Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:03 PM GMT

PDB ID	:	1N4P
Title	:	Protein Geranylgeranyltransferase type-I Complexed with Geranylgeranyl Diphosphate
Authors	:	Taylor, J.S.; Reid, T.S.; Casey, P.J.; Beese, L.S.
Deposited on	:	2002-11-01
Resolution	:	2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

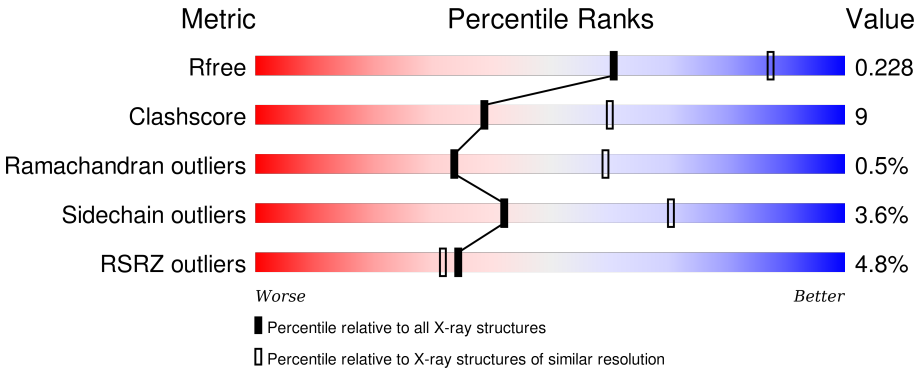
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	4% 67% 15% • 17%
1	C	377	3% 66% 17% • 17%
1	E	377	4% 64% 17% • 17%
1	G	377	3% 63% 20% • 17%
1	I	377	4% 64% 18% • 17%

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Mol	Chain	Length	Quality of chain
1	K	377	2% 69% 14% • 17%
2	B	377	5% 72% 19% • 8%
2	D	377	5% 72% 17% • 8%
2	F	377	5% 76% 15% • 8%
2	H	377	9% 69% 21% • 8%
2	J	377	5% 69% 21% • 8%
2	L	377	3% 73% 16% • 8%
3	M	11	27% 9% 27% 64%
3	N	11	18% 9% 27% 64%

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
5	CL	C	1705	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33443 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 protein farnesyltransferase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2629	1679	463	482	5			
1	C	314	Total	C	N	O	S	0	0	0
			2643	1689	461	488	5			
1	E	314	Total	C	N	O	S	0	0	0
			2642	1686	461	490	5			
1	G	314	Total	C	N	O	S	0	0	0
			2633	1683	459	486	5			
1	I	314	Total	C	N	O	S	0	0	0
			2656	1694	465	492	5			
1	K	314	Total	C	N	O	S	0	0	0
			2671	1703	467	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
			2697	1707	467	499	24			
2	D	346	Total	C	N	O	S	0	0	0
			2713	1715	472	502	24			
2	F	346	Total	C	N	O	S	0	0	0
			2718	1717	474	503	24			
2	H	346	Total	C	N	O	S	0	0	0
			2694	1706	464	500	24			
2	J	346	Total	C	N	O	S	0	0	0
			2711	1713	471	503	24			
2	L	346	Total	C	N	O	S	0	0	0
			2723	1720	473	506	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	4	Total	C	N	O	S	0	0	0
			30	20	4	5	1			
3	N	4	Total	C	N	O	S	0	0	0
			30	20	4	5	1			

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

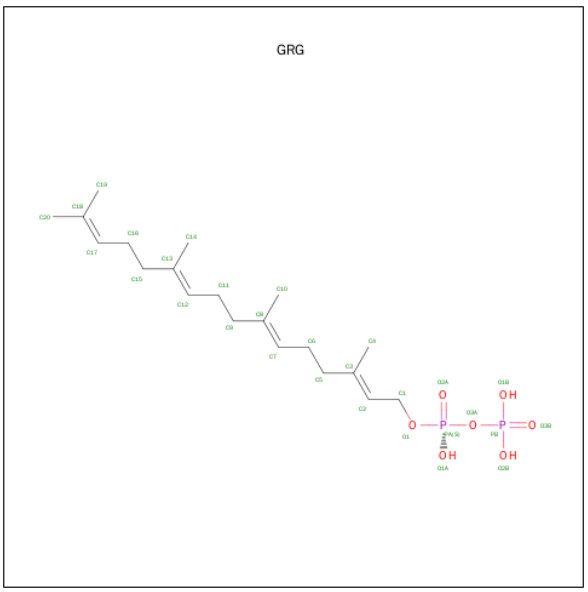
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

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

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

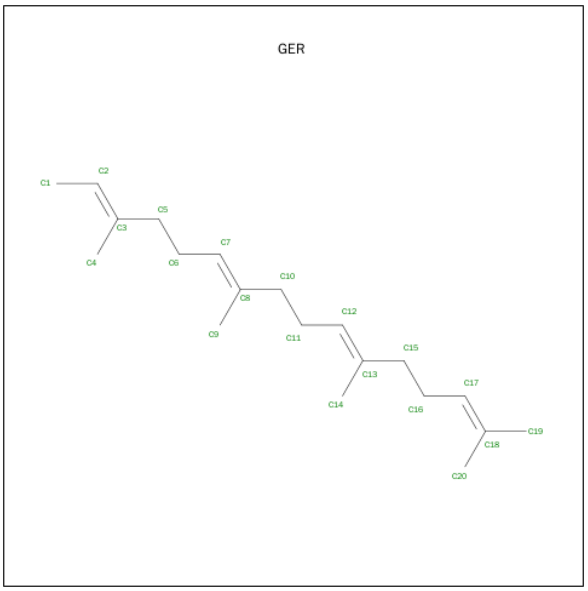
- Molecule 6 is GERANYLGERANYL DIPHOSPHATE (three-letter code: GRG) (formula:

$C_{20}H_{36}O_7P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	P	0	0
			29	20	7	2		
6	D	1	Total	C	O	P	0	0
			29	20	7	2		
6	F	1	Total	C	O	P	0	0
			29	20	7	2		
6	H	1	Total	C	O	P	0	0
			29	20	7	2		
6	J	1	Total	C	O	P	0	0
			29	20	7	2		
6	L	1	Total	C	O	P	0	0
			29	20	7	2		

- Molecule 7 is GERAN-8-YL GERAN (three-letter code: GER) (formula: $C_{20}H_{34}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total C 20 20	0	0
7	N	1	Total C 20 20	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	71	Total O 71 71	0	0
8	B	63	Total O 63 63	0	0
8	C	80	Total O 80 80	0	0
8	D	94	Total O 94 94	0	0
8	E	64	Total O 64 64	0	0
8	F	92	Total O 92 92	0	0
8	G	58	Total O 58 58	0	0
8	H	48	Total O 48 48	0	0
8	I	87	Total O 87 87	0	0
8	J	73	Total O 73 73	0	0

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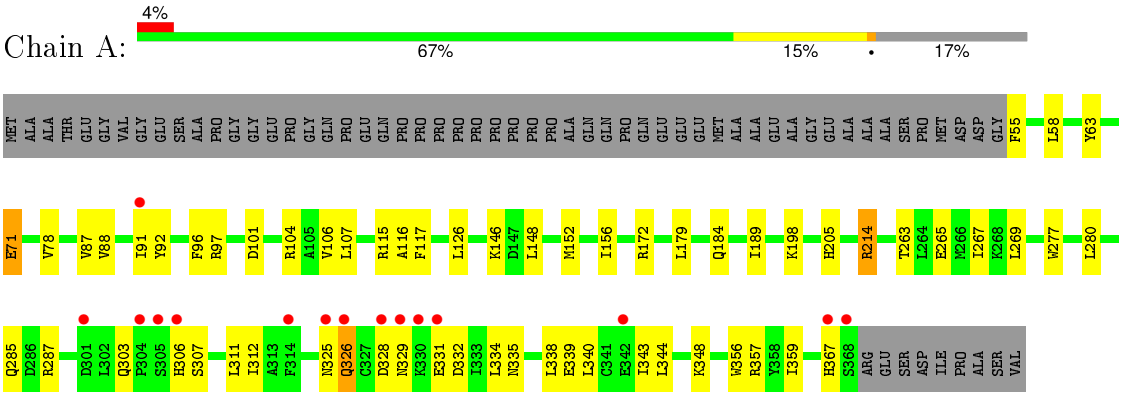
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	K	159	Total O 159 159	0	0
8	L	134	Total O 134 134	0	0
8	N	1	Total O 1 1	0	0

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.

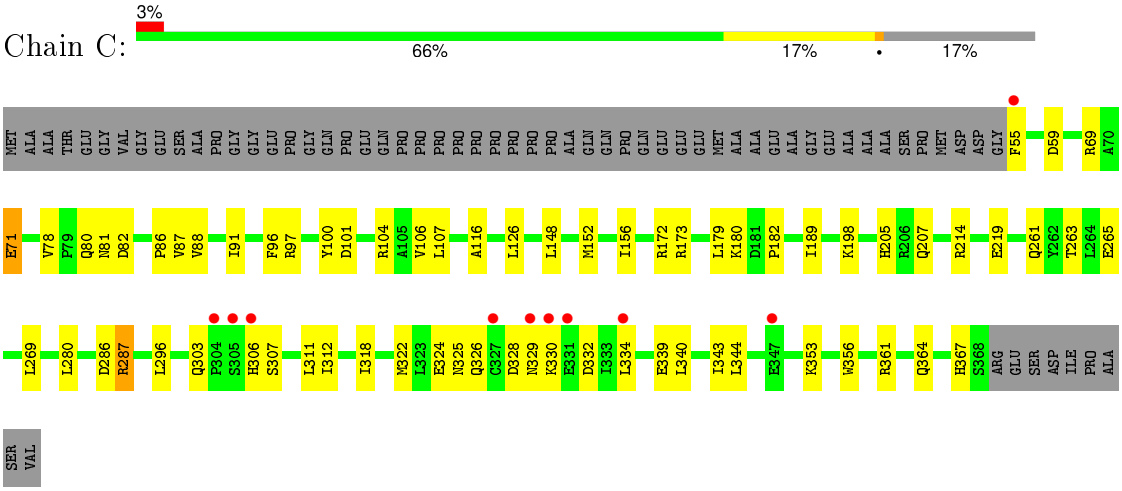
- Molecule 1: protein farnesyltransferase alpha subunit

Chain A:



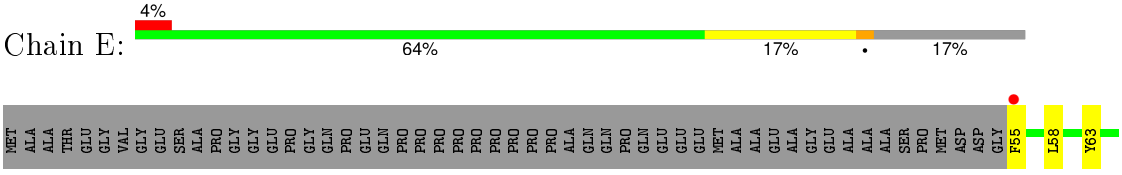
- Molecule 1: protein farnesyltransferase alpha subunit

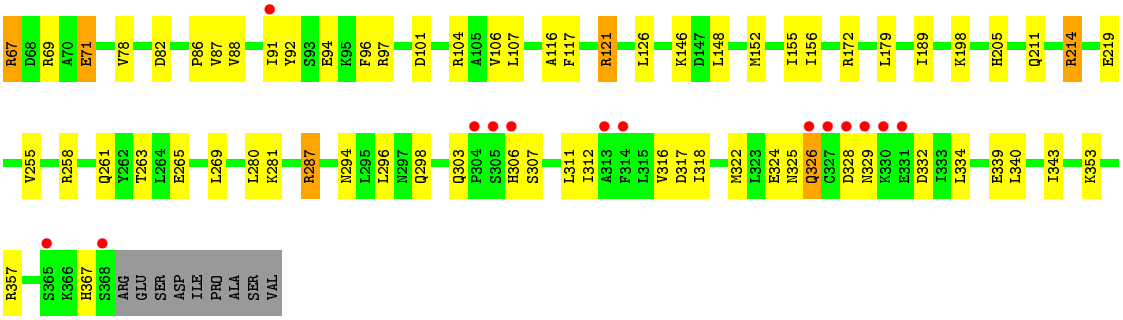
Chain C:



- Molecule 1: protein farnesyltransferase alpha subunit

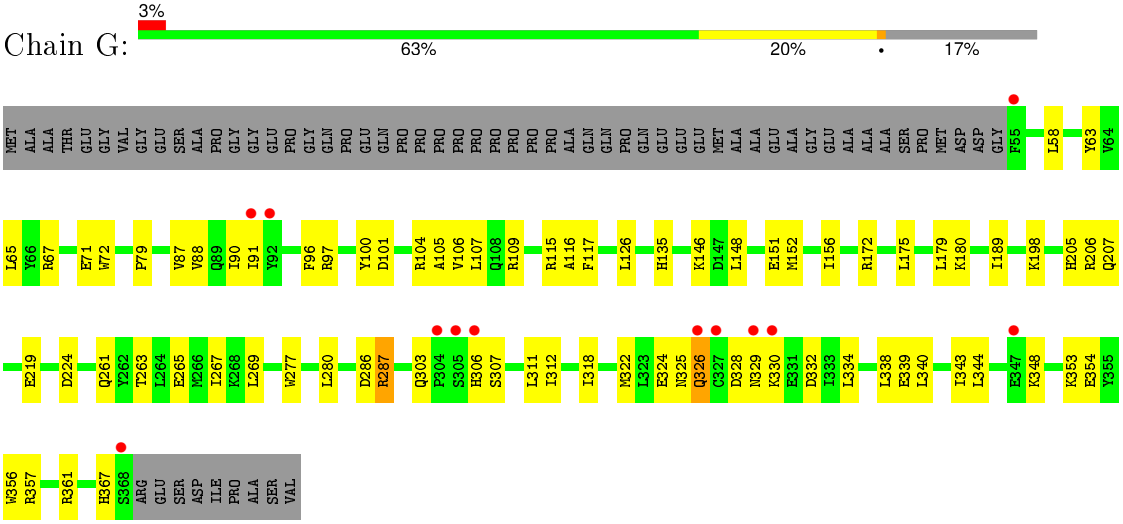
Chain E:





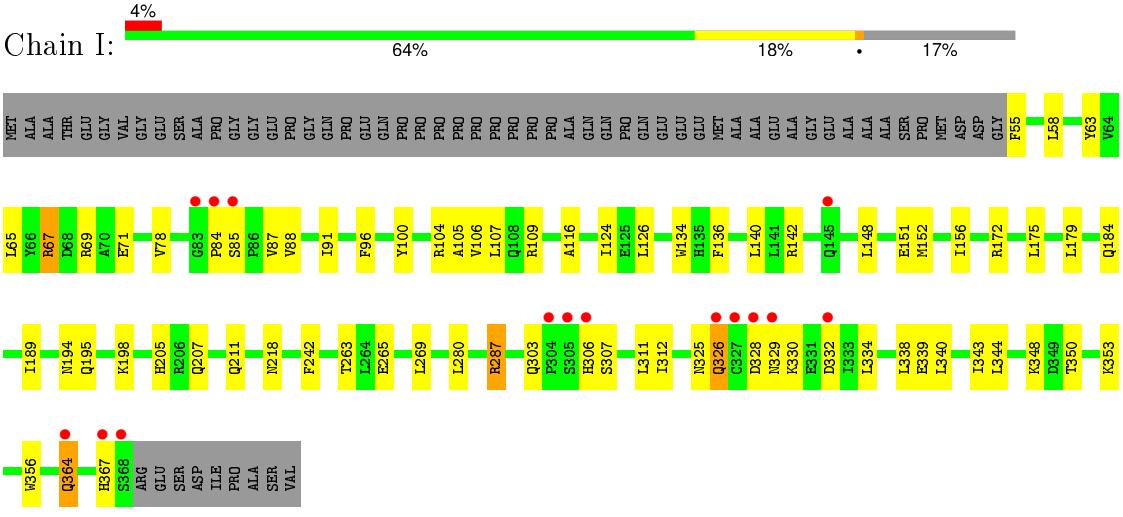
• Molecule 1: protein farnesyltransferase alpha subunit

Chain G:



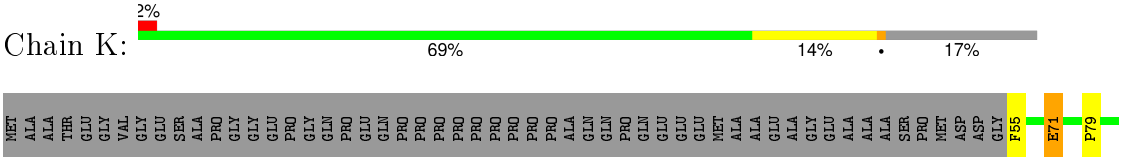
• Molecule 1: protein farnesyltransferase alpha subunit

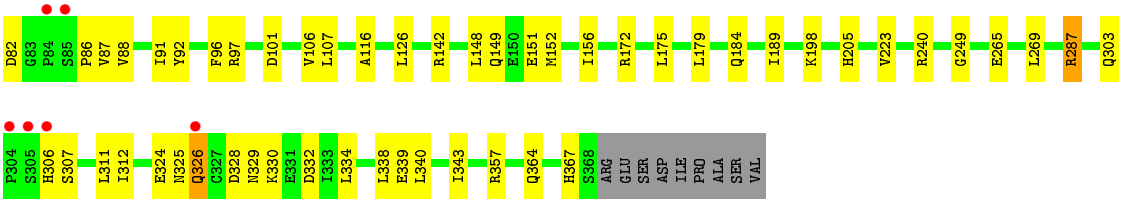
Chain I:



• Molecule 1: protein farnesyltransferase alpha subunit

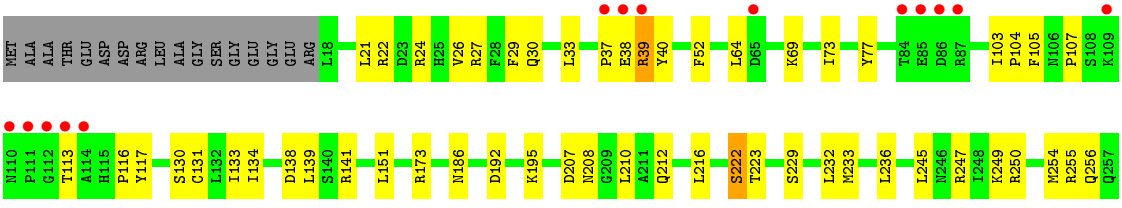
Chain K:

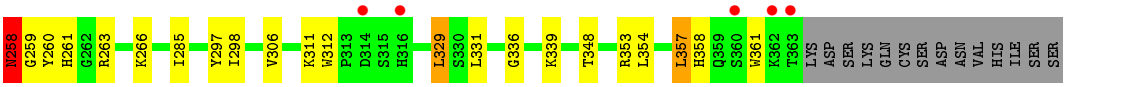




• Molecule 2: geranyltransferase type-I beta subunit

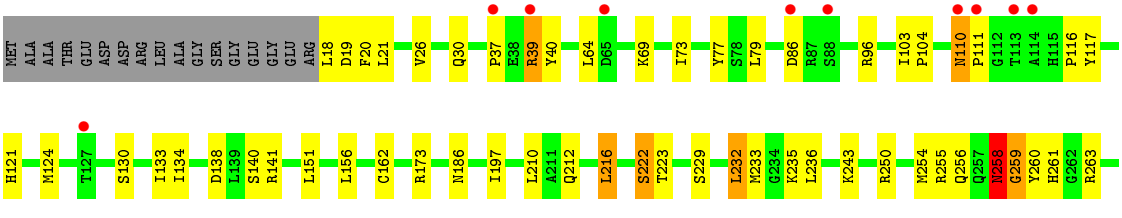
Chain B:

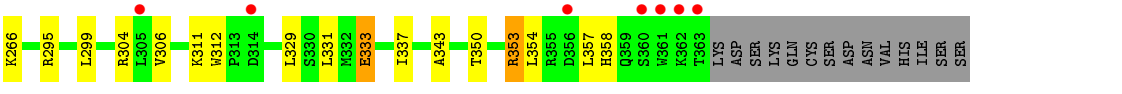




• Molecule 2: geranyltransferase type-I beta subunit

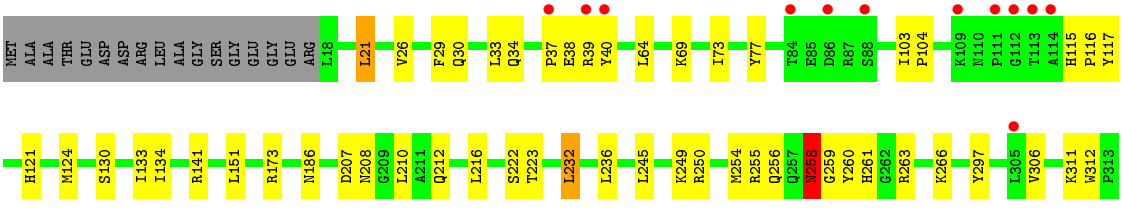
Chain D:

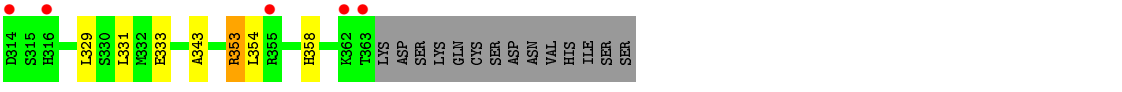




• Molecule 2: geranyltransferase type-I beta subunit

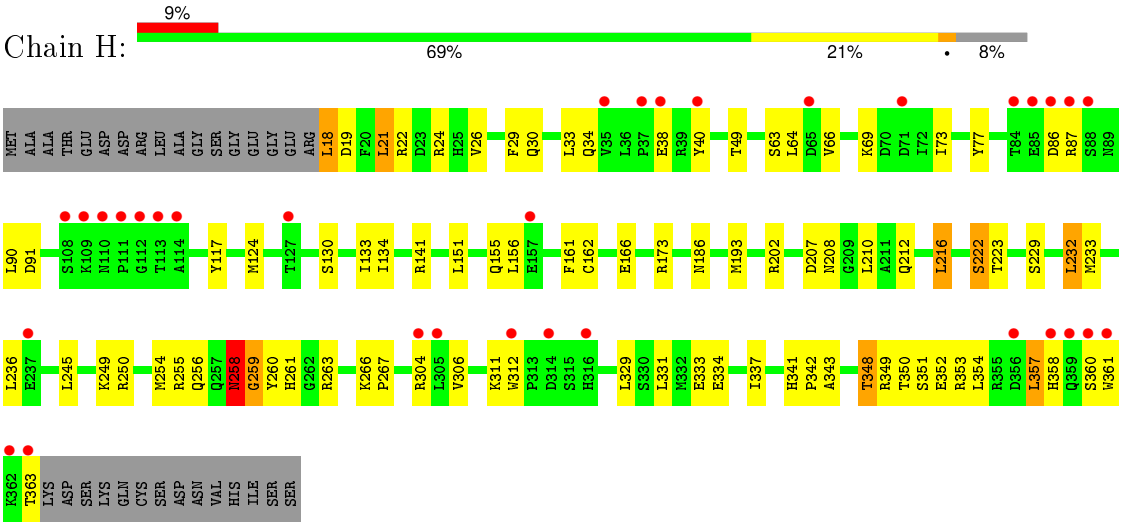
Chain F:





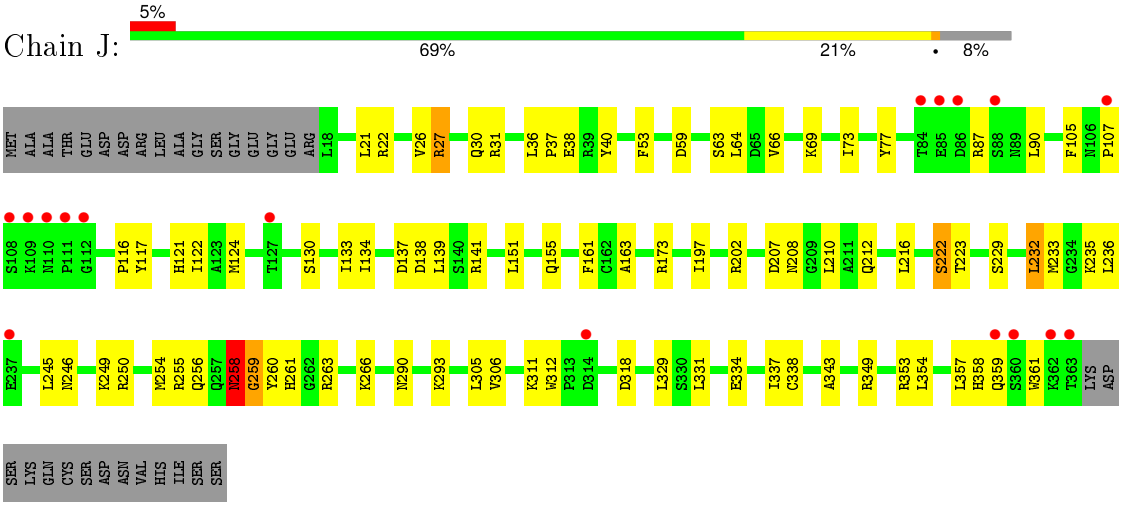
• Molecule 2: geranyltransferase type-I beta subunit

Chain H:



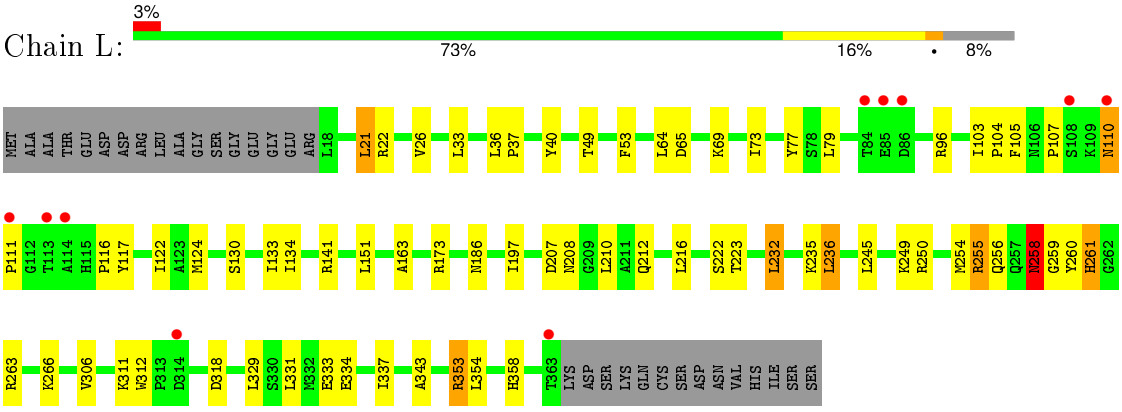
• Molecule 2: geranyltransferase type-I beta subunit

Chain J:



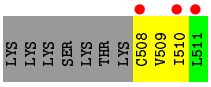
• Molecule 2: geranyltransferase type-I beta subunit

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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	272.34Å 271.57Å 185.43Å 90.00° 131.56° 90.00°	Depositor
Resolution (Å)	29.92 – 2.65 29.92 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.92-2.65) 98.7 (29.92-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.64Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.204 , 0.228 0.205 , 0.228	Depositor DCC
R_{free} test set	14292 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.7	EDS
Estimated twinning fraction	0.080 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 286743 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	33443	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: GRG, ZN, CL, GER

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	0/2695	0.52	0/3668
1	C	0.36	0/2709	0.53	0/3684
1	E	0.35	0/2708	0.53	0/3684
1	G	0.35	0/2699	0.53	0/3672
1	I	0.36	0/2722	0.53	0/3700
1	K	0.40	0/2737	0.55	0/3717
2	B	0.36	0/2759	0.60	2/3733 (0.1%)
2	D	0.37	0/2775	0.59	2/3752 (0.1%)
2	F	0.38	0/2780	0.60	2/3758 (0.1%)
2	H	0.35	0/2756	0.58	2/3729 (0.1%)
2	J	0.36	0/2773	0.59	2/3750 (0.1%)
2	L	0.40	0/2785	0.61	2/3764 (0.1%)
3	M	0.67	0/29	0.82	0/37
3	N	0.66	0/29	0.81	0/37
All	All	0.37	0/32956	0.56	12/44685 (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.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	259	GLY	N-CA-C	-6.01	98.07	113.10
2	F	259	GLY	N-CA-C	-5.96	98.20	113.10
2	D	259	GLY	N-CA-C	-5.84	98.49	113.10
2	J	259	GLY	N-CA-C	-5.83	98.51	113.10
2	L	259	GLY	N-CA-C	-5.77	98.68	113.10
2	B	259	GLY	N-CA-C	-5.76	98.70	113.10
2	L	258	ASN	N-CA-C	-5.46	96.25	111.00
2	J	258	ASN	N-CA-C	-5.42	96.36	111.00
2	B	258	ASN	N-CA-C	-5.32	96.63	111.00
2	D	258	ASN	N-CA-C	-5.31	96.67	111.00
2	H	258	ASN	N-CA-C	-5.29	96.72	111.00
2	F	258	ASN	N-CA-C	-5.25	96.84	111.00

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 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	2629	0	2520	48	0
1	C	2643	0	2540	44	0
1	E	2642	0	2534	57	0
1	G	2633	0	2524	55	0
1	I	2656	0	2560	44	0
1	K	2671	0	2588	39	0
2	B	2697	0	2600	50	0
2	D	2713	0	2628	52	0
2	F	2718	0	2635	37	0
2	H	2694	0	2590	67	0
2	J	2711	0	2616	51	0
2	L	2723	0	2643	45	0
3	M	30	0	34	3	0
3	N	30	0	34	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	1	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	1	0
5	L	1	0	0	0	0
6	B	29	0	33	1	0
6	D	29	0	33	1	0
6	F	29	0	33	2	0
6	H	29	0	33	1	0
6	J	29	0	33	1	0
6	L	29	0	33	1	0
7	M	20	0	33	5	0
7	N	20	0	33	5	0
8	A	71	0	0	1	0
8	B	63	0	0	0	0
8	C	80	0	0	3	0
8	D	94	0	0	1	0
8	E	64	0	0	0	0
8	F	92	0	0	2	0
8	G	58	0	0	2	0
8	H	48	0	0	2	0
8	I	87	0	0	4	0
8	J	73	0	0	2	0
8	K	159	0	0	4	0
8	L	134	0	0	2	0
8	N	1	0	0	0	0
All	All	33443	0	31310	573	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 9.

All (573) 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:I:156:ILE:HG12	1:I:172:ARG:HH12	1.10	1.15
1:E:156:ILE:HG12	1:E:172:ARG:HH12	1.09	1.11
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.03	1.08
1:K:156:ILE:HG12	1:K:172:ARG:HH12	0.99	1.08
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.17	1.04
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.17	1.04
2:F:212:GLN:HE21	2:F:222:SER:HB3	1.21	1.01
2:J:212:GLN:HE21	2:J:222:SER:HB3	1.29	0.96
1:K:156:ILE:HG12	1:K:172:ARG:NH1	1.81	0.95
2:H:21:LEU:HD21	2:H:304:ARG:HG2	1.47	0.95
2:F:212:GLN:NE2	2:F:222:SER:HB3	1.86	0.90
1:A:156:ILE:HG12	1:A:172:ARG:NH1	1.86	0.90
1:E:353:LYS:HE2	1:E:357:ARG:HH12	1.38	0.87
5:G:1711:CL:CL	8:G:383:HOH:O	2.31	0.86
2:H:18:LEU:HA	2:H:304:ARG:NH2	1.91	0.85
2:D:173:ARG:HG2	6:D:1722:GRG:H112	1.59	0.84
2:D:212:GLN:HE21	2:D:222:SER:HB3	1.41	0.84
2:L:173:ARG:HG2	6:L:1726:GRG:H112	1.59	0.83
1:E:255:VAL:HG13	1:E:258:ARG:HH21	1.42	0.83
1:G:152:MET:O	1:G:156:ILE:HG13	1.79	0.83
2:B:212:GLN:HE21	2:B:222:SER:HB3	1.44	0.83
2:D:39:ARG:H	2:D:39:ARG:HD2	1.42	0.82
2:D:212:GLN:NE2	2:D:222:SER:HB3	1.95	0.82
2:B:212:GLN:NE2	2:B:222:SER:HB3	1.95	0.82
2:H:348:THR:O	2:H:352:GLU:HG2	1.80	0.81
2:J:173:ARG:HG2	6:J:1725:GRG:H112	1.60	0.81
2:D:37:PRO:HB2	2:D:39:ARG:CD	2.11	0.81
1:A:152:MET:O	1:A:156:ILE:HG13	1.80	0.81
2:B:173:ARG:HG2	6:B:1721:GRG:H112	1.63	0.80
2:F:173:ARG:HG2	6:F:1723:GRG:H112	1.62	0.80
1:I:152:MET:O	1:I:156:ILE:HG13	1.82	0.79
1:E:152:MET:O	1:E:156:ILE:HG13	1.81	0.79
1:E:318:ILE:HG22	1:E:322:MET:HE3	1.65	0.79
1:K:330:LYS:HE2	1:K:367:HIS:HB3	1.66	0.77
2:D:37:PRO:HB2	2:D:39:ARG:HD2	1.67	0.77
2:H:173:ARG:HG2	6:H:1724:GRG:H112	1.67	0.76
2:H:186:ASN:HB2	2:H:358:HIS:CE1	2.20	0.76
1:C:152:MET:O	1:C:156:ILE:HG13	1.83	0.76
1:K:152:MET:O	1:K:156:ILE:HG13	1.85	0.76
1:E:156:ILE:HG12	1:E:172:ARG:NH1	1.94	0.75
1:E:255:VAL:HG13	1:E:258:ARG:NH2	2.01	0.75
2:H:212:GLN:NE2	2:H:222:SER:HB3	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:609:VAL:HG23	3:N:610:ILE:HG23	1.71	0.73
1:I:156:ILE:HG12	1:I:172:ARG:NH1	1.95	0.73
2:J:212:GLN:NE2	2:J:222:SER:HB3	2.02	0.73
1:G:97:ARG:HG2	1:G:101:ASP:OD2	1.89	0.72
1:K:156:ILE:CG1	1:K:172:ARG:HH12	1.90	0.72
2:H:229:SER:O	2:H:233:MET:HG3	1.90	0.71
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.56	0.71
1:E:156:ILE:CG1	1:E:172:ARG:HH12	1.98	0.71
3:M:509:VAL:HG23	3:M:510:ILE:HG23	1.71	0.71
5:K:1717:CL:CL	8:K:391:HOH:O	2.43	0.71
2:F:133:ILE:HD13	2:F:354:LEU:HD13	1.72	0.70
1:C:318:ILE:HG22	1:C:322:MET:HE3	1.73	0.70
2:L:212:GLN:HE21	2:L:222:SER:HB3	1.56	0.70
1:E:189:ILE:HD11	1:E:205:HIS:HD2	1.57	0.69
1:A:214:ARG:HG2	1:G:180:LYS:HB2	1.73	0.69
1:G:189:ILE:HD11	1:G:205:HIS:HD2	1.57	0.69
1:C:189:ILE:HD11	1:C:205:HIS:HD2	1.58	0.69
2:B:133:ILE:HD13	2:B:354:LEU:HD13	1.75	0.68
2:D:69:LYS:O	2:D:73:ILE:HG13	1.93	0.68
1:G:312:ILE:HG23	1:G:340:LEU:HD22	1.76	0.68
2:B:69:LYS:O	2:B:73:ILE:HG13	1.93	0.67
2:L:133:ILE:HD13	2:L:354:LEU:HD13	1.75	0.67
1:C:87:VAL:HG12	1:C:88:VAL:HG23	1.75	0.67
2:H:19:ASP:HB2	8:H:1494:HOH:O	1.96	0.66
2:D:37:PRO:HB2	2:D:39:ARG:HD3	1.77	0.66
1:K:91:ILE:O	1:K:91:ILE:HD12	1.95	0.66
1:K:189:ILE:HD11	1:K:205:HIS:HD2	1.60	0.65
2:H:212:GLN:HE21	2:H:222:SER:HB3	1.61	0.65
2:H:69:LYS:O	2:H:73:ILE:HG13	1.97	0.65
2:H:18:LEU:N	2:H:18:LEU:HD22	2.11	0.65
1:I:91:ILE:HD12	1:I:91:ILE:O	1.96	0.65
2:B:245:LEU:O	2:B:249:LYS:HG3	1.97	0.64
2:J:263:ARG:HG3	2:J:266:LYS:HG3	1.78	0.64
1:G:91:ILE:HD12	1:G:91:ILE:O	1.97	0.64
2:B:186:ASN:HB2	2:B:358:HIS:CE1	2.32	0.64
2:H:334:GLU:HB3	2:H:337:ILE:HD12	1.79	0.63
1:E:312:ILE:HG23	1:E:340:LEU:HD22	1.80	0.63
1:K:87:VAL:HG12	1:K:88:VAL:HG23	1.80	0.63
1:I:156:ILE:CG1	1:I:172:ARG:HH12	2.00	0.63
1:E:91:ILE:O	1:E:91:ILE:HD12	1.98	0.63
1:G:87:VAL:HG12	1:G:88:VAL:HG23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:GLN:O	1:G:265:GLU:HG2	1.99	0.63
2:B:353:ARG:HH11	2:B:353:ARG:HG2	1.62	0.63
1:I:189:ILE:HD11	1:I:205:HIS:HD2	1.62	0.63
1:I:87:VAL:HG12	1:I:88:VAL:HG23	1.80	0.63
2:D:263:ARG:HG3	2:D:266:LYS:HG3	1.80	0.62
2:H:21:LEU:CD2	2:H:304:ARG:HG2	2.25	0.62
2:D:295:ARG:CZ	2:D:299:LEU:HD11	2.29	0.62
2:F:69:LYS:O	2:F:73:ILE:HG13	1.99	0.62
1:A:91:ILE:O	1:A:91:ILE:HD12	2.00	0.62
2:H:263:ARG:HG3	2:H:266:LYS:HG3	1.81	0.62
2:B:39:ARG:HB3	2:B:39:ARG:HH11	1.65	0.62
1:E:353:LYS:CE	1:E:357:ARG:HH12	2.10	0.61
2:F:37:PRO:HD2	2:F:40:TYR:CD1	2.34	0.61
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.82	0.61
2:F:26:VAL:O	2:F:30:GLN:HG3	1.99	0.61
1:G:334:LEU:HD22	1:G:367:HIS:O	2.00	0.61
2:F:263:ARG:HG3	2:F:266:LYS:HG3	1.81	0.61
2:J:133:ILE:HD13	2:J:354:LEU:HD13	1.82	0.61
2:H:87:ARG:HH12	2:H:90:LEU:HD11	1.65	0.61
1:K:312:ILE:HG23	1:K:340:LEU:HD22	1.83	0.61
2:L:197:ILE:HD11	2:L:235:LYS:HD3	1.83	0.61
1:G:101:ASP:HA	1:G:104:ARG:NH1	2.15	0.60
1:G:100:TYR:O	1:G:104:ARG:HG3	2.01	0.60
1:G:198:LYS:HD3	2:H:266:LYS:HD3	1.81	0.60
1:C:91:ILE:O	1:C:91:ILE:HD12	2.01	0.60
1:C:330:LYS:HE2	1:C:367:HIS:HB3	1.83	0.60
2:B:263:ARG:HG3	2:B:266:LYS:HG3	1.82	0.60
1:A:78:VAL:O	1:A:104:ARG:HD2	2.01	0.60
1:G:357:ARG:O	1:G:361:ARG:HG3	2.01	0.60
2:H:232:LEU:HD13	2:H:343:ALA:HB1	1.84	0.60
1:I:156:ILE:HD11	1:I:172:ARG:HH22	1.67	0.59
2:H:21:LEU:HD23	2:H:24:ARG:HE	1.67	0.59
1:A:339:GLU:O	1:A:343:ILE:HG13	2.02	0.59
1:K:156:ILE:HD11	1:K:172:ARG:HH22	1.68	0.59
2:D:39:ARG:H	2:D:39:ARG:CD	2.14	0.59
2:H:193:MET:HE2	2:H:233:MET:HB3	1.85	0.59
2:B:26:VAL:O	2:B:30:GLN:HG3	2.01	0.59
1:A:97:ARG:HG2	1:A:101:ASP:OD2	2.02	0.59
1:K:107:LEU:HD22	2:L:117:TYR:CD2	2.37	0.59
1:C:303:GLN:O	1:C:307:SER:HB2	2.03	0.58
1:I:207:GLN:HG2	1:I:242:PHE:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:22:ARG:O	2:J:26:VAL:HG23	2.03	0.58
2:H:210:LEU:HB2	2:H:223:THR:HA	1.85	0.58
1:C:198:LYS:HD3	2:D:266:LYS:HD3	1.85	0.58
1:C:180:LYS:HB2	1:E:214:ARG:HG2	1.85	0.58
2:L:232:LEU:HD13	2:L:343:ALA:HB1	1.85	0.58
2:J:210:LEU:HB2	2:J:223:THR:HA	1.84	0.58
1:E:78:VAL:O	1:E:104:ARG:HD2	2.03	0.57
2:L:353:ARG:HD3	2:L:353:ARG:O	2.04	0.57
2:L:210:LEU:HB2	2:L:223:THR:HA	1.86	0.57
2:H:245:LEU:O	2:H:249:LYS:HG3	2.04	0.57
2:J:318:ASP:HB2	7:M:1727:GER:H71	1.87	0.57
1:G:334:LEU:O	1:G:338:LEU:HG	2.04	0.57
1:C:148:LEU:HB2	1:C:179:LEU:HD21	1.87	0.57
1:A:328:ASP:O	1:A:329:ASN:HB2	2.05	0.57
1:I:330:LYS:HE2	1:I:367:HIS:HB3	1.87	0.57
1:A:87:VAL:HG12	1:A:88:VAL:HG23	1.87	0.56
1:G:101:ASP:HA	1:G:104:ARG:HH11	1.69	0.56
1:A:214:ARG:O	1:A:214:ARG:HG3	2.05	0.56
2:H:22:ARG:HG2	2:H:22:ARG:HH11	1.70	0.56
2:D:210:LEU:HB2	2:D:223:THR:HA	1.86	0.56
2:J:338:CYS:SG	2:J:349:ARG:NH2	2.78	0.56
1:K:265:GLU:O	1:K:269:LEU:HD13	2.06	0.56
2:D:37:PRO:HB3	2:D:39:ARG:HH11	1.70	0.56
1:I:107:LEU:HD22	2:J:117:TYR:CD2	2.40	0.56
1:I:312:ILE:HG23	1:I:340:LEU:HD22	1.87	0.56
1:I:329:ASN:HB3	1:I:332:ASP:HB3	1.88	0.56
1:E:82:ASP:HB2	1:E:86:PRO:HB3	1.88	0.56
1:G:156:ILE:HG12	1:G:172:ARG:NH1	2.03	0.56
1:I:148:LEU:HB2	1:I:179:LEU:HD21	1.88	0.56
2:J:232:LEU:HD13	2:J:343:ALA:HB1	1.86	0.56
2:L:263:ARG:HG3	2:L:266:LYS:HG3	1.86	0.56
1:A:265:GLU:O	1:A:269:LEU:HD13	2.06	0.56
1:E:265:GLU:O	1:E:269:LEU:HD13	2.06	0.56
1:E:87:VAL:HG12	1:E:88:VAL:HG23	1.88	0.55
2:F:37:PRO:HD2	2:F:40:TYR:CE1	2.41	0.55
2:D:18:LEU:HD12	2:D:304:ARG:NH1	2.21	0.55
2:H:353:ARG:O	2:H:357:LEU:HB2	2.05	0.55
2:B:210:LEU:HB2	2:B:223:THR:HA	1.87	0.55
2:J:290:ASN:ND2	2:J:293:LYS:HD2	2.22	0.55
1:G:189:ILE:HD11	1:G:205:HIS:CD2	2.41	0.55
1:E:148:LEU:HB2	1:E:179:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:ILE:HD13	2:H:40:TYR:O	2.07	0.55
1:C:78:VAL:HB	1:C:104:ARG:HB3	1.89	0.55
1:G:148:LEU:HB2	1:G:179:LEU:HD21	1.87	0.55
2:H:64:LEU:HD11	2:H:134:ILE:HG22	1.88	0.55
1:C:334:LEU:HD22	1:C:367:HIS:O	2.07	0.55
2:F:210:LEU:HB2	2:F:223:THR:HA	1.88	0.55
2:B:336:GLY:HA2	2:J:305:LEU:HD13	1.89	0.55
1:E:261:GLN:O	1:E:265:GLU:HG2	2.06	0.55
1:C:82:ASP:HB2	1:C:86:PRO:HB3	1.89	0.55
1:C:261:GLN:O	1:C:265:GLU:HG2	2.07	0.55
1:E:353:LYS:HE2	1:E:357:ARG:NH1	2.17	0.55
2:D:133:ILE:HD13	2:D:354:LEU:HD13	1.89	0.55
1:K:97:ARG:HG2	1:K:101:ASP:OD2	2.07	0.55
1:E:121:ARG:NH1	1:E:121:ARG:HG3	2.21	0.55
2:F:186:ASN:HB2	2:F:358:HIS:NE2	2.22	0.54
1:E:353:LYS:HE3	1:E:357:ARG:HH22	1.73	0.54
1:A:357:ARG:HH11	1:A:357:ARG:HG3	1.72	0.54
2:L:212:GLN:NE2	2:L:222:SER:HB3	2.21	0.54
2:H:349:ARG:O	2:H:352:GLU:HB2	2.07	0.54
2:H:348:THR:HA	2:H:351:SER:OG	2.07	0.54
1:A:334:LEU:HD22	1:A:367:HIS:O	2.07	0.54
1:K:334:LEU:HD22	1:K:367:HIS:O	2.07	0.54
1:E:339:GLU:O	1:E:343:ILE:HG13	2.08	0.54
2:F:232:LEU:HD13	2:F:343:ALA:HB1	1.89	0.54
1:I:198:LYS:HD3	2:J:266:LYS:HD3	1.89	0.54
1:A:303:GLN:O	1:A:307:SER:HB2	2.08	0.54
2:B:250:ARG:O	2:B:254:MET:HG2	2.07	0.54
1:G:91:ILE:HD12	2:H:38:GLU:HB2	1.89	0.54
1:I:195:GLN:NE2	8:I:1500:HOH:O	2.41	0.53
2:J:197:ILE:HD11	2:J:235:LYS:HD3	1.91	0.53
2:D:212:GLN:HE21	2:D:222:SER:CB	2.18	0.53
1:K:198:LYS:HD3	2:L:266:LYS:HD3	1.90	0.53
1:I:344:LEU:HD13	1:I:356:TRP:CE2	2.44	0.53
1:E:294:ASN:O	1:E:298:GLN:HG3	2.08	0.53
1:C:339:GLU:O	1:C:343:ILE:HG13	2.09	0.53
2:H:186:ASN:HB2	2:H:358:HIS:NE2	2.24	0.53
2:L:318:ASP:HB2	7:N:1727:GER:H71	1.90	0.53
1:I:334:LEU:HD22	1:I:367:HIS:O	2.09	0.53
2:H:258:ASN:OD1	2:H:259:GLY:N	2.38	0.53
1:K:311:LEU:HD23	1:K:311:LEU:O	2.09	0.53
1:G:328:ASP:O	1:G:329:ASN:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:609:VAL:N	7:N:1727:GER:H11	2.23	0.52
1:C:328:ASP:O	1:C:329:ASN:HB2	2.09	0.52
1:I:339:GLU:O	1:I:343:ILE:HG13	2.08	0.52
2:J:202:ARG:HD2	8:J:384:HOH:O	2.09	0.52
2:B:339:LYS:O	2:B:348:THR:HG23	2.10	0.52
2:B:24:ARG:HD3	2:B:27:ARG:HH22	1.74	0.52
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.92	0.52
2:B:353:ARG:HG2	2:B:353:ARG:NH1	2.22	0.52
2:H:130:SER:O	2:H:134:ILE:HG13	2.10	0.52
2:B:229:SER:O	2:B:233:MET:HG3	2.09	0.52
1:G:303:GLN:O	1:G:307:SER:HB2	2.10	0.52
1:I:67:ARG:HD2	8:I:927:HOH:O	2.09	0.52
1:G:79:PRO:HA	1:G:101:ASP:OD1	2.11	0.51
1:K:338:LEU:HD11	1:K:364:GLN:HG2	1.92	0.51
2:J:87:ARG:HH12	2:J:90:LEU:HD11	1.75	0.51
1:K:148:LEU:HB2	1:K:179:LEU:HD21	1.92	0.51
1:E:198:LYS:HD3	2:F:266:LYS:HD3	1.92	0.51
1:C:78:VAL:O	1:C:104:ARG:HD2	2.11	0.51
1:I:265:GLU:O	1:I:269:LEU:HD13	2.10	0.51
1:A:189:ILE:HD11	1:A:205:HIS:CD2	2.41	0.51
1:I:328:ASP:O	1:I:329:ASN:HB2	2.10	0.51
1:K:311:LEU:HD23	1:K:311:LEU:C	2.30	0.51
2:H:267:PRO:HG2	8:H:1609:HOH:O	2.10	0.51
3:M:509:VAL:N	7:M:1727:GER:H11	2.25	0.51
2:J:105:PHE:CE2	2:J:107:PRO:HD3	2.46	0.51
2:J:77:TYR:CE1	2:J:141:ARG:HB2	2.45	0.51
1:I:106:VAL:HG11	1:I:116:ALA:HB1	1.93	0.51
1:G:343:ILE:HG22	1:G:348:LYS:HG3	1.93	0.51
2:L:334:GLU:HB3	2:L:337:ILE:HD12	1.93	0.51
1:E:318:ILE:HG22	1:E:322:MET:CE	2.38	0.51
2:J:63:SER:O	2:J:66:VAL:HG22	2.11	0.51
1:K:303:GLN:O	1:K:307:SER:HB2	2.11	0.51
2:F:250:ARG:O	2:F:254:MET:HG2	2.11	0.51
1:G:344:LEU:HD13	1:G:356:TRP:CE2	2.45	0.51
1:I:151:GLU:HG3	1:I:175:LEU:HD11	1.93	0.51
2:B:77:TYR:CZ	2:B:141:ARG:HB2	2.46	0.50
1:A:58:LEU:HD23	1:A:63:TYR:CZ	2.46	0.50
1:I:311:LEU:C	1:I:311:LEU:HD23	2.32	0.50
1:E:214:ARG:O	1:E:214:ARG:HG3	2.12	0.50
1:I:78:VAL:O	1:I:104:ARG:HD2	2.11	0.50
1:K:96:PHE:CE1	1:K:126:LEU:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:329:ASN:HB3	1:G:332:ASP:HB3	1.94	0.50
2:L:212:GLN:HE21	2:L:212:GLN:HA	1.76	0.50
2:D:232:LEU:HD13	2:D:343:ALA:HB1	1.92	0.50
1:C:69:ARG:HB3	1:C:71:GLU:OE1	2.12	0.50
1:E:92:TYR:O	1:E:97:ARG:NH2	2.45	0.50
1:G:311:LEU:HD23	1:G:311:LEU:C	2.32	0.50
2:F:207:ASP:O	2:F:208:ASN:HB2	2.11	0.49
2:D:333:GLU:HA	8:D:740:HOH:O	2.11	0.49
2:D:333:GLU:O	1:K:357:ARG:NH2	2.45	0.49
2:B:130:SER:O	2:B:134:ILE:HG13	2.11	0.49
2:F:256:GLN:HB2	2:F:260:TYR:CE2	2.47	0.49
2:J:27:ARG:HH12	2:J:30:GLN:NE2	2.09	0.49
2:H:202:ARG:HG3	2:H:202:ARG:HH11	1.77	0.49
2:F:130:SER:O	2:F:134:ILE:HG13	2.12	0.49
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.95	0.49
1:A:214:ARG:CG	1:A:214:ARG:O	2.59	0.49
2:F:38:GLU:O	2:F:38:GLU:HG2	2.13	0.49
1:C:100:TYR:HB3	1:C:104:ARG:HH21	1.78	0.49
2:J:334:GLU:HB3	2:J:337:ILE:HD12	1.93	0.49
2:B:29:PHE:O	2:B:33:LEU:HD22	2.12	0.49
2:D:250:ARG:O	2:D:254:MET:HG2	2.13	0.49
1:G:135:HIS:CD2	2:H:166:GLU:HG2	2.48	0.49
2:L:333:GLU:HA	8:L:1050:HOH:O	2.13	0.49
2:B:207:ASP:O	2:B:208:ASN:HB2	2.13	0.49
1:K:189:ILE:HD11	1:K:205:HIS:CD2	2.45	0.49
2:B:22:ARG:HH11	2:B:22:ARG:HG2	1.77	0.49
2:D:186:ASN:HB2	2:D:358:HIS:CE1	2.48	0.49
1:G:65:LEU:HD12	1:G:67:ARG:HH11	1.77	0.49
1:C:106:VAL:HG11	1:C:116:ALA:HB1	1.94	0.49
2:L:256:GLN:HB2	2:L:260:TYR:CE2	2.48	0.49
1:I:100:TYR:O	1:I:104:ARG:HG3	2.12	0.48
2:B:105:PHE:CE2	2:B:107:PRO:HD3	2.47	0.48
1:G:97:ARG:HH11	1:G:97:ARG:HB3	1.78	0.48
1:A:325:ASN:O	1:A:326:GLN:C	2.52	0.48
1:E:67:ARG:NH2	1:E:94:GLU:OE1	2.43	0.48
1:G:339:GLU:O	1:G:343:ILE:HG13	2.13	0.48
1:I:84:PRO:HG2	1:I:85:SER:H	1.79	0.48
1:E:303:GLN:O	1:E:307:SER:HB2	2.14	0.48
2:F:212:GLN:HE21	2:F:222:SER:CB	2.08	0.48
2:H:256:GLN:HB2	2:H:260:TYR:CE2	2.49	0.48
1:A:156:ILE:HD11	1:A:172:ARG:HH22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:22:ARG:O	2:H:26:VAL:HG23	2.14	0.48
1:I:303:GLN:O	1:I:307:SER:HB2	2.14	0.48
1:C:265:GLU:O	1:C:269:LEU:HD13	2.13	0.48
1:I:338:LEU:HD11	1:I:364:GLN:HG2	1.96	0.48
2:J:358:HIS:O	2:J:361:TRP:HB2	2.14	0.48
2:B:38:GLU:HG2	2:B:38:GLU:O	2.14	0.48
1:E:69:ARG:HB3	1:E:71:GLU:OE1	2.14	0.48
1:A:117:PHE:CE2	1:A:146:LYS:HE2	2.49	0.48
2:H:193:MET:HE2	2:H:233:MET:CG	2.44	0.48
1:E:121:ARG:HH11	1:E:121:ARG:HG3	1.78	0.48
1:E:296:LEU:HD22	1:E:322:MET:CE	2.44	0.47
1:G:219:GLU:OE1	1:G:219:GLU:HA	2.14	0.47
2:D:79:LEU:O	2:D:96:ARG:HG3	2.14	0.47
2:J:130:SER:O	2:J:134:ILE:HG13	2.14	0.47
1:A:184:GLN:HB2	8:A:379:HOH:O	2.14	0.47
2:L:105:PHE:CE2	2:L:107:PRO:HD3	2.49	0.47
2:L:110:ASN:HB3	2:L:111:PRO:HD2	1.96	0.47
1:C:311:LEU:HD23	1:C:311:LEU:C	2.34	0.47
2:D:197:ILE:HD11	2:D:235:LYS:HD3	1.95	0.47
1:I:189:ILE:HD11	1:I:205:HIS:CD2	2.47	0.47
2:J:229:SER:O	2:J:233:MET:HG3	2.14	0.47
1:E:96:PHE:CE1	1:E:126:LEU:HB3	2.49	0.47
1:I:184:GLN:HB2	8:I:378:HOH:O	2.15	0.47
1:G:265:GLU:O	1:G:269:LEU:HD13	2.14	0.47
2:B:256:GLN:HB2	2:B:260:TYR:CE2	2.50	0.47
1:C:173:ARG:NH1	8:C:412:HOH:O	2.46	0.47
1:E:106:VAL:HG11	1:E:116:ALA:HB1	1.96	0.47
1:E:58:LEU:HD23	1:E:63:TYR:CE2	2.50	0.47
2:J:258:ASN:OD1	2:J:259:GLY:N	2.42	0.47
2:H:311:LYS:HG3	2:H:312:TRP:CD2	2.49	0.47
1:G:117:PHE:CE2	1:G:146:LYS:HE2	2.49	0.47
2:J:69:LYS:O	2:J:73:ILE:HG13	2.13	0.47
1:K:249:GLY:HA3	8:K:640:HOH:O	2.14	0.47
1:C:312:ILE:HG23	1:C:340:LEU:HD22	1.97	0.47
1:G:156:ILE:HD11	1:G:172:ARG:HH22	1.80	0.47
2:F:311:LYS:HG3	2:F:312:TRP:CD2	2.50	0.47
2:D:37:PRO:CB	2:D:39:ARG:HH11	2.27	0.47
1:E:312:ILE:O	1:E:316:VAL:HG23	2.15	0.46
1:E:156:ILE:HD11	1:E:172:ARG:HH22	1.79	0.46
1:C:214:ARG:HG2	1:C:214:ARG:O	2.14	0.46
2:H:250:ARG:O	2:H:254:MET:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:130:SER:O	2:D:134:ILE:HG13	2.15	0.46
2:B:212:GLN:HE21	2:B:222:SER:CB	2.20	0.46
2:L:53:PHE:HE1	7:N:1727:GER:H42	1.80	0.46
2:H:30:GLN:OE1	2:H:66:VAL:HB	2.16	0.46
1:I:65:LEU:O	1:I:69:ARG:HG3	2.15	0.46
1:E:334:LEU:HD22	1:E:367:HIS:O	2.15	0.46
1:C:96:PHE:CE1	1:C:126:LEU:HB3	2.50	0.46
2:B:22:ARG:O	2:B:26:VAL:HG23	2.16	0.46
2:H:29:PHE:O	2:H:33:LEU:HD22	2.15	0.46
1:K:71:GLU:H	1:K:71:GLU:CD	2.18	0.46
1:G:325:ASN:O	1:G:326:GLN:C	2.54	0.46
1:C:189:ILE:HD11	1:C:205:HIS:CD2	2.44	0.46
2:L:133:ILE:CD1	2:L:354:LEU:HD13	2.42	0.46
2:D:311:LYS:HG3	2:D:312:TRP:CD2	2.50	0.46
1:G:106:VAL:HG11	1:G:116:ALA:HB1	1.97	0.46
2:H:22:ARG:HG2	2:H:22:ARG:NH1	2.29	0.46
2:D:138:ASP:OD1	2:D:140:SER:HB3	2.15	0.46
2:B:357:LEU:HD22	2:B:361:TRP:CE2	2.51	0.46
2:H:193:MET:HE2	2:H:233:MET:CB	2.46	0.46
1:A:198:LYS:HD3	2:B:266:LYS:HD3	1.97	0.46
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.51	0.46
1:E:263:THR:HG21	1:E:280:LEU:HB2	1.98	0.46
2:B:311:LYS:HG3	2:B:312:TRP:CD2	2.51	0.46
1:C:80:GLN:N	1:C:104:ARG:NH1	2.64	0.46
1:A:106:VAL:HG11	1:A:116:ALA:HB1	1.97	0.46
1:K:106:VAL:HG11	1:K:116:ALA:HB1	1.98	0.45
1:A:285:GLN:NE2	2:B:247:ARG:NH1	2.63	0.45
1:C:219:GLU:HA	1:C:219:GLU:OE1	2.16	0.45
2:L:22:ARG:NH1	2:L:22:ARG:HG2	2.30	0.45
2:B:37:PRO:HD2	2:B:40:TYR:CE1	2.51	0.45
1:I:263:THR:HG21	1:I:280:LEU:HB2	1.98	0.45
1:G:96:PHE:CE1	1:G:126:LEU:HB3	2.51	0.45
2:H:26:VAL:O	2:H:30:GLN:HG3	2.17	0.45
1:I:325:ASN:O	1:I:326:GLN:C	2.54	0.45
1:C:97:ARG:HG2	1:C:101:ASP:OD2	2.15	0.45
2:L:77:TYR:CZ	2:L:141:ARG:HB2	2.51	0.45
2:J:77:TYR:CZ	2:J:141:ARG:HB2	2.51	0.45
1:G:58:LEU:HD23	1:G:63:TYR:CZ	2.51	0.45
2:F:245:LEU:O	2:F:249:LYS:HG3	2.16	0.45
1:A:357:ARG:NH1	1:A:357:ARG:HG3	2.31	0.45
1:E:287:ARG:HG2	1:E:287:ARG:H	1.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:THR:HG21	1:A:280:LEU:HB2	1.98	0.45
2:J:311:LYS:HE2	2:J:312:TRP:CZ2	2.52	0.45
2:J:38:GLU:O	2:J:38:GLU:HG2	2.17	0.45
2:D:64:LEU:HD11	2:D:134:ILE:HG22	1.98	0.45
2:L:22:ARG:HH11	2:L:22:ARG:HG2	1.81	0.45
1:A:96:PHE:CE1	1:A:126:LEU:HB3	2.52	0.45
2:L:103:ILE:HG23	2:L:104:PRO:HD2	1.98	0.45
1:G:105:ALA:O	1:G:109:ARG:HG3	2.16	0.45
2:H:21:LEU:CD1	2:H:21:LEU:N	2.79	0.45
1:I:218:ASN:HB3	8:I:1242:HOH:O	2.16	0.45
1:E:281:LYS:NZ	1:E:317:ASP:OD1	2.37	0.45
2:B:311:LYS:HE2	2:B:312:TRP:CZ2	2.51	0.45
1:E:107:LEU:HD22	2:F:117:TYR:CD2	2.52	0.45
2:H:156:LEU:HD21	2:H:162:CYS:SG	2.57	0.45
1:G:286:ASP:HB2	8:G:618:HOH:O	2.16	0.45
1:K:325:ASN:O	1:K:326:GLN:C	2.55	0.45
1:G:318:ILE:HG22	1:G:322:MET:CE	2.47	0.45
1:E:91:ILE:HD12	2:F:38:GLU:HB2	1.99	0.45
1:A:91:ILE:HD11	2:B:38:GLU:H	1.81	0.45
2:B:103:ILE:HG23	2:B:104:PRO:HD2	1.99	0.44
1:A:71:GLU:O	1:A:115:ARG:NH1	2.50	0.44
1:I:105:ALA:O	1:I:109:ARG:HG3	2.17	0.44
1:A:198:LYS:CD	2:B:266:LYS:HD3	2.47	0.44
2:D:133:ILE:HG22	2:D:350:THR:HG23	1.98	0.44
1:A:58:LEU:HD23	1:A:63:TYR:CE2	2.52	0.44
2:J:256:GLN:HB2	2:J:260:TYR:CE2	2.52	0.44
1:E:189:ILE:HD11	1:E:205:HIS:CD2	2.44	0.44
1:C:344:LEU:HD13	1:C:356:TRP:CE2	2.52	0.44
1:E:328:ASP:O	1:E:329:ASN:HB2	2.18	0.44
2:D:19:ASP:OD2	2:D:19:ASP:N	2.44	0.44
2:D:295:ARG:NH2	2:D:299:LEU:HD11	2.33	0.44
2:J:207:ASP:O	2:J:208:ASN:HB2	2.18	0.44
1:C:263:THR:HG21	1:C:280:LEU:HB2	1.98	0.44
3:N:608:CYS:HA	7:N:1727:GER:C2	2.48	0.44
2:D:103:ILE:HG23	2:D:104:PRO:HD2	1.99	0.44
2:D:229:SER:O	2:D:233:MET:HG3	2.18	0.44
1:I:58:LEU:HD23	1:I:63:TYR:CZ	2.52	0.44
1:G:353:LYS:HG2	1:G:354:GLU:N	2.32	0.44
3:M:508:CYS:HA	7:M:1727:GER:C2	2.48	0.44
2:L:212:GLN:NE2	2:L:212:GLN:HA	2.33	0.44
2:H:24:ARG:HG3	2:H:24:ARG:HH11	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:116:PRO:HB2	2:J:117:TYR:CD2	2.53	0.44
1:A:334:LEU:O	1:A:338:LEU:HG	2.18	0.44
2:H:311:LYS:HE2	2:H:312:TRP:CZ2	2.52	0.44
2:H:77:TYR:CZ	2:H:141:ARG:HB2	2.53	0.44
2:H:360:SER:O	2:H:363:THR:HG23	2.18	0.44
2:L:207:ASP:O	2:L:208:ASN:HB2	2.18	0.44
1:G:107:LEU:HD22	2:H:117:TYR:CD2	2.53	0.44
2:H:24:ARG:NH1	2:H:24:ARG:HG3	2.32	0.43
2:D:295:ARG:NH1	2:D:299:LEU:CD1	2.81	0.43
1:K:92:TYR:O	1:K:97:ARG:NH2	2.52	0.43
2:B:116:PRO:HB2	2:B:117:TYR:CD2	2.53	0.43
1:C:207:GLN:OE1	2:D:216:LEU:HD13	2.18	0.43
1:K:79:PRO:HA	1:K:101:ASP:OD1	2.19	0.43
2:L:130:SER:O	2:L:134:ILE:HG13	2.18	0.43
2:J:311:LYS:HG3	2:J:312:TRP:CD2	2.53	0.43
1:I:96:PHE:CE1	1:I:126:LEU:HB3	2.53	0.43
1:G:263:THR:HG21	1:G:280:LEU:HB2	2.00	0.43
1:E:121:ARG:HH11	1:E:121:ARG:CG	2.32	0.43
2:F:29:PHE:O	2:F:33:LEU:HD22	2.19	0.43
2:H:207:ASP:O	2:H:208:ASN:HB2	2.18	0.43
1:K:328:ASP:O	1:K:329:ASN:HB2	2.18	0.43
1:E:117:PHE:CE2	1:E:146:LYS:HE2	2.54	0.43
2:F:333:GLU:HA	8:F:875:HOH:O	2.18	0.43
1:G:330:LYS:HE2	1:G:367:HIS:HB3	2.00	0.43
2:B:22:ARG:HG2	2:B:22:ARG:NH1	2.34	0.43
2:L:245:LEU:O	2:L:249:LYS:HG3	2.19	0.43
2:D:116:PRO:HB2	2:D:117:TYR:CD2	2.53	0.43
1:K:151:GLU:HG3	1:K:175:LEU:HD11	2.00	0.43
1:E:296:LEU:HD22	1:E:322:MET:HE1	2.00	0.43
2:F:30:GLN:O	2:F:34:GLN:HG3	2.19	0.43
2:D:110:ASN:HB3	2:D:111:PRO:HD2	2.01	0.43
2:L:311:LYS:HG3	2:L:312:TRP:CD2	2.54	0.43
1:K:223:VAL:HG11	1:K:240:ARG:HB2	2.01	0.43
2:F:21:LEU:N	2:F:21:LEU:CD1	2.82	0.43
2:H:18:LEU:N	2:H:18:LEU:CD2	2.81	0.43
2:J:53:PHE:HE1	7:M:1727:GER:H42	1.84	0.43
2:B:64:LEU:HD11	2:B:134:ILE:HG22	2.01	0.43
1:A:340:LEU:HD23	1:A:343:ILE:HD12	2.01	0.43
1:G:72:TRP:CZ2	1:G:115:ARG:HB2	2.53	0.43
2:L:250:ARG:O	2:L:254:MET:HG2	2.19	0.43
2:H:193:MET:HG3	2:H:233:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:21:LEU:HG	8:L:632:HOH:O	2.19	0.43
2:F:103:ILE:HG23	2:F:104:PRO:HD2	2.00	0.43
2:B:192:ASP:OD1	2:B:195:LYS:HE3	2.18	0.43
1:K:339:GLU:O	1:K:343:ILE:HG13	2.19	0.43
2:L:122:ILE:HG22	2:L:163:ALA:HA	2.01	0.43
1:E:97:ARG:HG2	1:E:101:ASP:OD2	2.18	0.43
1:C:361:ARG:HD3	8:C:1272:HOH:O	2.19	0.43
1:C:296:LEU:HD22	1:C:322:MET:CE	2.49	0.42
2:D:311:LYS:HE2	2:D:312:TRP:CZ2	2.54	0.42
2:F:116:PRO:HB2	2:F:117:TYR:CD2	2.54	0.42
1:G:267:ILE:HD13	1:G:277:TRP:CE2	2.54	0.42
2:D:77:TYR:CZ	2:D:141:ARG:HB2	2.54	0.42
1:E:325:ASN:O	1:E:326:GLN:C	2.56	0.42
1:C:286:ASP:HB2	8:C:621:HOH:O	2.18	0.42
2:H:354:LEU:HD11	2:H:358:HIS:NE2	2.34	0.42
1:E:329:ASN:HB3	1:E:332:ASP:HB3	2.00	0.42
2:D:86:ASP:N	2:D:86:ASP:OD2	2.48	0.42
2:J:36:LEU:HA	2:J:37:PRO:HD3	1.89	0.42
2:L:22:ARG:O	2:L:26:VAL:HG23	2.18	0.42
1:C:107:LEU:HD22	2:D:117:TYR:CD2	2.53	0.42
2:D:256:GLN:HB2	2:D:260:TYR:CE2	2.53	0.42
2:D:243:LYS:HE2	2:D:243:LYS:HB3	1.87	0.42
1:C:156:ILE:HD11	1:C:172:ARG:HH22	1.84	0.42
6:F:1723:GRG:HC62	6:F:1723:GRG:H101	1.91	0.42
1:K:329:ASN:HB3	1:K:332:ASP:HB3	2.02	0.42
1:G:318:ILE:HG22	1:G:322:MET:HE3	2.02	0.42
1:A:71:GLU:CD	1:A:71:GLU:H	2.17	0.42
2:L:186:ASN:HB2	2:L:358:HIS:CE1	2.55	0.42
1:A:267:ILE:HD13	1:A:277:TRP:CE2	2.55	0.42
2:L:79:LEU:O	2:L:96:ARG:HG3	2.19	0.42
1:I:287:ARG:H	1:I:287:ARG:HG2	1.59	0.42
1:A:348:LYS:HA	1:A:348:LYS:HD3	1.82	0.42
2:F:311:LYS:HE2	2:F:312:TRP:CZ2	2.54	0.42
2:D:121:HIS:HB3	2:D:124:MET:HG2	2.02	0.42
2:D:20:PHE:CZ	2:D:337:ILE:HD11	2.55	0.42
2:F:121:HIS:HB3	2:F:124:MET:HG2	2.02	0.42
2:F:353:ARG:NE	8:F:739:HOH:O	2.52	0.42
2:B:21:LEU:CD1	2:B:21:LEU:N	2.83	0.42
2:L:311:LYS:HE2	2:L:312:TRP:CZ2	2.55	0.42
1:A:311:LEU:HD23	1:A:311:LEU:C	2.40	0.42
2:H:87:ARG:HB3	2:H:87:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:63:SER:O	2:H:66:VAL:HG22	2.20	0.42
2:F:115:HIS:HA	2:F:116:PRO:HD3	1.91	0.42
2:J:122:ILE:HG22	2:J:163:ALA:HA	2.01	0.42
1:A:359:ILE:HD13	1:A:359:ILE:HA	1.92	0.42
2:J:59:ASP:OD2	2:J:349:ARG:NH1	2.53	0.41
2:F:77:TYR:CZ	2:F:141:ARG:HB2	2.54	0.41
2:D:37:PRO:HD2	2:D:40:TYR:CE1	2.55	0.41
2:L:69:LYS:O	2:L:73:ILE:HG13	2.20	0.41
1:E:219:GLU:HA	1:E:219:GLU:OE1	2.19	0.41
1:E:214:ARG:O	1:E:214:ARG:CG	2.68	0.41
2:J:138:ASP:O	2:J:139:LEU:HB2	2.20	0.41
1:K:82:ASP:HB2	1:K:86:PRO:HB3	2.03	0.41
2:F:37:PRO:HD2	2:F:40:TYR:HD1	1.85	0.41
1:G:287:ARG:HG2	1:G:287:ARG:H	1.54	0.41
2:B:77:TYR:CE1	2:B:141:ARG:HB2	2.55	0.41
2:B:37:PRO:HD2	2:B:40:TYR:CD1	2.55	0.41
1:C:325:ASN:O	1:C:326:GLN:C	2.59	0.41
2:J:246:ASN:ND2	8:J:395:HOH:O	2.54	0.41
2:J:155:GLN:HB2	2:J:161:PHE:CE2	2.56	0.41
1:E:311:LEU:HD23	1:E:311:LEU:C	2.41	0.41
7:M:1727:GER:H112	7:M:1727:GER:H91	1.88	0.41
2:D:26:VAL:O	2:D:30:GLN:HG3	2.21	0.41
2:D:353:ARG:NH1	2:D:357:LEU:HG	2.35	0.41
2:L:116:PRO:HB2	2:L:117:TYR:CD2	2.56	0.41
1:I:344:LEU:HA	1:I:348:LYS:HB2	2.02	0.41
1:C:329:ASN:HB3	1:C:332:ASP:HB3	2.01	0.41
2:J:359:GLN:C	2:J:361:TRP:H	2.24	0.41
2:J:37:PRO:HD2	2:J:40:TYR:CE1	2.55	0.41
1:I:136:PHE:CE2	1:I:140:LEU:HD11	2.55	0.41
1:K:149:GLN:HG3	8:K:1048:HOH:O	2.20	0.41
1:E:155:ILE:HD12	1:E:155:ILE:HA	1.94	0.41
2:L:37:PRO:HD2	2:L:40:TYR:CD1	2.56	0.41
1:A:92:TYR:O	1:A:97:ARG:NH2	2.54	0.41
1:C:100:TYR:HB3	1:C:104:ARG:NH2	2.36	0.41
2:J:121:HIS:HB3	2:J:124:MET:HG2	2.03	0.41
2:H:49:THR:HG23	2:H:124:MET:SD	2.61	0.41
1:E:353:LYS:CE	1:E:357:ARG:HH22	2.34	0.41
2:D:37:PRO:HD2	2:D:40:TYR:CD1	2.55	0.41
2:H:352:GLU:HA	2:H:352:GLU:OE2	2.20	0.41
2:L:36:LEU:HA	2:L:37:PRO:HD3	1.93	0.41
2:L:40:TYR:CE2	7:N:1727:GER:H101	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:ILE:HG21	1:G:206:ARG:HB2	2.03	0.41
2:H:30:GLN:O	2:H:34:GLN:HG3	2.21	0.41
2:F:64:LEU:HD23	2:F:64:LEU:HA	1.84	0.41
2:L:236:LEU:HD22	2:L:245:LEU:HD21	2.03	0.41
1:C:353:LYS:HE3	1:K:339:GLU:HG3	2.03	0.41
2:B:138:ASP:O	2:B:139:LEU:HB2	2.20	0.41
2:H:341:HIS:HA	2:H:342:PRO:HD2	1.81	0.41
2:H:133:ILE:HG22	2:H:350:THR:HG23	2.02	0.41
2:J:250:ARG:O	2:J:254:MET:HG2	2.20	0.41
2:L:255:ARG:HD3	2:L:261:HIS:CD2	2.55	0.41
2:J:77:TYR:HE2	2:J:137:ASP:OD2	2.04	0.41
1:A:331:GLU:O	1:A:335:ASN:ND2	2.54	0.41
2:J:245:LEU:O	2:J:249:LYS:HG3	2.21	0.41
1:K:184:GLN:HB2	8:K:382:HOH:O	2.20	0.41
2:B:52:PHE:HA	2:B:131:CYS:SG	2.61	0.41
2:B:249:LYS:HB3	2:B:285:ILE:HD13	2.03	0.40
2:D:156:LEU:HD21	2:D:162:CYS:SG	2.61	0.40
1:G:207:GLN:OE1	2:H:216:LEU:HD13	2.21	0.40
2:L:49:THR:HG23	2:L:124:MET:SD	2.61	0.40
2:D:258:ASN:OD1	2:D:259:GLY:N	2.42	0.40
1:C:287:ARG:H	1:C:287:ARG:HG2	1.64	0.40
1:K:287:ARG:HG2	1:K:287:ARG:H	1.63	0.40
2:B:64:LEU:HB3	2:B:69:LYS:HE2	2.03	0.40
2:J:133:ILE:CD1	2:J:354:LEU:HD13	2.49	0.40
1:G:58:LEU:HD23	1:G:63:TYR:CE2	2.56	0.40
1:I:350:THR:O	1:I:353:LYS:HB3	2.21	0.40
2:L:64:LEU:HD23	2:L:64:LEU:HA	1.90	0.40
1:A:156:ILE:CD1	1:A:172:ARG:HH22	2.35	0.40
2:B:298:ILE:HD12	2:B:329:LEU:HD13	2.04	0.40
1:G:151:GLU:HG3	1:G:175:LEU:HD11	2.02	0.40
2:H:357:LEU:HD22	2:H:361:TRP:CZ2	2.56	0.40
2:J:30:GLN:HE21	2:J:30:GLN:HB3	1.65	0.40
2:F:64:LEU:HD11	2:F:134:ILE:HG22	2.04	0.40
2:J:64:LEU:HB3	2:J:69:LYS:HE2	2.03	0.40
1:A:107:LEU:HD22	2:B:117:TYR:CD2	2.56	0.40
2:J:37:PRO:HD2	2:J:40:TYR:CD1	2.57	0.40
1:I:124:ILE:HD13	1:I:134:TRP:CH2	2.57	0.40
2:H:155:GLN:HB2	2:H:161:PHE:CE2	2.56	0.40
2:H:86:ASP:N	2:H:86:ASP:OD2	2.50	0.40

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%)	287 (92%)	23 (7%)	2 (1%)	30	54
1	C	312/377 (83%)	289 (93%)	22 (7%)	1 (0%)	46	72
1	E	312/377 (83%)	289 (93%)	21 (7%)	2 (1%)	30	54
1	G	312/377 (83%)	291 (93%)	19 (6%)	2 (1%)	30	54
1	I	312/377 (83%)	289 (93%)	21 (7%)	2 (1%)	30	54
1	K	312/377 (83%)	293 (94%)	17 (5%)	2 (1%)	30	54
2	B	344/377 (91%)	329 (96%)	14 (4%)	1 (0%)	46	72
2	D	344/377 (91%)	329 (96%)	13 (4%)	2 (1%)	30	54
2	F	344/377 (91%)	328 (95%)	15 (4%)	1 (0%)	46	72
2	H	344/377 (91%)	323 (94%)	19 (6%)	2 (1%)	30	54
2	J	344/377 (91%)	324 (94%)	19 (6%)	1 (0%)	46	72
2	L	344/377 (91%)	330 (96%)	13 (4%)	1 (0%)	46	72
3	M	2/11 (18%)	2 (100%)	0	0	100	100
3	N	2/11 (18%)	2 (100%)	0	0	100	100
All	All	3940/4546 (87%)	3705 (94%)	216 (6%)	19 (0%)	34	59

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	258	ASN
1	G	306	HIS
1	G	326	GLN
2	H	258	ASN
1	I	306	HIS
2	J	258	ASN
1	K	306	HIS
2	L	258	ASN
1	A	306	HIS

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Mol	Chain	Res	Type
1	A	326	GLN
2	D	258	ASN
2	F	258	ASN
1	I	326	GLN
1	K	326	GLN
1	C	306	HIS
2	D	333	GLU
1	E	306	HIS
2	H	333	GLU
1	E	326	GLN

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	280/338 (83%)	276 (99%)	4 (1%)	74	91
1	C	283/338 (84%)	275 (97%)	8 (3%)	51	79
1	E	284/338 (84%)	276 (97%)	8 (3%)	51	79
1	G	281/338 (83%)	277 (99%)	4 (1%)	74	91
1	I	287/338 (85%)	279 (97%)	8 (3%)	51	79
1	K	291/338 (86%)	286 (98%)	5 (2%)	68	88
2	B	289/326 (89%)	275 (95%)	14 (5%)	31	59
2	D	293/326 (90%)	278 (95%)	15 (5%)	29	55
2	F	294/326 (90%)	281 (96%)	13 (4%)	35	62
2	H	288/326 (88%)	272 (94%)	16 (6%)	26	50
2	J	292/326 (90%)	276 (94%)	16 (6%)	27	51
2	L	296/326 (91%)	281 (95%)	15 (5%)	29	55
3	M	4/11 (36%)	4 (100%)	0	100	100
3	N	4/11 (36%)	4 (100%)	0	100	100
All	All	3466/4006 (86%)	3340 (96%)	126 (4%)	42	70

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	PHE
1	A	71	GLU
1	A	214	ARG
1	A	287	ARG
2	B	39	ARG
2	B	113	THR
2	B	151	LEU
2	B	216	LEU
2	B	222	SER
2	B	232	LEU
2	B	236	LEU
2	B	255	ARG
2	B	258	ASN
2	B	261	HIS
2	B	306	VAL
2	B	329	LEU
2	B	331	LEU
2	B	357	LEU
1	C	55	PHE
1	C	59	ASP
1	C	71	GLU
1	C	81	ASN
1	C	182	PRO
1	C	287	ARG
1	C	324	GLU
1	C	364	GLN
2	D	21	LEU
2	D	39	ARG
2	D	110	ASN
2	D	151	LEU
2	D	216	LEU
2	D	222	SER
2	D	232	LEU
2	D	236	LEU
2	D	255	ARG
2	D	258	ASN
2	D	261	HIS
2	D	306	VAL
2	D	329	LEU
2	D	331	LEU
2	D	353	ARG
1	E	55	PHE

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Mol	Chain	Res	Type
1	E	67	ARG
1	E	71	GLU
1	E	121	ARG
1	E	211	GLN
1	E	214	ARG
1	E	287	ARG
1	E	324	GLU
2	F	21	LEU
2	F	39	ARG
2	F	151	LEU
2	F	216	LEU
2	F	232	LEU
2	F	236	LEU
2	F	255	ARG
2	F	258	ASN
2	F	261	HIS
2	F	306	VAL
2	F	329	LEU
2	F	331	LEU
2	F	353	ARG
1	G	71	GLU
1	G	224	ASP
1	G	287	ARG
1	G	324	GLU
2	H	18	LEU
2	H	21	LEU
2	H	91	ASP
2	H	151	LEU
2	H	216	LEU
2	H	222	SER
2	H	232	LEU
2	H	236	LEU
2	H	255	ARG
2	H	258	ASN
2	H	261	HIS
2	H	306	VAL
2	H	329	LEU
2	H	331	LEU
2	H	348	THR
2	H	357	LEU
1	I	55	PHE
1	I	67	ARG

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Mol	Chain	Res	Type
1	I	71	GLU
1	I	142	ARG
1	I	194	ASN
1	I	211	GLN
1	I	287	ARG
1	I	364	GLN
2	J	21	LEU
2	J	27	ARG
2	J	31	ARG
2	J	151	LEU
2	J	216	LEU
2	J	222	SER
2	J	232	LEU
2	J	236	LEU
2	J	255	ARG
2	J	258	ASN
2	J	261	HIS
2	J	306	VAL
2	J	329	LEU
2	J	331	LEU
2	J	353	ARG
2	J	357	LEU
1	K	55	PHE
1	K	71	GLU
1	K	142	ARG
1	K	287	ARG
1	K	324	GLU
2	L	21	LEU
2	L	33	LEU
2	L	65	ASP
2	L	110	ASN
2	L	151	LEU
2	L	216	LEU
2	L	232	LEU
2	L	236	LEU
2	L	255	ARG
2	L	258	ASN
2	L	261	HIS
2	L	306	VAL
2	L	329	LEU
2	L	331	LEU
2	L	353	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	201	HIS
1	A	278	ASN
1	A	329	ASN
1	A	335	ASN
2	B	212	GLN
1	C	108	GLN
1	C	184	GLN
1	C	218	ASN
1	C	298	GLN
1	C	335	ASN
1	C	364	GLN
2	D	212	GLN
2	D	246	ASN
1	E	184	GLN
1	E	201	HIS
1	E	298	GLN
2	F	212	GLN
2	F	246	ASN
1	G	80	GLN
1	G	89	GLN
1	G	162	GLN
1	G	201	HIS
1	G	297	ASN
1	G	325	ASN
2	H	212	GLN
2	H	296	ASN
1	I	89	GLN
1	I	135	HIS
1	I	285	GLN
1	I	364	GLN
2	J	30	GLN
2	J	208	ASN
2	J	212	GLN
2	J	246	ASN
1	K	135	HIS
1	K	218	ASN
1	K	298	GLN
2	L	212	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 15 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
6	GRG	B	1721	-	26,28,28	0.81	0	33,37,37	0.85	0
6	GRG	D	1722	-	26,28,28	0.87	1 (3%)	33,37,37	0.82	0
6	GRG	F	1723	-	26,28,28	0.81	0	33,37,37	0.82	0
6	GRG	H	1724	-	26,28,28	0.77	0	33,37,37	0.84	0
6	GRG	J	1725	-	26,28,28	0.80	1 (3%)	33,37,37	0.82	0
6	GRG	L	1726	-	26,28,28	0.77	0	33,37,37	0.84	0
7	GER	M	1727	-	19,19,19	0.96	2 (10%)	22,22,22	0.74	0
7	GER	N	1727	-	19,19,19	0.99	2 (10%)	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
6	GRG	B	1721	-	-	0/31/31/31	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GRG	D	1722	-	-	0/31/31/31	0/0/0/0
6	GRG	F	1723	-	-	0/31/31/31	0/0/0/0
6	GRG	H	1724	-	-	0/31/31/31	0/0/0/0
6	GRG	J	1725	-	-	0/31/31/31	0/0/0/0
6	GRG	L	1726	-	-	0/31/31/31	0/0/0/0
7	GER	M	1727	-	-	0/20/20/20	0/0/0/0
7	GER	N	1727	-	-	0/20/20/20	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1727	GER	C7-C8	2.00	1.36	1.33
6	J	1725	GRG	C7-C8	2.05	1.37	1.33
6	D	1722	GRG	C7-C8	2.05	1.37	1.33
7	N	1727	GER	C7-C8	2.08	1.37	1.33
7	M	1727	GER	C12-C13	2.13	1.37	1.33
7	N	1727	GER	C12-C13	2.16	1.37	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1721	GRG	1	0
6	D	1722	GRG	1	0
6	F	1723	GRG	2	0
6	H	1724	GRG	1	0
6	J	1725	GRG	1	0
6	L	1726	GRG	1	0
7	M	1727	GER	5	0
7	N	1727	GER	5	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%)	0.05	15 (4%)	34	32	35, 57, 92, 110	0
1	C	314/377 (83%)	-0.01	10 (3%)	51	50	33, 54, 80, 97	0
1	E	314/377 (83%)	0.19	15 (4%)	34	32	35, 59, 86, 103	0
1	G	314/377 (83%)	0.16	12 (3%)	44	42	35, 59, 87, 102	0
1	I	314/377 (83%)	0.01	15 (4%)	34	32	29, 52, 84, 95	0
1	K	314/377 (83%)	-0.20	6 (1%)	70	69	23, 41, 67, 81	0
2	B	346/377 (91%)	0.03	19 (5%)	29	26	35, 52, 75, 100	0
2	D	346/377 (91%)	0.04	17 (4%)	33	31	32, 46, 71, 95	0
2	F	346/377 (91%)	0.04	17 (4%)	33	31	34, 47, 74, 101	0
2	H	346/377 (91%)	0.45	33 (9%)	10	8	36, 65, 95, 112	0
2	J	346/377 (91%)	0.12	17 (4%)	33	31	30, 50, 80, 104	0
2	L	346/377 (91%)	-0.01	10 (2%)	55	53	25, 40, 65, 93	0
3	M	4/11 (36%)	2.79	3 (75%)	0	0	60, 65, 73, 79	4 (100%)
3	N	4/11 (36%)	2.40	2 (50%)	0	0	59, 65, 74, 80	4 (100%)
All	All	3968/4546 (87%)	0.08	191 (4%)	34	32	23, 52, 84, 112	8 (0%)

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	306	HIS	6.0
1	G	306	HIS	5.4
1	G	305	SER	5.3
2	D	363	THR	5.2
2	H	363	THR	5.1
1	C	304	PRO	4.8
2	B	363	THR	4.8
1	G	304	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
2	J	108	SER	4.7
2	F	112	GLY	4.7
2	H	112	GLY	4.7
1	E	306	HIS	4.7
1	E	91	ILE	4.6
1	G	55	PHE	4.5
2	H	361	TRP	4.5
2	H	65	ASP	4.4
2	H	304	ARG	4.3
1	A	304	PRO	4.2
2	J	111	PRO	4.2
1	C	305	SER	4.2
2	H	111	PRO	4.0
2	F	113	THR	4.0
2	J	86	ASP	4.0
3	M	508	CYS	4.0
1	I	328	ASP	3.9
2	F	363	THR	3.9
2	H	86	ASP	3.9
2	J	84	THR	3.8
2	H	38	GLU	3.8
2	H	360	SER	3.8
1	I	306	HIS	3.7
1	E	304	PRO	3.7
2	F	88	SER	3.7
1	A	306	HIS	3.6
2	L	363	THR	3.6
2	B	113	THR	3.5
2	D	110	ASN	3.5
2	H	88	SER	3.5
2	H	108	SER	3.5
2	B	86	ASP	3.5
2	H	362	LYS	3.5
1	I	305	SER	3.4
1	A	328	ASP	3.4
2	D	111	PRO	3.4
1	K	306	HIS	3.4
2	L	86	ASP	3.4
2	L	113	THR	3.3
2	B	37	PRO	3.3
2	H	314	ASP	3.3
1	E	368	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	91	ILE	3.2
2	B	362	LYS	3.2
2	J	112	GLY	3.1
2	J	363	THR	3.1
1	E	328	ASP	3.1
2	H	305	LEU	3.1
2	D	362	LYS	3.1
1	G	91	ILE	3.1
3	M	510	ILE	3.1
1	I	368	SER	3.1
2	L	111	PRO	3.0
1	E	305	SER	3.0
1	I	304	PRO	3.0
2	B	111	PRO	3.0
2	L	84	THR	3.0
2	F	37	PRO	3.0
1	G	329	ASN	3.0
1	K	305	SER	3.0
1	A	329	ASN	3.0
1	E	314	PHE	3.0
2	J	110	ASN	3.0
1	E	331	GLU	2.9
1	E	326	GLN	2.9
2	B	110	ASN	2.9
3	N	609	VAL	2.9
2	H	71	ASP	2.9
2	H	84	THR	2.9
2	H	40	TYR	2.9
2	F	111	PRO	2.9
1	C	329	ASN	2.9
1	G	330	LYS	2.9
1	C	55	PHE	2.8
2	L	110	ASN	2.8
2	H	87	ARG	2.8
2	J	85	GLU	2.8
3	M	511	LEU	2.8
1	E	55	PHE	2.8
2	J	88	SER	2.8
2	J	360	SER	2.8
1	G	326	GLN	2.7
2	H	37	PRO	2.7
3	N	608	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	65	ASP	2.7
2	H	316	HIS	2.7
2	F	86	ASP	2.7
2	F	84	THR	2.7
1	I	329	ASN	2.7
1	I	83	GLY	2.7
2	H	35	VAL	2.7
2	B	84	THR	2.7
2	H	85	GLU	2.7
1	E	313	ALA	2.7
2	H	110	ASN	2.6
1	A	301	ASP	2.6
1	I	84	PRO	2.6
2	L	108	SER	2.6
1	C	327	CYS	2.6
2	F	39	ARG	2.6
1	C	330	LYS	2.6
2	B	360	SER	2.6
2	B	114	ALA	2.6
2	H	127	THR	2.6
2	D	305	LEU	2.5
1	A	326	GLN	2.5
2	F	362	LYS	2.5
2	J	237	GLU	2.5
1	E	365	SER	2.5
1	G	92	TYR	2.5
1	I	326	GLN	2.5
1	A	330	LYS	2.5
1	A	305	SER	2.5
1	A	331	GLU	2.5
2	H	114	ALA	2.4
1	C	331	GLU	2.4
2	D	86	ASP	2.4
2	D	314	ASP	2.4
2	F	314	ASP	2.4
1	E	330	LYS	2.4
2	D	113	THR	2.4
2	J	109	LYS	2.4
2	H	356	ASP	2.4
1	A	342	GLU	2.4
2	L	85	GLU	2.3
2	D	37	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	368	SER	2.3
2	H	237	GLU	2.3
1	G	327	CYS	2.3
1	K	304	PRO	2.3
1	A	367	HIS	2.3
1	C	347	GLU	2.3
2	B	87	ARG	2.3
2	B	112	GLY	2.3
1	A	314	PHE	2.3
2	F	305	LEU	2.3
2	H	359	GLN	2.3
1	K	85	SER	2.3
2	B	85	GLU	2.3
2	B	109	LYS	2.3
2	F	109	LYS	2.3
2	H	109	LYS	2.3
1	G	368	SER	2.2
2	D	360	SER	2.2
2	L	314	ASP	2.2
2	B	65	ASP	2.2
1	I	85	SER	2.2
2	F	114	ALA	2.2
2	J	107	PRO	2.2
2	B	316	HIS	2.2
2	D	39	ARG	2.2
2	H	157	GLU	2.2
2	J	127	THR	2.2
2	J	362	LYS	2.2
2	H	358	HIS	2.1
2	D	127	THR	2.1
1	A	325	ASN	2.1
1	E	329	ASN	2.1
2	B	39	ARG	2.1
2	F	355	ARG	2.1
1	C	334	LEU	2.1
1	I	327	CYS	2.1
1	K	84	PRO	2.1
1	K	326	GLN	2.1
2	F	316	HIS	2.1
2	D	356	ASP	2.1
2	J	359	GLN	2.1
1	I	332	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	38	GLU	2.1
1	I	364	GLN	2.1
2	D	361	TRP	2.1
2	H	312	TRP	2.1
2	J	314	ASP	2.1
2	H	113	THR	2.1
2	B	314	ASP	2.1
2	D	88	SER	2.1
2	L	114	ALA	2.1
2	F	40	TYR	2.0
1	I	145	GLN	2.0
1	I	367	HIS	2.0
2	D	114	ALA	2.0
1	G	347	GLU	2.0
1	E	327	CYS	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^{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	CL	C	1705	1/1	0.97	0.25	5.38	55,55,55,55	0
7	GER	N	1727	20/20	0.79	0.37	1.83	63,70,82,82	20
5	CL	G	1711	1/1	0.97	0.19	1.74	55,55,55,55	0
7	GER	M	1727	20/20	0.82	0.33	1.11	67,74,81,82	20
6	GRG	B	1721	29/29	0.96	0.18	0.28	48,53,59,60	0
6	GRG	F	1723	29/29	0.96	0.17	0.27	47,52,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	GRG	L	1726	29/29	0.95	0.23	0.26	37,42,53,58	0
6	GRG	J	1725	29/29	0.96	0.21	-0.03	38,44,55,58	0
6	GRG	D	1722	29/29	0.95	0.17	-0.15	42,48,55,57	0
6	GRG	H	1724	29/29	0.95	0.18	-0.17	52,57,72,73	0
5	CL	F	1709	1/1	0.99	0.11	-0.78	46,46,46,46	0
4	ZN	B	378	1/1	1.00	0.10	-1.26	38,38,38,38	0
4	ZN	D	378	1/1	1.00	0.09	-1.29	37,37,37,37	0
4	ZN	H	378	1/1	0.98	0.10	-1.44	54,54,54,54	0
5	CL	D	1706	1/1	0.98	0.07	-1.54	41,41,41,41	0
4	ZN	F	378	1/1	1.00	0.08	-1.69	40,40,40,40	0
4	ZN	J	378	1/1	0.99	0.10	-1.83	35,35,35,35	0
5	CL	L	1718	1/1	0.99	0.06	-1.89	43,43,43,43	0
5	CL	K	1717	1/1	0.98	0.10	-2.04	55,55,55,55	0
5	CL	J	1715	1/1	0.97	0.07	-2.11	58,58,58,58	0
5	CL	B	1702	1/1	0.97	0.07	-2.17	64,64,64,64	0
5	CL	H	1712	1/1	0.97	0.06	-2.58	58,58,58,58	0
4	ZN	L	378	1/1	1.00	0.09	-2.64	27,27,27,27	0

6.5 Other polymers

There are no such residues in this entry.