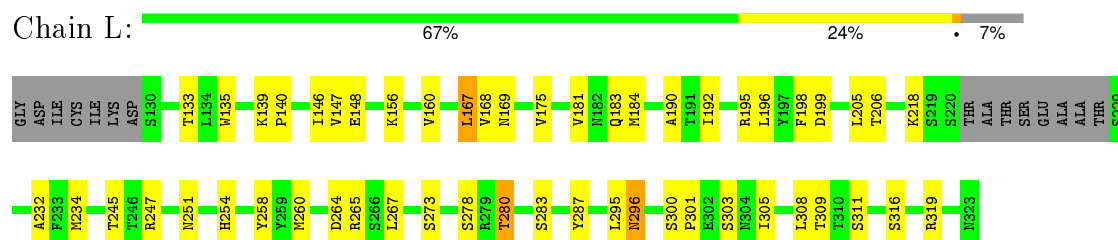
- Molecule 1: Fiber protein



- Molecule 1: Fiber protein



- Molecule 1: Fiber protein



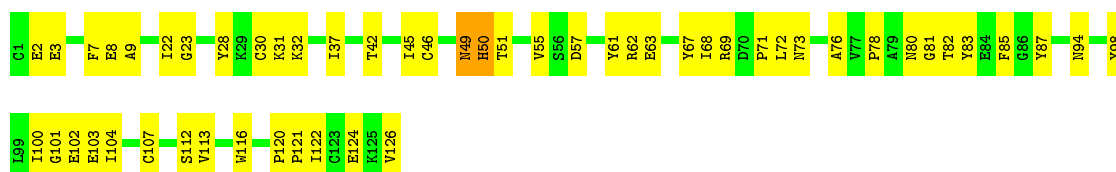
- Molecule 2: Membrane cofactor protein





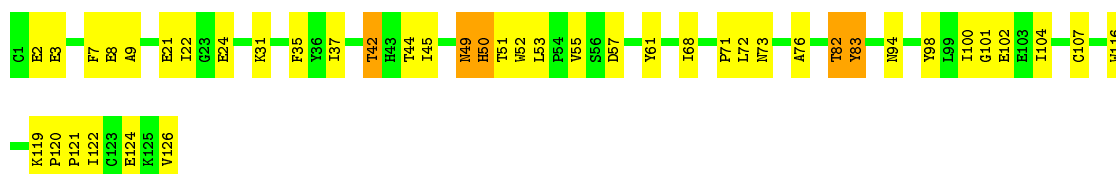
• Molecule 2: Membrane cofactor protein

Chain N: 58% 40%



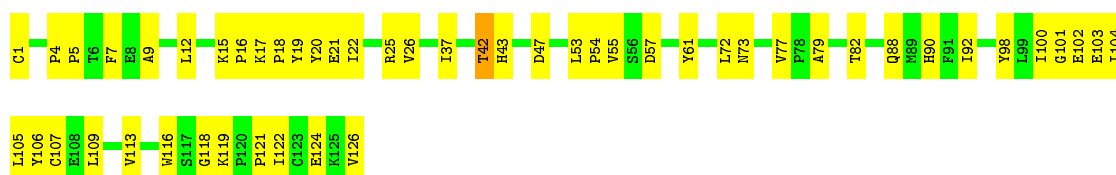
• Molecule 2: Membrane cofactor protein

Chain O: 66% 30%



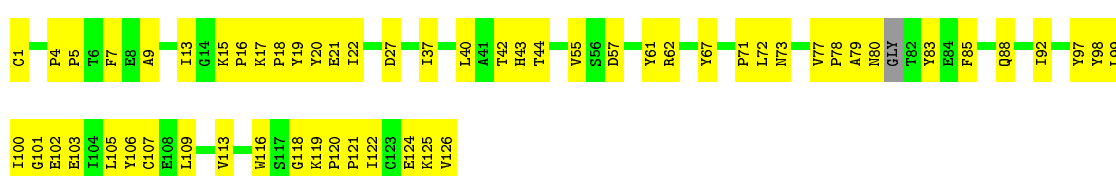
• Molecule 2: Membrane cofactor protein

Chain P: 60% 40%



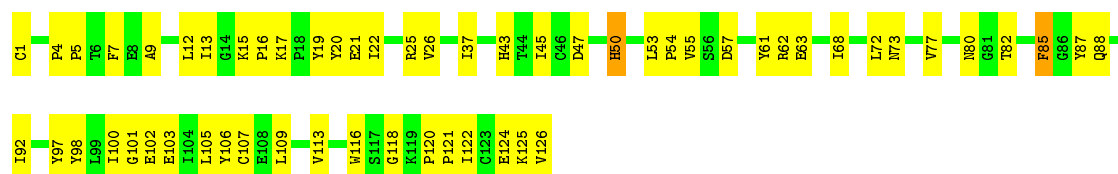
• Molecule 2: Membrane cofactor protein

Chain Q: 54% 45%

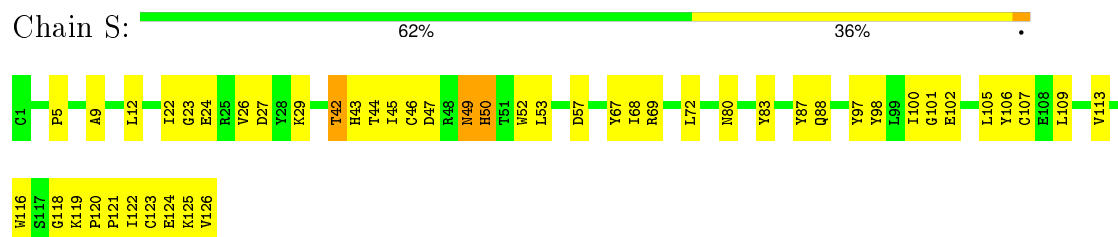


• Molecule 2: Membrane cofactor protein

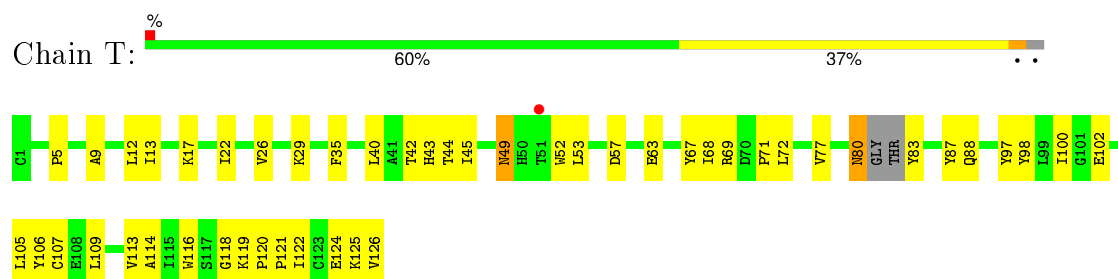
Chain R: 55% 44%



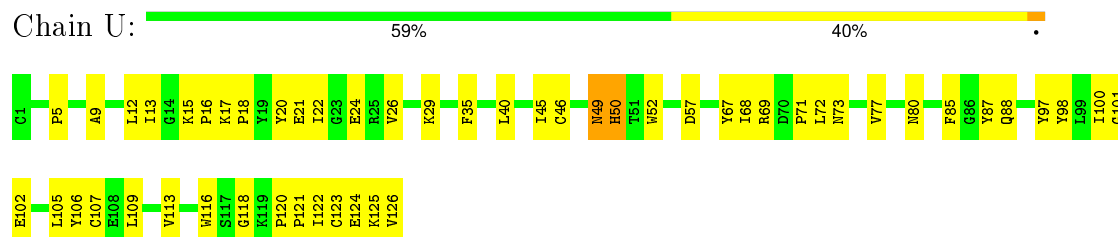
• Molecule 2: Membrane cofactor protein



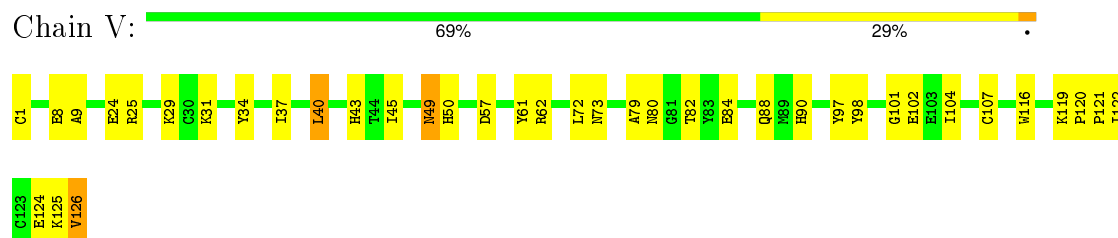
• Molecule 2: Membrane cofactor protein



• Molecule 2: Membrane cofactor protein



• Molecule 2: Membrane cofactor protein

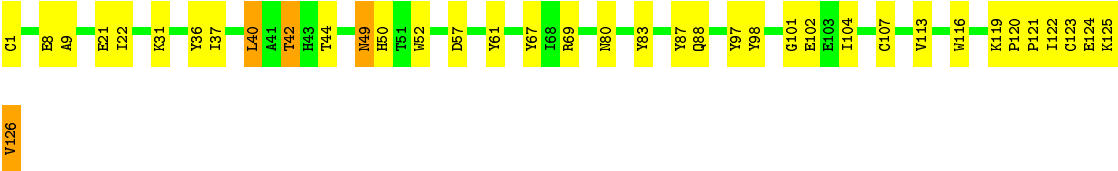


• Molecule 2: Membrane cofactor protein





● Molecule 2: Membrane cofactor protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.53Å 107.71Å 154.10Å 90.01° 90.10° 104.70°	Depositor
Resolution (Å)	47.99 – 3.50 47.99 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.3 (47.99-3.50) 95.8 (47.99-3.50)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.73 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _288)	Depositor
R, $R_{free}$	0.204 , 0.239 0.194 , 0.229	Depositor DCC
$R_{free}$ test set	3574 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.6	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 9.1	EDS
Estimated twinning fraction	0.419 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 71363 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	29017	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.29	0/1439	0.47	0/1961
1	B	0.29	0/1457	0.47	0/1986
1	C	0.29	0/1455	0.47	0/1983
1	D	0.29	0/1443	0.48	0/1966
1	E	0.29	0/1463	0.48	0/1994
1	F	0.29	0/1466	0.48	0/1998
1	G	0.28	0/1447	0.49	0/1969
1	H	0.28	0/1456	0.48	0/1982
1	I	0.30	0/1476	0.49	0/2011
1	J	0.28	0/1446	0.49	0/1969
1	K	0.28	0/1457	0.48	0/1986
1	L	0.28	0/1470	0.49	0/2004
2	M	0.29	0/1021	0.45	0/1396
2	N	0.29	0/1024	0.46	0/1397
2	O	0.30	0/1045	0.45	0/1424
2	P	0.29	0/1009	0.45	0/1380
2	Q	0.29	0/993	0.46	0/1355
2	R	0.29	0/1031	0.44	0/1408
2	S	0.29	0/1008	0.44	0/1377
2	T	0.29	0/988	0.45	0/1348
2	U	0.28	0/1030	0.45	0/1406
2	V	0.28	0/1025	0.47	0/1399
2	W	0.28	0/1015	0.47	0/1385
2	X	0.29	0/1035	0.45	0/1411
All	All	0.29	0/29699	0.47	0/40495

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 ⓘ

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	1411	0	1357	31	0
1	B	1428	0	1382	36	0
1	C	1426	0	1377	38	0
1	D	1415	0	1364	51	0
1	E	1434	0	1391	57	0
1	F	1437	0	1391	51	0
1	G	1419	0	1383	54	0
1	H	1428	0	1382	55	0
1	I	1447	0	1404	55	0
1	J	1417	0	1378	46	0
1	K	1428	0	1377	47	0
1	L	1441	0	1395	42	0
2	M	987	0	903	35	0
2	N	991	0	908	46	0
2	O	1011	0	942	38	0
2	P	977	0	888	41	0
2	Q	962	0	864	51	0
2	R	997	0	916	55	0
2	S	976	0	888	42	0
2	T	958	0	873	40	0
2	U	996	0	916	47	0
2	V	991	0	904	32	0
2	W	983	0	907	28	0
2	X	1001	0	934	35	0
3	M	14	0	13	2	0
3	P	14	0	13	0	0
3	S	14	0	13	0	0
3	V	14	0	13	3	0
All	All	29017	0	27476	920	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 16.

The worst 5 of 920 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:67:TYR:HA	2:Q:83:TYR:HE1	1.33	0.93
2:R:25:ARG:HB2	2:R:45:ILE:HG12	1.49	0.93
1:E:303:SER:HB2	2:P:122:ILE:HD11	1.53	0.88
1:F:303:SER:HB2	2:Q:122:ILE:HD11	1.55	0.86
1:A:251:ASN:HD22	1:A:278:SER:HB2	1.41	0.84

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	177/201 (88%)	164 (93%)	11 (6%)	2 (1%)	17	63
1	B	180/201 (90%)	168 (93%)	12 (7%)	0	100	100
1	C	180/201 (90%)	167 (93%)	12 (7%)	1 (1%)	30	75
1	D	177/201 (88%)	168 (95%)	6 (3%)	3 (2%)	11	54
1	E	180/201 (90%)	169 (94%)	9 (5%)	2 (1%)	17	63
1	F	181/201 (90%)	169 (93%)	8 (4%)	4 (2%)	8	49
1	G	176/201 (88%)	165 (94%)	10 (6%)	1 (1%)	30	75
1	H	177/201 (88%)	165 (93%)	11 (6%)	1 (1%)	30	75
1	I	182/201 (90%)	166 (91%)	13 (7%)	3 (2%)	12	55
1	J	178/201 (89%)	169 (95%)	8 (4%)	1 (1%)	30	75
1	K	181/201 (90%)	169 (93%)	9 (5%)	3 (2%)	11	54
1	L	182/201 (90%)	172 (94%)	8 (4%)	2 (1%)	17	63
2	M	124/126 (98%)	114 (92%)	7 (6%)	3 (2%)	7	47
2	N	124/126 (98%)	113 (91%)	9 (7%)	2 (2%)	12	55
2	O	124/126 (98%)	114 (92%)	7 (6%)	3 (2%)	7	47
2	P	124/126 (98%)	112 (90%)	12 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	121/126 (96%)	107 (88%)	13 (11%)	1 (1%)	24	70
2	R	124/126 (98%)	111 (90%)	13 (10%)	0	100	100
2	S	124/126 (98%)	112 (90%)	12 (10%)	0	100	100
2	T	120/126 (95%)	107 (89%)	13 (11%)	0	100	100
2	U	124/126 (98%)	112 (90%)	12 (10%)	0	100	100
2	V	124/126 (98%)	114 (92%)	9 (7%)	1 (1%)	24	70
2	W	121/126 (96%)	111 (92%)	8 (7%)	2 (2%)	11	54
2	X	124/126 (98%)	116 (94%)	7 (6%)	1 (1%)	24	70
All	All	3629/3924 (92%)	3354 (92%)	239 (7%)	36 (1%)	19	66

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	131	ILE
1	E	148	GLU
1	I	148	GLU
1	L	245	THR
2	W	21	GLU

### 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	159/182 (87%)	153 (96%)	6 (4%)	40	76
1	B	163/182 (90%)	156 (96%)	7 (4%)	35	74
1	C	162/182 (89%)	155 (96%)	7 (4%)	35	74
1	D	161/182 (88%)	153 (95%)	8 (5%)	30	69
1	E	165/182 (91%)	157 (95%)	8 (5%)	31	71
1	F	165/182 (91%)	154 (93%)	11 (7%)	20	61
1	G	162/182 (89%)	156 (96%)	6 (4%)	41	76
1	H	164/182 (90%)	159 (97%)	5 (3%)	48	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	166/182 (91%)	159 (96%)	7 (4%)	36	74
1	J	162/182 (89%)	157 (97%)	5 (3%)	47	81
1	K	161/182 (88%)	158 (98%)	3 (2%)	65	87
1	L	164/182 (90%)	160 (98%)	4 (2%)	57	85
2	M	102/110 (93%)	98 (96%)	4 (4%)	39	76
2	N	103/110 (94%)	100 (97%)	3 (3%)	50	81
2	O	108/110 (98%)	103 (95%)	5 (5%)	33	72
2	P	101/110 (92%)	99 (98%)	2 (2%)	63	87
2	Q	97/110 (88%)	96 (99%)	1 (1%)	82	93
2	R	105/110 (96%)	101 (96%)	4 (4%)	40	76
2	S	101/110 (92%)	97 (96%)	4 (4%)	38	75
2	T	99/110 (90%)	95 (96%)	4 (4%)	38	75
2	U	105/110 (96%)	102 (97%)	3 (3%)	50	81
2	V	103/110 (94%)	99 (96%)	4 (4%)	39	76
2	W	103/110 (94%)	98 (95%)	5 (5%)	31	70
2	X	106/110 (96%)	101 (95%)	5 (5%)	32	72
All	All	3187/3504 (91%)	3066 (96%)	121 (4%)	40	76

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	208	GLU
1	J	167	LEU
2	W	1	CYS
1	H	296	ASN
1	I	280	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	254	HIS
1	K	132	ASN
2	W	43	HIS
1	I	290	GLN
1	J	217	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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$
3	NAG	M	1080	2	14,14,15	0.44	0	15,19,21	0.86	0
3	NAG	P	1080	2	14,14,15	0.44	0	15,19,21	0.87	0
3	NAG	S	1080	2	14,14,15	0.49	0	15,19,21	1.00	1 (6%)
3	NAG	V	1080	2	14,14,15	0.47	0	15,19,21	1.01	1 (6%)

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
3	NAG	M	1080	2	-	0/6/23/26	0/1/1/1
3	NAG	P	1080	2	-	0/6/23/26	0/1/1/1
3	NAG	S	1080	2	-	0/6/23/26	0/1/1/1
3	NAG	V	1080	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	1080	NAG	C1-O5-C5	-2.41	109.19	112.25
3	V	1080	NAG	C2-N2-C7	-2.22	120.18	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1080	NAG	2	0
3	V	1080	NAG	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	183/201 (91%)	-0.21	0 100 100	34, 49, 74, 90	0
1	B	184/201 (91%)	-0.24	1 (0%) 91 88	34, 48, 75, 92	0
1	C	184/201 (91%)	-0.26	0 100 100	34, 49, 68, 85	0
1	D	183/201 (91%)	-0.20	0 100 100	36, 50, 72, 90	0
1	E	184/201 (91%)	-0.25	0 100 100	35, 50, 77, 92	0
1	F	185/201 (92%)	-0.19	0 100 100	35, 49, 74, 87	0
1	G	182/201 (90%)	-0.15	0 100 100	35, 50, 72, 83	0
1	H	183/201 (91%)	-0.25	0 100 100	35, 51, 72, 94	0
1	I	186/201 (92%)	-0.21	0 100 100	35, 50, 71, 89	0
1	J	182/201 (90%)	-0.21	0 100 100	34, 49, 74, 90	0
1	K	185/201 (92%)	-0.26	0 100 100	33, 49, 77, 91	0
1	L	186/201 (92%)	-0.20	0 100 100	34, 49, 73, 86	0
2	M	126/126 (100%)	-0.14	0 100 100	45, 64, 93, 99	0
2	N	126/126 (100%)	-0.19	0 100 100	46, 65, 85, 98	0
2	O	126/126 (100%)	-0.25	0 100 100	46, 64, 92, 98	0
2	P	126/126 (100%)	-0.14	0 100 100	43, 67, 106, 117	0
2	Q	125/126 (99%)	-0.02	0 100 100	43, 70, 114, 121	0
2	R	126/126 (100%)	-0.12	0 100 100	43, 67, 100, 117	0
2	S	126/126 (100%)	-0.16	0 100 100	44, 66, 107, 119	0
2	T	124/126 (98%)	0.03	1 (0%) 87 80	45, 69, 117, 120	0
2	U	126/126 (100%)	-0.02	0 100 100	44, 67, 102, 118	0
2	V	126/126 (100%)	-0.19	0 100 100	44, 63, 89, 96	0
2	W	125/126 (99%)	-0.19	1 (0%) 87 80	44, 64, 82, 96	0
2	X	126/126 (100%)	-0.19	0 100 100	44, 64, 84, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3715/3924 (94%)	-0.18	3 (0%) 95 94	33, 56, 90, 121	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	W	80	ASN	2.4
1	B	245	THR	2.0
2	T	51	THR	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 carbohydrates 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. 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	S	1080	14/15	0.91	0.27	0.24	54,60,64,64	0
3	NAG	V	1080	14/15	0.93	0.29	0.13	62,65,72,73	0
3	NAG	M	1080	14/15	0.91	0.23	-0.43	61,64,70,75	0
3	NAG	P	1080	14/15	0.90	0.21	-1.01	52,59,62,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.