wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:31 PM GMT

PDB ID	:	1TNB
Title	:	Rat Protein Geranylgeranyltransferase Type-I Complexed with a GGPP analog and a substrate KKSKTKCVIF Peptide Derived from TC21
Authors	:	Reid, T.S.; Terry, K.L.; Casey, P.J.; Beese, L.S.
Deposited on	:	2004-06-11
Resolution	:	2.85 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:

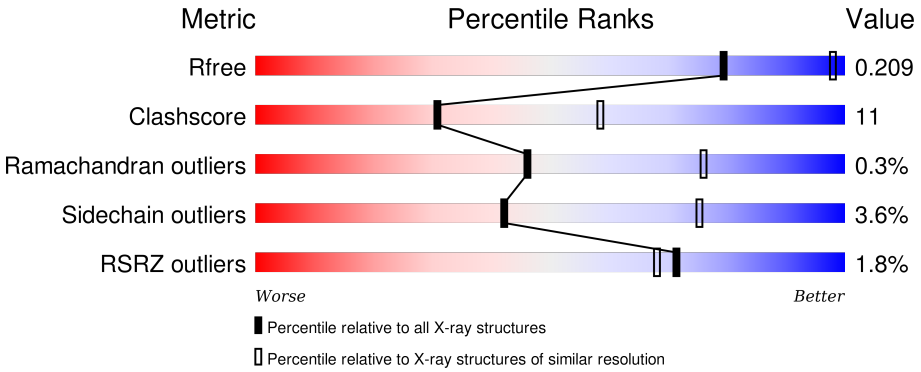
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	377	2% 60% 21% • 17%
1	C	377	2% 64% 19% • 17%
1	E	377	2% 62% 21% • 17%
1	G	377	2% 64% 19% • 17%
1	I	377	2% 64% 19% • 17%

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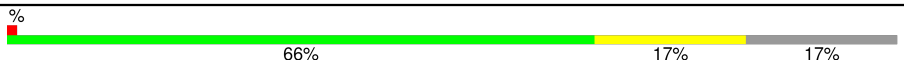
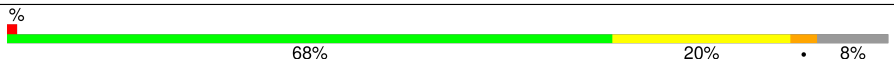
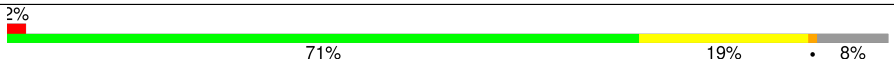
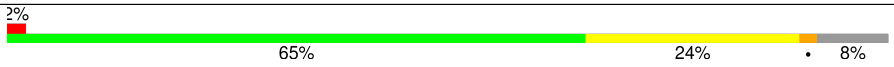
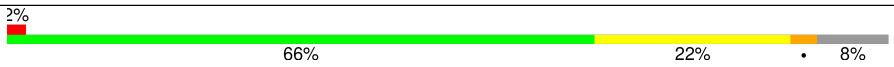
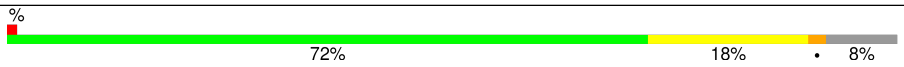
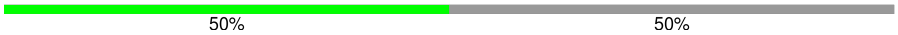
Mol	Chain	Length	Quality of chain
1	K	377	
2	B	377	
2	D	377	
2	F	377	
2	H	377	
2	J	377	
2	L	377	
3	M	10	
3	N	10	
3	O	10	
3	P	10	
3	Q	10	
3	R	10	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33504 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 geranylgeranyltransferase type I alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2636	1682	463	486	5			
1	C	314	Total	C	N	O	S	0	0	0
			2655	1695	465	490	5			
1	E	314	Total	C	N	O	S	0	0	0
			2664	1698	466	495	5			
1	G	314	Total	C	N	O	S	0	0	0
			2651	1694	465	487	5			
1	I	314	Total	C	N	O	S	0	0	0
			2648	1691	461	491	5			
1	K	314	Total	C	N	O	S	0	0	0
			2675	1705	468	497	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2703	1709	468	502	24			
2	D	346	Total	C	N	O	S	0	0	0
			2706	1713	467	502	24			
2	F	346	Total	C	N	O	S	0	0	0
			2717	1716	473	504	24			
2	H	346	Total	C	N	O	S	0	0	0
			2694	1705	464	501	24			
2	J	346	Total	C	N	O	S	0	0	0
			2708	1711	471	502	24			
2	L	346	Total	C	N	O	S	0	0	0
			2719	1718	473	504	24			

- Molecule 3 is a protein called Fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	5	Total	C	N	O	S	0	0	0
			42	29	6	6	1			
3	N	5	Total	C	N	O	S	0	0	0
			42	29	6	6	1			
3	O	5	Total	C	N	O	S	0	0	0
			42	29	6	6	1			
3	P	5	Total	C	N	O	S	0	0	0
			42	29	6	6	1			
3	Q	5	Total	C	N	O	S	0	0	0
			42	29	6	6	1			
3	R	5	Total	C	N	O	S	0	0	0
			42	29	6	6	1			

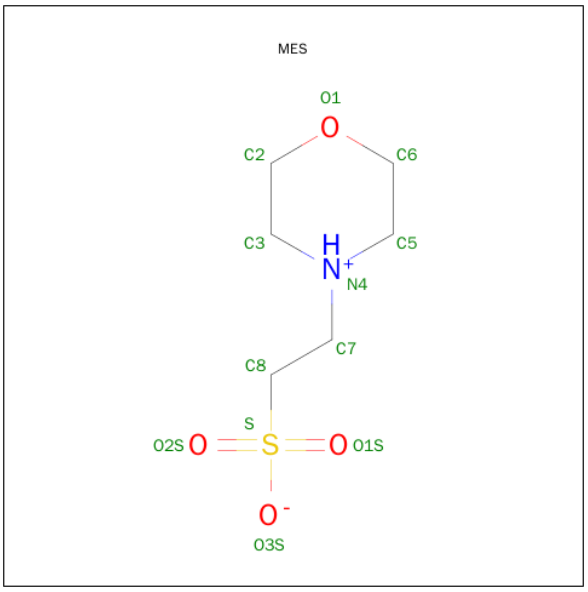
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

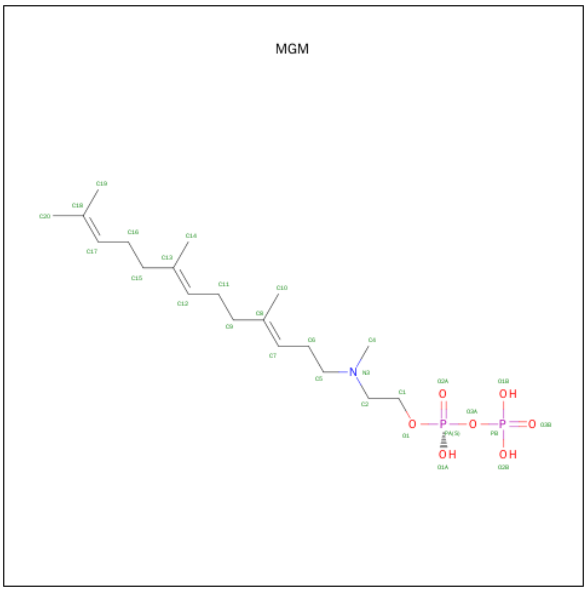
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	F	1	Total	Cl	0	0
			1	1		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 7 is 2-[METHYL-(5-GERANYL-4-METHYL-PENT-3-ENYL)-AMINO]-ETHYL-DIPHOSPHATE (three-letter code: MGM) (formula: $C_{19}H_{37}NO_7P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
7	D	1	Total	C	N	O	P	0	0
			29	19	1	7	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	F	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
7	H	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
7	J	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
7	L	1	Total	C	N	O	P	0	0
			29	19	1	7	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	56	Total	O	0	0
			56	56		
8	B	55	Total	O	0	0
			55	55		
8	C	64	Total	O	0	0
			64	64		
8	D	70	Total	O	0	0
			70	70		
8	E	60	Total	O	0	0
			60	60		
8	F	77	Total	O	0	0
			77	77		
8	G	57	Total	O	0	0
			57	57		
8	H	49	Total	O	0	0
			49	49		
8	I	62	Total	O	0	0
			62	62		
8	J	59	Total	O	0	0
			59	59		
8	K	128	Total	O	0	0
			128	128		
8	L	110	Total	O	0	0
			110	110		
8	M	9	Total	O	0	0
			9	9		
8	N	7	Total	O	0	0
			7	7		
8	O	2	Total	O	0	0
			2	2		

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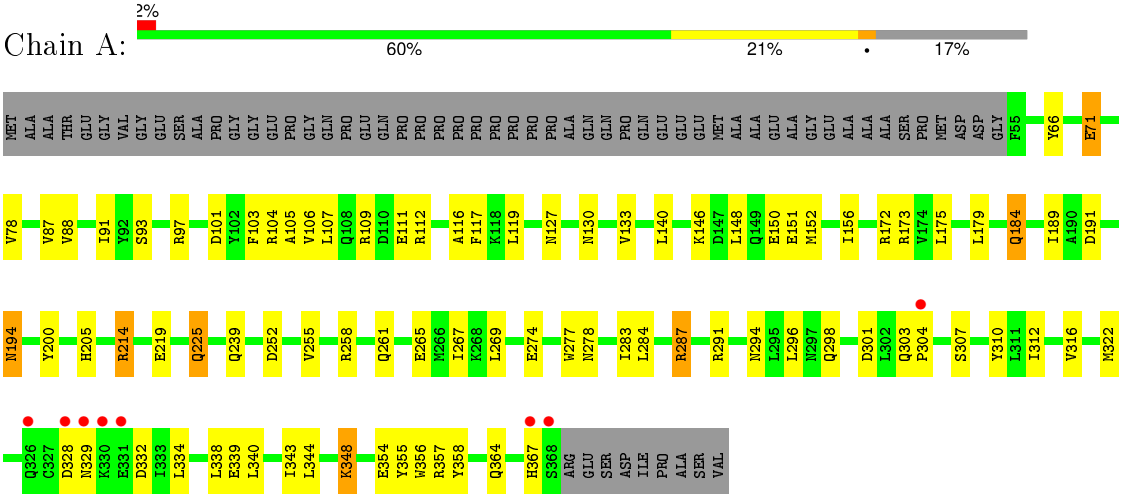
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	P	4	Total O 4 4	0	0
8	Q	6	Total O 6 6	0	0
8	R	6	Total O 6 6	0	0

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.

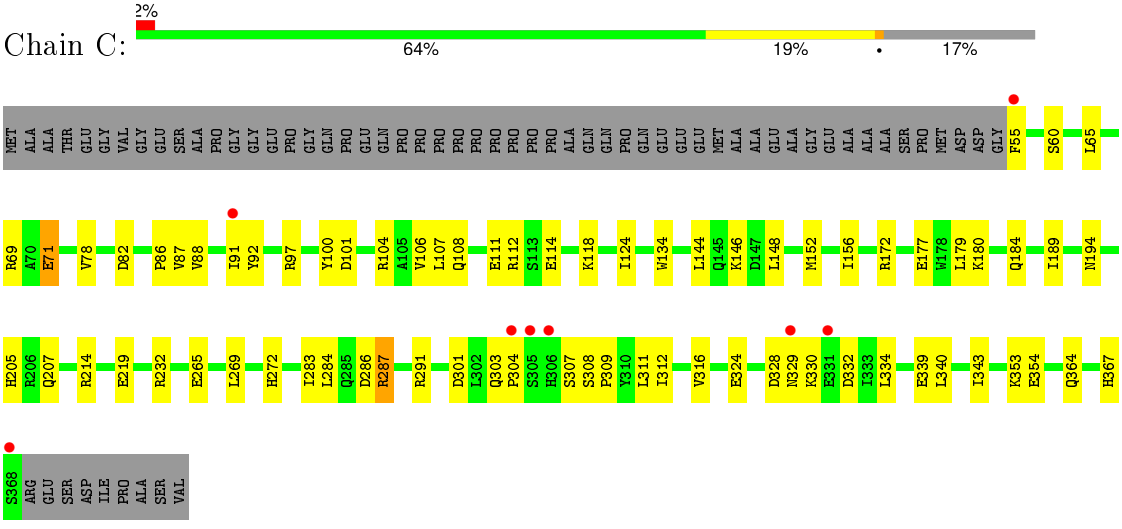
- Molecule 1: geranylgeranyltransferase type I alpha subunit

Chain A:



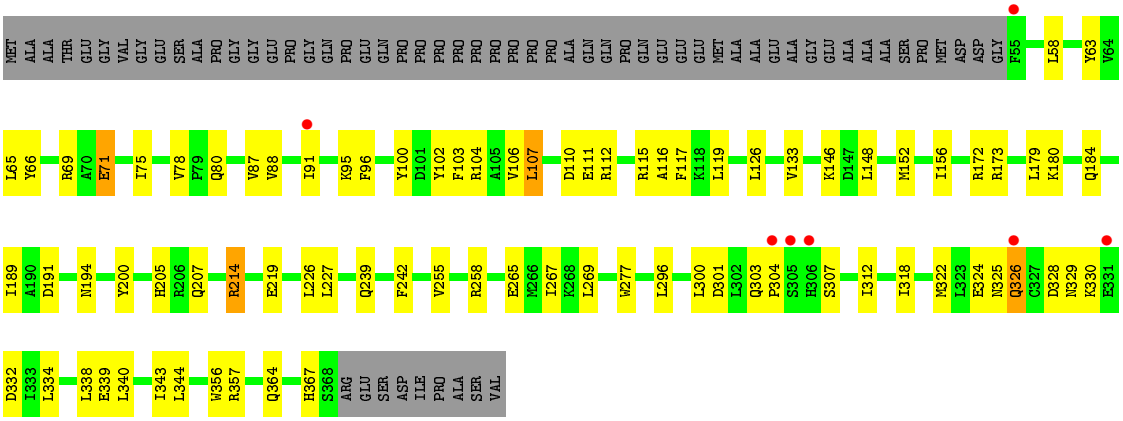
- Molecule 1: geranylgeranyltransferase type I alpha subunit

Chain C:



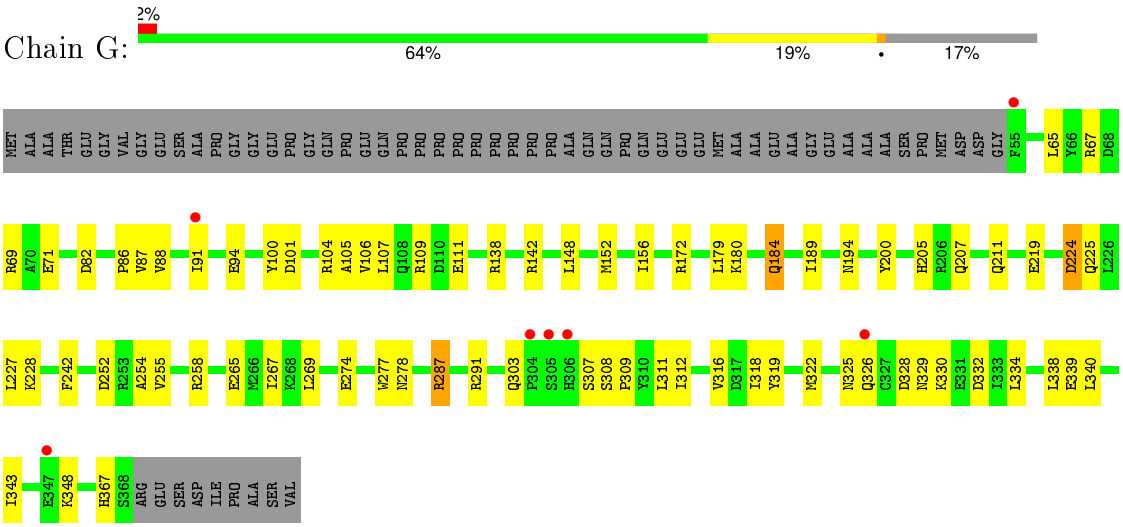
- Molecule 1: geranylgeranyltransferase type I alpha subunit

Chain E:



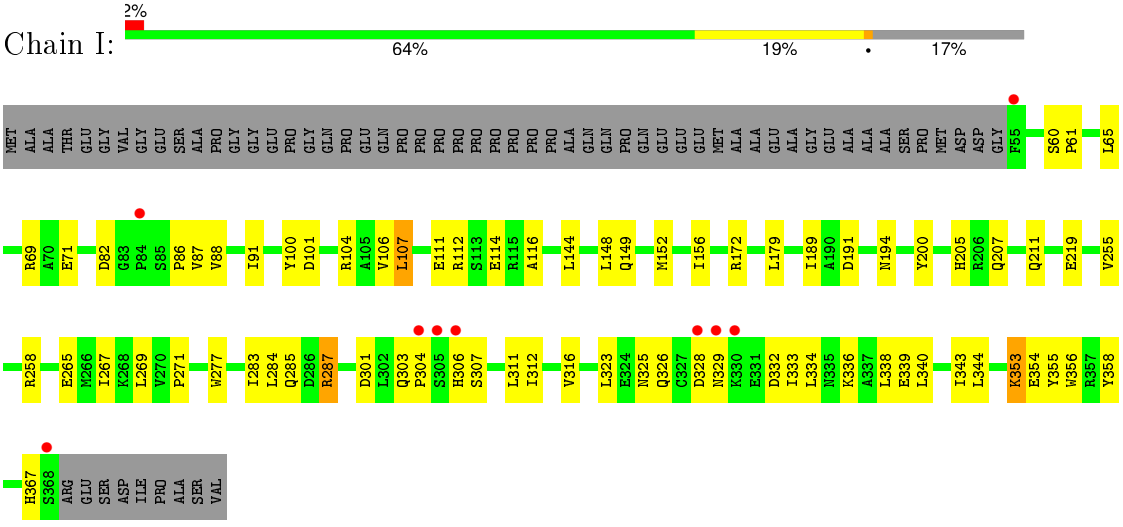
• Molecule 1: geranylgeranyltransferase type I alpha subunit

Chain G:



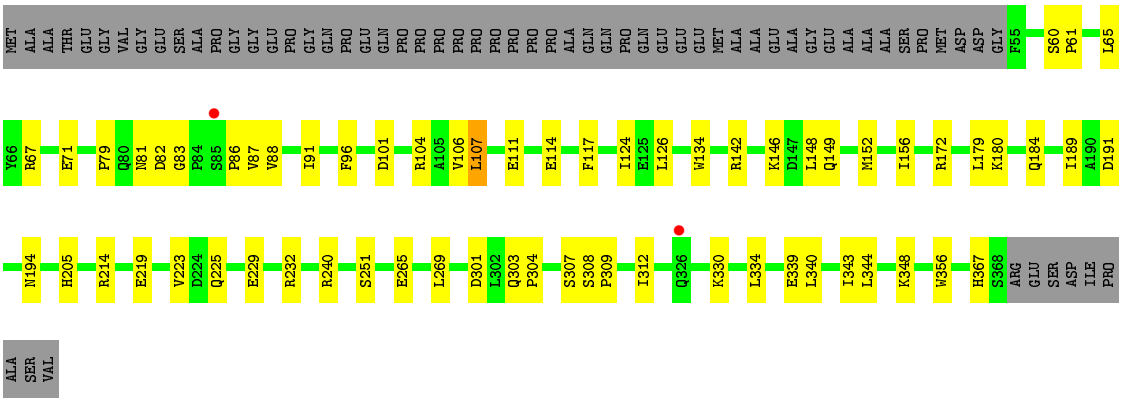
• Molecule 1: geranylgeranyltransferase type I alpha subunit

Chain I:



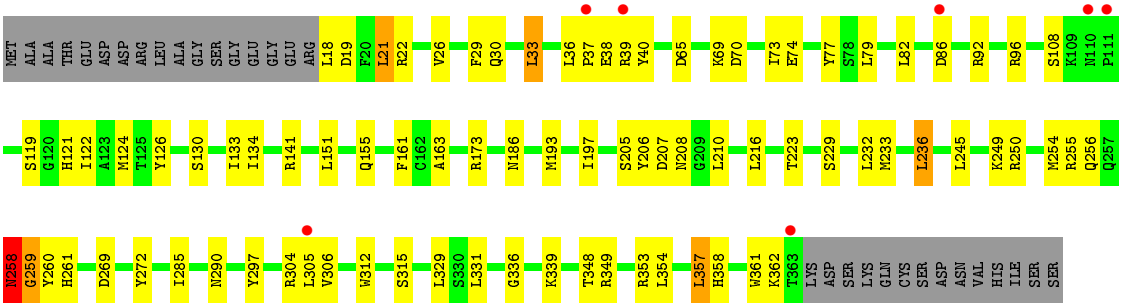
• Molecule 1: geranylgeranyltransferase type I alpha subunit

Chain K:



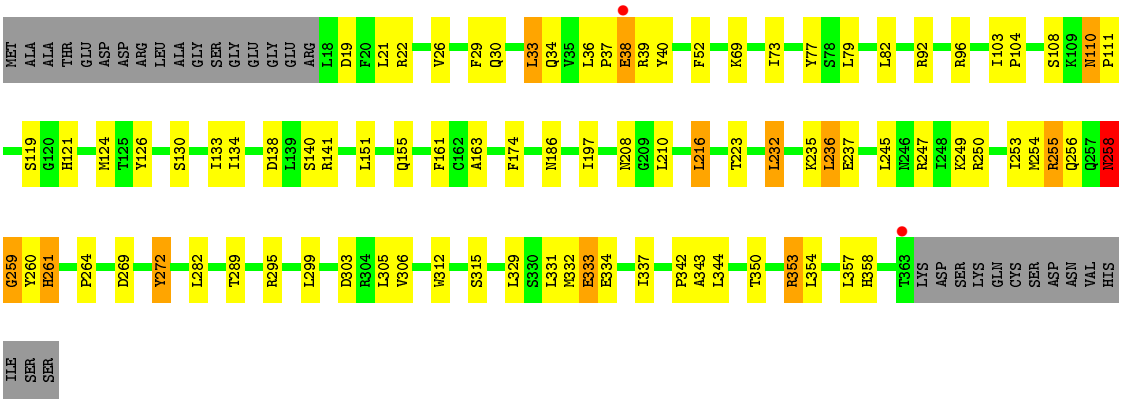
• Molecule 2: Geranylgeranyl transferase type I beta subunit

Chain B:



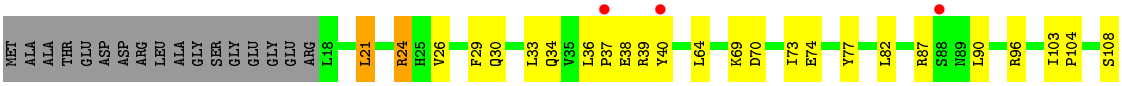
• Molecule 2: Geranylgeranyl transferase type I beta subunit

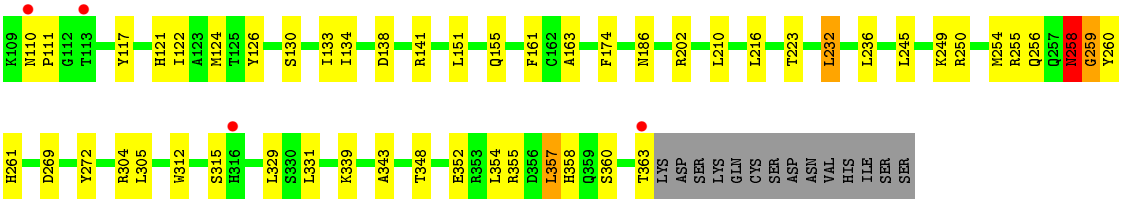
Chain D:



• Molecule 2: Geranylgeranyl transferase type I beta subunit

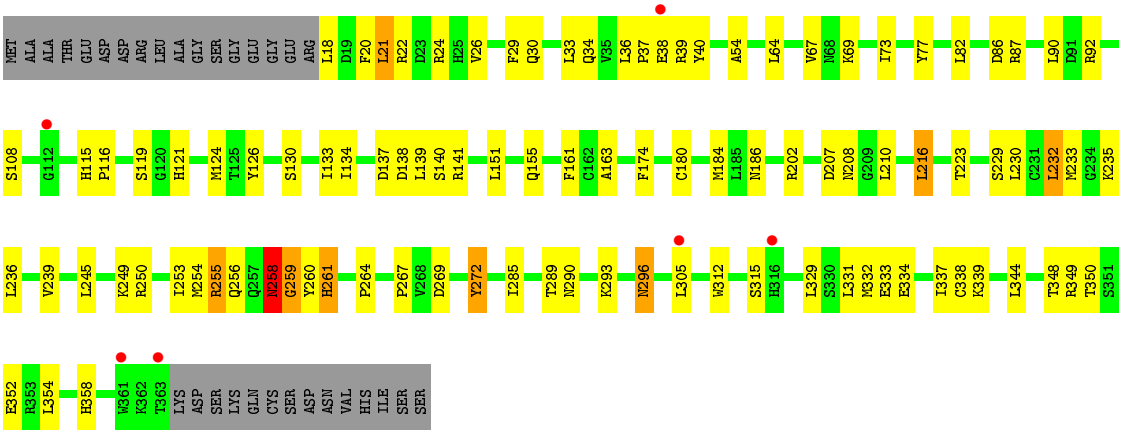
Chain F:





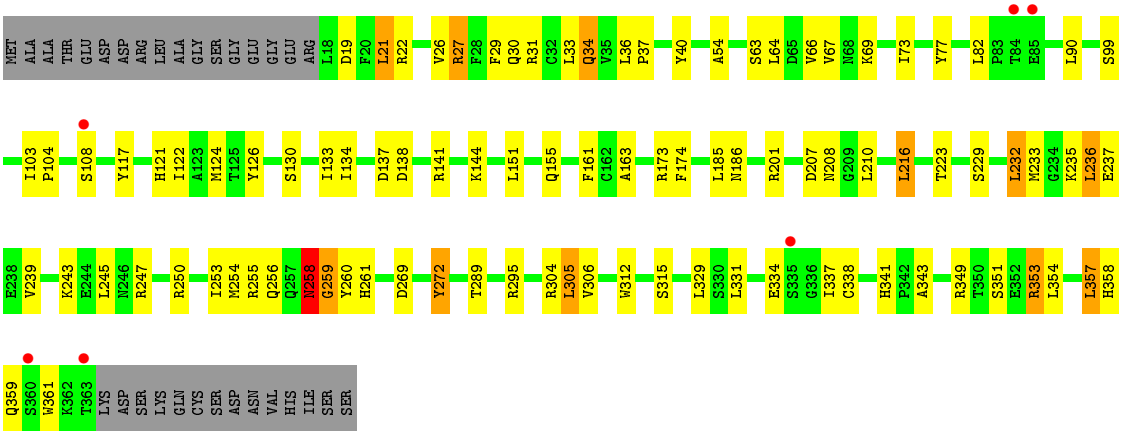
• Molecule 2: Geranylgeranyl transferase type I beta subunit

Chain H:



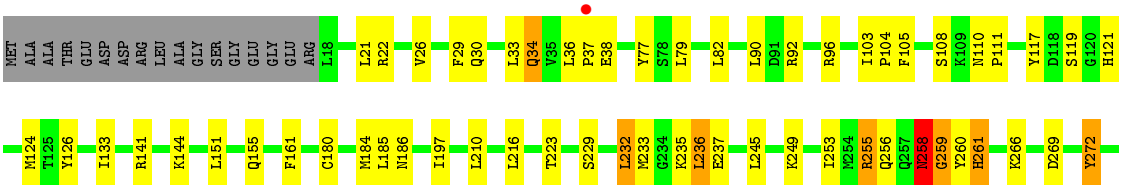
• Molecule 2: Geranylgeranyl transferase type I beta subunit

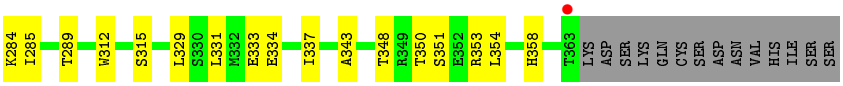
Chain J:



• Molecule 2: Geranylgeranyl transferase type I beta subunit

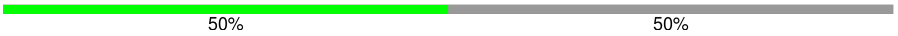
Chain L:





- Molecule 3: Fusion protein

Chain M:



- Molecule 3: Fusion protein

Chain N:

- Molecule 3: Fusion protein

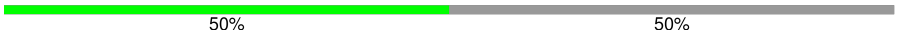
Chain O:

- Molecule 3: Fusion protein

Chain P:

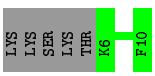
- Molecule 3: Fusion protein

Chain Q:



- Molecule 3: Fusion protein

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	271.13Å 266.72Å 185.14Å 90.00° 131.68° 90.00°	Depositor
Resolution (Å)	27.66 – 2.85 27.66 – 2.85	Depositor EDS
% Data completeness (in resolution range)	93.6 (27.66-2.85) 93.7 (27.66-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.85Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.189 , 0.210 0.188 , 0.209	Depositor DCC
R_{free} test set	10767 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 60.3	EDS
Estimated twinning fraction	0.087 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 213442 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	33504	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: ZN, MGM, 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	0.34	0/2702	0.52	0/3677
1	C	0.36	0/2721	0.54	0/3698
1	E	0.35	0/2730	0.54	0/3710
1	G	0.37	0/2717	0.54	0/3692
1	I	0.36	0/2714	0.53	0/3690
1	K	0.38	0/2741	0.55	0/3722
2	B	0.37	0/2765	0.59	2/3741 (0.1%)
2	D	0.38	0/2768	0.59	2/3743 (0.1%)
2	F	0.39	0/2779	0.60	2/3757 (0.1%)
2	H	0.36	0/2755	0.58	2/3727 (0.1%)
2	J	0.35	0/2769	0.59	2/3744 (0.1%)
2	L	0.38	0/2781	0.61	2/3759 (0.1%)
3	M	0.64	0/42	0.55	0/53
3	N	0.59	0/42	0.55	0/53
3	O	0.63	0/42	0.59	0/53
3	P	0.69	0/42	0.58	0/53
3	Q	0.71	0/42	0.60	0/53
3	R	0.71	0/42	0.64	0/53
All	All	0.37	0/33194	0.57	12/44978 (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
1	E	0	1
2	B	0	1
2	D	0	1
2	H	0	1
2	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
All	All	0	6

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	259	GLY	N-CA-C	-6.25	97.48	113.10
2	D	259	GLY	N-CA-C	-6.14	97.75	113.10
2	H	259	GLY	N-CA-C	-6.07	97.92	113.10
2	L	259	GLY	N-CA-C	-6.05	97.98	113.10
2	F	259	GLY	N-CA-C	-6.03	98.04	113.10

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	297	TYR	Sidechain
2	D	272	TYR	Sidechain
1	E	102	TYR	Sidechain
2	H	272	TYR	Sidechain
2	J	272	TYR	Sidechain

5.2 Too-close contacts (i)

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	2636	0	2526	76	0
1	C	2655	0	2562	56	0
1	E	2664	0	2570	68	0
1	G	2651	0	2563	58	0
1	I	2648	0	2547	49	0
1	K	2675	0	2594	55	0
2	B	2703	0	2606	57	0
2	D	2706	0	2616	68	0
2	F	2717	0	2635	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	2694	0	2589	75	0
2	J	2708	0	2613	69	0
2	L	2719	0	2639	52	0
3	M	42	0	45	0	0
3	N	42	0	45	0	0
3	O	42	0	45	0	0
3	P	42	0	45	0	0
3	Q	42	0	45	0	0
3	R	42	0	45	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	L	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
6	F	12	0	13	0	0
7	B	29	0	34	2	0
7	D	29	0	34	0	0
7	F	29	0	34	2	0
7	H	29	0	34	1	0
7	J	29	0	34	2	0
7	L	29	0	34	0	0
8	A	56	0	0	4	0
8	B	55	0	0	0	0
8	C	64	0	0	2	0
8	D	70	0	0	1	0
8	E	60	0	0	1	0
8	F	77	0	0	3	0
8	G	57	0	0	1	0
8	H	49	0	0	2	0
8	I	62	0	0	2	0
8	J	59	0	0	0	0
8	K	128	0	0	5	0
8	L	110	0	0	2	0
8	M	9	0	0	0	0
8	N	7	0	0	0	0
8	O	2	0	0	0	0
8	P	4	0	0	0	0
8	Q	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	R	6	0	0	0	0
All	All	33504	0	31547	698	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 11.

The worst 5 of 698 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:156:ILE:HG12	1:A:172:ARG:HH12	1.12	1.14
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.15	1.08
1:K:156:ILE:HG12	1:K:172:ARG:HH12	0.98	1.08
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.12	1.07
1:E:156:ILE:HG12	1:E:172:ARG:HH12	1.17	1.04

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	312/377 (83%)	288 (92%)	24 (8%)	0	100	100
1	C	312/377 (83%)	290 (93%)	22 (7%)	0	100	100
1	E	312/377 (83%)	289 (93%)	23 (7%)	0	100	100
1	G	312/377 (83%)	289 (93%)	23 (7%)	0	100	100
1	I	312/377 (83%)	290 (93%)	22 (7%)	0	100	100
1	K	312/377 (83%)	293 (94%)	19 (6%)	0	100	100
2	B	344/377 (91%)	326 (95%)	16 (5%)	2 (1%)	30	63
2	D	344/377 (91%)	329 (96%)	12 (4%)	3 (1%)	21	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	F	344/377 (91%)	327 (95%)	16 (5%)	1 (0%)	46 76
2	H	344/377 (91%)	326 (95%)	17 (5%)	1 (0%)	46 76
2	J	344/377 (91%)	322 (94%)	20 (6%)	2 (1%)	30 63
2	L	344/377 (91%)	328 (95%)	14 (4%)	2 (1%)	30 63
3	M	3/10 (30%)	3 (100%)	0	0	100 100
3	N	3/10 (30%)	3 (100%)	0	0	100 100
3	O	3/10 (30%)	3 (100%)	0	0	100 100
3	P	3/10 (30%)	3 (100%)	0	0	100 100
3	Q	3/10 (30%)	3 (100%)	0	0	100 100
3	R	3/10 (30%)	3 (100%)	0	0	100 100
All	All	3954/4584 (86%)	3715 (94%)	228 (6%)	11 (0%)	46 76

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	38	GLU
2	B	258	ASN
2	D	258	ASN
2	F	258	ASN
2	H	258	ASN

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	282/338 (83%)	273 (97%)	9 (3%)	46 79
1	C	286/338 (85%)	278 (97%)	8 (3%)	51 82
1	E	289/338 (86%)	281 (97%)	8 (3%)	51 82
1	G	285/338 (84%)	278 (98%)	7 (2%)	55 84
1	I	285/338 (84%)	280 (98%)	5 (2%)	66 89
1	K	292/338 (86%)	289 (99%)	3 (1%)	82 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	291/326 (89%)	276 (95%)	15 (5%)	29	60
2	D	291/326 (89%)	276 (95%)	15 (5%)	29	60
2	F	295/326 (90%)	281 (95%)	14 (5%)	32	66
2	H	288/326 (88%)	276 (96%)	12 (4%)	36	70
2	J	291/326 (89%)	273 (94%)	18 (6%)	23	51
2	L	295/326 (90%)	283 (96%)	12 (4%)	37	71
3	M	5/10 (50%)	5 (100%)	0	100	100
3	N	5/10 (50%)	5 (100%)	0	100	100
3	O	5/10 (50%)	5 (100%)	0	100	100
3	P	5/10 (50%)	5 (100%)	0	100	100
3	Q	5/10 (50%)	5 (100%)	0	100	100
3	R	5/10 (50%)	5 (100%)	0	100	100
All	All	3500/4044 (86%)	3374 (96%)	126 (4%)	42	75

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	24	ARG
1	G	184	GLN
2	L	151	LEU
2	F	151	LEU
2	F	258	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	246	ASN
1	G	278	ASN
1	K	325	ASN
1	G	81	ASN
1	G	170	HIS

5.3.3 RNA

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)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
7	MGM	B	379	-	26,28,28	1.11	2 (7%)	33,37,37	1.89	5 (15%)
7	MGM	D	380	-	26,28,28	1.03	2 (7%)	33,37,37	1.89	5 (15%)
6	MES	F	380	-	11,12,12	6.44	7 (63%)	14,16,16	3.00	5 (35%)
7	MGM	F	381	-	26,28,28	1.12	2 (7%)	33,37,37	1.94	6 (18%)
7	MGM	H	380	-	26,28,28	1.05	2 (7%)	33,37,37	1.87	5 (15%)
7	MGM	J	379	-	26,28,28	1.08	2 (7%)	33,37,37	1.91	6 (18%)
7	MGM	L	379	-	26,28,28	1.13	2 (7%)	33,37,37	1.89	6 (18%)

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
7	MGM	B	379	-	-	0/31/31/31	0/0/0/0
7	MGM	D	380	-	-	0/31/31/31	0/0/0/0
6	MES	F	380	-	-	0/6/14/14	0/1/1/1
7	MGM	F	381	-	-	0/31/31/31	0/0/0/0
7	MGM	H	380	-	-	0/31/31/31	0/0/0/0
7	MGM	J	379	-	-	0/31/31/31	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MGM	L	379	-	-	0/31/31/31	0/0/0/0

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	380	MES	C7-C8	-3.62	1.39	1.52
6	F	380	MES	C3-C2	-2.60	1.39	1.50
6	F	380	MES	C7-N4	-2.46	1.41	1.47
6	F	380	MES	C5-C6	-2.42	1.40	1.50
7	F	381	MGM	C12-C13	2.39	1.37	1.33

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	380	MES	O3S-S-O2S	-2.88	104.89	111.61
7	B	379	MGM	C10-C8-C9	-2.41	111.72	115.41
7	F	381	MGM	C10-C8-C9	-2.33	111.84	115.41
7	H	380	MGM	C10-C8-C9	-2.32	111.86	115.41
7	J	379	MGM	C10-C8-C9	-2.28	111.93	115.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	379	MGM	2	0
7	F	381	MGM	2	0
7	H	380	MGM	1	0
7	J	379	MGM	2	0

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, 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	314/377 (83%)	-0.21	8 (2%)	61	56	31, 53, 86, 100	0
1	C	314/377 (83%)	-0.29	8 (2%)	61	56	28, 49, 77, 98	0
1	E	314/377 (83%)	-0.25	7 (2%)	65	61	28, 51, 77, 95	0
1	G	314/377 (83%)	-0.27	7 (2%)	65	61	29, 49, 76, 98	0
1	I	314/377 (83%)	-0.24	9 (2%)	55	49	27, 52, 82, 96	0
1	K	314/377 (83%)	-0.49	2 (0%)	90	89	21, 37, 63, 75	0
2	B	346/377 (91%)	-0.31	7 (2%)	68	64	30, 45, 67, 91	0
2	D	346/377 (91%)	-0.39	2 (0%)	90	89	26, 39, 62, 76	0
2	F	346/377 (91%)	-0.39	7 (2%)	68	64	24, 38, 64, 85	0
2	H	346/377 (91%)	-0.22	6 (1%)	73	70	30, 50, 74, 96	0
2	J	346/377 (91%)	-0.27	6 (1%)	73	70	28, 48, 74, 94	0
2	L	346/377 (91%)	-0.45	2 (0%)	90	89	21, 34, 54, 77	0
3	M	5/10 (50%)	-0.76	0	100	100	35, 35, 43, 53	0
3	N	5/10 (50%)	-0.82	0	100	100	35, 39, 41, 53	0
3	O	5/10 (50%)	-0.77	0	100	100	34, 35, 41, 52	0
3	P	5/10 (50%)	-0.71	0	100	100	41, 41, 47, 59	0
3	Q	5/10 (50%)	-0.83	0	100	100	38, 39, 42, 54	0
3	R	5/10 (50%)	-1.02	0	100	100	33, 34, 39, 51	0
All	All	3990/4584 (87%)	-0.32	71 (1%)	71	68	21, 45, 73, 100	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	55	PHE	5.3
1	C	55	PHE	4.2
1	C	306	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	I	305	SER	3.9
2	J	108	SER	3.8

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^{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
6	MES	F	380	12/12	0.92	0.29	1.76	72,77,79,79	0
7	MGM	L	379	29/29	0.96	0.17	0.45	18,29,42,44	0
7	MGM	B	379	29/29	0.96	0.19	0.43	33,40,53,54	0
7	MGM	D	380	29/29	0.95	0.17	0.32	29,35,47,47	0
7	MGM	F	381	29/29	0.96	0.16	0.26	27,39,47,47	0
7	MGM	H	380	29/29	0.96	0.17	0.01	30,38,53,54	0
7	MGM	J	379	29/29	0.96	0.16	0.00	24,34,43,44	0
5	CL	D	379	1/1	0.98	0.10	-0.93	37,37,37,37	0
5	CL	F	379	1/1	0.99	0.08	-1.10	35,35,35,35	0
4	ZN	L	378	1/1	1.00	0.07	-1.82	29,29,29,29	0
5	CL	H	379	1/1	0.97	0.08	-1.85	47,47,47,47	0
4	ZN	B	378	1/1	1.00	0.06	-2.09	33,33,33,33	0
4	ZN	F	378	1/1	1.00	0.05	-2.19	32,32,32,32	0
4	ZN	D	378	1/1	0.99	0.07	-2.36	31,31,31,31	0
4	ZN	H	378	1/1	1.00	0.07	-2.63	43,43,43,43	0
4	ZN	J	378	1/1	1.00	0.06	-2.79	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.