



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 07:44 PM GMT

PDB ID : 1N4R
Title : Protein Geranylgeranyltransferasetype-I Complexed with a Geranylgeranylated KKKSKTKCVIL Peptide Product
Authors : Taylor, J.S.; Reid, T.S.; Casey, P.J.; Beese, L.S.
Deposited on : 2002-11-01
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

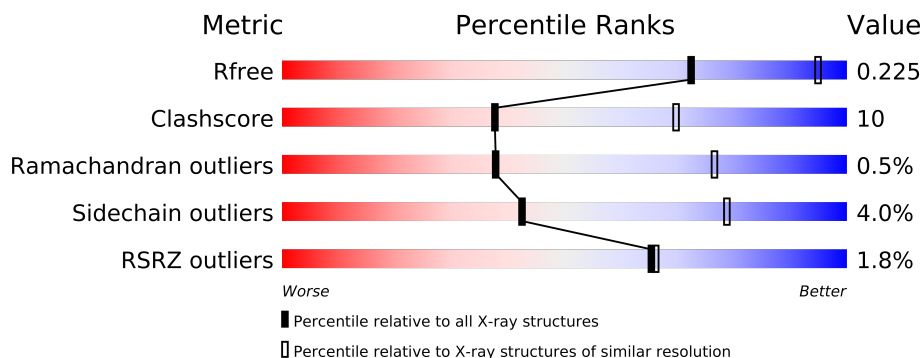
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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.





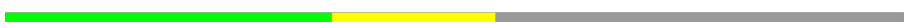

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	377	
1	C	377	
1	E	377	
1	G	377	
1	I	377	
1	K	377	
2	B	377	
2	D	377	
2	F	377	
2	H	377	
2	J	377	
2	L	377	
3	M	11	
3	N	11	

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Mol	Chain	Length	Quality of chain
3	O	11	
3	P	11	
3	Q	11	
3	R	11	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MES	A	901	X	X
4	MES	C	902	X	X
4	MES	E	903	X	X
4	MES	G	904	X	X
4	MES	I	905	X	X
4	MES	K	906	X	X
8	GER	R	1608	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 33129 atoms, of which 0 are hydrogen and 0 are deuterium.

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 protein farnesyltransferase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2614	1673	458	478	5			
1	C	314	Total	C	N	O	S	0	0	0
			2648	1691	462	490	5			
1	E	314	Total	C	N	O	S	0	0	0
			2630	1682	460	483	5			
1	G	314	Total	C	N	O	S	0	0	0
			2632	1683	459	485	5			
1	I	314	Total	C	N	O	S	0	0	0
			2654	1693	461	495	5			
1	K	314	Total	C	N	O	S	0	0	0
			2667	1700	466	496	5			

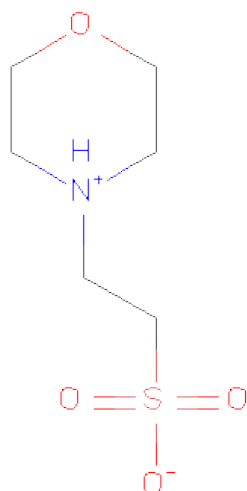
- Molecule 2 is a protein called geranyltransferase type-I beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2689	1702	467	496	24			
2	D	346	Total	C	N	O	S	0	0	0
			2693	1704	467	498	24			
2	F	346	Total	C	N	O	S	0	0	0
			2708	1711	471	502	24			
2	H	346	Total	C	N	O	S	0	0	0
			2670	1692	458	496	24			
2	J	346	Total	C	N	O	S	0	0	0
			2709	1711	471	503	24			
2	L	346	Total	C	N	O	S	0	0	0
			2714	1715	471	504	24			

- Molecule 3 is a protein called Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	6	Total	C	N	O	S	0	0	0
			46	30	7	8	1			
3	N	6	Total	C	N	O	S	0	0	0
			46	30	7	8	1			
3	O	6	Total	C	N	O	S	0	0	0
			46	30	7	8	1			
3	P	6	Total	C	N	O	S	0	0	0
			46	30	7	8	1			
3	Q	6	Total	C	N	O	S	0	0	0
			46	30	7	8	1			
3	R	6	Total	C	N	O	S	0	0	0
			46	30	7	8	1			

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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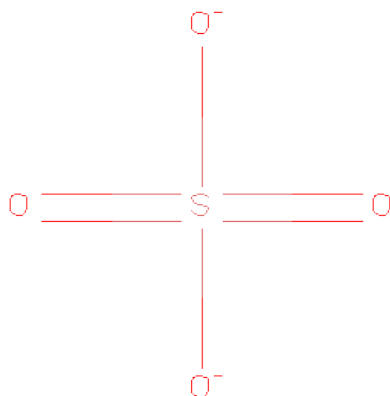
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		
5	H	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		
5	L	1	Total	Zn	0	0
			1	1		
5	F	1	Total	Zn	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

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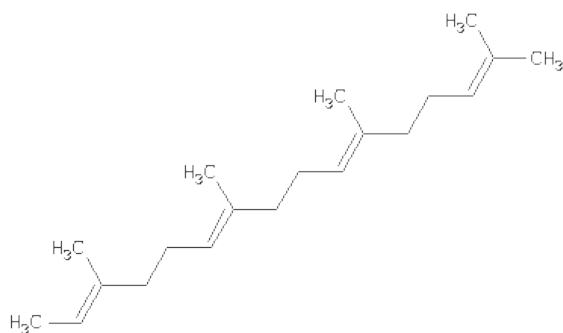
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Cl	0	0
			1	1		
7	J	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		
7	K	1	Total	Cl	0	0
			1	1		
7	H	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		
7	F	1	Total	Cl	0	0
			1	1		

- Molecule 8 is GERAN-8-YL GERAN (three-letter code: GER) (formula: C₂₀H₃₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total C 20 20	0	0
8	N	1	Total C 20 20	0	0
8	O	1	Total C 20 20	0	0
8	P	1	Total C 20 20	0	0
8	Q	1	Total C 20 20	0	0
8	R	1	Total C 20 20	0	0

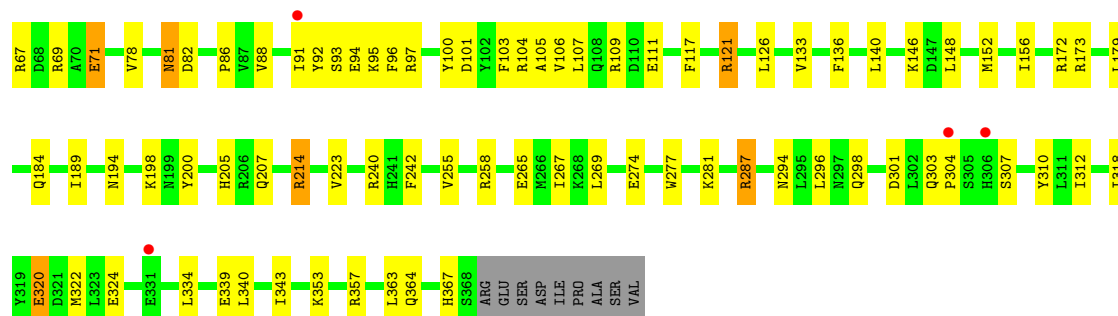
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	45	Total O 45 45	0	0
9	B	35	Total O 35 35	0	0
9	C	49	Total O 49 49	0	0
9	D	45	Total O 45 45	0	0
9	E	40	Total O 40 40	0	0
9	F	51	Total O 51 51	0	0

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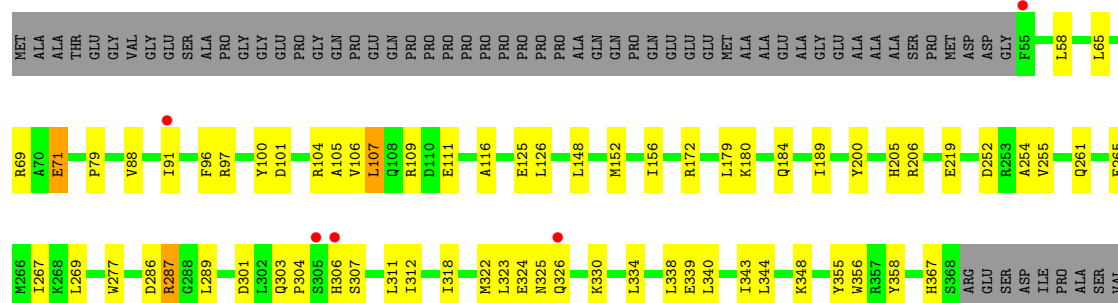
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	40	Total 40	O 40	0	0
9	H	23	Total 23	O 23	0	0
9	I	52	Total 52	O 52	0	0
9	J	36	Total 36	O 36	0	0
9	K	101	Total 101	O 101	0	0
9	L	60	Total 60	O 60	0	0
9	M	1	Total 1	O 1	0	0
9	N	3	Total 3	O 3	0	0
9	O	1	Total 1	O 1	0	0
9	Q	3	Total 3	O 3	0	0
9	R	5	Total 5	O 5	0	0



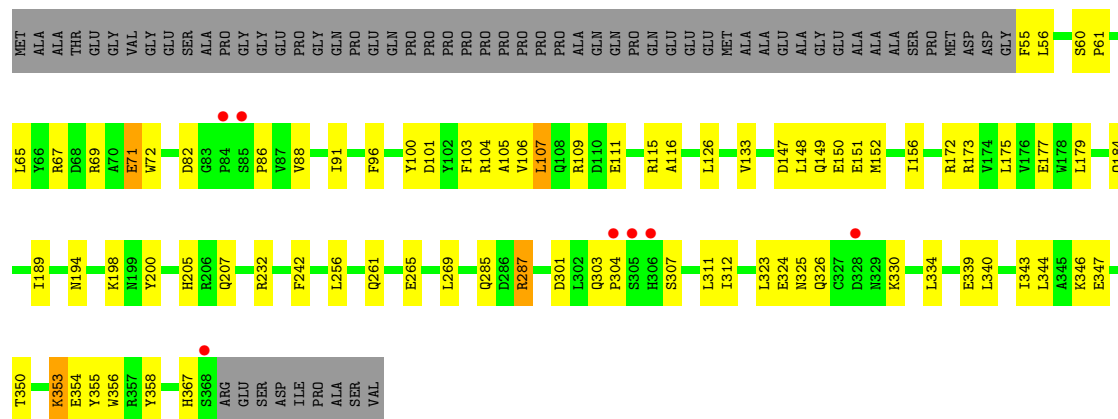
- Molecule 1: protein farnesyltransferase alpha subunit

Chain G:



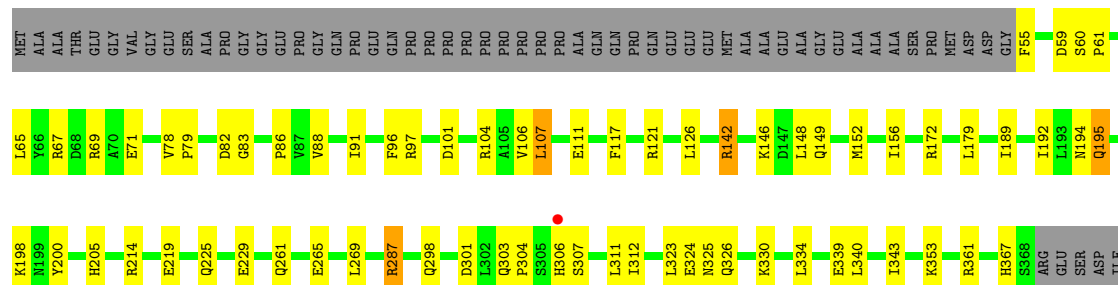
- Molecule 1: protein farnesyltransferase alpha subunit

Chain I:



- Molecule 1: protein farnesyltransferase alpha subunit

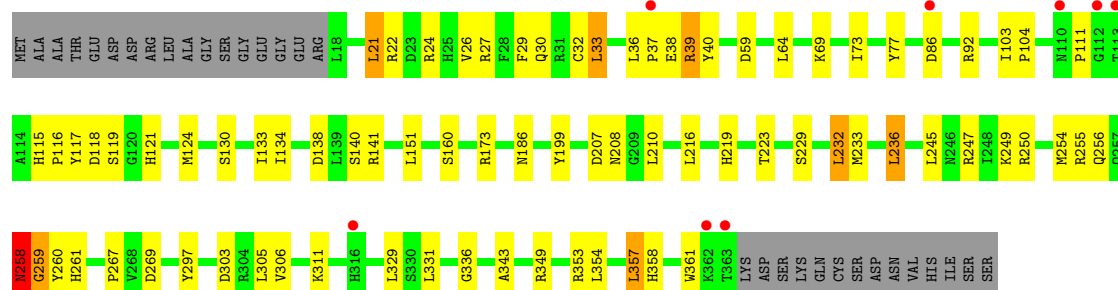
Chain K:



PRO
ALA
SER
VAL

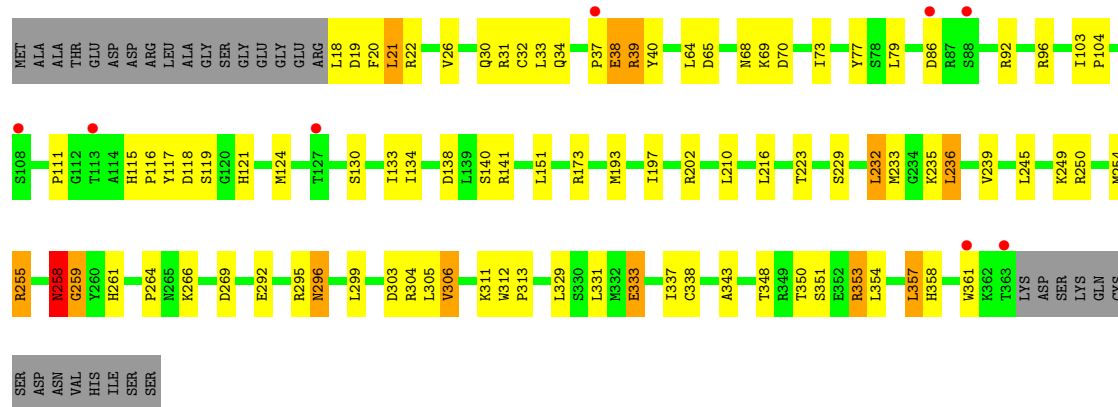
- Molecule 2: geranyltransferase type-I beta subunit

Chain B:



- Molecule 2: geranyltransferase type-I beta subunit

Chain D:



- Molecule 2: geranyltransferase type-I beta subunit

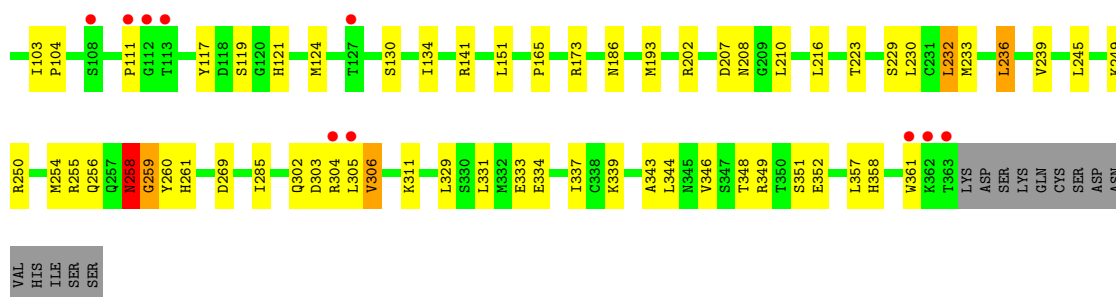
Chain F:



- Molecule 2: geranyltransferase type-I beta subunit

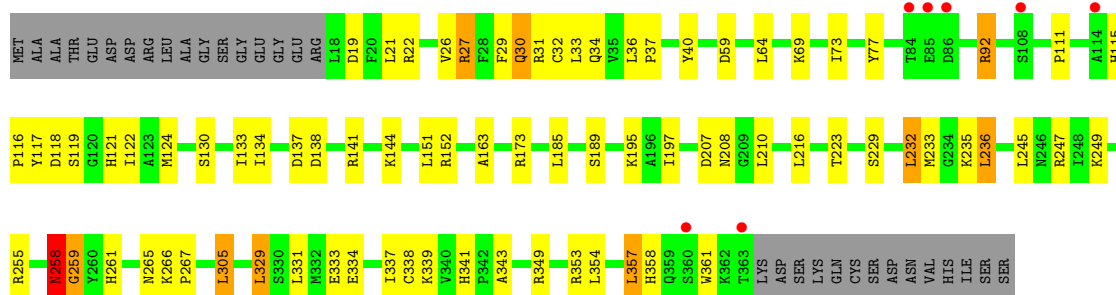
Chain H:





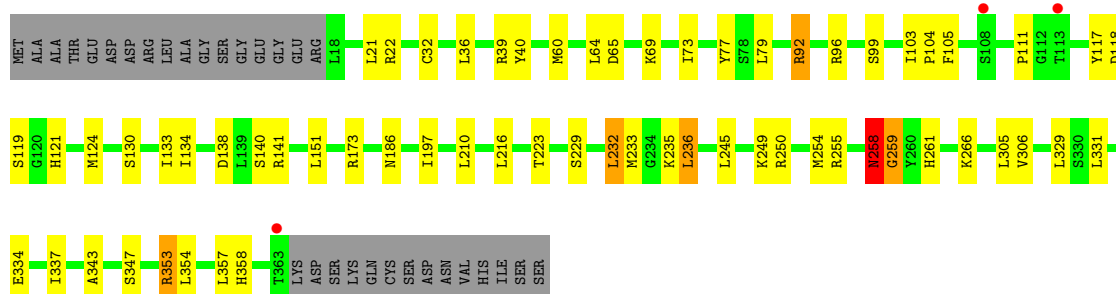
- Molecule 2: geranyltransferase type-I beta subunit

Chain J:



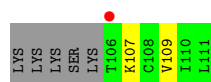
- Molecule 2: geranyltransferase type-I beta subunit

Chain L:



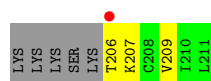
- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain M:



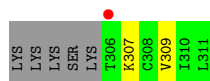
- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain N:



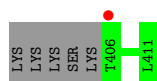
- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain O: 



- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain P: 



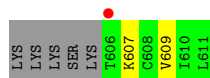
- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain Q: 



- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain R: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	272.07Å 268.80Å 185.31Å 90.00° 131.55° 90.00°	Depositor
Resolution (Å)	29.86 – 2.80 29.86 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.86-2.80) 95.3 (29.86-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.200 , 0.218 0.209 , 0.225	Depositor DCC
R_{free} test set	12101 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.0	EDS
Estimated twinning fraction	0.085 for -h-2*1,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 288709 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33129	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GER, ZN, SO4, MES, CL

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	0/2680	0.52	0/3649
1	C	0.36	0/2714	0.53	0/3690
1	E	0.35	0/2696	0.53	0/3668
1	G	0.36	0/2698	0.53	0/3670
1	I	0.36	0/2720	0.54	0/3698
1	K	0.39	0/2733	0.56	0/3713
2	B	0.36	0/2750	0.60	2/3720 (0.1%)
2	D	0.37	0/2754	0.59	2/3725 (0.1%)
2	F	0.38	0/2769	0.60	2/3743 (0.1%)
2	H	0.35	0/2730	0.58	2/3696 (0.1%)
2	J	0.36	0/2770	0.59	2/3745 (0.1%)
2	L	0.39	0/2775	0.61	2/3750 (0.1%)
3	M	0.54	0/45	0.50	0/58
3	N	0.52	0/45	0.51	0/58
3	O	0.54	0/45	0.53	0/58
3	P	0.50	0/45	0.51	0/58
3	Q	0.55	0/45	0.52	0/58
3	R	0.56	0/45	0.53	0/58
All	All	0.37	0/33059	0.57	12/44815 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	F	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	259	GLY	N-CA-C	-5.88	98.40	113.10
2	F	259	GLY	N-CA-C	-5.80	98.61	113.10
2	L	259	GLY	N-CA-C	-5.79	98.62	113.10
2	H	259	GLY	N-CA-C	-5.75	98.73	113.10
2	D	259	GLY	N-CA-C	-5.65	98.97	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	297	TYR	Sidechain
2	F	297	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2614	0	2499	58	0
1	C	2648	0	2549	50	0
1	E	2630	0	2524	69	0
1	G	2632	0	2527	57	0
1	I	2654	0	2551	54	0
1	K	2667	0	2577	54	0
2	B	2689	0	2585	55	0
2	D	2693	0	2589	64	0
2	F	2708	0	2613	48	0
2	H	2670	0	2551	66	0
2	J	2709	0	2610	46	0
2	L	2714	0	2621	39	0
3	M	46	0	54	1	0
3	N	46	0	54	2	0
3	O	46	0	54	1	0
3	P	46	0	54	0	0
3	Q	46	0	54	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	46	0	54	1	0
4	A	12	0	13	3	0
4	C	12	0	13	1	0
4	E	12	0	13	2	0
4	G	12	0	13	2	0
4	I	12	0	13	2	0
4	K	12	0	13	1	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
6	B	5	0	0	0	0
6	D	5	0	0	0	0
6	F	5	0	0	0	0
6	H	5	0	0	0	0
6	J	5	0	0	0	0
6	L	5	0	0	0	0
7	C	1	0	0	1	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	2	0
7	H	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	1	0
8	M	20	0	32	1	0
8	N	20	0	32	1	0
8	O	20	0	32	1	0
8	P	20	0	32	1	0
8	Q	20	0	32	1	0
8	R	20	0	32	2	0
9	A	45	0	0	3	0
9	B	35	0	0	1	0
9	C	49	0	0	2	0
9	D	45	0	0	2	0
9	E	40	0	0	2	0
9	F	51	0	0	2	0
9	G	40	0	0	4	0
9	H	23	0	0	0	0
9	I	52	0	0	0	0
9	J	36	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	101	0	0	4	0
9	L	60	0	0	0	0
9	M	1	0	0	0	0
9	N	3	0	0	0	0
9	O	1	0	0	0	0
9	Q	3	0	0	0	0
9	R	5	0	0	0	0
All	All	33129	0	31390	639	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

The worst 5 of 639 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:156:ILE:HG12	1:E:172:ARG:HH12	1.12	1.14
1:K:156:ILE:HG12	1:K:172:ARG:HH12	0.99	1.14
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.12	1.12
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.15	1.11
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.16	1.09

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/377 (83%)	288 (92%)	23 (7%)	1 (0%)	50	84
1	C	312/377 (83%)	292 (94%)	20 (6%)	0	100	100
1	E	312/377 (83%)	291 (93%)	21 (7%)	0	100	100
1	G	312/377 (83%)	287 (92%)	24 (8%)	1 (0%)	50	84
1	I	312/377 (83%)	290 (93%)	22 (7%)	0	100	100
1	K	312/377 (83%)	292 (94%)	19 (6%)	1 (0%)	50	84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	344/377 (91%)	324 (94%)	18 (5%)	2 (1%)	33	72
2	D	344/377 (91%)	326 (95%)	14 (4%)	4 (1%)	19	54
2	F	344/377 (91%)	323 (94%)	19 (6%)	2 (1%)	33	72
2	H	344/377 (91%)	318 (92%)	22 (6%)	4 (1%)	19	54
2	J	344/377 (91%)	324 (94%)	17 (5%)	3 (1%)	25	63
2	L	344/377 (91%)	325 (94%)	17 (5%)	2 (1%)	33	72
3	M	4/11 (36%)	4 (100%)	0	0	100	100
3	N	4/11 (36%)	4 (100%)	0	0	100	100
3	O	4/11 (36%)	4 (100%)	0	0	100	100
3	P	4/11 (36%)	4 (100%)	0	0	100	100
3	Q	4/11 (36%)	4 (100%)	0	0	100	100
3	R	4/11 (36%)	4 (100%)	0	0	100	100
All	All	3960/4590 (86%)	3704 (94%)	236 (6%)	20 (0%)	38	76

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	111	PRO
2	B	258	ASN
2	D	111	PRO
2	D	258	ASN
2	F	111	PRO

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	276/338 (82%)	270 (98%)	6 (2%)	64	92
1	C	285/338 (84%)	275 (96%)	10 (4%)	48	83
1	E	280/338 (83%)	269 (96%)	11 (4%)	43	80
1	G	281/338 (83%)	276 (98%)	5 (2%)	71	94
1	I	287/338 (85%)	278 (97%)	9 (3%)	52	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	290/338 (86%)	279 (96%)	11 (4%)	44	80
2	B	286/326 (88%)	273 (96%)	13 (4%)	38	74
2	D	287/326 (88%)	270 (94%)	17 (6%)	28	62
2	F	291/326 (89%)	276 (95%)	15 (5%)	32	68
2	H	282/326 (86%)	271 (96%)	11 (4%)	43	80
2	J	291/326 (89%)	274 (94%)	17 (6%)	28	63
2	L	292/326 (90%)	279 (96%)	13 (4%)	38	74
3	M	6/11 (54%)	6 (100%)	0	100	100
3	N	6/11 (54%)	6 (100%)	0	100	100
3	O	6/11 (54%)	6 (100%)	0	100	100
3	P	6/11 (54%)	6 (100%)	0	100	100
3	Q	6/11 (54%)	6 (100%)	0	100	100
3	R	6/11 (54%)	6 (100%)	0	100	100
All	All	3464/4050 (86%)	3326 (96%)	138 (4%)	42	79

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	232	LEU
2	H	21	LEU
2	L	92	ARG
2	F	255	ARG
2	F	353	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	30	GLN
1	G	162	GLN
1	K	184	GLN
2	F	246	ASN
1	G	80	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 31 ligands modelled in this entry, 13 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	MES	A	901	-	12,12,12	9.63	9 (75%)	16,16,16	2.62	9 (56%)
6	SO4	B	810	-	4,4,4	0.14	0	6,6,6	0.11	0
4	MES	C	902	-	12,12,12	9.53	9 (75%)	16,16,16	2.64	9 (56%)
6	SO4	D	811	-	4,4,4	0.16	0	6,6,6	0.14	0
4	MES	E	903	-	12,12,12	9.56	9 (75%)	16,16,16	2.65	9 (56%)
6	SO4	F	812	-	4,4,4	0.24	0	6,6,6	0.12	0
4	MES	G	904	-	12,12,12	9.51	9 (75%)	16,16,16	2.67	9 (56%)
6	SO4	H	813	-	4,4,4	0.18	0	6,6,6	0.18	0
4	MES	I	905	-	12,12,12	9.44	9 (75%)	16,16,16	2.73	9 (56%)
6	SO4	J	814	-	4,4,4	0.19	0	6,6,6	0.20	0
4	MES	K	906	-	12,12,12	9.46	8 (66%)	16,16,16	2.67	10 (62%)
6	SO4	L	815	-	4,4,4	0.13	0	6,6,6	0.25	0
8	GER	M	1108	3	19,19,19	0.73	0	22,22,22	0.74	0
8	GER	N	1208	3	19,19,19	0.68	0	22,22,22	0.74	0
8	GER	O	1308	3	19,19,19	0.70	0	22,22,22	0.76	0
8	GER	P	1408	3	19,19,19	0.62	0	22,22,22	0.75	0
8	GER	Q	1508	3	19,19,19	0.69	0	22,22,22	0.76	0
8	GER	R	1608	3	19,19,19	0.68	0	22,22,22	0.76	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
4	MES	A	901	-	-	0/6/14/14	0/1/1/1
6	SO4	B	810	-	-	0/0/0/0	0/0/0/0
4	MES	C	902	-	-	0/6/14/14	0/1/1/1
6	SO4	D	811	-	-	0/0/0/0	0/0/0/0
4	MES	E	903	-	-	0/6/14/14	0/1/1/1
6	SO4	F	812	-	-	0/0/0/0	0/0/0/0
4	MES	G	904	-	-	0/6/14/14	0/1/1/1
6	SO4	H	813	-	-	0/0/0/0	0/0/0/0
4	MES	I	905	-	-	0/6/14/14	0/1/1/1
6	SO4	J	814	-	-	0/0/0/0	0/0/0/0
4	MES	K	906	-	-	0/6/14/14	0/1/1/1
6	SO4	L	815	-	-	0/0/0/0	0/0/0/0
8	GER	M	1108	3	-	0/20/20/20	0/0/0/0
8	GER	N	1208	3	-	0/20/20/20	0/0/0/0
8	GER	O	1308	3	-	0/20/20/20	0/0/0/0
8	GER	P	1408	3	-	0/20/20/20	0/0/0/0
8	GER	Q	1508	3	-	0/20/20/20	0/0/0/0
8	GER	R	1608	3	-	0/20/20/20	0/0/0/0

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	906	MES	C8-S	-19.24	1.44	1.78
4	A	901	MES	C8-S	-19.22	1.44	1.78
4	G	904	MES	C8-S	-18.84	1.44	1.78
4	E	903	MES	C8-S	-18.81	1.44	1.78
4	C	902	MES	C8-S	-18.77	1.44	1.78

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	902	MES	C7-C8-S	4.80	125.55	112.49
4	K	906	MES	C7-C8-S	4.79	125.52	112.49
4	G	904	MES	C7-C8-S	4.76	125.45	112.49
4	I	905	MES	C8-C7-N4	4.63	120.36	112.44
4	I	905	MES	C7-C8-S	4.60	125.00	112.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	314/377 (83%)	-0.37	2 (0%) 86 88	36, 57, 91, 105	0
1	C	314/377 (83%)	-0.39	4 (1%) 74 75	35, 55, 81, 99	0
1	E	314/377 (83%)	-0.36	4 (1%) 74 75	34, 57, 83, 103	0
1	G	314/377 (83%)	-0.32	5 (1%) 68 69	38, 58, 85, 104	0
1	I	314/377 (83%)	-0.41	7 (2%) 59 60	32, 52, 80, 91	0
1	K	314/377 (83%)	-0.58	1 (0%) 91 93	25, 43, 67, 82	0
2	B	346/377 (91%)	-0.33	8 (2%) 57 58	36, 52, 78, 100	0
2	D	346/377 (91%)	-0.28	8 (2%) 57 58	34, 48, 78, 92	0
2	F	346/377 (91%)	-0.32	5 (1%) 72 72	32, 48, 77, 103	0
2	H	346/377 (91%)	-0.01	13 (3%) 38 38	37, 64, 92, 111	0
2	J	346/377 (91%)	-0.30	7 (2%) 62 63	31, 50, 79, 102	0
2	L	346/377 (91%)	-0.43	3 (0%) 81 81	27, 42, 66, 88	0
3	M	6/11 (54%)	0.17	1 (16%) 2 2	52, 58, 82, 89	0
3	N	6/11 (54%)	0.14	1 (16%) 2 2	56, 61, 79, 85	0
3	O	6/11 (54%)	0.11	1 (16%) 2 2	52, 59, 78, 84	0
3	P	6/11 (54%)	0.36	1 (16%) 2 2	64, 68, 89, 92	0
3	Q	6/11 (54%)	0.03	0 100 100	51, 56, 72, 79	0
3	R	6/11 (54%)	-0.03	1 (16%) 2 2	51, 57, 71, 76	0
All	All	3996/4590 (87%)	-0.33	72 (1%) 65 66	25, 52, 83, 111	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	363	THR	5.3
2	H	108	SER	5.1
2	B	363	THR	4.0

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Mol	Chain	Res	Type	RSRZ
2	J	108	SER	4.0
2	J	363	THR	3.9

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 carbohydrates 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. 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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MES	A	901	12/12	0.31	10.92	96,103,106,106	0
4	MES	G	904	12/12	0.35	7.51	97,101,104,104	0
4	MES	C	902	12/12	0.31	5.35	86,93,95,96	0
4	MES	E	903	12/12	0.25	5.14	84,90,94,94	0
4	MES	I	905	12/12	0.28	4.41	78,84,88,89	0
4	MES	K	906	12/12	0.24	2.87	65,77,83,84	0
8	GER	R	1608	20/20	0.31	2.62	47,50,54,54	0
8	GER	M	1108	20/20	0.25	1.34	48,52,61,61	0
8	GER	Q	1508	20/20	0.26	1.21	47,50,55,56	0
8	GER	P	1408	20/20	0.28	1.18	61,66,73,73	0
8	GER	O	1308	20/20	0.23	1.04	48,51,58,60	0
8	GER	N	1208	20/20	0.25	0.88	49,53,58,59	0
6	SO4	F	812	5/5	0.13	0.26	67,67,68,69	0
6	SO4	B	810	5/5	0.14	0.18	67,68,68,69	0
6	SO4	D	811	5/5	0.14	0.16	66,66,67,67	0
7	CL	C	801	1/1	0.14	-0.05	53,53,53,53	0
6	SO4	L	815	5/5	0.15	-0.19	54,54,56,56	0
6	SO4	J	814	5/5	0.12	-0.55	52,52,54,55	0
6	SO4	H	813	5/5	0.11	-0.74	68,69,69,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	CL	G	804	1/1	0.10	-1.13	52,52,52,52	0
7	CL	H	805	1/1	0.10	-1.56	60,60,60,60	0
7	CL	D	802	1/1	0.05	-2.29	45,45,45,45	0
7	CL	J	806	1/1	0.06	-2.35	58,58,58,58	0
7	CL	K	807	1/1	0.07	-2.46	44,44,44,44	0
5	ZN	H	378	1/1	0.04	-2.63	87,87,87,87	0
5	ZN	L	378	1/1	0.05	-2.64	58,58,58,58	0
5	ZN	D	378	1/1	0.04	-2.87	66,66,66,66	0
5	ZN	F	378	1/1	0.05	-2.88	78,78,78,78	0
5	ZN	J	378	1/1	0.05	-2.90	68,68,68,68	0
5	ZN	B	378	1/1	0.03	-2.93	77,77,77,77	0
7	CL	F	803	1/1	0.04	-4.55	51,51,51,51	0

6.5 Other polymers ⓘ

There are no such residues in this entry.